NUCLEAR REACTOR ANALYSIS

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PREFACE

During recent years nuclear fission reactors have become an economically competitive source of electrical power. It is now widely recognized that nuclear power generation is an absolute necessity if we are to meet the ever-growing demand for electrical power while preserving our natural environment. Both the maturation of the nuclear power industry, as well as the national commitment to fast breeder reactor development, have created a substantial and growing demand for well-trained nuclear engineers at the B.S. and M.S. degree levels. In response to this demand, universities are shifting their attention from the training of Ph.D. nuclear engineers to the development of programs more geared to the present and future needs of the nuclear power industry.

It is therefore surprising to find that, almost without exception, such programs are based upon material that lags many years behind techniques used in modern nuclear reactor analysis. The availability of large, fast digital computers has revolutionized methods of reactor analysis and design. In most cases, such modern methods of reactor analysis bear little resemblance to the pre-computer techniques of earlier years. And yet, most contemporary courses on nuclear reactor analysis are based almost entirely on these outdated techniques, stressing as they do analytical methods to the near exclusion of numerical techniques and digital computation.

Furthermore, it is vital to coordinate nuclear reactor theory courses with parallel courses in thermal-hydraulics and structural analysis in order to present a complete picture of nuclear core analysis. Finally, the traditional pre-occupation of nuclear engineering programs with light water moderated thermal reactors must be balanced with a detailed study of fast breeder reactors and high temperature, gas-cooled reactors, since these latter types of reactors are expected to play important roles in the nuclear power industry of the 1980's.

These lecture notes represent one attempt at developing an introductory course in nuclear reactor analysis which meets these goals. Since these notes are also intended to be the preliminary draft of a text on nuclear reactor theory, they contain considerably more detail than it is possible to cover in a one or two-term course on this subject. They are incomplete as they stand, and they will be supplemented occasionally with further references, detailed examples, and, of course, problem sets.

We would also hasten to add that these notes have not been carefully edited (or censored, for that matter) and hence probably contain numerous errors (as well as other items of little redeeming social value). Caveat emptor!

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TABLE OF CONTENTS

Preface

Part I: Introductory Concepts of Nuclear Reactor Analysis

Chapter 1: Introduction

Chapter 2: The Interaction of Neutrons with Matter

Chapter 3: Fission Chain Reactions and Nuclear Reactors: An Introduction

Chapter 4: Neutron Transport

Part II: The One-Speed Diffusion Model of a Nuclear Reactor

Chapter 5: The One-Speed Diffusion Theory Model

IV. Reactor Criticality Calculations

Chapter 6: Nuclear Reactor Kinetics

III. Solution of the Point Reactor Kinetics Equations

D. Approximate Solutions

IV. Reactivity Feedback

V. Fission Product Poisoning

Part III: The Multigroup Diffusion Method

Chapter 7: Multigroup Diffusion Theory

Chapter 8: Fast Spectrum Calculations and Fast Group Constants

Chapter 9: Thermal Spectra and Thermal Group Constants

Part IV: An Introduction To The Design Of Nuclear Power Reactors

Chapter 10: General Aspects of Core Design

Chapter 11: Calculation Of Reactor Criticality And Power Distributions

Chapter 12: Control Studies

I. Control Rod Analysis and Design
  A. Qualitative Discussion of Rod Worth, Calibration, Control Requirements
  B. Perturbation Theory
  C. Calculation and Measurements of Rod Worth
II. Burnable Poisons and Mechanical Shim
III. Chemical Shim
IV. Feedback Effects and Reactivity Coefficients
  A. Calculation of Temperature Feedback Coefficients
  B. Void Coefficients
  C. Measurement of Power Coefficients

Chapter 13: Design Studies of Reactor Operation

I. Core Lifetime Studies
II. Startup and Shutdown (Reactivity Margins, etc.)
III. Power Level Changes--Load Following
IV. Safety Studies--Accident Analysis

Chapter 14: Nuclear Fuel Management

I. Introduction (Overview of Fuel Cycle)
II. Head-End Fuel Management
  A. Mining, Refining, Processing
  B. Isotope Separation
  C. Fuel Fabrication
III. In-Core Fuel Management
  A. Analytical Models of Fuel Cycles
  B. Depletion Analysis Revisited
  C. Fuel Loading Schemes
IV. Tail-End Fuel Management
V. Isotope Buildup and Decay
VI. Fuel Cycle Economics

Chapter 15: Nuclear Power Plants

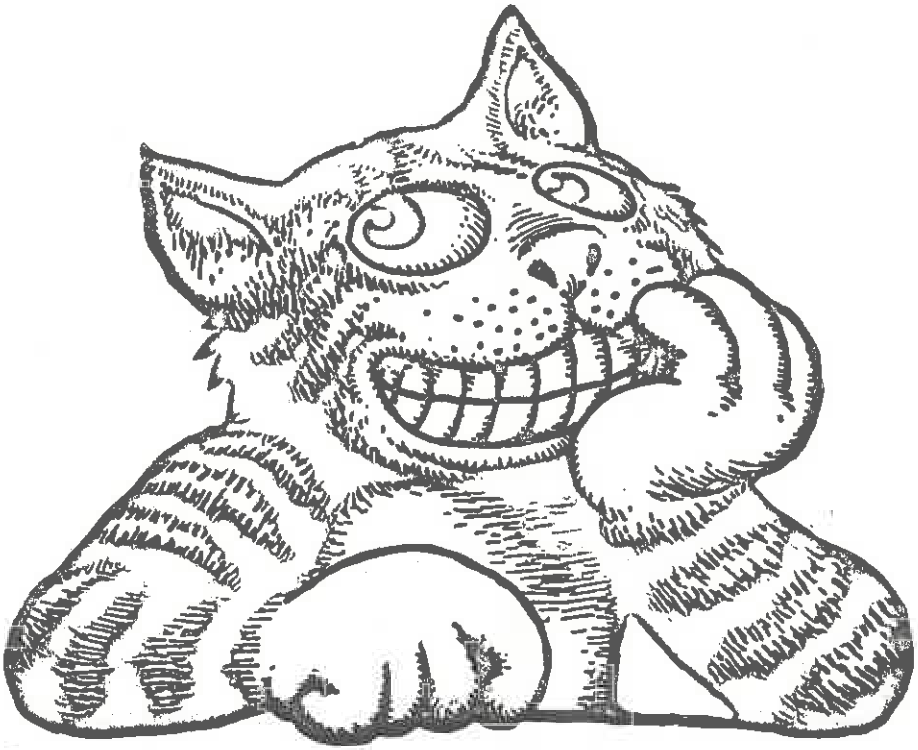
I. An Overview of Central Station Power Plants
  A. Major Systems
  B. Auxiliary Systems
  C. Engineered Safeguards
II. Nuclear Plant Operation
III. Licensing of Nuclear Power Plants

Appendices:

  A. Kinematics of Two-Body Collisions
  B. The ENDF/B Cross Section System
  C. The Zoology of Special Functions
  D. Step Functions, Delta Functions, and other Exotic Beasts
  E. Some Assorted Facts on Linear Operators
  F. An Introduction to Matrices and Matrix Algebra
  G. Some Topics in Numerical Analysis
  H. Integral Transforms

PART I

INTRODUCTORY CONCEPTS OF NUCLEAR REACTOR ANALYSIS



CHAPTER 1: INTRODUCTION

The generation of power using nuclear fission reactors can be expected to continue its dominance until well into the next century, if one recognizes that roughly 50 years are needed to shift the energy industry from one type of fuel to another, due to the long operating lifetime of power machinery and the long lead time for redirecting manufacturing capability. Hence even though there appear to be attractive alternatives to nuclear fission power such as solar power or power generated by controlled thermonuclear fusion reactions, the practical implementation of such alternatives will not occur for several decades to come--at the earliest. Hence nuclear fission reactors will comprise the dominant source of electrical power during the productive lifetimes of the present generation of engineering students.

A very central role in the development and application of nuclear energy will be played by the nuclear engineer who is uniquely characterized by his ability to assist in boththe nuclear design of fission reactors, as well as in their integration into large power plants. In the early days of the reactor industry, a nuclear engineer was usually thought of as a Ph.D. level reactor physicist, primarily concerned with nuclear reactor core research and design. Today, however, nuclear engineers are needed not only by research laboratories and reactor manufacturers to design and develop reactor cores, but as well by the electrical utilities who buy and operate the nuclear power plants and by the engineering companies who build the power plants and service them during their operating lifetime. Hence an understanding of core physics is not enough for today's nuclear engineer. He must learn how to interface his specialized knowledge of core theory and design with the myriad of other engineering demands made upon a nuclear power reactor, such as thermal analysis, materials limitations, mechanical core design, the economics of reactor operation, and so on. In this sense, he must recognize that nuclear core design is only one facet to be considered in nuclear power engineering. To study and master it out of the context of these other disciplines would be highly undesirable.

Our concern in this text will be the study of the theory of nuclear fission reactors, particularly as it relates to the engineering analysis and design of nuclear reactor cores. However it is our intent to develop this theory as much as possible within the context of the other considertions involved in nuclear reactor analysis, such as thermal-hydraulic analysis or nuclear fuel economics, for example. We must admit a certain preoccupation with nuclear power reactors simply because most nuclear engineers will find themselves involved in the nuclear power industry. This will be particularly apparent in the examples we have chosen to discuss and the problems we have emphasized. Of course, most of the topics we develop have a much broader range of validity and would apply equally well to the analysis of other types of nuclear reactors.

II. WHAT IS A NUCLEAR FISSION REACTOR?

The term "nuclear reactor" will be used in this text to refer to devices in which controlled nuclear fission chain reactions can be achieved. (This restricted definition may offend the segment of the nuclear community involved in nuclear fusion research, but since an honest-to-God working nuclear fusion reactor seems several years away, no confusion should result.) In a very narrow sense then, a nuclear reactor is simply a mass of fissionable material (e.g., U^{235} or Pu^{239}) in which a controlled fission chain reaction can be sustained.

In actuality, of course, a nuclear reactor is much more complex. It must not only contain a lattice of very carefully refined and fabricated nuclear fuel, but as well must provide for cooling this fuel during the course of the chain reaction, maintaining the fuel in a very precise geometrical arrangement with structural materials. controlling the chain reaction, and shielding the surroundings of the reactor from the intense nuclear radiation generated during the fission reactions. If the reactor is to produce power in a useful fashion, it must as well be designed so that it will operate as economically and as safely as possible. Such engineering constraints make the actual nuclear reactor configuration quite complex indeed, as the example shown in Figure 1 indicates.

Nuclear reactors have been used for over 20 years in a variety of applications. They are particularly valuable tools for nuclear research since they produce copious amounts of nuclear radiation, primarily in the form of neutrons or gamma rays. Such radiation can be used in fundamental investigations of the microscopic structure and dynamics of matter.

The radiation produced by reactors can also be used to transmute nuclei in such a fashion as to produce artificial isotopes which can then be used, for example, as radioactive tracers in nuclear medicine. Reactors can use the same scheme to produce nuclear fuel. Such "converter" production reactors produce the plutonium fuels for fission reactors. In fact, a nuclear reactor can be used to produce its own fuel as in the fast breeder reactors currently being developed for commercial application in the next decade.

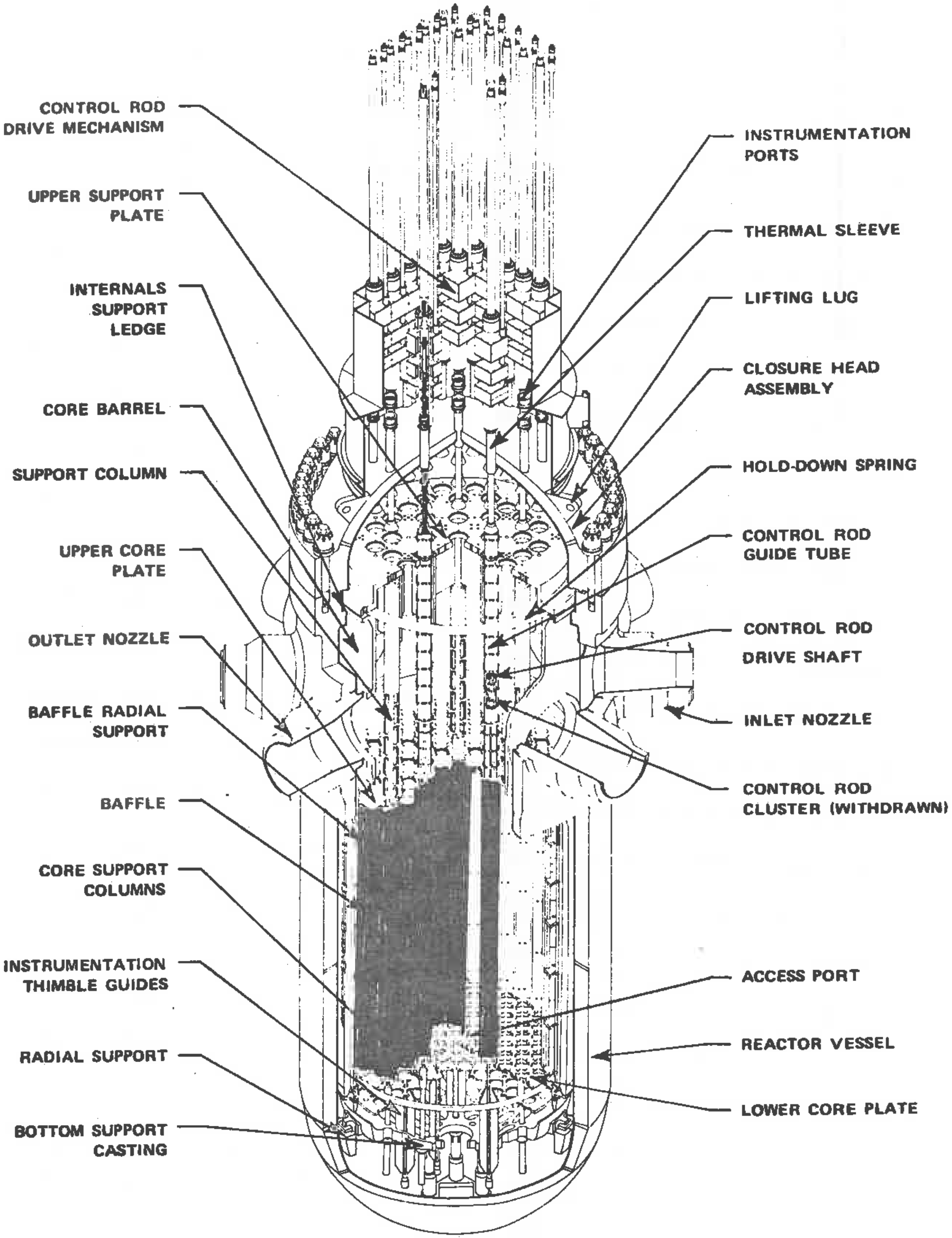


FIGURE 1-1: A Modern Nuclear Reactor (in this case, a Pressurized Water Peactor manufactured by Westinghouse)

Small, compact reactors have been used for propulsion in submarines, ships, aircraft, and rocket vehicles. (Indeed, the present generation of light water reactors are little more than very big brothers of the propulsion reactors used in nuclear submarines.) They can also be used as small sources of power in satellites (or on the moon).

But by far the most significant application of nuclear fission reactors is in large, central station power plants. The level of effort--both in manpower and money--for this application far exceeds other uses of nuclear reactors. A nuclear power plant is actually very similar to a fossil fuel power plant--except that it replaces the coal or oil-fired boiler by a nuclear reactor, which generates heat by sustaining a chain reaction of nuclear fission events in a suitable lattice of fuel material. Of course there are some dramatic differences between a nuclear reactor, and say, a coal-fired boiler. But the useful quantity produced by each is high temperature, high pressure steam which can then be used to run turbo-generators. Hence at the center of a modern nuclear power plant is the <u>n</u>uclear <u>s</u>team <u>s</u>upply <u>s</u>ystem (NSSS), composed of the nuclear reactor, its associated coolant loops and pumps, and steam generators. A typical NSSS is shown in Figure 2. The remainder of the power plant is fairly conventional as indicated by the diagram of a typical large nuclear power plant in Figure 3.

Actually, the NSSS contributes only a relatively small fraction of the total capital cost of a nuclear power plant (presently, about 12%). Nevertheless, it is of central concern since it not only dictates the detailed design of the remainder of the plant, but through its low fuel costs, is responsible as well for the economic advantages enjoyed by nuclear power generation.

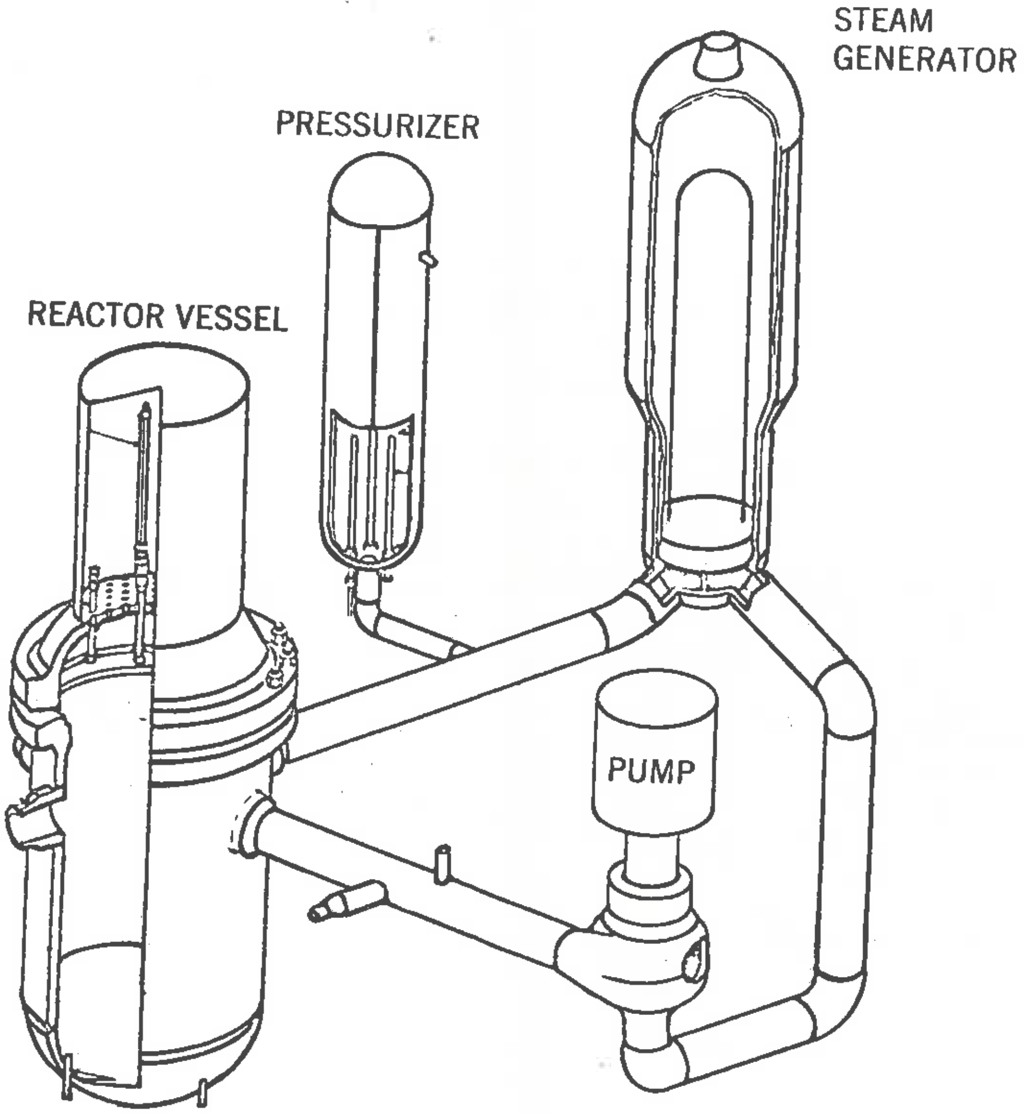


FIGURE 1-2: A Nuclear Steam Supply System including a nuclear reactor, a coolant loop, and a steam generator

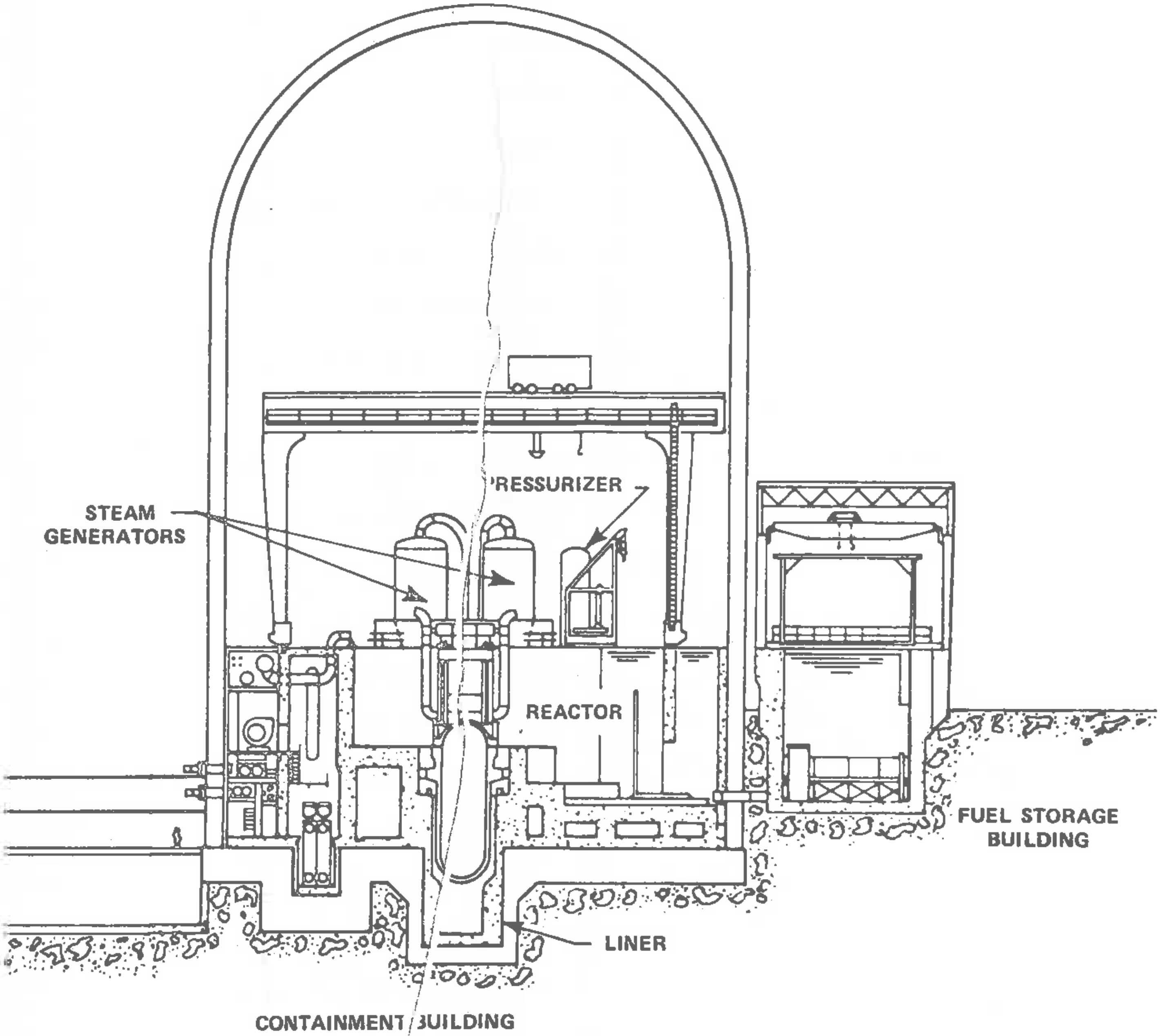


FIGURE I-3a: Cross Section of a Typical Nuclear Power Plant

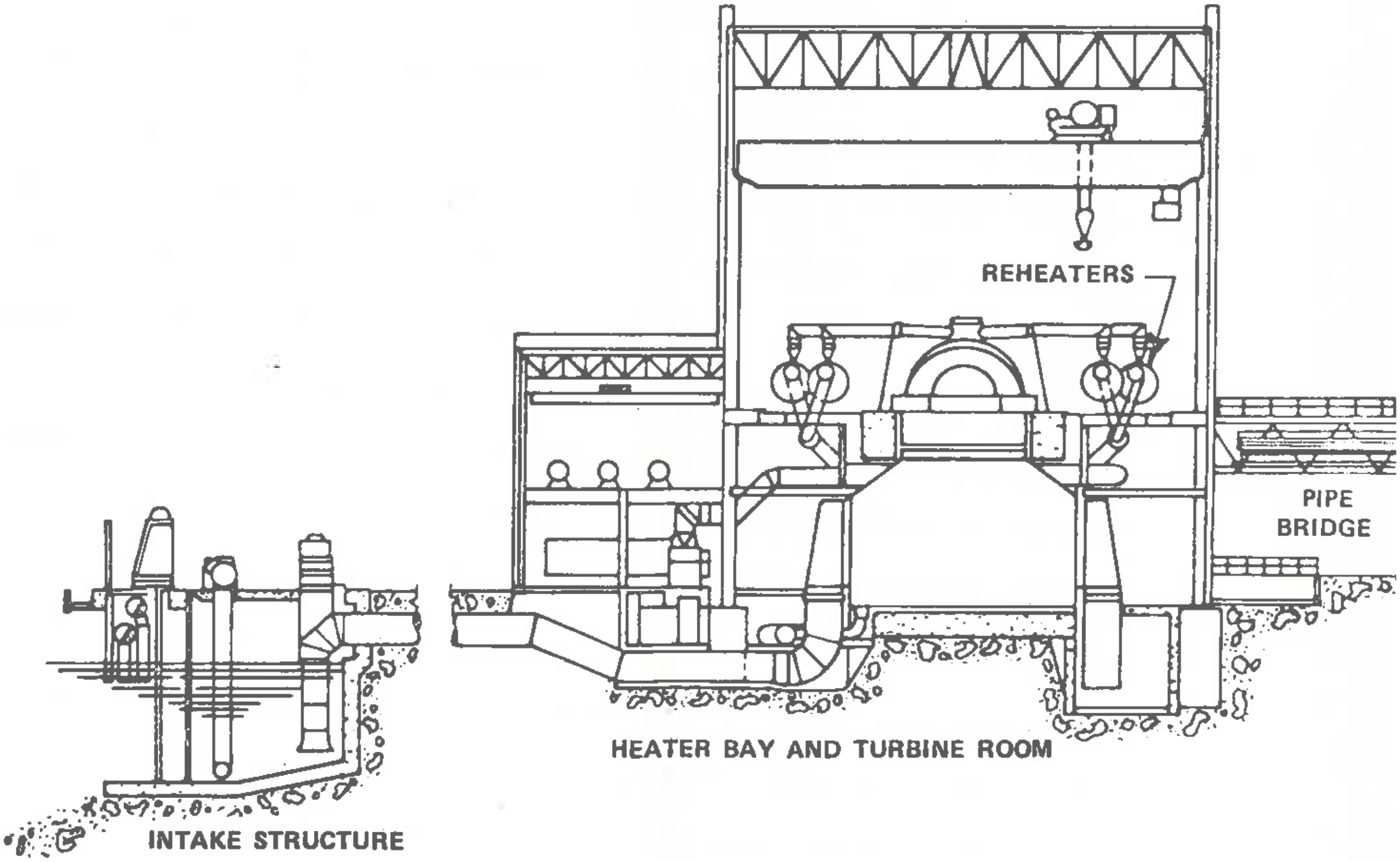


FIGURE 1-3b: continued

At the heart of the NSSS is the nuclear reactor itself. A rather wide variety of nuclear reactors are in operation today or have been proposed for future development. Reactor types can be characterized by a number of features. One usually distinguishes between those reactors whose chain reactions are maintained by neutrons with characteristic energy comparable to the energy of thermal vibration of the atoms comprising the reactor core (so-called "thermal" reactors) or reactors in which the average neutron energy is more characteristic of the much higher energy neutrons released in a nuclear fission reaction ("fast" reactors). Yet another common distinction refers to the type of coolant used in the reactor. In the United States, and indeed throughout the world, the most popular of the present generation of reactors uses ordinary water as a coolant--so-called light water reactors (LWR). By way of contrast, heavy water (D_2O) is used as a coolant in several of the Canadian reactors. Liquid metals can also be used as coolants when efficient heat transfer is at a premium, and sodium has been chosen as the coolant for the fast breeder reactor (the liquid metal fast breeder reactor or LMFBR). Gases have also been used as coolants. The early British reactors used CO_2 as a coolant. More recently, high pressure helium is being used in the high temperature gas cooled reactor (HTGR) being developed in the United States and the advanced gas cooled reactors (AGR) under development in Great Britian.

Numerous other types of reactors have been proposed and studied--some even involving exotic concepts such as liquid or gaseous fuels. Although much of the analysis presented in this text will be applicable to such reactors, our dominant concern will be with the solid-fuel reactors cooled by either water, sodium, or helium, since these will comprise the vast majority of the power reactors installed during the next several decades.

III. THE NUCLEAR POWER INDUSTRY

It is commonly recognized that high technology nations are today facing "energy crisis" in which shortages of various types of energy will become more common, and the price of energy will rapidly increase. There are actually two aspects to this problem in the public mind:

(i) First, the common belief that we are running out of conventional fuels. (This is technically true, but probably on a much longer time scale than most people realize.)

(ii) Secondly, the "rate" problem--that is, keeping up with the soaring demand for energy. (That this is certainly a significant problem can be readily testified to by anyone who has experienced a "brownout" or a gasolene shortage.)

Projected world energy requirements are usually measured in a unit of energy called the "Q". One Q is equal to 10^{18} BTU's, and as a reference point, the current worldwide consumption of energy is 0.15 Q per year. By the year 2000 this is expected to rise to 1 Q, and by the year 2100 to level off at 16 Q.

These energy requirements should be compared to present estimates of recoverable fossil fuel reserves which range between 40 and 400 Q, and uranium reserves which amount to 160 Q (if the breeder reactor is not introduced). These magnitudes indicate that for the immediate future, the problem of energy supply will remain a problem of introducing sufficient new capacity to meet the growing demand rather than a depletion of fuel reserves. However, fossil fuel resources will come under increasing pressure in the course of the next century. This will be particularly true of liquid fuels, whose price trends are already increasing at a rapid rate.

In order to solve the longer term problem of energy resources, one is forced to new sources of energy such as the fast breeder reactor. Then the available uranium reserves are rapidly multiplied to the order of 10,000 Q. The successful development of controlled thermonuclear fusion would solve the world energy problem for a practically indefinite period of time.

Of course, one could adopt the alternative viewpoint and consider restricting the usage and hence the demand for energy. Such an approach seems highly undesirable--at least for the long term--since one finds a rather linear relation between the per capita consumption of energy and the per capita gross national produce of various countries (see Figure 4). In fact, in order to meet the food requirements and assure a minimally reasonable quality of life in the fact of present world population growth, an adequate growth in energy supply seems mandatory.

Hence the issue is not whether energy production for the world should be increased, but rather how to increase it without harmful side effects. It is furthermore vitally necessary to meet the present demand for energy, and this can only be accomplished, at least in the immediate future, with present technology. At the present time, it appears that this demand can only be met via the large-scale introduction of nuclear power plants.

This recognition, when combined with the growing economic advantages of nuclear power, has led to a rapid growth of the nuclear power industry. Although the gradual phasing in of nuclear power plants has not led to

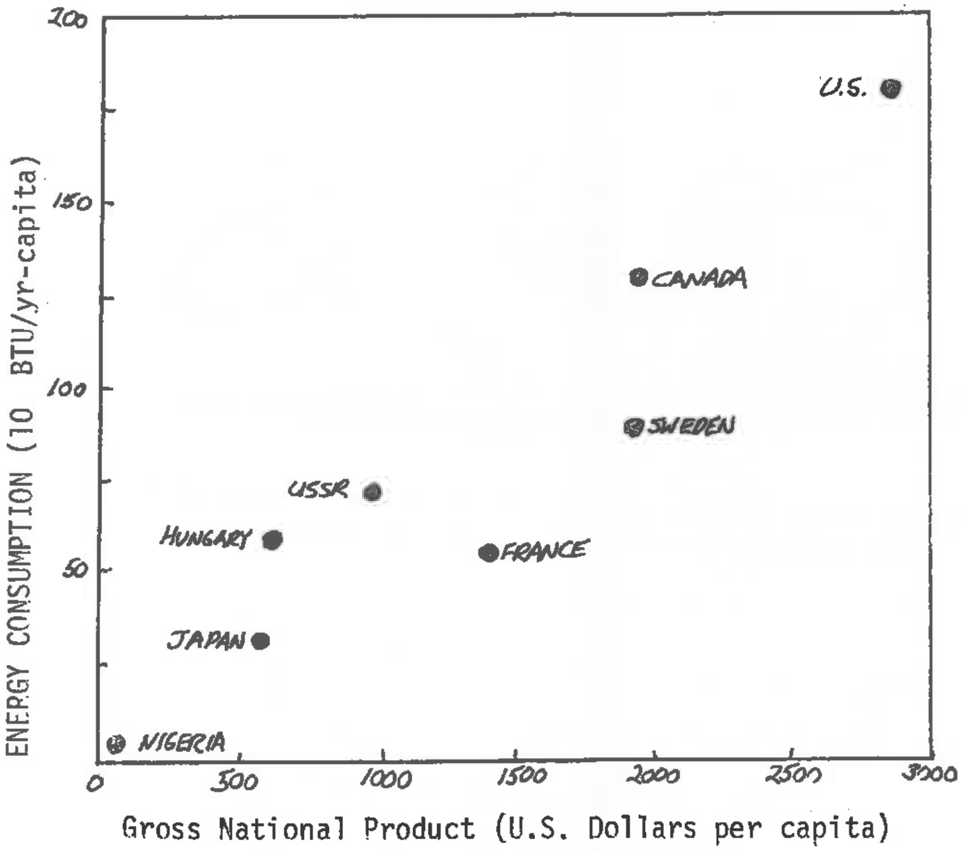


FIGURE 4: Commercial Energy Use and Gross National Product

"By standing upright, we free our hands for making tools and weapons, building cities, creating civilization!"

the abrupt revolution of the nuclear age that many predicted during the early years of atomic energy, most countries are relying more and more upon nuclear power generation as a major source of electrical energy. The growth of the nuclear power industry can easily be seen in Figure 5. We have also listed in Table 1 the present status of nuclear plant construction in the United States.

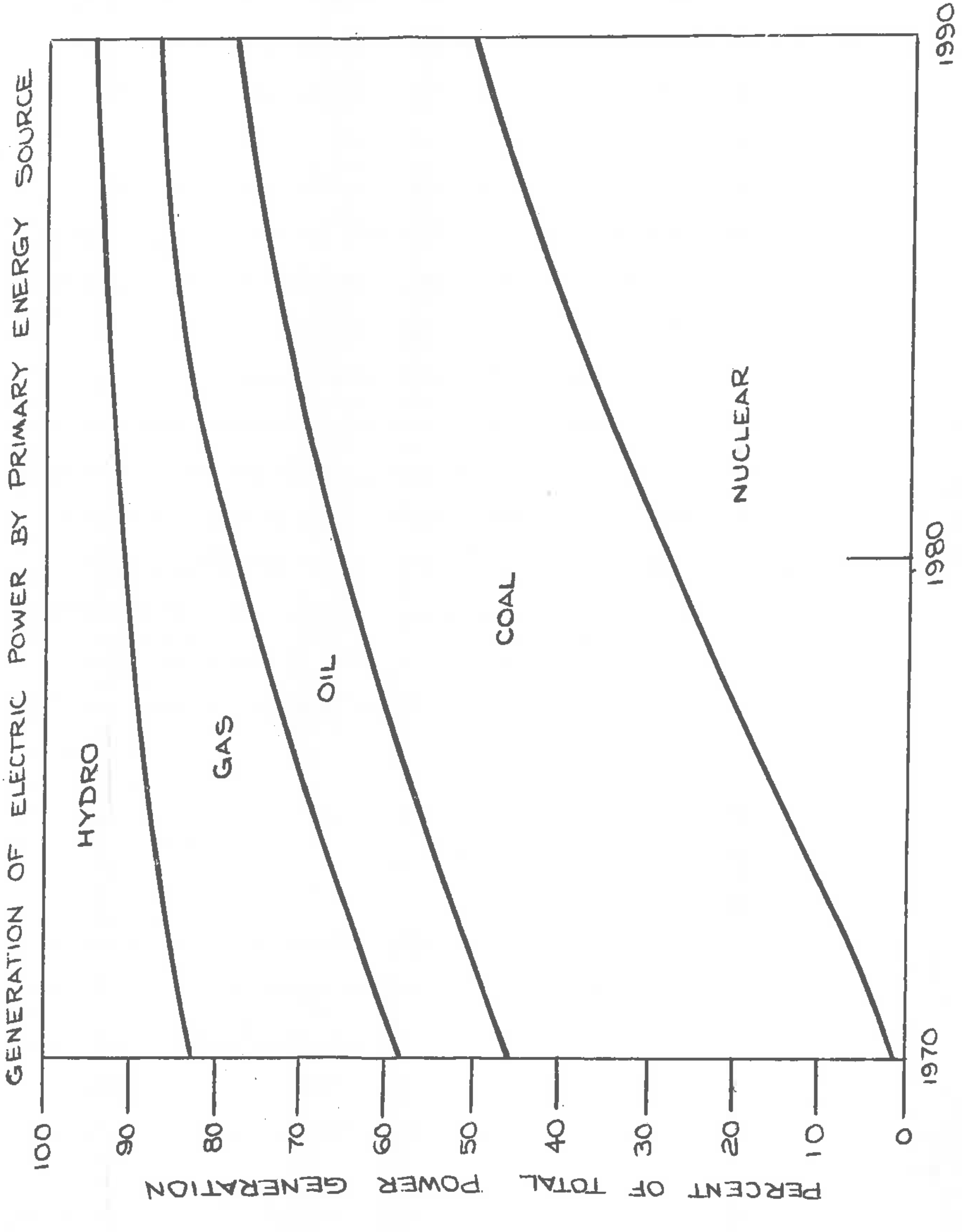
For nuclear plants to be economically competitive, they must utilize their lower fuel costs to compensate for their somewhat larger capital costs over fossil fueled plants. This has resulted in a gradual increase in plant size--from early plants in the 200-300 Mwe size to plants being ordered today in the 1200-1600 Mwe range.

Today's nuclear power industry is based primarily on the light water reactors--both the pressurized water reactor and the boiling water reactor. To stabilize the soaring capital costs of such plants (now ranging in the $300/kw-installed range), reactor manufacturers are making every effort to standarize design features. This is significant in that it tends to downplay research in favor of more slowly paced engineering development. But at the center of either of these activities is the nuclear engineer.

IV. THE ROLE OF THE NUCLEAR ENGINEER

The maturation of the nuclear power industry has also substantially changed the need of the industry for nuclear engineers. No longer does the manufacturer require large staffs of Ph.D. reactor physicists. Indeed, much of the core physics of the present generation of thermal reactors is quite well understood--and even the development of the fast breeder

FIGURE 1-5



GENERATION OF ELECTRIC POWER BY PRIMARY ENERGY SOURCE

TABLE 1-1

U.S. Central Station Nuclear Power Plants

Operable, Under Construction, or on Order (175 MWe and Over) as of December 31, 1972

	Net MWe Capacity	Type	Reactor Supplier	Generator Supplier	Architect Engineer	Constructor	Construction Stage (%)	Start
NEW ENGLAND & MIDDLE ATLANTIC								
Boston Edison Co.								
Pilgrim	654	BWR	GE	GE	Bechtel	Bechtel	100	1972
#Pilgrim No. 2	1150	PWR	C-E		Bechtel	Bechtel	0	1978
Connecticut Yankee Atomic Power Co.								
Connecticut Yankee	575	PWR	W	W	Utility	Utility	100	1967
Consolidated Edison Co. (N.Y.)								
Indian Point No. 1	265	PWR	B&W	W	Utility	Utility	100	1963
Indian Point No. 2	873	PWR	W	W	UE&C	UE&C/Jones	100	1973
Indian Point No. 3	965	PWR	W	W	UE&C	UE&C/Jones	75	1975
Delmarva Power & Light (Del.)								
Unit 1	770	HTGR	GGA	Allis	UE&C		0	1979
Unit 2	770	HTGR	GGA	Allis	UE&C		0	1982
Duquesne Light Co. (Pa.)								
Beaver Valley No. 1	847	PWR	W	W	Utility/S&W	Utility/S&W	56	1974
Beaver Valley No. 2	847	PWR	W				0	1978
Jersey Central P&L Co.								
Forked River No. 1	1140	PWR	C-E	BB	B&R	SR	0	1978
Oyster Creek No. 1	530	BWR	GE	GE	B&R	B&R/Jones	100	1969
Three Mile Island No. 2	810	PWR	B&W	W	B&R/Gilbert	UE&C	35	1976
Long Island Lighting Co.								
Shoreham	819	BWR	GE	GE	S&W	S&W	0	1977
Maine Yankee Atomic Power Co.								
Maine Yankee	790	PWR	C-E	W	S&W	S&W	100	1972
Metropolitan Edison Co. (Pa.)								
Three Mile Island No. 1	810	PWR	B&W	GE	Gilbert	UE&C	92	1972
New England Electric (R.I.)								
Rome Point No. 1*	900	PWR	W		S&W			
Rome Point No. 2*	900	PWR	W		S&W			
New York Power Authority and Niagara Mohawk Power Corp.								
FitzPatrick	821	BWR	GE	GE	S&W	S&W	80	1973
ew York State Electric & Gas Corp.								
#Lansing*	830	BWR	GE				0	early '80's
#Somerset*	1200	BWR	GE				0	early '80's
Niagara Mohawk Power Corp. (N.Y.)								
Nine Mile Point No. 1	625	BWR	GE	GE	Utility	S&W	100	1970
Nine Mile Point No. 2	1100	BWR	GE	GE	S&W	S&W	0	1978
Northeast Utilities (Conn.)								
Millstone No. 1	652	BWR	GE	GE	Ebasco	Ebasco	100	1971
Millstone No. 2	828	PWR	C-E	GE	Bechtel	Bechtel	52	1974
Pennsylvania Power & Light								
Susquehanna No. 1	1052	BWR	GE	GE	Bechtel	Bechtel	0	1979
Susquehanna No. 2	1052	BWR	GE	GE	Bechtel	Bechtel	0	1981
Philadelphia Electric Co.								
Peach Bottom No. 2	1065	BWR	GE	GE	Bechtel	Bechtel	93	1973
Peach Bottom No. 3	1065	BWR	GE	GE	Bechtel	Bechtel	55	1974
Limerick No. 1	1065	BWR	GE	GE	Bechtel	Bechtel	5	1978
Limerick No. 2	1065	BWR	GE	GE	Bechtel	Bechtel	5	1980
Site Undesignated, No. 1	1140	HTGR	GGA	W	S&W	S&W	0	1979
Site Undesignated, No. 2	1140	HTGR	GGA	W	S&W	S&W	0	1981
Public Service Co. of New Hampshire								
#Seabrook No. 1	1100	PWR	W		UE&C		0	1979
#Seabrook No. 2	1100	PWR	W		UE&C		0	1981
Public Service Electric & Gas Co. (N.J.)								
Salem No. 1	1050	PWR	W	W	Utility	UE&C	75	1973
Salem No. 2	1050	PWR	W	W	Utility	UE&C	42	1974
Newbold Island No. 1	1088	BWR	GE	GE	Utility	UE&C	0	1975
Newbold Island No. 2	1088	BWR	GE	GE	Utility	UE&C	0	1977
#Atlantic No. 1	1150	PWR	W	W	Offshore (PS)	OPS	0	1980
#Atlantic No. 2	1150	PWR	W	W	Offshore (PS)	OPS	0	1981
Rochester Gas & Electric Co.								
Robert E. Ginna	420	PWR	W	W	Gilbert	Bechtel	100	1969
Vermont Yankee Nuclear Power Corp.								
Vermont Yankee	514	BWR	GE	GE	Ebasco	Ebasco	100	1972
ankee Atomic Electric Co. (Mass.)								
Yankee-Rowe	175	PWR	W	W	S&W	S&W	100	1961
Total (45 units)	**39,000**							

#Units sold in 1972. *Letter of intent

CONTINUED ON NEXT PAGE

TABLE 1-1 (continued)

Central Station Nuclear Plants—continued	Net MWe Capacity	Type	Reactor Supplier	Generator Supplier	Architect Engineer	Constructor	Construction Stage (%)	Start
EAST NORTH CENTRAL, WEST NORTH CENTRAL & MOUNTAIN STATES								
Cincinnati Gas & Electric Co.								
Zimmer No. 1	810	BWR	GE	W	S&L	Kaiser	0	1977
Cleveland Electric Illuminating								
#Perry No. 1	1100	BWR	GE	GE	Gilbert		0	1979
#Perry No. 2	1100	BWR	GE	GE	Gilbert		0	1980
Commonwealth Edison Co. (Ill.)								
Dresden No. 1	200	BWR	GE	GE	Bechtel	Bechtel	100	1960
Dresden No. 2	809	BWR	GE	GE	S&L	UE&C	100	1970
Dresden No. 3	809	BWR	GE	GE	S&L	UE&C	100	1971
LaSalle No. 1	1078	BWR	GE	GE	S&L	Utility	0	1977
LaSalle No. 2	1078	BWR	GE	GE	S&L	Utility	0	1978
Zion No. 1	1050	PWR	W	W	S&L	Utility	98	1973
Zion No. 2	1050	PWR	W	W	S&L	Utility	85	1973
Byron No. 1	1100	PWR	W	W	S&L		0	1979
Byron No. 2	1100	PWR	W	W	S&L		0	1980
#Braidwood No. 1	1100	PWR	W	W	S&L		0	1980
#Braidwood No. 2	1100	PWR	W	W	S&L		0	1981
Commonwealth Edison Co. and Iowa-Illinois Gas & Electric Co.								
Quad Cities No. 1	809	BWR	GE	GE	S&L	UE&C	100	1972
Quad Cities No. 2	809	BWR	GE	GE	S&L	UE&C	100	1972
Consumers Power Co. (Mich.)								
Palisades	700	PWR	C-E	W	Bechtel	Bechtel	100	1971
Midland No. 1	492	PWR	B&W	GE	Bechtel	Bechtel	0	1976
Midland No. 2	818	PWR	B&W	GE	Bechtel	Bechtel	0	1977
#Quanicassee No. 1	1150	PWR	W					1981
#Quanicassee No. 2	1150	PWR	W					1982
Consumers Public Power District (Nebr.)								
Cooper	778	BWR	GE	W	B&R	B&R.	89	1973
Detroit Edison Co.								
Fermi No. 2	1126	BWR	GE	EE	Utility, S&L	Parsons	27	1975
#Fermi No. 3	1150	BWR	GE	GE	Utility/S&L		0	1981
#Greenwood No. 2	1150	PWR	B&W		Bechtel		0	1979
#Greenwood No. 3	1150	PWR	B&W		Bechtel		0	1981
Indiana & Michigan Electric Co. (Mich.)								
Donald C. Cook No. 1	1054	PWR	W	GE	AEPSC	Jones	84	1973
Donald C. Cook No. 2	1060	PWR	W	BB	AEPSC	Jones	25	1974
Iowa Electric Light & Power Co.								
Duane Arnold	545	BWR	GE	GE	Bechtel	Bechtel	75	1974
Northern Indiana Public Service Co.								
Bailly	660	BWR	GE	GE	S&L		0	1977
Northern States Power Co. (Minn.)								
Monticello	545	BWR	GE	GE	Bechtel	Bechtel	100	1971
Prairie Island No. 1	530	PWR	W	W	PS&E	Utility	90	1973
Prairie Island No. 2	530	PWR	W	W	PS&E	Utility	35	1974
Omaha Public Power District								
Fort Calhoun	457	PWR	C-E	GE	G&H/D&R	G&H/D&R	99	1973
Potomac Electric Power Co.								
#Douglas Pt. No. 1	1100	BWR	GE	Ebasco	Ebasco		0	1980
#Douglas Pt. No. 2	1100	BWR	GE	Ebasco	Ebasco		0	1981
Public Service Company of Colorado								
Fort St. Vrain	330	HTGR	GGA	GE	S&L	Ebasco	100	1973
Toledo Edison Co.								
Davis-Besse	872	PWR	B&W	GE	Bechtel	Bechtel	45	1975
Wisconsin Michigan Power Co. (Wisc.)								
Point Beach No. 1	497	PWR	W	W	Bechtel	Bechtel	100	1971
Point Beach No. 2	497	PWR	W	W	Bechtel	Bechtel	100	1973
Wisconsin Public Service Co.								
Kewaunee	527	PWR	W	W	PS&E	PS&E	96	1973
Total (41 units)	**35,070**							
SOUTH ATLANTIC & EAST SOUTH CENTRAL STATES (& PUERTO RICO)								
Alabama Power Company								
Joseph M. Farley No. 1	829	PWR	W	W	SS/Bechtel	Daniel	35	1975
Joseph M. Farley No. 2	829	PWR	W	W	SS/Bechtel	Daniel	5	1977
#Central Alabama No. 1	1200	BWR	GE	GE	SS		0	1981
#Central Alabama No. 2	1200	BWR	GE	GE	SS		0	1982
Arkansas Power & Light Co.								
Nuclear One	820	PWR	B&W	W	Bechtel	Bechtel	90	1973
Nuclear Two	950	PWR	C-E		Bechtel	Bechtel	8	1976

#Units sold in 1972.

TABLE 1-1 (continued)

Central Station Nuclear Plants—continued	Net MWe Capacity	Type	Reactor Supplier	Generator Supplier	Architect Engineer	Constructor	Construction Stage (%)	Start
SOUTH ATLANTIC & EAST SOUTH CENTRAL STATES continued								
ltimore Gas & Electric Co.								
Calvert Cliffs No. 1	800	PWR	C-E	GE	Bechtel	Bechtel	75	1973
Calvert Cliffs No. 2	800	PWR	C-E	W	Bechtel	Bechtel	62	1974
Carolina Power & Light Co. (N.C.)								
Brunswick No. 1	821	BWR	GE	GE	UE&C	Brown	70	1974
Brunswick No. 2	821	BWR	GE	GE	UE&C	Brown	35	1975
Shearon Harris No. 1	900	PWR	W	W	Ebasco	Daniels	0	1977
Shearon Harris No. 2	900	PWR	W	W	Ebasco	Daniels	0	1978
Shearon Harris No. 3	900	PWR	W	W	Ebasco	Daniels	0	1979
Shearon Harris No. 4	900	PWR	W	W	Ebasco	Daniels	0	1980
Carolina Power & Light Co. (S.C.)								
Robinson No. 2	700	PWR	W	W	Ebasco	Ebasco	100	1971
Duke Power Co. (S.C.)								
Oconee No. 1	841	PWR	B&W	GE	Utility/Bechtel	Utility	100	1973
Oconee No. 2	886	PWR	B&W	GE	Utility/Bechtel	Utility	85	1973
Oconee No. 3	886	PWR	B&W	GE	Utility/Bechtel	Utility	50	1974
McGuire No. 1	1150	PWR	W	W	Utility	Utility	7	1975
McGuire No. 2	1150	PWR	W	W	Utility	Utility	5	1977
#Catawba No. 1	1180	PWR	W	W	Utility	Utility	0	1979
#Catawba No. 2	1180	PWR	W	W	Utility	Utility	0	1980
Florida Power & Light Co.								
Turkey Point No. 3	652	PWR	W	W	Bechtel	Bechtel	100	1972
Turkey Point No. 4	652	PWR	W	W	Bechtel	Bechtel	99	1973
St. Lucie No. 1	813	PWR	C-E	W	Ebasco	Ebasco	43	1975
#St. Lucie No. 2	890	PWR	C-E		Ebasco	Ebasco	0	1979
Florida Power Corp.								
Crystal River No. 3	858	PWR	B&W	W	Gilbert	Jones	60	1974
Georgia Power Co.								
Edwin I. Hatch No. 1	786	BWR	GE	GE	SS/Bechtel	Utility	70	1974
Edwin I. Hatch No. 2	786	BWR	GE	GE	SS/Bechtel	Utility	15	1976
Vogtle 1	1100	PWR	W	GE	Bechtel	Utility	0	1978
Vogtle 2	1100	PWR	W	GE	Bechtel	Utility	0	1979
Gulf States Utility Co.								
#River Bend	940	BWR	GE	Allis	S&W	S&W	0	1979
ouisiana Power & Light Co.								
Waterford No. 3	1140	PWR	C-E	W	Ebasco	Ebasco	0	1977
Mississippi Power & Light								
Grand Gulf	1250	BWR	GE		Bechtel	Bechtel	0	1979
Puerto Rico Water Resources Authority								
Aguirre	583	PWR	W	W	G&H	UE&C	1	1977
South Carolina Electric & Gas Co.								
Virgil C. Summer No. 1	890	PWR	W	W	Gilbert	Daniels	0	1977
Tennessee Valley Authority								
Browns Ferry No. 1	1064	BWR	GE	GE	Utility	Utility	99	1973
Browns Ferry No. 2	1064	BWR	GE	GE	Utility	Utility	75	1974
Browns Ferry No. 3	1065	BWR	GE	GE	Utility	Utility	50	1974
Sequoyah No. 1	1124	PWR	W	W	Utility	Utility	50	1975
Sequoyah No. 2	1124	PWR	W	W	Utility	Utility	40	1975
Watts Bar No. 1	1130	PWR	W	W	Utility	Utility	0	1977
Watts Bar No. 2	1130	PWR	W	W	Utility	Utility	0	1978
Unit 8	1176	PWR	B&W	BB	Utility	Utility	0	1977
Unit 9	1176	PWR	B&W	BB	Utility	Utility	0	1978
#Unit 10	1200	BWR	GE		Utility	Utility	0	1980
#Unit 11	1200	BWR	GE		Utility	Utility	0	1981
#Unit 12	1200	BWR	GE		Utility	Utility	0	1981
#Unit 13	1200	BWR	GE		Utility	Utility	0	1982
#LMFBR Demo Plant*	400	LMFBR	W		B&R		0	1980
Texas Utilities								
#Comanche Peak No. 1	1150	PWR	W		G&H		0	1980
#Comanche Peak No. 2	1150	PWR	W		G&H		0	1982
Virginia Electric & Power Co.								
Surry No. 1	780	PWR	W	W	S&W	S&W	100	1972
Surry No. 2	780	PWR	W	W	S&W	S&W	99	1973
North Anna No. 1	845	PWR	W	W	S&W	S&W	53	1975
North Anna No. 2	845	PWR	W	W	S&W	S&W	28	1975
North Anna No. 3	940	PWR	B&W	W	S&W	S&W	0	1977
North Anna No. 4	940	PWR	B&W	W	S&W	S&W	0	1978
#Site undesignated No. 1	900	PWR	B&W				0	1980
#Site undesignated No. 2	900	PWR	B&W				0	1981
Total (49 units)	**57,576**							

#Units sold in 1972. *Letter of intent

CONTINUED ON NEXT PAGE

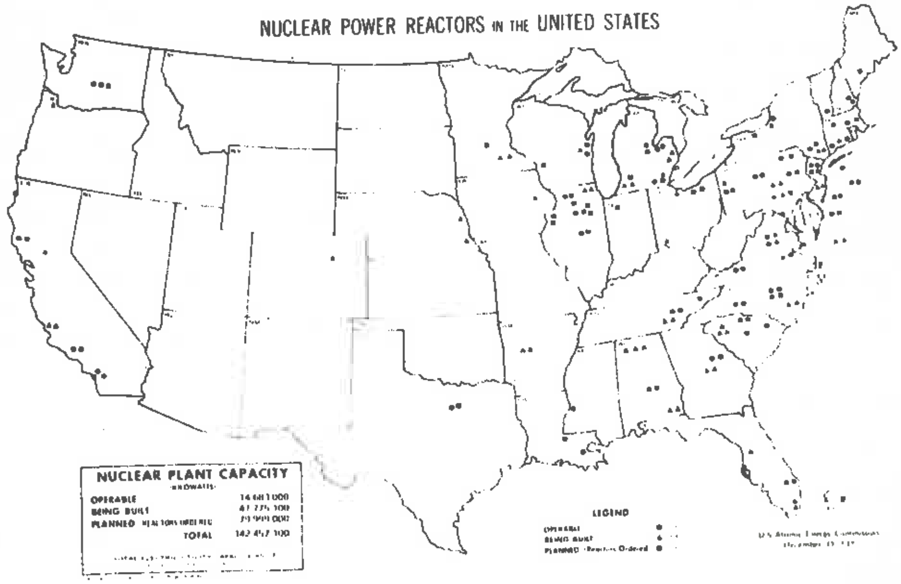
TABLE 1-1 (continued)

Central Station Nuclear Plants—continued	Net MWe Capacity	Type	Reactor Supplier	Generator Supplier	Architect Engineer	Constructor	Est. Cost (millions)	Start
PACIFIC STATES								
Pacific Gas & Electric Co. (Calif.)								
Diablo Canyon No. 1	1060	PWR	W	W	Utility	Utility	60	1975
Diablo Canyon No. 2	1060	PWR	W	W	Utility	Utility	20	1975
Mendocino No. 1	1100	BWR	GE	GE	Utility		0	1977
Mendocino No. 2	1100	BWR	GE	GE	Utility		0	1979
Portland General Electric Co.								
Trojan	1130	PWR	W	GE	Bechtel	Bechtel	57	1975
Sacramento Municipal Utility District								
Rancho Seco	804	PWR	B&W	W	Bechtel	Bechtel	80	1974
Southern California Edison								
#Unit 1	770	HTGR	GGA				0	1981
#Unit 2	770	HTGR	GGA				0	1982
Southern California Edison and San Diego Gas Co. & Electric Co.								
San Onofre No. 1	430	PWR	B&W	W	Bechtel	Bechtel	100	1967
San Onofre No. 2	1140	PWR	C-E	EE	Bechtel		0	1978
San Onofre No. 3	1140	PWR	C-E	EE	Bechtel		0	1979
Washington Public Power Supply System								
Hanford-N	790	BWR	GE	GE	B&R	B&R	100	1966
WPPSS No. 2	1135	BWR	GE	W	B&R	B&R	0	1977
#WPPSS No. 1	1200	PWR	B&W		UE&C		0	1980
Total (15 units)	**13,629**							
GRAND TOTAL (159 units)	**145,275**							

#Units sold in 1972. *Letter of intent

Abbreviations used in table

AEPSC	American Electric Power Service Corp.
AEI	Associated Electric Industries (Engl.)
Allis	Allis-Chalmers
B&W	Babcock & Wilcox Co.
Bechtel	Bechtel Corp.
Brown	Brown & Root, Inc.
BB	Brown Boveri (of Switzerland)
B&R	Burns & Roe, Inc.
C-E	Combustion Engineering, Inc.
Daniel	Daniel Construction Co.
D&R	Durham & Richardson
Ebasco	Ebasco Services, Inc.
EE	English Electric (of England)
GE	General Electric Co.
G&H	Gibbs & Hill, Inc.
Gilbert	Gilbert Associates, Inc.
GGA	Gulf General Atomic
Jones	J. A. Jones Construction Co.
Kaiser	Kaiser Engineers
OPS	Offshore Power Systems
Parsons	Ralph M. Parsons Co.
PS&E	Pioneer Services & Engineering Co.
S&L	Sargent & Lundy Engineers
SS	Southern Services, Inc.
SR	Stearns-Roger Corp.
S&W	Stone & Webster Engineering Corp.
UE&C	United Engineers & Constructors
W	Westinghouse Electric Corp.
#	Units sold in 1972.

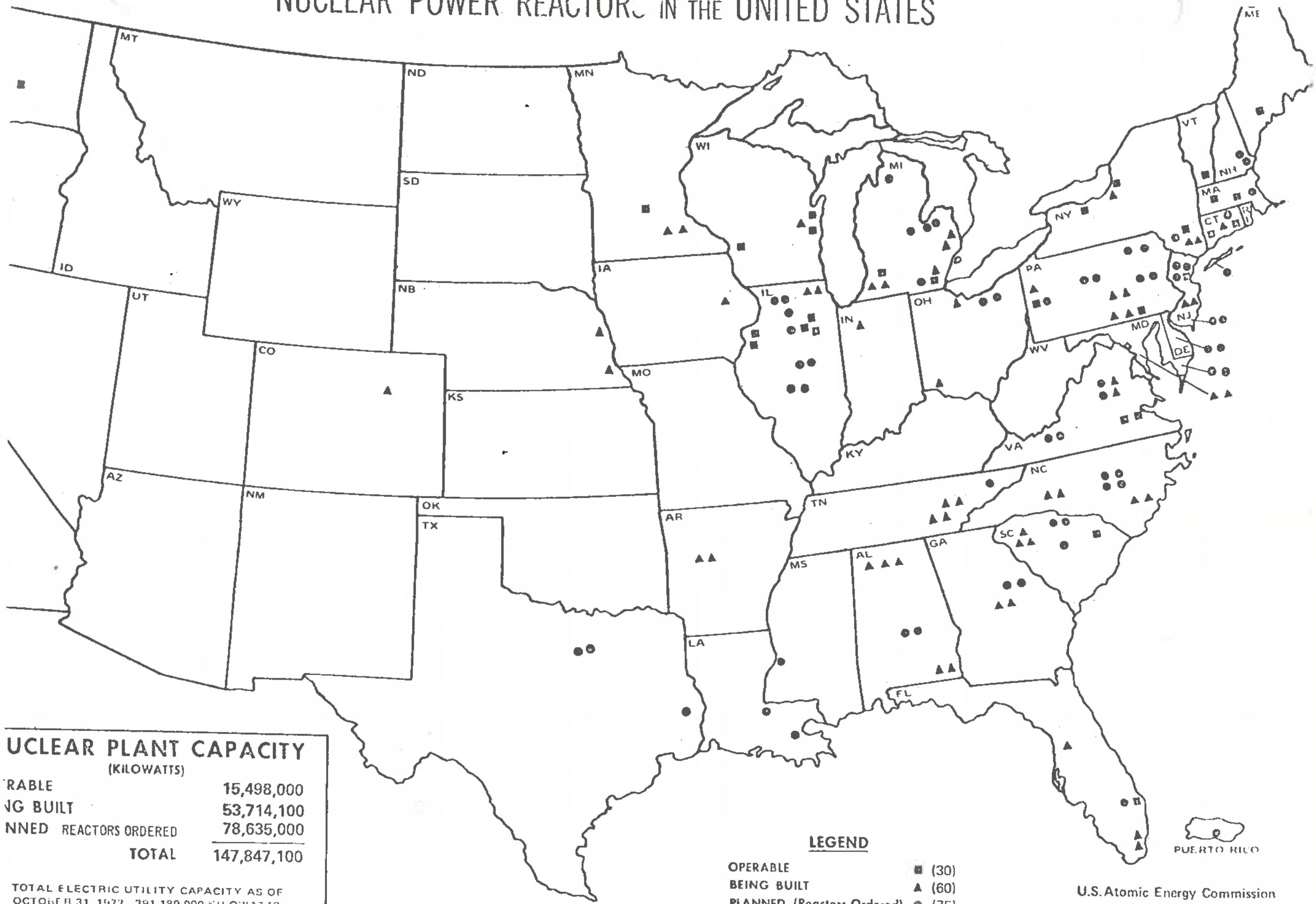


This AEC map shows the locations of the nuclear power reactors that were operable, being built, or planned (reactors ordered) as of December 31, 1972.

Domestic Reactor Sales by Vendors

	Units	Capacity Mwe	% Cap.
Babcock & Wilcox	21	18,694	13
Combustion Engineering	14	12,738	9
General Electric	55	51,813	35
Gulf General Atomic	7	5,690	4
Westinghouse	62	56,340	39
Total	159	145,275	100

NUCLEAR POWER REACTORS IN THE UNITED STATES



UCLEAR PLANT CAPACITY

(KILOWATTS)

'RABLE	15,498,000
NG BUILT	53,714,100
NNED REACTORS ORDERED	78,635,000
TOTAL	147,847,100

TOTAL ELECTRIC UTILITY CAPACITY AS OF OCTOBER 31, 1972. 391,180,000 KILOWATTS

of Information Center, Oak Ridge, Tennessee

LEGEND

OPERABLE	■	(30)
BEING BUILT	▲	(60)
PLANNED (Reactors Ordered)	●	(75)

(over)

U.S. Atomic Energy Commission
March 31, 1973

will require only a limited number of research reactor physicists. Rather the nuclear power industry is more directly in need of more broadly trained nuclear engineers who can combine their specialized knowledge of nuclear design with other aspects of nuclear reactor design, such as thermal analysis, mechanical design, materials problems, and fuel economics.

Hence the nuclear engineer must learn to interact with a variety of other disciplines, including mechanical engineering, electrical engineering, civil engineering, metallurgy, and even economists and accountants. Although the bulk of the newly trained nuclear engineers still end up with reactor manufacturers, more and more will find themselves as the resident nuclear expert in an electrical utility or an engineering firm engaged in the construction or servicing of nuclear power plants.

The problems faced by future nuclear engineers are complex and overlap a wide range of considerations. One of the most significant areas of problems concerns nuclear reactor safety. Although a large number of nuclear power plants have been successfully constructed and operated for years without incident, there still remain a number of important unanswered questions about nuclear reactor safety. These questions will be accentuated with the introduction of the fast breeder reactor later in this decade.

A related problem area concerns the impact of nuclear power plants upon their environment. Perhaps of most general concern has been the limitation of release of low level radioactivity, and the restrictions placed upon the release of waste heat. These releases can certainly be controlled (although with a certain economic penalty) to almost any desirable limit. Of more serious concern is the handling of the radioactive waste (spent fuel) produced in the reactor. This problem, although not serious at the present time, will require substantial attention as the number of nuclear plants grows.

And, of course, the nuclear engineer must always be concerned with the economic design and operation of the plant, since such plants must produce electrical energy as cheaply as possible. And all of these problems must be confronted and handled in the public arena.

V. THE SCOPE OF THE TEXT

Our goal in this text is to develop in some detail the underlying theory of nuclear fission reactors. Our intent is to begin always with the fundamental scientific principles governing nuclear fission chain reactions, and to carry these fundamental concepts through to the level of realistic engineering applications in reactor core design. During this development, however, it is important not to lose sight that any realistic nuclear analysis of a reactor core cannot be decoupled from a parallel non-nuclear analysis--including considerations of thermal-hydraulic behavior, materials limitations, and so on.

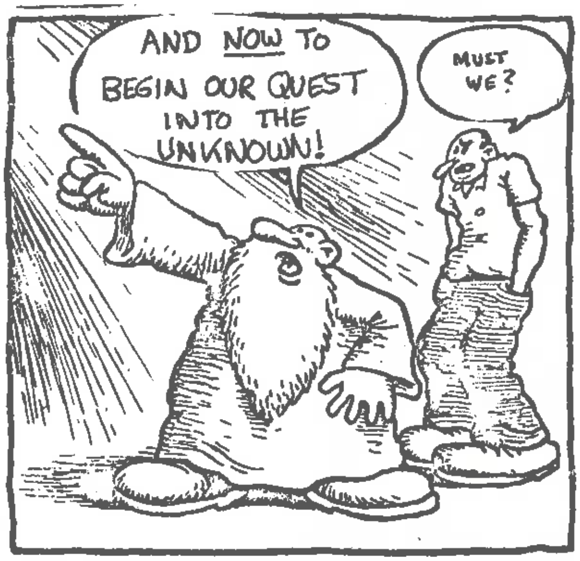
The basic program involves four progressive stages. We will first give a very brief introduction to those concepts from nuclear physics which are relevant to nuclear fission reactors. These include not only some of the details of the nuclear fission reaction, but as well a consideration of the various ways in which neutrons (which act as the carrier of the chain reaction) interact with nuclei. It should be stressed that this brief introduction is not intended to be complete in itself, but to serve rather as a review and a point of departure for the further development.) We then consider from a qualitative viewpoint the general concepts involved in studying nuclear chain reactions. The introductory section then ends with an overview of nuclear reactor engineering, including a consideration of both the components and the various types of modern nuclear reactors, as well as a qualitative discussion of nuclear reactor design.

The latter three sections of the text are intended to develop the fundamental scientific principles underlying nuclear reactor analysis and then to apply these principles to derive the most common analytical tools used in contemporary reactor design. By way of illustration, these tools are then applied to analyze several of the more common and significant problems which face nuclear engineers.

The second section develops the mathematical theory of neutron transport in a reactor core. It begins with the most general description based upon the neutron transport equation, and briefly reviews qualitatively) the standard approximations to this equation. After this brief discussion, we turn quickly to the development of the simplest nontrivial model of a nuclear fission reactor--that based upon one-speed neutron diffusion theory. This model is used to analyze both the steady state and time dependent behavior of nuclear reactors, since although the model has very limited validity in practical reactor calculations, it does illustrate most of the concepts as well as the calculational techniques used in actual reactor design.

In the third section, we develop the principal tool of modern reactor design, the multigroup diffusion model. Particular attention is devoted to the calculation of the group constants appearing in these equations, as well as to the practical numerical solution of the equations themselves.

In the final section, we attempt to give an overview of methods used in nuclear reactor design. In particular, we consider the application of the concepts and tools developed in the earlier sections to a variety of problems faced by the nuclear engineer (such as criticality calculations, burnup and control studies, fuel management, etc.). We then conclude with a more detailed description of the manner in which the nuclear reactor interfaces with the design of a modern nuclear power plant.



CHAPTER 2: THE INTERACTION OF NEUTRONS WITH MATTER

I. A REVIEW OF NUCLEAR PHYSICS

It is useful to begin our development of the theory of nuclear fission reactors with a very brief review of nuclear physics. It should be stressed that this review is not intended to be complete but rather to remind the student of those features of nuclear physics which are significant in discussing nuclear fission chain reactions. Students who are not familar with the material in this chapter should consult one of the standard references[1] on introductory nuclear physics which contain substantially more thorough discussions of these topics.

A. Nuclear Structure

The atomic nucleus is composed of two types of subnuclear particles, the proton and the neutron, whose respective mass and charge are:

proton: $m_p = 1.67252 \times 10^{-24}$ gm, charge = + 1

neutron: $m_n = 1.67482 \times 10^{-24}$ gm, charge = neutral

These particles, called nucleons, are packed tightly together in a roughly spherical structure of essentially uniform density to form the atomic nucleus. The Coulomb repulsion forces between the positively charged protons are counteracted by strong, short range nuclear forces which attract the nucleons together and bind them into the nucleus. The respective number of neutrons and protons in a given nucleus classify nuclei. It is customary to define:

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[1] I. Kaplan, Nuclear Physics (Addison-Wesley, 1963), Second Edition O. Oldenberg and N. Rasmussen, Modern Physics for Engineers (McGraw-Hill, 1966) R. D. Evans, The Atomic Nucleus (McGraw-Hill, 1955)

Number of protons:	Z	(atomic number)
Number of neutrons:	N	
Number of nucleons:	$A = N + Z$	(mass number)

The notation most frequently used to label a specific nucleus or nuclide is

$${}_{Z}X^{A}$$

where A is the mass number, Z is the atomic number, and X is the chemical symbol for the atom of interest. For example, ${}_{1}H^{1}$, ${}_{6}C^{12}$, or ${}_{92}U^{235}$ are notations for three such nuclides. A couple of useful terms are "isotopes" which refer to nuclei of the same Z, but different A [e.g., ${}_{92}U^{233}$, ${}_{92}U^{234}$, ${}_{92}U^{235}$, ${}_{92}U^{238}$] and "isomer" in which both Z and A are the same, but the nucleus may be in an excited state. [We usually denote this excited state by an asterisk, e.g., ${}_{92}U^{235*}$.]

The attractive nuclear forces which tend to bind the nucleons together tend to saturate. This leads to an essentially uniform nuclear density, regardless of the type of nuclide. Hence one finds that the nuclear volume, $V = 4/3\,\pi R^3$, goes essentially as the number of nucleons, A. If we assume the nucleus is essentially spherical in shape, then the effective radius of the nucleus is given by

$$R = 1.5 \times 10^{-13} A^{1/3} \text{ cm}$$

This estimate of nuclear size should be compared to the size of an atom which is typically 10^{-8} cm. This size difference will be very significant when we later compare nuclear reactions against the more familiar atomic (or "chemical") reactions.

B. Nuclear Binding Energies

Experiments indicate that the sum of the masses of the individual nucleons comprising a nucleus is always greater than the actual mass of the nucleus. This is easily understood in terms of the important result from the theory of relativity:

$$E = m\,c^2 \tag{2-3}$$

Hence, this mass difference can be interpreted as the binding energy holding the nucleus together. If one defines the "mass defect"*, Δ,

$$\Delta \equiv [A\,m_p + (A-Z)\,m_n] - M_A \tag{2-4}$$

where M_A is the mass of the nucleus of interest, then the corresponding binding energy for this nucleus is

$$E_b = \Delta\,c^2 \tag{2-5}$$

This binding energy which holds the nucleus together is the principal quantity we exploit in nuclear power generation. Suppose we compute the average binding energy per nucleon for each nucleus and plot it versus mass number A. Then one finds the curve shown in Figure 2-1.

One can interpret E_b/A as the net gain in binding energy attributable to the addition of a single nucleon to the nucleus. There is actually a "fine structure" superimposed upon this curve and caused by the fact that

---

*Technical Note: One should actually add in the mass of the electrons, since then one can use atomic masses:

$$\Delta = \underbrace{Z(m_p + m_e)}_{H\ \text{atom}} + (A-Z)\,m_n - \underbrace{(M_A + Z m_e)}_{A\ \text{atom}}$$

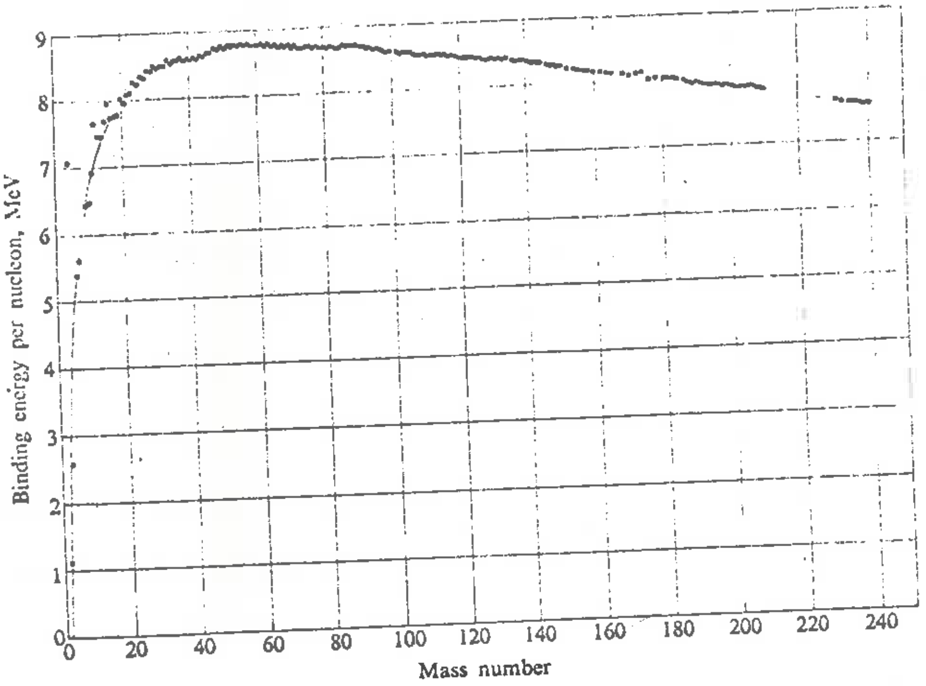


FIGURE 2-1: Binding Energy per Nucleon as a Function of Mass Number

certain nuclei are more stable than others (e.g., the nuclei with either N or Z equal to a "magic number", 2, 6, 8, 14, 20, 28, 50, 82, or 126). These nuclear systematics are closely analogous to the "shell" structure interpretation of the periodic table which orders atoms.

For the present, however, we are more concerned with the general trend of this curve. Suppose first we combine or "fuse" together two light nuclei to make a heavier nucleus. Then the average binding energy per nucleon increases, which implies a net energy release. An important example of such a <u>nuclear fusion</u> reaction is

$$ {}_1D^2 + {}_1T^3 \longrightarrow {}_2He^4 + {}_0n^1 + 17 \text{ MeV} \tag{2-6} $$

Such reactions are of considerable interest in achieving net energy production using controlled fusion reactions. Unfortunately these light nuclei are charged and strongly repel one another. One must heat them up to sufficiently high temperatures (and hence velocities) that the Coulomb repulsion will be overcome. Unfortunately net energy release from such "thermonuclear" fusion reactions as yet to be achieved. (Although, an uncontrolled application of such reactions has been achieved--the H-bomb).

One can take an alternative tact, and try to split up or "fission" very heavy nuclei to produce two lighter nuclei, each with a larger binding energy per nucleon. Then one could achieve a net energy production by means of such <u>nuclear fission</u> reactions.

But how do we split up a heavy nucleus? Well, from the discussion of fusion reactions, it is apparent that we can't just slam two nuclei together since their charges would strongly repel one another. An alternative idea is to slam a neutral particle into a big, "overweight" nucleus, and hope that this splits it. An ideal candidate for the incident particle is the neutron. Indeed, experiments have shown that certain nuclei have an enormous appetite for neutrons, but after swallowing them, run into a case of violent indigestion which causes them to fission. As an example of such a reaction, consider

$$ {}_0n^1 + {}_{92}U^{235} \longrightarrow \text{fission products + more neutrons} \qquad (2\text{-}7)$$

The fission products (i.e., the lighter nuclei) emerge with very large energies (~ 190 MeV) which can then be converted into heat energy. But just as significantly, the fission reaction kicks loose a few neutrons which can then go on to induce more fission reactions. Hence we can use the neutrons to propagate a "chain" of fission reactions. This, of course, is the principal topic of this course.

C. Radioactive Decay

Certain nuclei are unstable in the sense that they may spontaneously undergo a transformation into a different nuclide--usually accompanied by the emission of energetic particles. Such a spontaneous nuclear transformation is referred to as "radioactive decay". Only three types of radioactive decay are found in naturally occurring nuclides--alpha-decay which corresponds to the emission of an helium nucleus, ${}_2He^4$, beta-decay which corresponds to the internal conversion of a neutron in the nucleus into a proton, with the corresponding emission of an electron and a neutrino, and gamma-decay, the change of a nucleus from one isomeric state to a lower isomeric state with the accompanying emission of a photon.

Other types of radioactive decay are possible in a nuclear reactor, however, since there will be many unstable nuclides produced which do not occur in nature. For example, certain nuclei decay by emitting a neutron (we will find that this decay process is of particular importance for reactor applications).

The basic law describing radioactive decay is based upon the experimental observation that the probability that a nucleus will decay in a given time interval is constant--independent of the age of the nucleus or its environment, dependent only upon the type of the nucleus itself. Hence the time rate of change of the number of original nuclei of a given type must be proportional to the number of nuclei present at that time

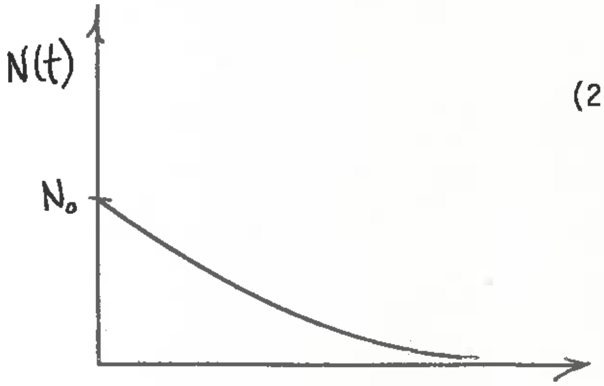
$$\text{rate of decay} \quad \propto \quad \text{number of nuclei} \tag{2-8}$$

Let us call the proportionality constant λ. Then if N is the number of original nuclei left at a time t, we find

$$-\frac{dN}{dt} = \lambda N(t) \; . \tag{2-9}$$

Here, λ is referred to as the radioactive decay constant characteristic of the nucleus and has units of inverse time. If we initially have N_o nuclei present, then at any later time the number of nuclei present will be given by an exponential law:

$$N(t) = N_o e^{-\lambda t} \tag{2-10}$$



Now the rate that which nuclei are decaying is given (from Eq. 2-8)

$$\text{rate} = \lambda N_0 e^{-\lambda t} \quad . \tag{2-11}$$

From this time behavior, it is apparent that the probability that a given nucleus will decay in a time interval t to t + dt is just

$$p(t)\, dt = \lambda e^{-\lambda t} dt \quad . \tag{2-12}$$

Since radioactive decay is a statistical phenomenon, we cannot predict with any certainty precisely when a given nucleus will decay. However we can calculate the mean lifetime of the nucleus, t, before decay using our expression for p(t) in Eq. (2-11):

$$\bar{t} \equiv \int_0^\infty dt\, t\, p(t) = \lambda \int_0^\infty dt\, t e^{-\lambda t} = 1/\lambda \; . \tag{2-13}$$

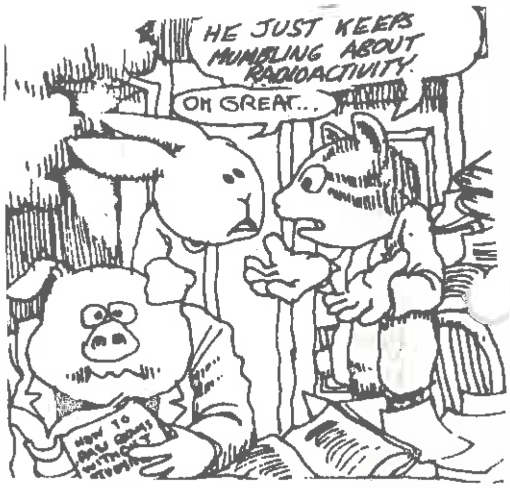
Hence, on the average, a given nucleus will decay after a time $1/\lambda$.

A closely related quantity is the length of time necessary for half of the original number of nuclei to decay away. Such a time, $T_{1/2}$, is referred to as a radioactive "half-life" for the nucleus and can be calculated from its definition by noting

$$N(T_{1/2}) = N_0/2 = N_0 e^{-\lambda T_{1/2}} \tag{2-14}$$

or

$$T_{1/2} = \frac{\ln 2}{\lambda} \quad .$$



One most frequently finds the radioactive half-lives of various unstable nuclei tabulated, rather than the mean life $\bar{t}$ or the decay constant λ.

A final definition of importance is the "activity" of a sample of radioactive nuclei. This is simply the total number of disintegrations occurring per second--that is,

$$\text{activity} = \lambda N$$

where N is the number of nuclei present at the time of interest. Activities are usually measured in units of "curies", where one curie (Ci) is defined to be that quantity of radioactivity nuclide in which the number of disintegrations per second is 3.7000 x 10^{10}. (This is roughly the activity of 1 g of radium.)

Most radioactive decay processes are somewhat more complicated than those described by Eq. (2-9). For example, the decaying nuclide may itself be produced by some type of source of, say, R(t) nuclei/sec. Then the nuclide balance equation becomes

$$\frac{dN}{dt} = -\lambda N(t) + R(t) . \qquad (2\text{-}16)$$

We can also write similar equations which describe several nuclear isotopes each of which decays into another. Consider, by way of example, the radioactive decay "chain"

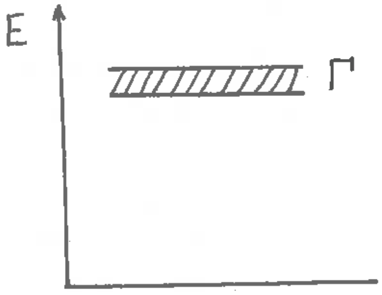
$$X \xrightarrow{\lambda_x} Y \xrightarrow{\lambda_y} Z \xrightarrow{\lambda_z} \qquad (2\text{-}17)$$

Then the appropriate equations describing the number of nuclides of each type present are

$$
\begin{aligned}
\frac{dN_x}{dt} &= -\lambda_x N_x + R_x \\
\frac{dN_y}{dt} &= -\lambda_y N_y + \lambda_x N_x + R_y \\
\frac{dN_z}{dt} &= -\lambda_z N_z + \lambda_y N_y + R_z \quad .
\end{aligned}
\tag{2-18}
$$

where $R_x(t)$ is the production term for the X-nuclide, and so on. Since this is just a system of linear first-order ordinary differential equations with constant coefficients, it can easily be solved in the usual manner, and hence, we will defer further discussion to the problems at the end of the chapter.

Very similar considerations also held for the transitionof nuclei between different isomeric states. Such states represent the quantum levels available to the nucleus. We can again characterize the probability that the nucleus will "decay" out of one excited state into a lower state by a decay constant λ --hence again developing the concept of a mean lifetime for the excited state, $\bar{t}$. A useful related concept here is the uncertainty of "width" Γ of the energy characterizing the excited state. This width is related to the mean lifetime of the state by the Heisenberg uncertainty relation



$$\Delta t \, \Delta E > \hbar \quad . \tag{2-19}$$

Hence the width of the state can be expressed in terms of its decay constant by

$$\Gamma = \Delta E = \hbar / \Delta t = \hbar \lambda \quad . \tag{2-20}$$

D. Nuclear Reactions

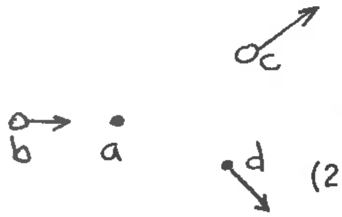
Nuclear reactions are very similar to chemical reactions--except for the fact that they occur with far smaller probability. This is a consequence of the relative sizes of the nuclei compared to atomic (10^{-12} cm versus 10^{-8} cm). In a sense, one can predict that since the effective "cross sectional areas" of nuclei are some 10^{-8} those of atoms, we would require nuclei to run into each other some 10^{8} times more frequently to achieve the same rate of reactions as obtained with atoms.

A notation very similar to that used to describe chemical reactions is used for nuclear reactions

$$a + b \longrightarrow c + d \qquad (2\text{-}21)$$

However, since in nuclear reactions, one particle is usually considered as a projectile while the other is taken as a target, one sometimes uses the more detailed notation

$$\underset{\text{target}}{\underset{\uparrow}{a}}(\underset{\text{projectile}}{\underset{\uparrow}{b}},c)\,d \qquad (2\text{-}22)$$



As an example, the reaction

$${}_8O^{16} + {}_0n^1 \longrightarrow {}_7N^{16} + p \qquad (2\text{-}23)$$

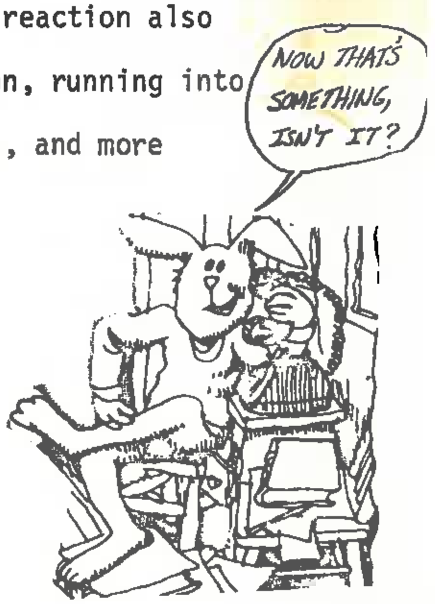
would be written as

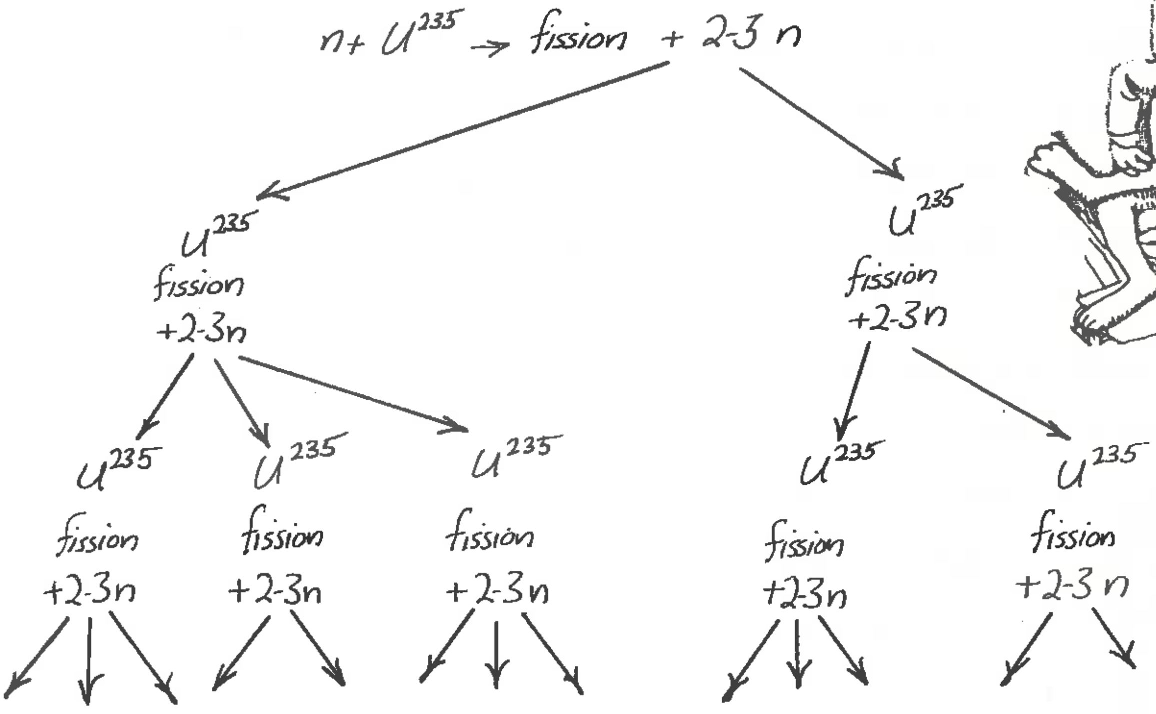
$${}_8O^{16}\,(n,p)\,{}_7N^{16} \,. \qquad (2\text{-}24)$$

The third reaction of importance is scattering. In this reaction, the neutron simply scatters off of the nucleus (although in some cases, it may first combine with the nucleus to form a compound nucleus for a short time before being reemitted). Both radiative capture and scattering are extremely important reactions in nuclear reactors, and we will return to discuss them in more detail later in this chapter.

E. Nuclear Fission Chain Reactions

The energy released in nuclear fission reactions is the prime objective in a nuclear reactor. However the key element in the successful liberation of this energy is the neutron. Not only does the neutron induce the fission reaction, but in addition it serves to propagate a chain of such reactions from one nucleus to another. A general schematic involves an initial neutron incident upon, say a U^{235}, nucleus, which induces a fission reaction. As we have seen, the fission reaction also produces from 2 to 3 new neutrons which can now continue on, running into more uranium nuclei and hence inducing still more fissions, and more neutrons, and so on.





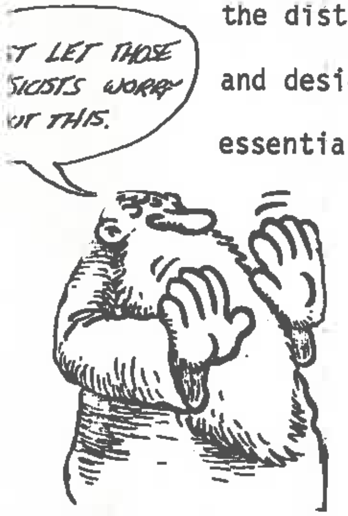
In this sense, the neutrons act as the "chain carriers" which propagate a fission chain reaction.

But of course there are other possible nuclear reactions a neutron can undergo which do not lead to fission and hence are unproductive in nature. For example, the neutrons could be captured by a nucleus in a (n, γ) reaction. Or the neutron could scatter off a nucleus and fly out of the uranium core of the reactor. Either process removes neutrons from the chain, thereby inhibiting the chain reaction.

Hence there are evidently two tasks which we must direct our attention to if we are to build a nuclear fission reactor. First we must learn how to determine the neutron population in the reactor, since this will determine whether a chain reaction is possible. The job of following the neutron "economy" in order to assure a stable chain reaction is usually addressed by a nuclear engineer and is referred to as <u>nuclear reactor theory</u>. It is the subject of this text.

However, even if we can maintain a stable chain of fission reactions, we must still learn how to extract and use the energy liberated in these reactions. This task involves the subjects of heat transfer, fluid flow, stress and materials analysis, and power systems analysis and interacts strongly with the nuclear analysis of a reactor core.

The principal goal of nuclear reactor theory, then, will be to predict the distribution of neutrons in a chunk of material in order to understand and design a fission chain reaction system. We will need to consider essentially two subjects:



(i) The probabilities of occurrence of various neutron-nuclear reactions, which are given in terms of so-called nuclear "cross sections",

(ii) The derivation and solution of an equation which uses these "cross sections" to determine the neutron density in a nuclear reactor core. This is known as the <u>neutron transport equation</u>.

II. CROSS SECTIONS AND REACTION RATES

A. Microscopic Cross Sections

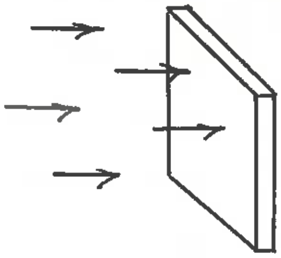
The probability for a neutron-nuclear reaction to occur is related to the concept of a "nuclear cross section". Let us first define this quantity operationally by considering a thin target (say, one atomic layer thick) upon which is incident a beam of monoenergetic, monodirectional neutrons. Such an experiment would then find that the rate at which neutron-nuclear reactions occur in the sample is proportional to

(i) number of neutrons incident upon the target per unit time and per unit area $\equiv I$

(ii) cross sectional area of the target $\equiv a$

(iii) target thickness $\equiv x$

(iv) atomic density of target $\equiv N$



If we call the constant of proportionality σ, then we can write the rate at which reactions occur as

$$\underset{[\#/\text{sec}]}{\text{rate}} = \underset{[\text{cm}^2]}{\sigma}\quad \underset{[\#/\text{cm}^2\text{-sec}]}{I}\quad \underset{[\#/\text{cm}^3]}{N}\quad \underset{[\text{cm}^2]}{a}\quad \underset{[\text{cm}]}{x} \tag{2-26}$$

We have indicated the units of each of these quantities, since they imply that σ must have the units of an area. More generally then, we define the microscopic cross section σ by

$$\sigma \equiv \frac{\text{\# of events of given kind/nucleus/sec}}{\text{\# of incident neutrons/cm}^2\text{/sec}} = \frac{\text{rate}}{\left(Nax/I\right)} \quad . \qquad (2\text{-}27)$$

In this sense, then, we can interpret

$$\frac{\sigma}{a} = \text{probability per nucleus that a neutron in the beam will interact with it} \qquad (2\text{-}28)$$

One might think of σ as the effective cross sectional area present by the nucleus to the beam of neutrons. Since the nuclear radius is roughly

$$R \sim 10^{-12} \text{ cm}$$

then the geometric area of the nucleus is roughly 10^{-24} cm^2. Hence one might expect that nuclear cross sections are of the order of 10^{-24} cm^2. In fact, microscopic cross sections are usually measured in units of barns, where 1 barn $\equiv 10^{-24}$ cm^2. The geometrical interpretation of a nuclear cross section can frequently be misleading, however, since σ can be much larger than the geometrical cross section of the nucleus (as large as 10^6 barns, in fact) due to resonance effects (which, in turn, are a consequence of quantum mechanics and the wave nature of the incident neutron).

One can define a different cross section for each type of neutron-nuclear reaction and each type of nuclide. For example, some common types of cross sections include:

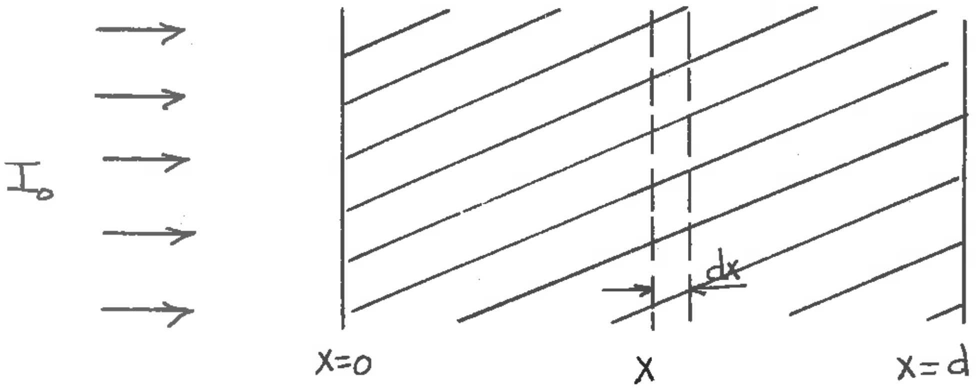
σ_s elastic scattering

σ_i inelastic scattering

σ_γ or σ_c	radiative capture
σ_f	fission
σ_t	total $\equiv \sigma_s + \sigma_i + \sigma_\gamma + \sigma_f + \cdots$
σ_a	absorption $\equiv \sigma_\gamma + \sigma_f$
σ_{ne}	nonelastic $\equiv \sigma_t - \sigma_e$

B. Macroscopic Cross Sections

Thus far we have considered a beam of neutrons incident upon a very thin target. This was done so as to insure that each nucleus in the target would be exposed to the same beam intensity. If the target were thicker, then the nuclei deeper into the target would tend to be shielded from the beam by the nuclei on the surface of the sample, since interactions remove neutrons from the incident beam. To account for such finite thickness effects, let us now consider a neutron beam incident upon the surface of a target of arbitrary thickness d.



We will now derive an equation for the "virgin" beam intensity I(x) at any point x in the target. By virgin beam, we are here referring to that portion of the beam neutrons which have not interacted with target nuclei. Consider a differential thickness of target between x and x + dx. Then since dx is infinitesmal, we know the results from our study of thin targets can be used to calculated the interaction rate in dx.

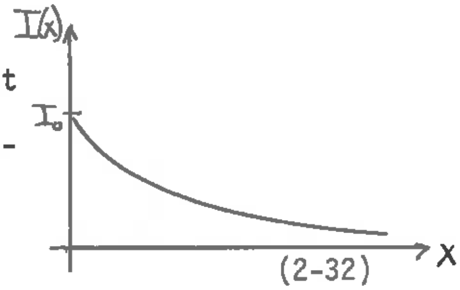
$$\text{interaction rate in } dx = \sigma I N a\, dx \ . \qquad (2\text{-}29)$$

But the decrease in the beam intensity between x and x + dx is just

$$-dI(x) = -\left[I(x+dx) - I(x)\right] = \frac{\sigma I(x) N a\, dx}{a} \ . \qquad (2\text{-}30)$$

If we divide by dx, we find a differential equation for I(x):

$$\frac{dI}{dx} = -N\sigma I(x) \ . \qquad (2\text{-}31)$$

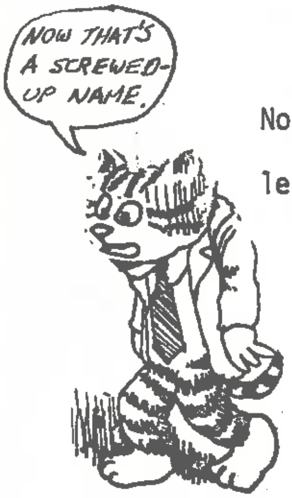


If we solve this equation, subject to an incident beam intensity of I_0 at x=0, we find an exponential attenuation of the incident beam

$$I(x) = I_0 e^{-N\sigma x} \ . \qquad (2\text{-}32)$$

It is convenient to define the produce of atomic density, N, and the microscopic cross section, σ , as a new quantity, the <u>macroscopic cross section</u>

$$\Sigma \equiv N\sigma = \left[\#/\text{cm}^3\right]\left[\text{cm}^2\right] = \left[\text{cm}^{-1}\right] \ . \qquad (2\text{-}33)$$



Notice that Σ is really not a "cross section" since its units are inverse length. In fact, if we write

$$\Sigma = -\frac{dI}{dx}\Big/ I = -\frac{dI}{I}\Big/ dx \ , \qquad (2\text{-}34)$$

then we can interpret Σ as the probability per unit path length traveled that the neutron will undergo a reaction with a nucleus in the sample.

In this sense, then

$e^{-\Sigma x} \equiv$ probability that neutron moves a distance dx without interaction

$\Sigma e^{-\Sigma x} dx \equiv$ probability that neutron has its first interaction in dx

$\equiv$ $p(x)\,dx$

With this probability, we can calculate the mean distance a neutron travels before interacting with a nucleus in the sample as

$$\bar{x} \equiv \int_0^\infty dx\, x\, p(x) = \Sigma \int_0^\infty dx\, x\, e^{-\Sigma x} = 1/\Sigma \tag{2-35}$$

$\equiv$ "mean free path"

Notice the similarity of this analysis to our treatment of radioactive decay. Both the spatial attentuation of a neutron beam passing through a sample of material as well as the temporal attentuation of a sample of radioactive nuclei are statistical pheonmena. It should be stressed that both the mean free path as well as the mean life time for decay are very much average quantities. In general, there will be fluctuations about these mean values.

If we note that Σ is the probability per unit path length that a neutron will undergo a reaction, while the neutron speed v is the distance traveled by the neutron in a unit time, then evidently

$$v\Sigma = \left[\frac{cm}{sec}\right]\left[\frac{1}{cm}\right] = \left[\frac{1}{sec}\right] \equiv \text{frequency with which reactions occur} \tag{2-36}$$

$\equiv$ "collision frequency"

In the same sense,

$$\frac{1}{v\Sigma} = [\mathrm{sec}] \equiv \text{mean time between reactions} \qquad (2\text{-}37)$$

Thus far we have avoided specifying precisely what type of neutron-nuclear reaction we are talking about. In fact, this analysis can be used to define the macroscopic cross section for any specific reaction,

$$\Sigma_f = N\sigma_f \;,\quad \Sigma_a = N\sigma_a \;,\quad \Sigma_t = N\sigma_t \;,\ldots \qquad (2\text{-}38)$$

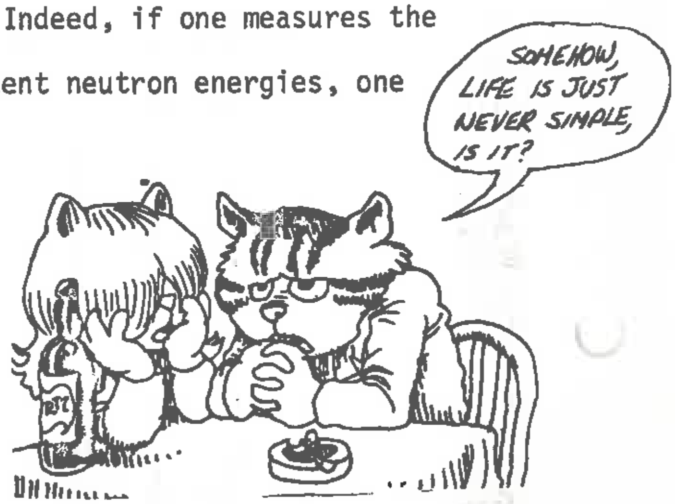
It can also be generalized to define the macroscopic cross sectons for homogeneous mixtures of nuclides. For example, if we have a homogeneous mixture of materials X, Y, and Z, with respective atomic densities N_X, N_Y, and N_Z, then the total macroscopic cross section, for example, is given by

$$\Sigma_t = N_X \sigma_t^X + N_Y \sigma_t^Y + N_Z \sigma_t^Z \qquad (2\text{-}39)$$

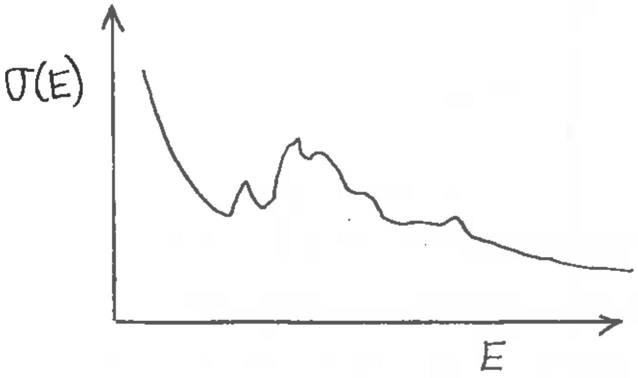
where σ_t^X is the microscopic total cross section for nuclide X, etc.

C. Some Generalizations

Thus far we have defined cross sections for monoenergetic, monodirectional beams of neutrons incident upon homogeneous media. It is certainly conceivable that such cross sections will vary, depending upon the incident neutron energy or direction. Indeed, if one measures the microscopic cross section for various incident neutron energies, one finds a strong energy dependence:

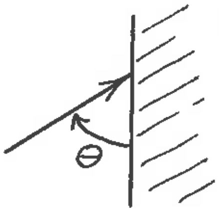


$$\sigma \rightarrow \sigma(E)$$



There may also be a dependence upon the incident neutron angle, say

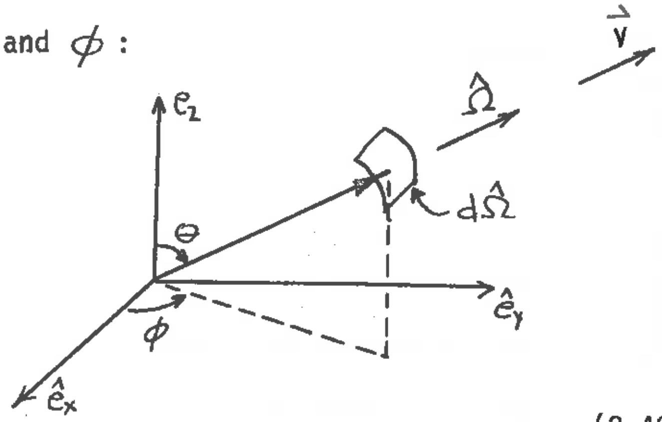
$$\sigma \rightarrow \sigma(\theta)$$



--but, fortunately, this angular dependence can usually be neglected in nuclear reaction applications.

There is a generalization of the cross section σ_s for scattering of a neutron from a nucleus which does depend upon angle, however. This is known as the "differential scattering cross section" and describes the probability that a neutron is scattered from a nucleus through a certain angle, say θ .

To be more precise, let $\hat{\Omega}$ be a unit vector in the direction of the neutron motion. We usually write $\hat{\Omega}$ in terms of the spherical coordinate angles θ and ϕ :



$$\hat{\Omega} = \hat{e}_x \sin\theta \cos\phi + \hat{e}_y \sin\theta \sin\phi + \hat{e}_z \cos\theta \, . \tag{2-40}$$

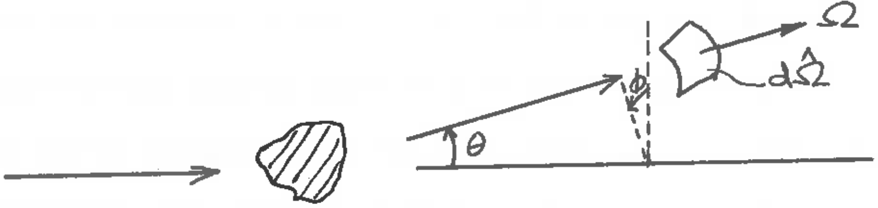
Note that the velocity of the neutron can then be written as

$$\vec{v} = v\hat{\Omega} \quad \text{or} \quad \hat{\Omega} = \vec{v}/|\vec{v}| \qquad (2\text{-}41)$$

The differential of $\hat{\Omega}$, $d\hat{\Omega}$, corresponds to a differential solid angle. One usually specifies the direction of motion in terms of spherical coordinates, θ and ϕ. Then, more explicitly,

$$d\hat{\Omega} = \sin\theta \, d\theta \, d\phi \qquad (2\text{-}42)$$

With these definitions, let us now consider the number of neutrons scattered per second into a solid angle $d\hat{\Omega}$ about $\hat{\Omega} = (\theta, \phi)$:



This scattering rate will again be proportional to the incident beam intensity I, the atomic number density N, the sample area A, the sample thickness x, and in addition, the solid angle $d\hat{\Omega}$. The proportionality constant will be defined as the differential scattering cross section

$$\#\text{ scattered into } d\hat{\Omega}\text{ /sec} = \sigma_s(\theta,\phi)\, I N a x \, d\hat{\Omega} \qquad (2\text{-}43)$$

Actually, for most materials, $\sigma_s(\theta,\phi)$ depends only upon the cosine of the scattering angle, θ, and not upon the azimuthal angle ϕ. If we consider a neutron incident from an initial direction $\hat{\Omega}$ and scattered into a final direction $\hat{\Omega}'$:

then obviously, $\cos\theta = \hat{\Omega}\cdot\hat{\Omega}'$, and we can write

$$\sigma_s(\theta) = \sigma_s(\hat{\Omega}\cdot\hat{\Omega}') \, . \qquad (2\text{-}44)$$

There are several alternative notations for the differential scattering cross section, including

$$\frac{d\sigma_s}{d\Omega}(\hat{\Omega}\rightarrow\hat{\Omega}') \quad \text{or} \quad \sigma_s(\hat{\Omega}\rightarrow\hat{\Omega}') \qquad (2\text{-}45)$$

We can similarly introduce the concept of a differential scattering cross section describing the probability of scattering from an incident energy E to a final energy E'

$$\frac{d\sigma_s}{dE}(E\rightarrow E')$$

or

$$\sigma_s(E\rightarrow E')$$

(2-46)

Finally, one can combine these ideas to define a "double differential scattering cross section" which characterizes scattering from an incident direction $\hat{\Omega}$, energy E, to a final direction $\hat{\Omega}'$, energy E':

$$\frac{d^2\sigma_s}{d\Omega\, dE}(\hat{\Omega}, E\rightarrow\hat{\Omega}', E')$$

or

$$\sigma_s(\hat{\Omega}, E\rightarrow\hat{\Omega}', E')$$

or

$$\sigma_s(E\rightarrow E', \hat{\Omega}\rightarrow\hat{\Omega}')$$

Notice that

$$\sigma_s(E\to E') = \int_{4\pi} d\hat{\Omega}\, \sigma_s(E\to E',\hat{\Omega}\to\hat{\Omega}') , \qquad (2\text{-}48)$$

$$\left[\int_{4\pi} d\hat{\Omega} \equiv \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\phi\right]$$

or

$$\sigma_s(E,\hat{\Omega}\to\hat{\Omega}') = \int_0^{\infty} dE'\, \sigma_s(E\to E',\hat{\Omega}\to\hat{\Omega}') , \qquad (2\text{-}49)$$

or

$$\sigma_s(E) = \int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE'\, \sigma_s(E\to E',\hat{\Omega}\to\hat{\Omega}') . \qquad (2\text{-}50)$$

We have explicitly noted in Eqs. (2-48) and (2-50) that while the scattering cross section usually depends upon the incident neutron energy, it does not normally depend upon its direction $\hat{\Omega}$. Only the differential scattering cross section depends strongly upon angle, and this dependence is upon the scattering angle itself, $\cos^{-1}(\hat{\Omega}\cdot\hat{\Omega}')$.

The concept of a differential scattering cross section can also be applied to macroscopic cross sections by merely multiplying by atomic number density N:

$$\Sigma_s(E\to E',\hat{\Omega}\to\hat{\Omega}') = N\sigma_s(E\to E',\hat{\Omega}\to\hat{\Omega}')$$

$$\Sigma_s(E\to E') = N\sigma_s(E\to E') \qquad (2\text{-}51)$$

$$\Sigma_s(\hat{\Omega}\to\hat{\Omega}') = N\sigma_s(\hat{\Omega}\to\hat{\Omega}')$$

It should be noted that macroscopic cross sections can have one additional dependence. Suppose the target material does not have a uniform or homogeneous density. Then N will depend upon the position $\vec{r}$ in the sample, and hence the macroscopic cross sections will be space dependent

$$\Sigma(\vec{r}) = N(\vec{r})\sigma \quad (2\text{-}52)$$

This situation arises very frequently in reactor studies.

Hence we have seen that nuclear cross sections can be used to characterize the probability of various types of neutron-nuclear reactions occurring. They obviously will be a very basic ingredient in any calculation of the neutron distribution in a reactor. For this reason, a very important facet of nuclear engineering is involved with measuring or calculating nuclear cross sections.

D. Characteristics of Neutron-Nuclear Cross Sections

The direct calculation of neutron cross sections involves two aspects:

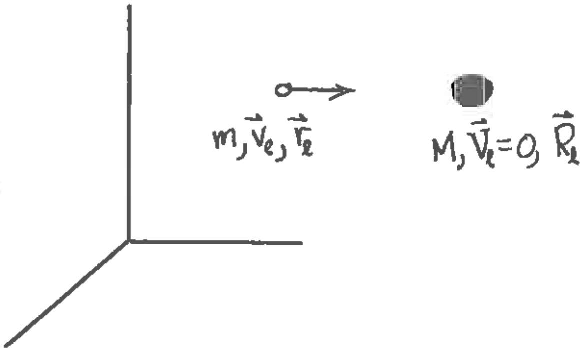
(i) the kinematics of two-particle collisions

(ii) the dynamics of nuclear reactions

The kinematics of two body collisions (i.e., the application of the laws of conservation of momentum and energy to such a collision) should be very familiar to the reader from introductory courses in mechanics or modern physics. However, for completeness, the kinematics of such collisions has been included in Appendix A. We will only review the results of such an analysis here.

1. Two-Body Kinematics

To be specific, consider the elastic scattering of a neutron from a stationary nucleus



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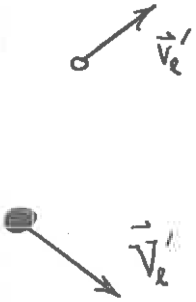
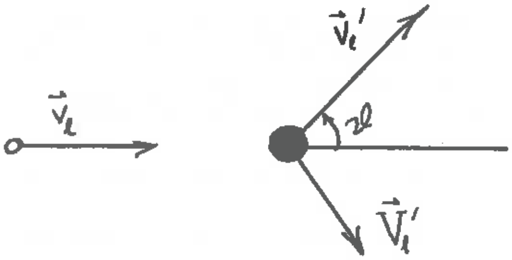
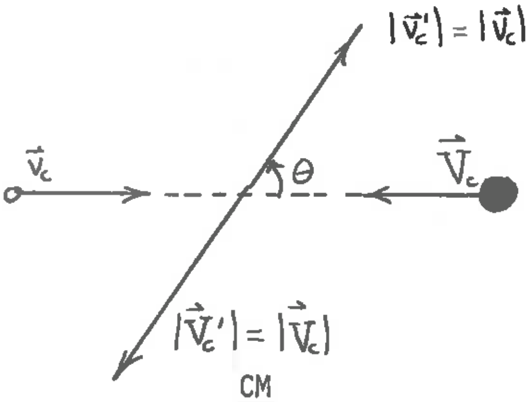


after

It is much more convenient when analyzing such collisions to transform from laboratory (LAB) to center of mass (CM) coordinates



LAB



CM

The energy, E_c , available for a nuclear reaction to occur in the CM system is given in terms of the incident neutron energy, E_ℓ , as

$$E_c = \frac{M}{m+M} E_\ell = \frac{A}{1+A} E_\ell . \qquad (2-53)$$

Note $E_c < E_\ell$, with the remainder of the energy appearing as the kinetic energy of the motion of the center of mass.

One can relate the two scattering angles by

$$\tan \vartheta = \frac{\sin \Theta}{\frac{1}{A} + \cos \Theta} \tag{2-54}$$

[In the more general case of inelastic scattering,

$$\tan \vartheta = \frac{\sin\Theta}{\gamma + \cos\Theta} \;, \quad \gamma = \frac{V_{CM}}{V_c'} \tag{2-55}$$

or

$$\cos\vartheta = \frac{\gamma + \cos\Theta}{\sqrt{\gamma^2 + 2\gamma\cos\Theta + 1}} \;. \;] \tag{2-56}$$

These relationships are of use in relating the differential scattering cross section in the LAB system to that in the CM system:

$$\sigma_L(\vartheta)\, d\hat{\Omega}_L = \sigma_c(\Theta)\, d\hat{\Omega}_c \tag{2-57}$$

or

$$\sigma_L(\vartheta) \sin\vartheta \, d\vartheta = \sigma_c(\Theta) \sin\Theta \, d\Theta \;. \tag{2-58}$$

Using (2-56) and some algebra yields

$$\sigma_L(\vartheta) = \sigma_c(\Theta) \frac{(\gamma^2 + 2\gamma\cos\Theta + 1)^{3/2}}{1 + \gamma\cos\Theta} \;. \tag{2-59}$$

It is important to note here that even though the differential scattering cross section as calculated in the CM system may be angle-independent, $\sigma_c \neq \sigma_c(\theta)$ [we refer to such a cross section as isotropic since it implies equal probabilities for scattering through any angle θ], the LAB differential scattering cross section will in general be angle dependence, i.e., anisotropic.

These topics are quite important, since cross sections are usually

(i) calculated in the CM system
(ii) measured in the LAB system
(iii) applied to reactor analysis in the LAB system

2. Mechanisms of Neutron-Nucleus Interactions

a. Compound nucleus formation

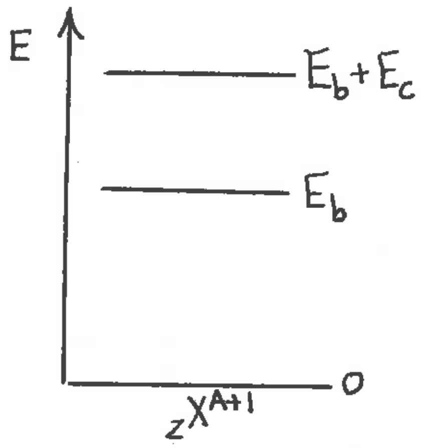
The general idea in such reactions is that the incident neutron is first absorbed by the nucleus ${}_ZX^A$ to create a new, "compound" nucleus ${}_ZX^{A+1}$. This compound nucleus later decays into a new nucleus.

The formation of a compound nucleus actually corresponds to a resonance reaction in which the incident neutron energy matches one of the virtual levels in the compound nucleus. [Since nuclei involve a number ofnucleons, it is possible to have excited states above the binding energy of a single nucleon, since this energy can be distributed among several nucleus so that no single nucleon has sufficient energy to be ejected. Such states are referred to as "virtual" states.] Consider a neutron incident upon a nuclide ${}_ZX^A$.

The energy available for such a reaction is the CM energy

$$E_c = \frac{1}{2}\left(\frac{mM}{m+M}\right) v_e^2 . \tag{2-60}$$

The actual energy of the excited level is much higher, due to the additional binding energy of the added neutron. This level will correspond to a virtual state since its energy is greater than the binding energy by E_c. The compound nucleus may remain in this virtual state for some time before decaying.



The second stage of the process is the decay of the compound nucleus state. This decay may occur in a variety of ways

$${}_0n^1 + {}_ZX^A \rightarrow ({}_ZX^{A+1})^* \rightarrow \begin{cases} {}_0n^1 + {}_ZX^A & \text{resonance elastic scattering} \\ {}_0n^1 + ({}_ZX^A)^* & \text{inelastic scattering} \\ {}_ZX^{A+1} + \gamma & \text{radiative capture} \\ {}_{Z_1}X_1^{A_1} + {}_{Z_2}X_2^{A_2} + \nu\,{}_0n^1 & \text{fission} \end{cases}$$

If $E_c + E_b$ is very close to a virtual nuclear energy level of the compound nucleus ${}_ZX^{A+1}$, one expects the probability for compound nucleus formation to be much larger than if $E_c + E_b$ doesn't "match" this energy level. Hence, we expect the cross sections for such compound nuclear reactions to

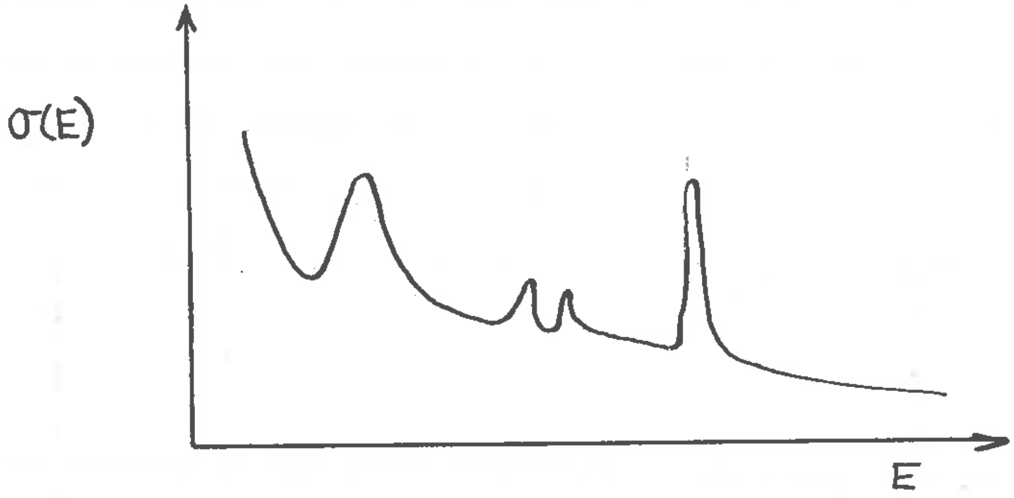
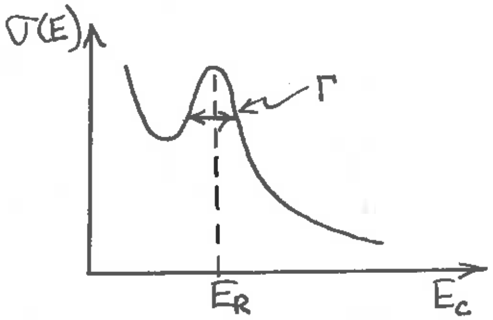


exhibit <u>resonances</u> at energy E_ℓ such that $E_c + E_b$ is close to a virtual energy level of ${}_ZX^{A+1}$.

A simple empirical expression can be written for the energy dependence of a cross section in the neighborhood of a single resonance:



$$\sigma(E_c) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_R}{E_c}} \; \frac{1}{4\frac{(E_c - E_R)^2}{\Gamma^2} + 1} \tag{2-62}$$

and

Γ = level width = (level decay constant) x $\hbar = \lambda\hbar$

Γ_n = line width for gamma emission

σ_0 = cross section at resonance

(2-63)

while

E_c = center of mass energy

E_R = resonance energy

This formula, known as the Breit-Wigner formula can be "derived" using arguments from nuclear physics.[1] It will prove quite useful in our later studies.

Most "interesting" neutron-nuclear reactions involve compound nucleus formation, including

radiation capture,
fission, and
inelastic scattering

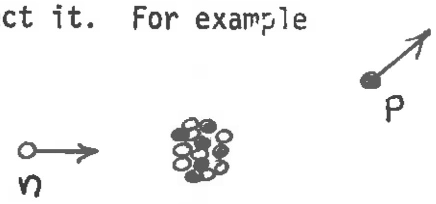
b. Potential scattering

Another type of reaction of considerable importance in reactor design is potential scattering in which the neutron scatters elastically off the nuclear potential, much as two billiard balls collide. In contrast to compound nucleus formation in which the neutron is absorbed by the nucleus, in potential scattering the neutron does not even penetrate the nucleus.

c. Direct interactions

At high energies ($\gtrsim 10$ MeV), the neutron can interact directly with a single nucleon in the nucleus and eject it. For example

(n,p)



and

(n,n')

are examples of such direct interactions. These reactions are usually of secondary importance in reactors however, since they require rather large incident energies.

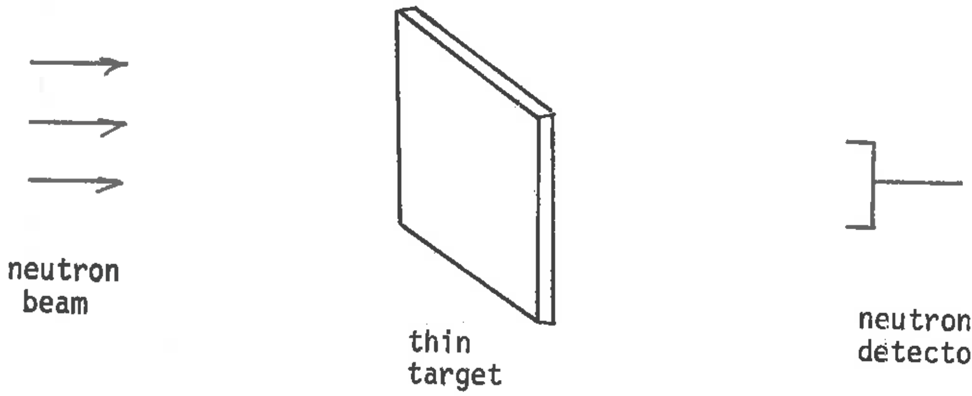
3. Qualitative Discussion of Neutron Cross Sections

a. Total neutron cross sections

Recall that we defined the total cross section for neutron-nuclear reactions as the sum of the cross sections for each type of reaction

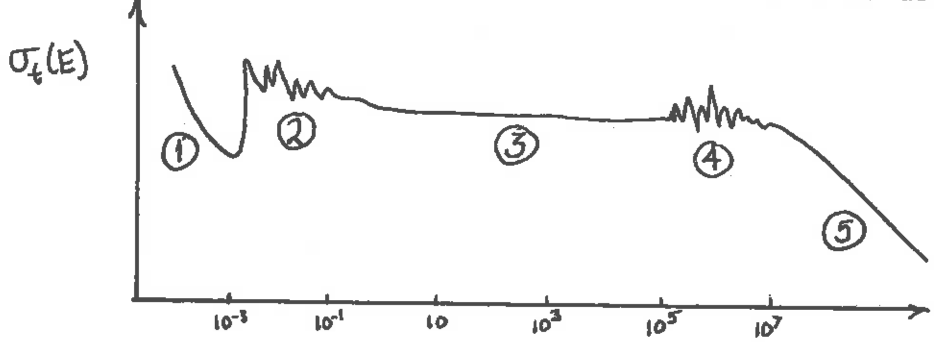
$$\sigma_t = \sigma_s + \sigma_{in} + \sigma_\gamma + \sigma_f + \cdots \tag{2-64}$$

Such cross sections can be measured rather directly by performing transmission experiments such as those used to define the cross section--that is, shooting a monoenergetic beam of neutrons of energy E at a thin target, and then measuring the fraction of the incident beam which penetrates the sample.



It is of considerable interest to study the dependence of such cross sections on the incident neutron energy. Consider a very typical example:

EXAMPLE: graphite C^{12}: The total cross section for graphite is given in Figure 2-3 and is sketched below as well



There are several features of interest in this cross section.

(1) For very low energies, the cross section rises as $\frac{1}{\sqrt{E}}$:

$$\sigma_t(E) \sim C_1 + C_2/\sqrt{E}$$

(2) There is a very jagged behavior near 10^{-3} eV.

(3) The cross section smooths out to a flat behavior near $10^{-1} < E < 10^{5}$.

(4) The jagged behavior reappears in MeV region.

(5) For very high energies, the cross section drops off.

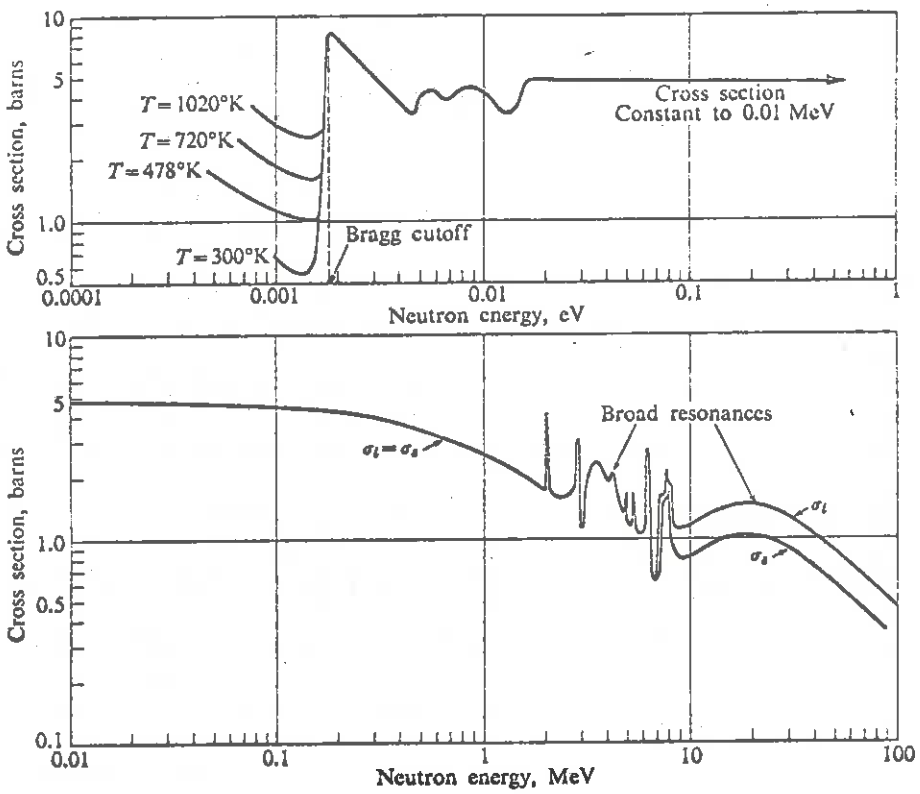


FIGURE 2-3: The total cross section of C^{12}

Let's consider the nuclear physics behind each of these trends which are present in most cross section behavior:

Region 3: For intermediate neutron energies, one usually finds potential scattering. The cross section is essentially just the geometric area presented to the neutron by the nucleus, and hence one expects a smooth, relatively flat cross section.

Region 4: The jagged behavior in the MeV region corresponds to resonant cross section behavior. The resonance behavior for heavier nuclei arises at lower energies (indeed, down to the eV range in nuclei such as ${}_{92}U^{235}$).

Region 5: If we recall the neutron wavelength

$$\lambda = h/p = h/\sqrt{2mE}$$

decreases with increasing energy, then it is apparent that for sufficiently high energies, the neutron will pass through the nucleus without interacting. [Such very high energy behavior is of no consequence in nuclear reactors, however.]

Region 2: The jagged behavior at low energies ($\sim 10^{-3}$ eV) is also a wavelength effect. For sufficient small energies, the wavelength becomes comparable to the interatomic spacing. If the material has a regular structure (such as the crystalline structure of graphite) the neutron will be diffracted, just as x-rays passing through a crystal. For even smaller energies, λ becomes so large that diffraction becomes impossible and the cross section becomes smoothly varying again.

Region 1: The behavior at low energies is attributable to two effects

(i) the neutron energy is now less than the chemical binding energy of the sample, and hence the neutron interacts with an aggregate of nuclei. It can excite the internal modes of the sample (e.g., crystal lattice vibrations).

(ii) For these low energies, the thermal motion of the nuclei becomes important. [More specifically, for $E \sim .025$ eV.] Now one must average $\sigma_t(E)$ over a distribution of nuclear speeds. For very small $v_t << \bar{V}_\ell$, the nuclear reaction rate $v\sigma_t$ = constant, which implies $\sigma_t(E) \sim 1/v \sim 1/\sqrt{E}$ for small E.

b. Elastic scattering cross sections (potential scattering)

Elastic scattering is extremely important in reactors which utilize slow neutrons to induce fission reactions, since fast neutrons scattering off of light nuclei (such as ${}_1H^1$) rapidly slow down. [See Figure 2-4 for the total cross section of H_2O.] The differential scattering cross section for such scattering, $\sigma_s^{CM}(\Theta)$, is either angle-independent or linearly anisotropic for most energies of interest. One can give a simple quantum mechanical argument that for neutron wavelengths greater than a nuclear radius, the CM cross section is constant. For light nuclei, this corresponds to:

$$E < 0.1 \text{ MeV}, \quad \sigma_{CM}(\Theta) = constant = \frac{\sigma_s}{4\pi} \qquad \text{"s-wave"}$$

For larger neutron energies (small or wavelengths), angular dependence begins to appear. For example, for ${}_1H^1$

$$0.1 \text{ MeV} < E < 10 \text{ MeV}, \quad \sigma_{CM}(\Theta) = \frac{\sigma_s}{\pi} \cos\Theta \qquad \text{"p-wave"}$$

For most applications, we will assume s-wave scattering so that the differential scattering cross section is isotropic in the CM system. Of course, it will not generally be isotropic in the LAB system unless the nuclei of interest are very heavy. In particular, for hydrogen, s-wave scattering implies

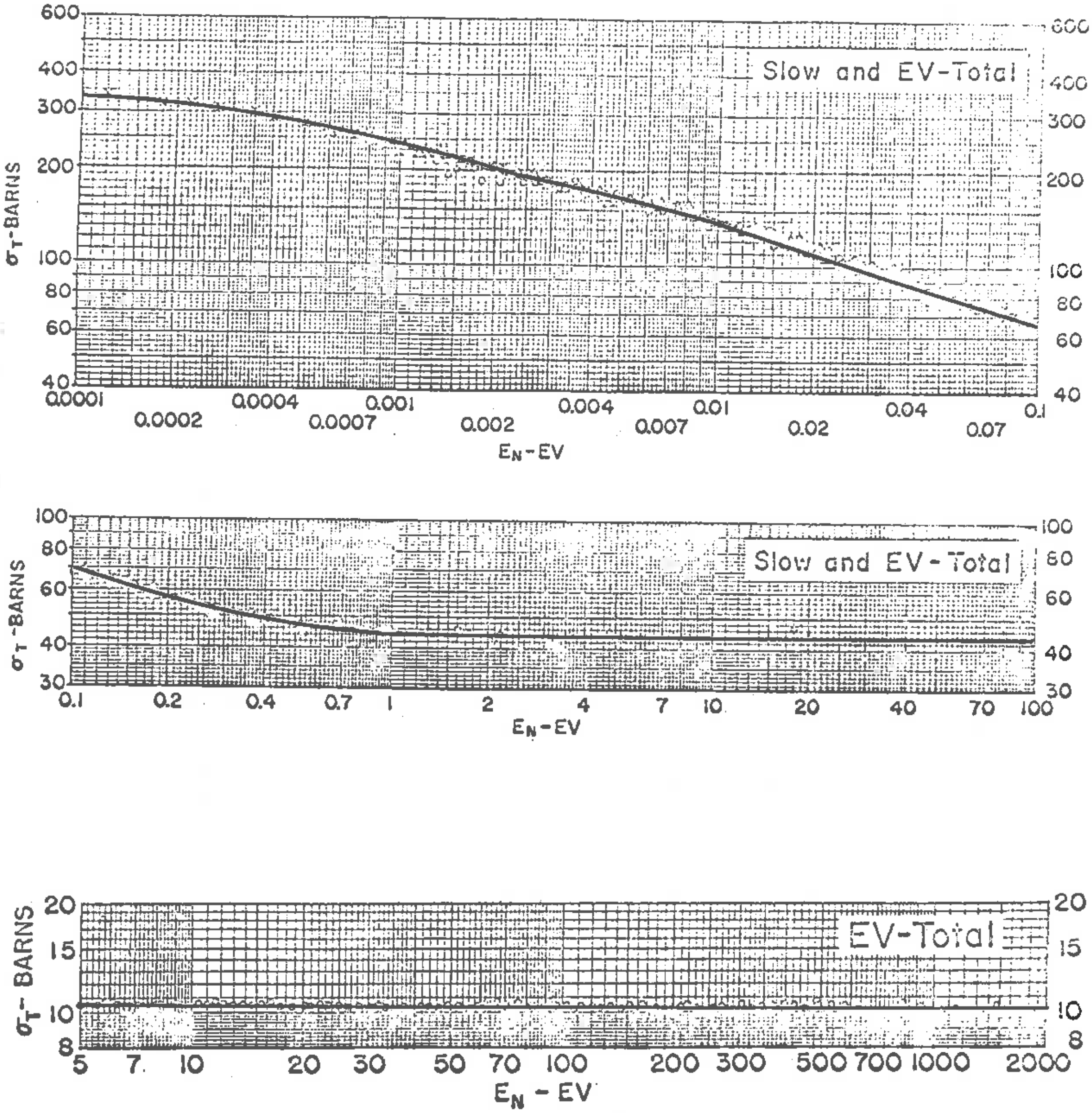
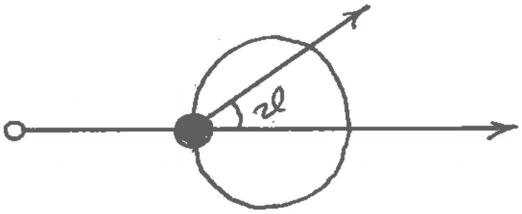


FIGURE 2-4: The total cross section for H_2O

$$\sigma_{CM}(\theta) = \frac{\sigma_s}{4\pi} \quad \Longrightarrow \quad \sigma_s(\vartheta) = \frac{\sigma_s}{\pi}\cos\vartheta$$

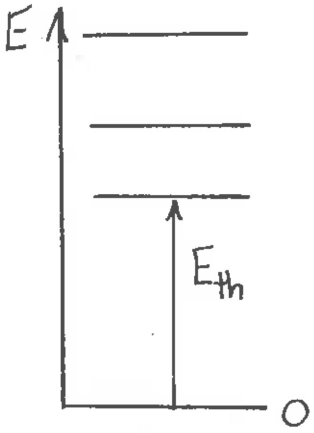
which yields very forward scattering (with no backscatter).



Our more general development later will allow for higher order scattering (e.g., p-wave, etc.)

c. Inelastic scattering (compound nucleus formation)

Inelastic scattering is very significant at the higher neutron energies found in fast reactors. In fact, the neutron must exceed a certain threshold energy E_{th} in order to excite the first nuclear level of the compound nucleus. An example of this behavior is shown in the inelastic scattering cross section of U^{238} in Figure 2-5 .



d. Absorption reactions

Absorption reactions are quite significant for reactor analysis since they remove neutrons from the chain reaction. Radiative capture is the most common such reaction and is most probable at lower energies in heavier nuclei. Since it is a resonance reaction, the energy dependence of the absorption cross section can frequently be described by the Breit-Wigner formula

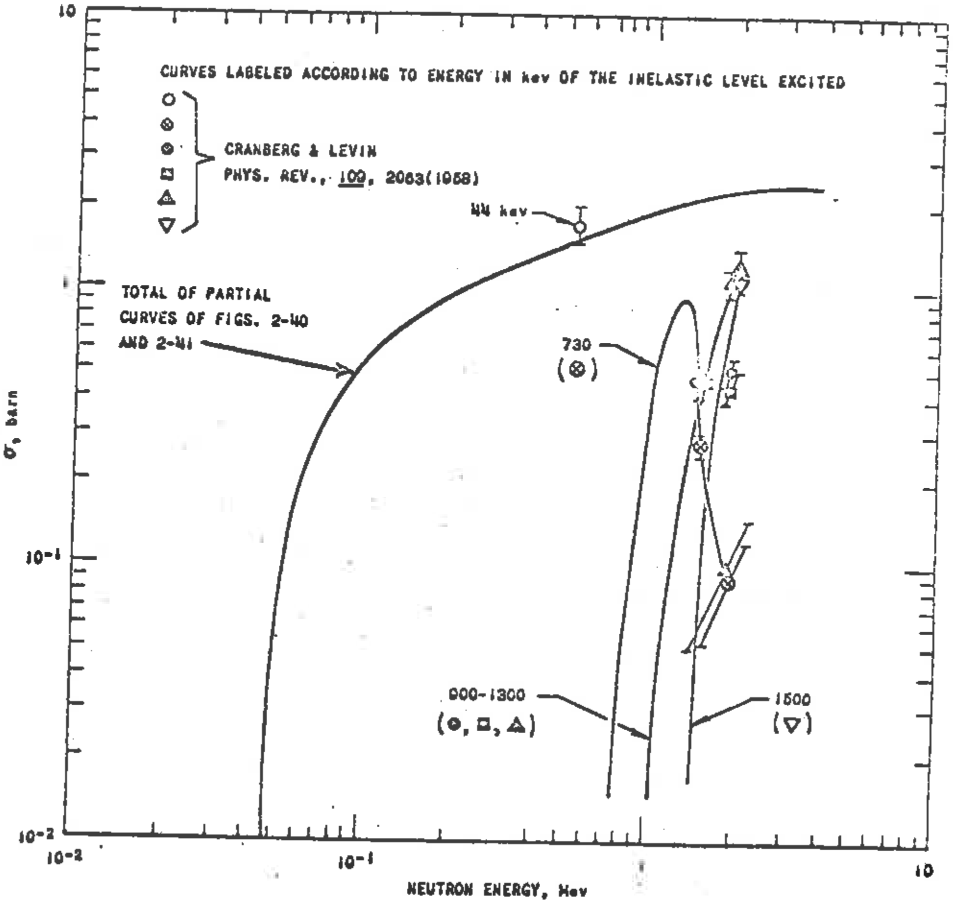


FIGURE 2-5: The inelastic scattering cross sections for the excitations of various energy levels in U^{238}. Notice the thresholds for these reactions.

$$\sigma_\gamma(E_c) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_R}{E_c}}\,\frac{1}{4\frac{(E_c-E_R)^2}{\Gamma^2}+1}$$

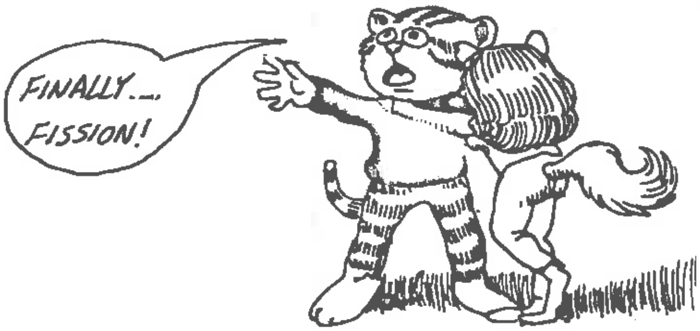
[Notice that for low E, $\sigma_\gamma(E) \sim \frac{1}{\sqrt{E}}$ --just as in scattering.] The absorption cross section for Cd is given in Figure 2-6.

There are other absorption reactions such as (n,p) or (n,α), but these are not significant for the neutron energies found in a reactor [$0 < E < 10$ MeV].

Of course, the most significant absorption reaction is nuclear fission. We shall discuss the fission reaction in some detail momentarily.

e. Other reactions

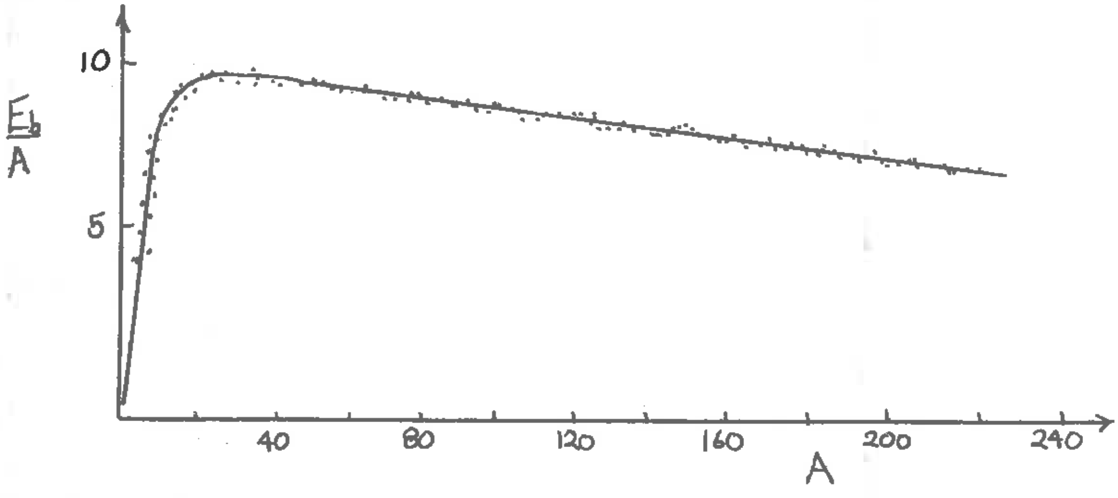
There are several other reactions of minor importance in certain reactors such as (n, 2n), (n, 3n), or (γ, n) which add neutrons to the chain. However because of their low cross sections, we will avoid a discussion of such reactions here.



III. NUCLEAR FISSION

A. Fission Physics

Recall our plot of the average energy per nucleons versus mass number A



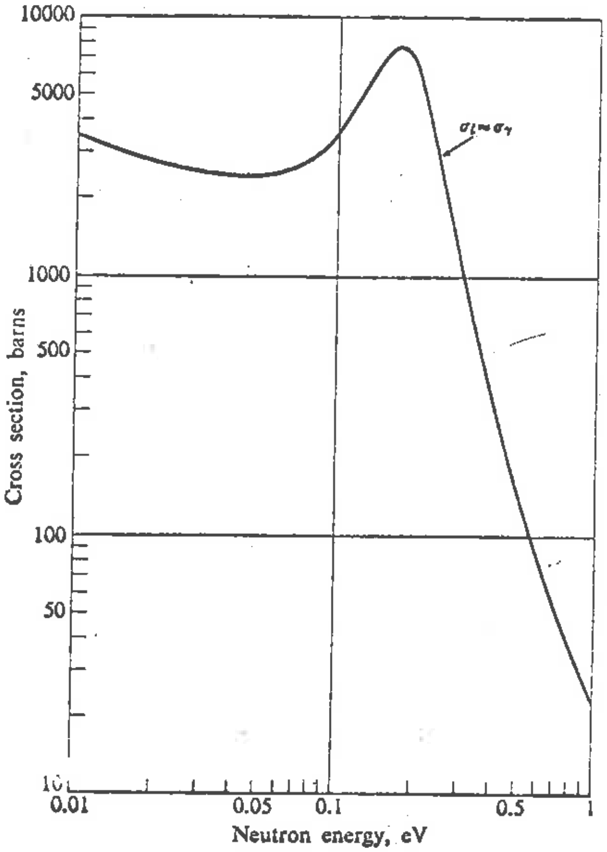
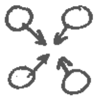


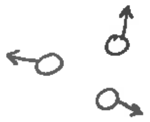
FIGURE 2-6: The total cross section of cadmium (which is almost entirely attributable to radiative capture)

From this plot one might expect fission to occur spontaneously for any nucleus with $A > 50$. What prevents this? A barrier to the fission reaction. There are two types of forces between nucleons

(i) nuclear attraction (short range)



(ii) Coulomb repulsion (long range)



In a bound nucleus, the nuclear forces dominate to bind the nucleons together. But if the nucleons can be separated far enough apart, the longer range Coulomb forces will take over and push them away from each other.

We can get more of an idea of the balance between these forces if we plot the potential energy of two nuclei of Z_1, A_1, and Z_2, A_2 versus their distance of separation r:

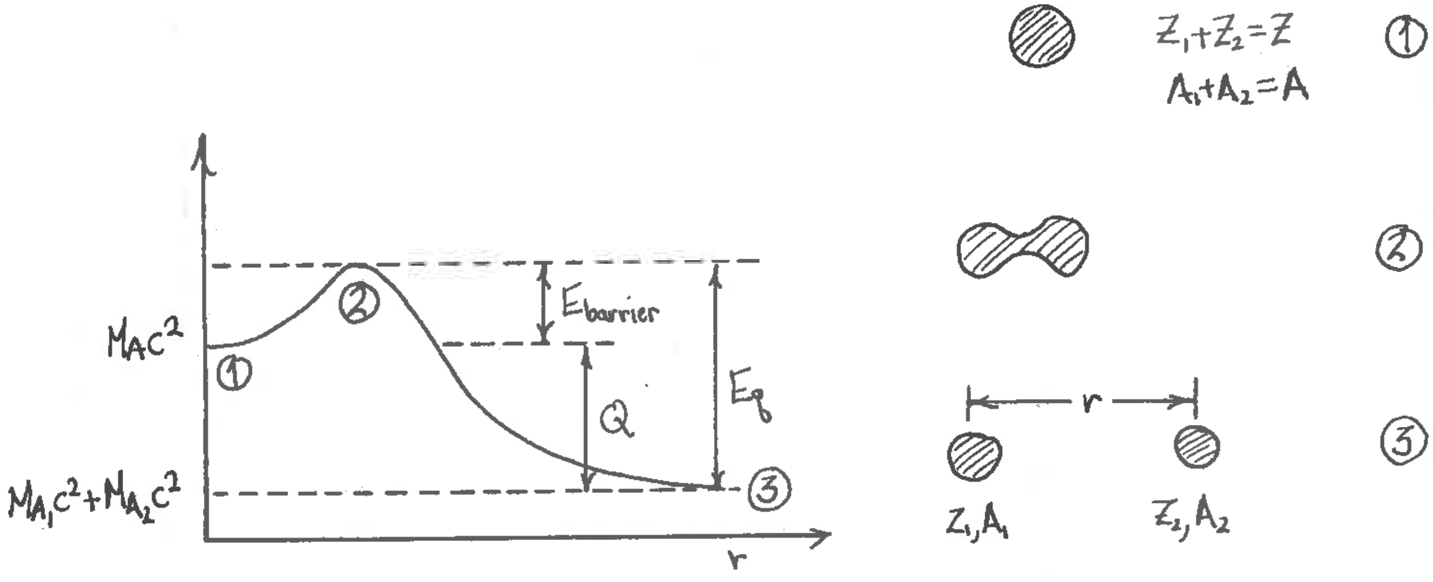


FIGURE 2-7

The energy of the potential barrier, $E_{barrier}$, which must be overcome to pass from one potential minimum to another is

$$E_{barrier} = E_{q} - Q ,$$

where

$$E_{q} = \frac{Z_1 Z_2 e^2}{R_1 + R_2} \qquad \text{Coulomb repulsion energy when nuclei are just touching}$$

For symmetric fission, $Z_1 = Z_2$, $A_1 = A_2$, one finds

$$E_{q} = \frac{0.16 Z^2}{A^{1/3}} \cong 218 \text{ MeV} \quad \text{for} \quad {}_{92}U^{238}$$

Now Q, the energy involved in the exothermic fission reaction is

$$Q = [M_A - (M_{A_1} + M_{A_2})]c^2 \cong 212 \text{ MeV}.$$

Hence the additional energy we must add to overcome the potential barrier is

$$E_{barrier} = E_{q} - Q \cong 218 - 212 = 6 \text{ MeV}.$$

Thus we must somehow figure out a way to add this energy to the nucleus Z, A to induce it to fission. Of course we could try to do this by merely slamming a 6 MeV (actually a bit higher because we need CM energy $E_c > E_{barrier}$) projectile into the nucleus. But there is a much easier way. First we notice that since a neutron has no charge, it can easily penetrate the nucleus. Furthermore, if it is absorbed by the nucleus, it will add its binding energy E_b/A. If this binding energy of the extra neutron exceeds the fission barrier energy, $E_{barrier}$, the nucleus will fission.

The details of neutron induced fission are a bit more complicated and depend upon nuclear systematics. [Indeed, the fission barrier for certain isotopes is double humped.] In Table 2-1, we give the fission barriers for a number of heavy nuclei, along with the binding energy of the last neutron in these nuclei:

TABLE 2-1

Nucleus	$E_{barrier}$	E_b/A of last neutron
Th^{232}	5.9	*
Th^{233}	6.5	5.1
U^{233}	5.5	*
U^{234}	4.6	6.6
U^{235}	5.75	*
U^{236}	5.3	6.4
U^{238}	5.85	*
U^{239}	5.5	4.9
Pu^{239}	5.5	*
Pu^{240}	4.0	6.4

EXAMPLE: As several examples of how we can use this information, consider

$${}_0n^1 + {}_{91}Th^{232} \Rightarrow \frac{E_b}{A} = 5.1 < E_{barrier} = 6.5 \Rightarrow \text{ no fission}$$

$${}_0n^1 + {}_{92}U^{235} \Rightarrow \frac{E_b}{A} = 6.4 > 5.3 \Rightarrow \text{ fission}$$

$${}_0n^1 + {}_{92}U^{238} \Rightarrow \frac{E_b}{A} = 4.9 < 5.5 \Rightarrow \text{ no fission}$$

---

*cannot be formed by neutron absorption

In this way, we conclude that neutron induced fission is possible in

$$_{92}U^{233}, \qquad _{92}U^{235}, \qquad _{93}Pu^{239}$$

These are referred to as the "fissile" isotopes.

Of course if we could add a bit of kinetic energy to the incident neutrons, then we could overcome the fission barrier even in isotopes like $_{92}U^{238}$. It is apparent that this would require neutrons of kinetic energy $E > .6$ Mev--which are referred to as "fast" neutrons in contrast to "thermal" neutrons of energy $E < 1$ eV. Such nuclides which can be fissioned by fast neutrons are referred to as "fissionable" isotopes.

Finally, we should note that most of these nuclei can also fission spontaneously via the "barrier penetration" mechanism familar from quantum mechanics. However the lifetime for such spontaneous fission is usually very long in typical nuclear fuels.

B. Nuclear Reactor Fuels

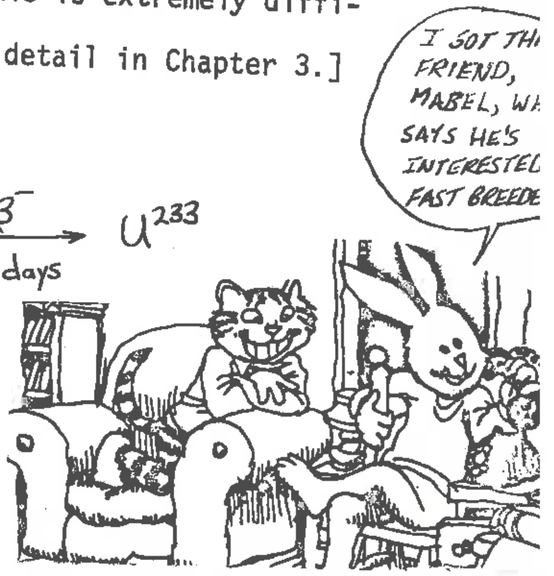
At present, one must use one of the three fissile isotopes to fuel a reactor

$$U^{233}, \qquad U^{235}, \qquad Pu^{239}$$

only U^{235} occurs naturally, and then only as 0.71% of natural uranium (which is predominantly U^{238}). This small percentage of fissile isotope implies one must separate out U^{235} from U^{238}. This is extremely difficult and expensive. [We will discuss it in more detail in Chapter 3.]

To produce U^{233}, one must transmute Th^{232}

$$Th^{232}(n,\gamma)Th^{233} \xrightarrow[22\,\text{min}]{\beta^-} Pa^{233} \xrightarrow[27\,\text{days}]{\beta^-} U^{233}$$



This scheme is under investigation for the fuel cycle of the high temperature gas cooled reactor.

One uses a very similar transmutation sequence to produce Pu^{239} from U^{238}

$$U^{238}(n,\gamma)U^{239} \xrightarrow{\beta^-} Np^{239} \xrightarrow{\beta^-} Pu^{239}$$

Large quantities of plutonium have been and are continually being produced as a byproduct in U^{235}-U^{238} fueled (enriched uranium) reactors. However, plutonium is still quite expensive for large scale power production (although it is now being recycled into power reactor cores). It is also an extremely toxic and dangerous material to fabricate into fuel elements, requiring elaborate fabrication facilities.

C. Fission Cross Sections

Neutrons can not only induce fission reactions in a fissile isotope, but as well can be absorbed in radiative capture reactions. The relative balance between fission and radiative capture in a fuel isotope is expressed in terms of the capture to fission ratio,

$$\alpha = \frac{\sigma_\gamma}{\sigma_f}$$

Obviously one wants α to be as small as possible. Figure 2-8 shows the capture to fission ratio α for the three fissile isotopes, U^{233}, U^{235}, and Pu^{239} plotted versus energy.

Figure 2-9 to 2-11 shows the fission cross sections for each of these isotopes. It should be noted that the fission cross section is largest for slow neutrons ($<$ 1 eV). Hence, since the probability of fission is highest at low energies, it should be easiest to maintain a

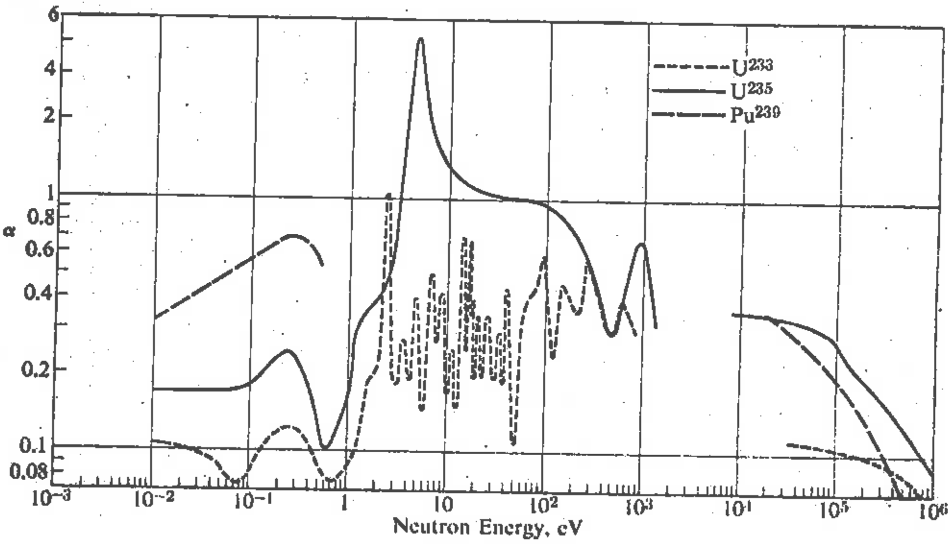


FIGURE 2-8: Variation of α with energy for U^{233}, U^{235}, and Pu^{239}.

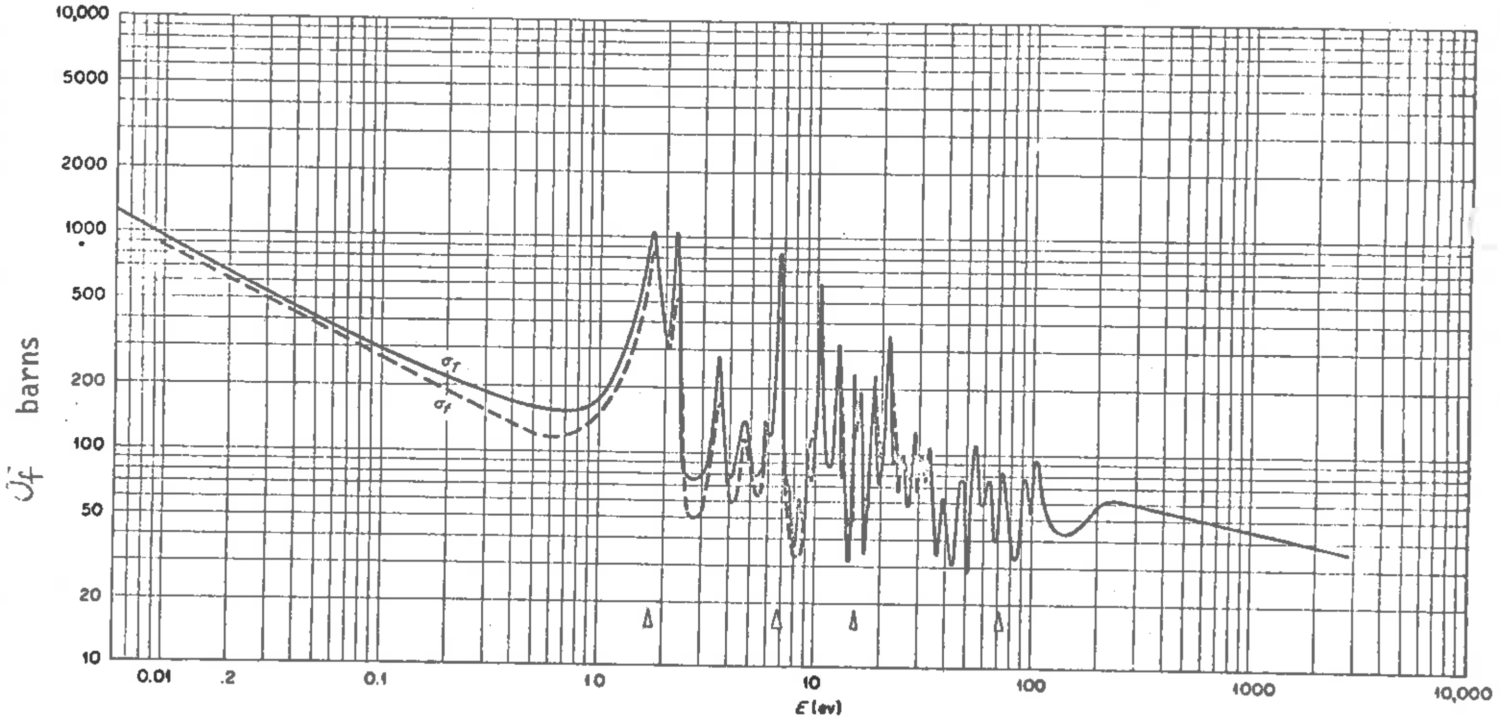


FIGURE 2-9: The fission cross section of U^{233}

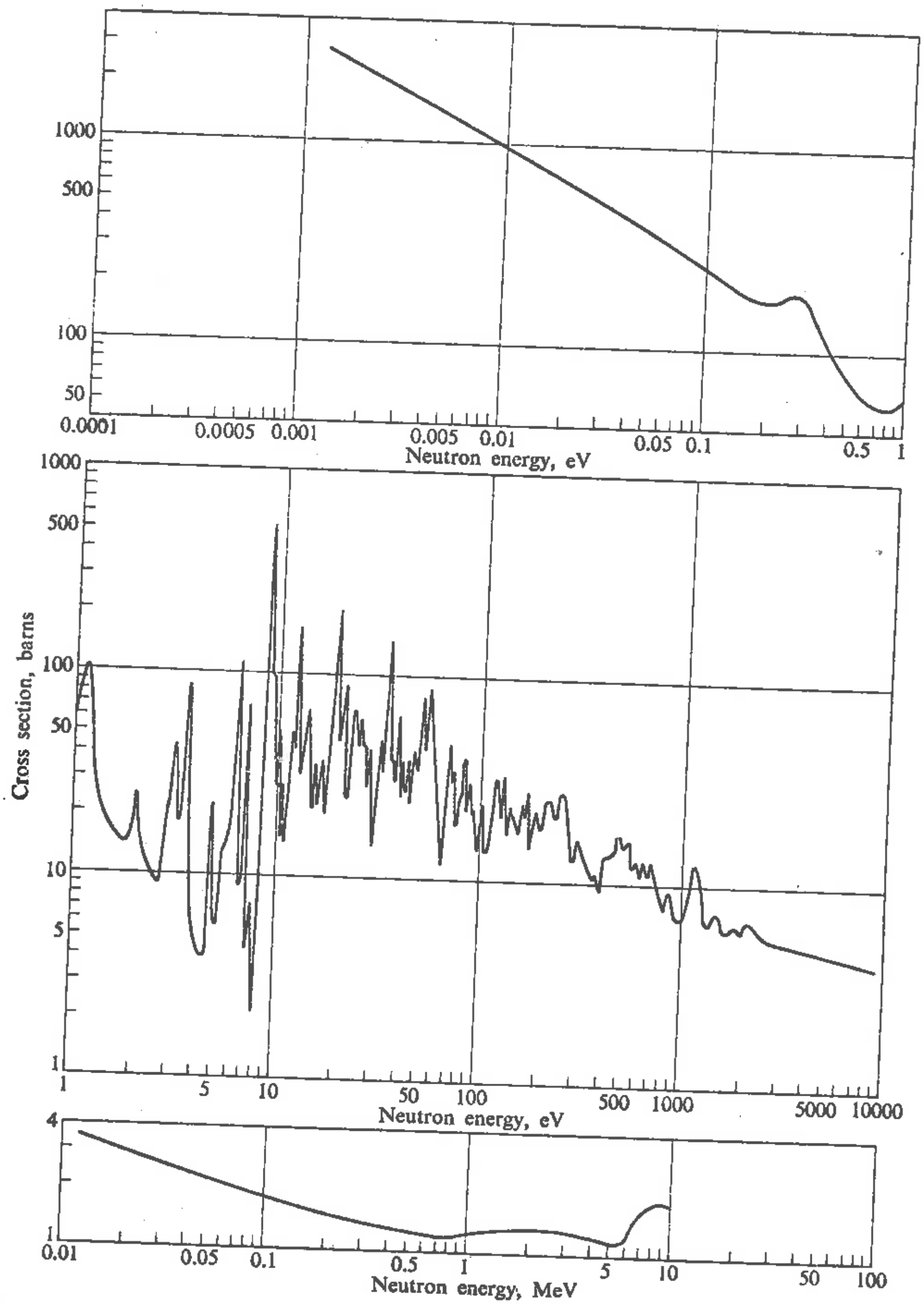


FIGURE 2-10: The fission cross section of U^{235}

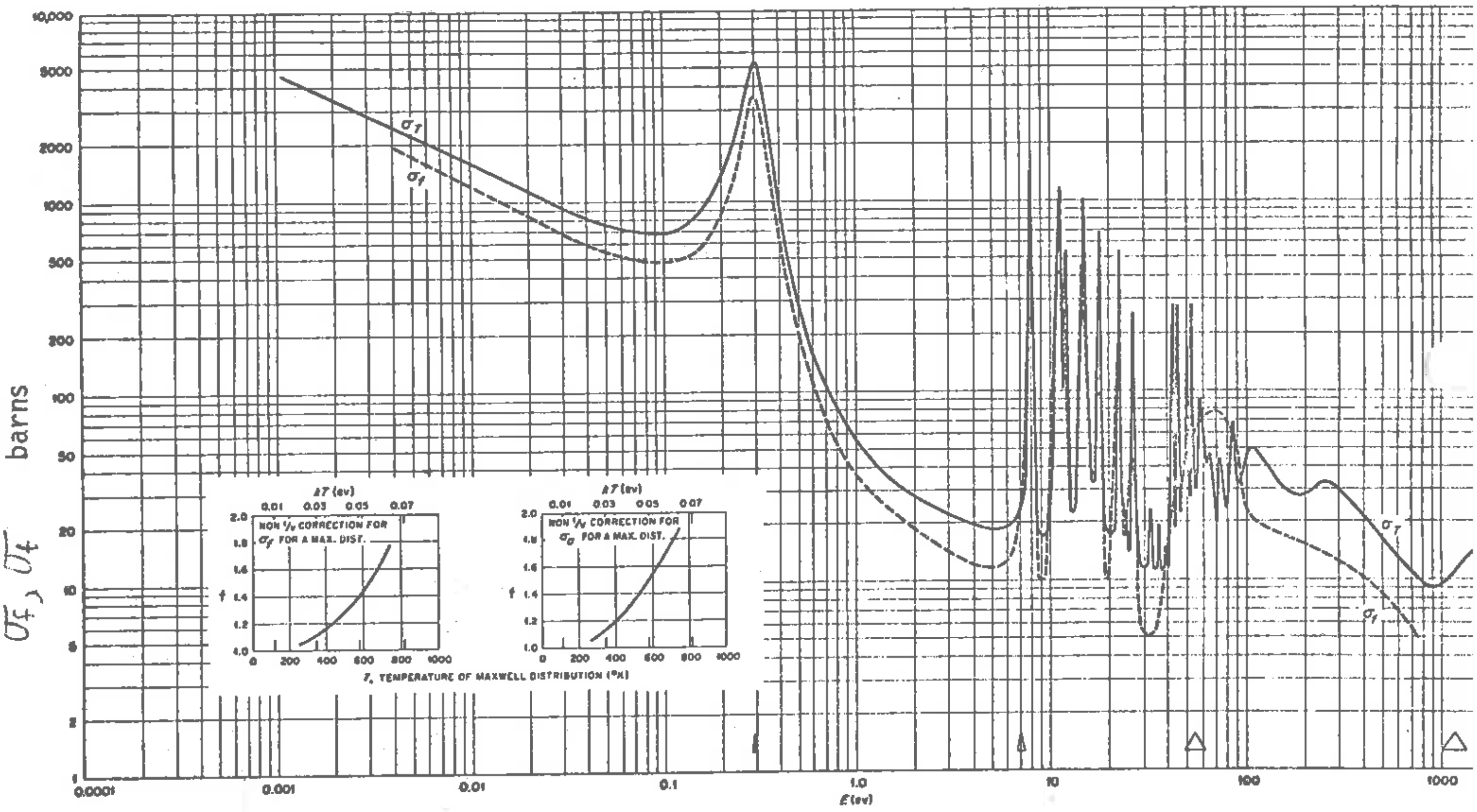


FIGURE 2-11: The fission cross section of Pu^{239}

fission chain reaction in an assembly which rapidly slows down the energetic fission neutrons ($E > 1$ Mev) to thermal energy ($E \sim kT = .025$ eV).

However, one must be careful in using arguments based upon the fission cross section alone. Indeed, α is largest for energies for above 1 eV. We will later see that there are certain advantages to maintaining a chain reaction using fast neutrons with energies $E > 1$ keV.

The fission cross section for U^{238}, Pu^{240}, and Th^{232} is given in Figure 2-12 (note only fast fission is possible in these isotopes because of the large fission barrier).

D. Fission Products

A fission reaction spews out a large variety of reaction products:

Fission fragment nuclei
neutrons
γ-rays
β-rays
neutrons

Most of these products are emitted essentially instantaneously (within 10^{-17} sec) and are referred to as prompt events. However a few reaction products may be emitted sometime after the fission reaction due to the subsequent decay of unstable fission fragments. Of particular interest are the "delayed neutrons" emitted by decaying fission fragments some time after the fission reaction. Although comprising only a small fraction of the neutrons emitted ($< 1\%$), such delayed neutrons turn out to be vital for the effective control of the nuclear chain reaction.

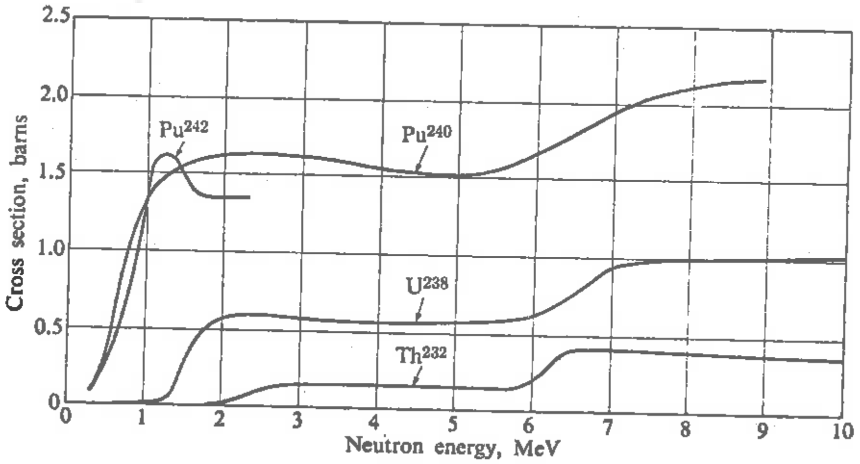


FIGURE 2-12: The fission cross sections of Th^{232}, U^{238}, Pu^{240} and Pu^{242}.

Let us define

$\nu \equiv$ average number of neutrons released per fission

ν is usually small, from 2 to 3, although it is dependent upon the incident neutron energy and the isotope involved. [See Figure 2-13] Occasionally one combines ν with α to define*

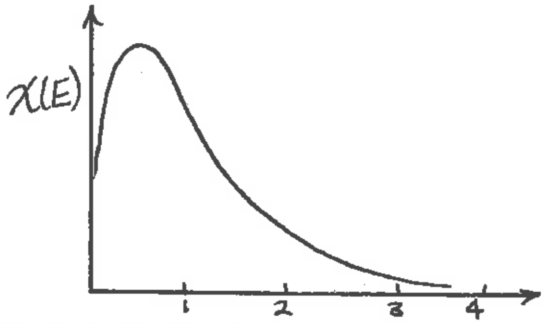
$$\eta \equiv \frac{\nu}{1+\alpha} = \nu\frac{\sigma_f}{\sigma_a} = \frac{\text{ave. no. of neutrons emitted in fission}}{\text{no. of neutrons absorbed in fuel}}$$

This very important parameter is plotted in Figure 2-14.

The neutrons emitted in a fission reaction emerge with various energies. The energy spectrum characterizing fission neutrons can frequently be taken as

$$\chi(E) = 0.453\, e^{-1.036E} \sinh\sqrt{2.29E}$$

which peaks at about 2 MeV:



[See Figure 2-15 for more detailed plots.]

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*There is an important exception to this definition. For a mixture of uranium isotopes (U^{235} and U^{238}) one uses

$$\eta = \nu_{235}\frac{N_{235}\,\sigma_f^{235}}{N_{235}\,\sigma_f^{235} + N_{238}\,\sigma_f^{238}}$$

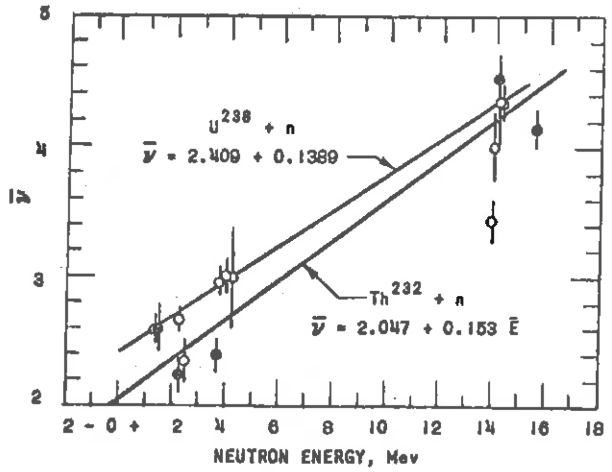


Fig. 1-8—Dependence of $\bar{\nu}(U^{238})$ and $\bar{\nu}(Th^{232})$ on incident neutron energy.

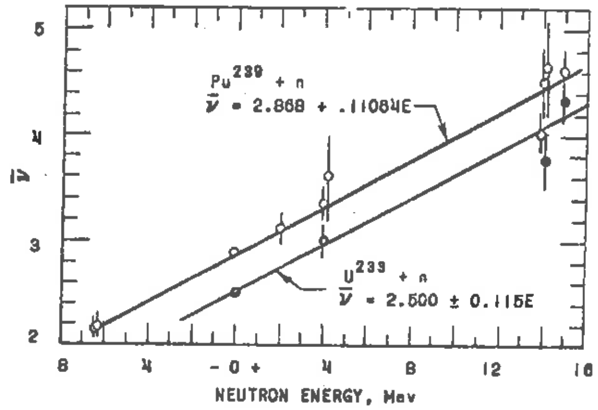


Fig. 1-9—Dependence of $\bar{\nu}(Pu^{239})$ and $\bar{\nu}(U^{233})$ on incident neutron energy.

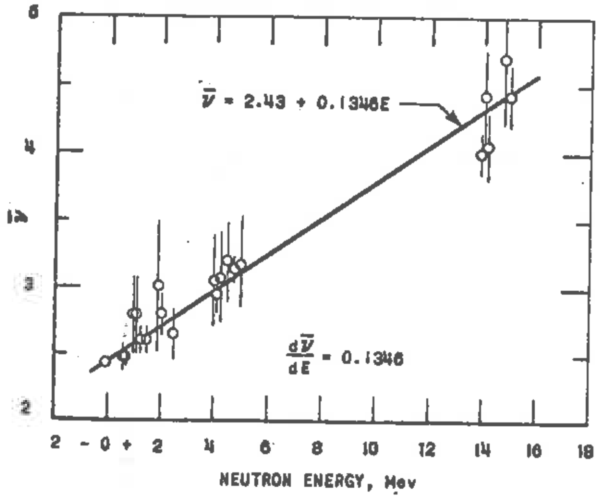


Fig. 1-10—Dependence of $\bar{\nu}(U^{235})$ on incident neutron energy.

Table 1-23—CONSTANTS FOR THE EXPRESSION $\bar{\nu}(E) = \bar{\nu}(\text{thermal}) + (d\bar{\nu}/dE)\,dE$

Isotope	$\bar{\nu}$(thermal)	$d\bar{\nu}/dE$, Mev^{-1}
U^{233} + n	2.500	0.115
U^{235} + n	2.43	0.1346
U^{238} + n	2.409	0.1385
Pu^{239} + n	2.868	0.1106
Th^{232} + n	2.047	0.153

FIGURE 2-13: The energy dependence of $\nu(E)$

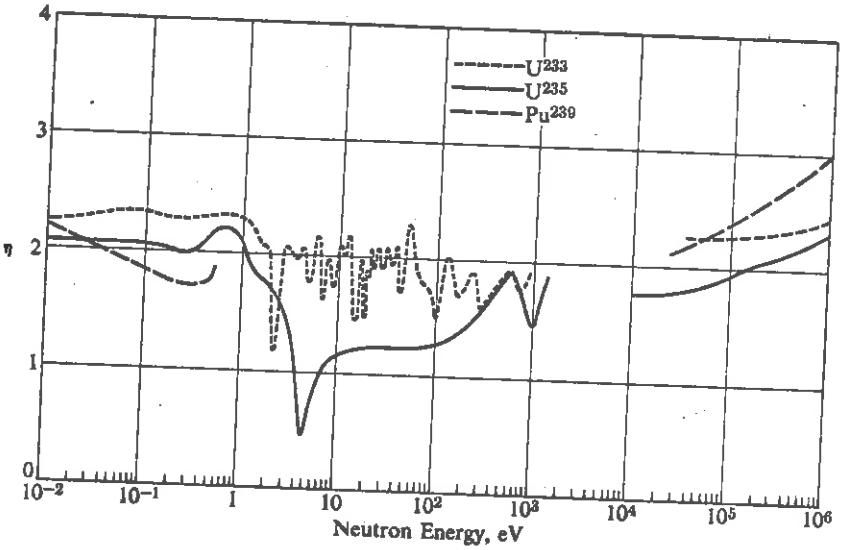


FIGURE 2-14: Variation of η with energy for U^{233}, U^{235}, and Pu^{239}.

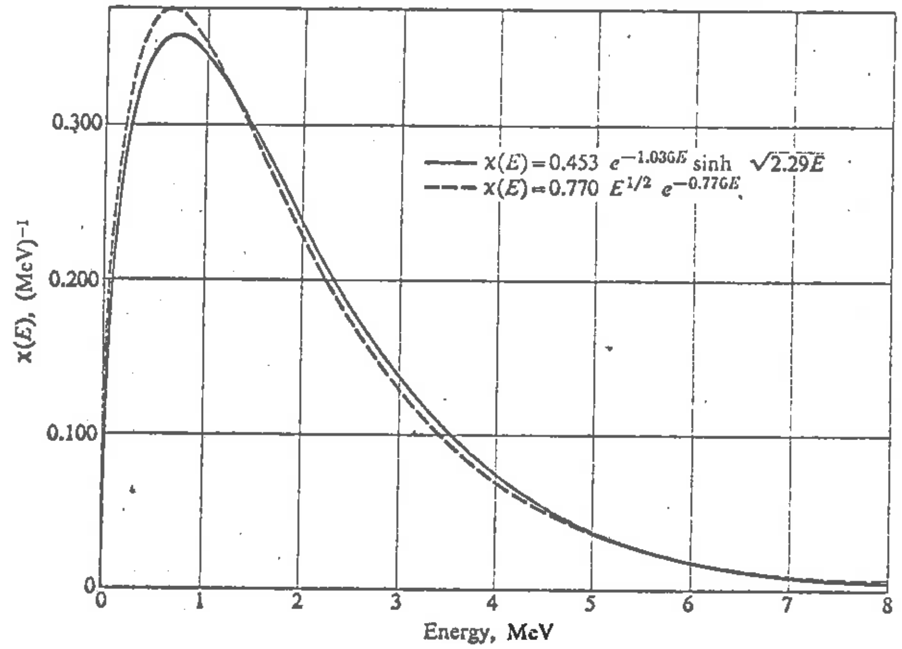


FIGURE 2-15: The fission spectrum for U^{235}

E. Energy Release From Fission

The fission reactions occurring in a nuclear reactor core release a considerable amount of energy. This energy is distributed among a number of different fission products:

Type	% of total reactor energy	Time delay	Range
Kinetic energy of fission fragments	80.5%	instantaneous	very short
Kinetic energy of prompt neutrons	2.5%	"	medium
γ energy released with fission	2.5%	"	long
Kinetic energy of delayed neutrons	.02%	delayed	medium
β decay of fission products	3.0%	"	short
neutrinos	5.0%	"	nonrecoverable
γ energy of fission products	3.0%	"	long
Nonfission reactions	3.5%	"	variable

Here we have taken care to distinguish between energy released instantaneously in the fission reaction and that which appears after some appreciable time delay due to radioactive decay. This is quite important, since 3-4% of the energy appears in the form of such decay heat. If the reactor were to be suddenly shut down, this decay heat would continue to be produced and would have to be removed (otherwise the reactor core temperature would rise dramatically, causing fuel element melting and failure).

It is evident that most of the fission energy appears in short range fission fragments which deposit this energy in the form of heat as they slow down in the fuel. Since the range of these fragments is so short ($\sim$ .01 cm), most of the fission energy ($\sim$ 90%) can be assumed to be liberated as heat at the same point at which the fission reaction occurs.

On the average, some 203 MeV of energy is released in each fission reaction. If we recall that 1 MeV = 1.6×10^{-13} joules, then

$$1 \text{ fission} = 3.25 \times 10^{-11} \text{ watt-sec}$$

We can convert this into energy released per mass of uranium fissioned to find

$$1 \text{ gm of fuel fissioned} = 1 \text{ MW-day of energy}$$

which corresponds to 3.1×10^{10} BTU released per pound. By way of contrast, a pound of coal releases some 10^4 BtU. Hence nuclear energy is some million times more concentrated than fossil fuel energy.

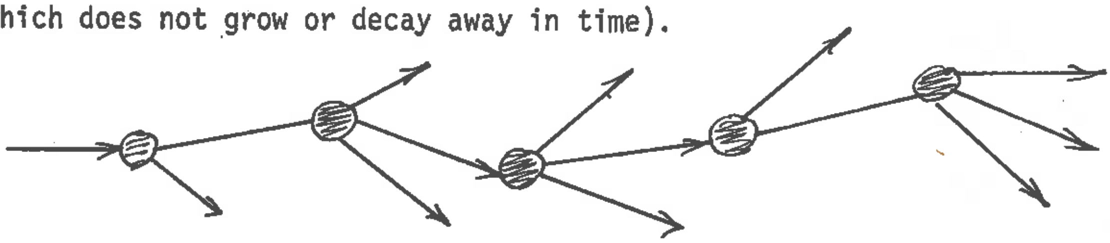
"I'm afraid I've forgotten why I asked you all here today."

CHAPTER 3: FISSION CHAIN REACTIONS AND NUCLEAR REACTORS --AN INTRODUCTION

I. THE MULTIPLICATION FACTOR AND NUCLEAR CRITICALITY

A. The Multiplication Factor

In the preceding chapter we indicated that an essential idea involved in tapping the energy released in nuclear fission was to use the fission neutrons from one fission reaction to induce yet another reaction, hence propagating a chain of fission reactions by using the neutron as a chain carrier. Physically, it is apparent that we wish for precisely one neutron from each fission to induce another fission in order to maintain a stable or steady-state chain reaction (i.e., one which does not grow or decay away in time).



It is desirable to express this requirement in mathematical form. This can be done by defining the "multiplication factor k" characterizing the chain reaction:

$$k \equiv \text{multiplication factor} \equiv \frac{\text{\# of fissions in one generation}}{\text{\# of fissions in preceding generation}} \qquad (3\text{-}1)$$

The term generation is used to refer to the average time elapsing between the "birth" of a neutron in a fission reaction and its eventual "death" via absorption or leakage out of the sample of fissile material. Actually, in the above definition, we could as well have merely calculated the ratio of the number of neutrons in the system for two consecutive generations, since this number is merely ν times the number of fissions.

Now notice that if k = 1, the number of fissions in each generation remains constant, and the chain reaction is time-independent. We refer to such a chain reaction as being "critical". In a similar fashion, if $k < 1$, the number of neutrons decreases from generation to generation, and the chain reaction dies out. We then refer to the system as being "subcritical". Finally, if $k > 1$, the chain reaction grows without bound, and we refer to the system as being "supercritical". In summary then,

$$\begin{aligned} k < 1 &\Longrightarrow \text{subcritical} \\ k = 1 &\Longrightarrow \text{critical} \qquad (3\text{-}2) \\ k > 1 &\Longrightarrow \text{supercritical} \end{aligned}$$

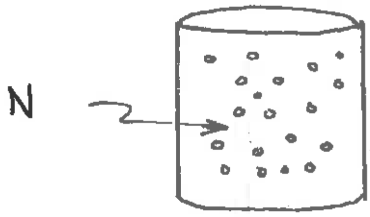
Hence the first objective of the nuclear engineer is to design the nuclear reactor so as to achieve a critical system. One approach would be to choose a particular reactor material composition and configuration, then calculate k for this choice, and if k is not unity, readjust the reactor design until the "criticality" condition:

$$k = 1 \qquad (3\text{-}3)$$

is achieved. Hence the calculation of the multiplication factor k becomes a very important objective in the analysis of a nuclear reactor, and much of our attention here will be devoted to describing various procedures for performing this calculation. Before beginning our discussions of these procedures, we will first discuss several other simple ideas associated with fission chain reactions.

B. Simple Kinetics of Chain Reactions

Imagine that somehow we can count the number of neutrons in a nuclear reactor at a time t, and we find



this number to be N(t). Now using our definition of k, we can calculate the increase in the number of neutrons from one generation to the next as:

$$k\,N(t) - N(t) = \text{increase in number of neutrons from one generation to the next} \tag{3-4}$$

But we are interested in the change in the neutron population in the reactor as a function of time, not generation. Hence we define

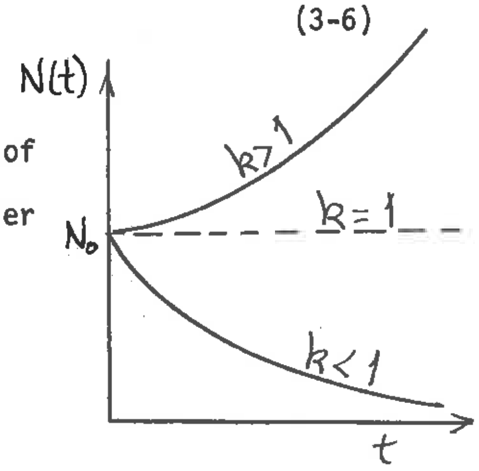
$$\ell \equiv \begin{cases} \text{mean life of a neutron in a generation (i.e., from its birth} \\ \text{to its death via absorption or leakage from the system)} \end{cases}$$

This, of course, is only a formal definition at this point--we will later discuss methods which allow the calculations of ℓ. Using the neutron lifetime ℓ, we can now compute the time rate of increase of the neutron population at a time t as

$$\frac{dN}{dt} = \left(\frac{k-1}{\ell}\right) N(t) \tag{3-5}$$

If there are N_0 neutrons in the reactor at a time t = 0, then we can solve for the neutron population at any future time as

$$N(t) = N_0\, e^{\left(\frac{k-1}{\ell}\right)t} \tag{3-6}$$



In particular, note that this very simple model of "nuclear reactor kinetics" agrees with our earlier definition of criticality in terms of k. The growth or decay of the neutron population in a reactor core obeys an exponential growth law.

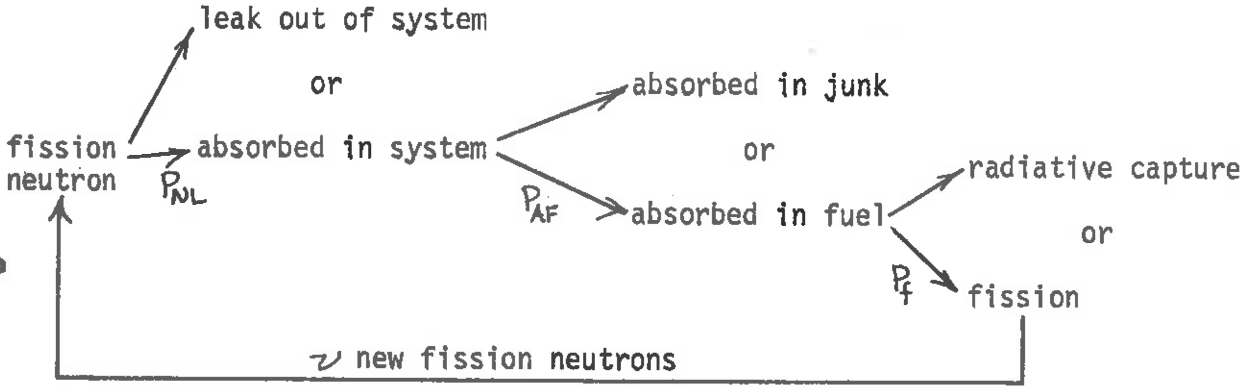
Such exponential growth is quite commonly found in the study of population dynamics. Indeed, the study of the "neutron" population in a reactor core is mathematically rather similar to the study of biological populations--and hence the terminology of the latter field is frequently adopted to reactor physics [e.g., generation, birth, life, death, virgin, father, daughter, mutha, etc.] The time constant characterizing this exponential behavior is referred to as the "reactor period" T

$$T \equiv \frac{\ell}{k-1} \equiv \text{time required for neutron population to change by a factor of } e \qquad (3\text{-}7)$$

In particular, it should be noted that as the multiplication constant k approaches unity, the reactor period T approaches infinity--corresponding to a time-independent neutron population in the reactor.

C. A Formal Calculation of k--the 4-Factor Formula

Let's now turn our attention to the calculation of the multiplication factor, for say, a lump of uranium that one wishes to make into a nuclear reactor, with perhaps some structural material to hold the core together. [We will assume, however, that for now we can treat these materials as intimately and homogeneously mixed.] It is evident that one must trace out the various possible destinies of a neutron in the system. In the simplest sense, we know the neutron has only a few available alternatives: Of course it can leak out of the system. If it does not leak out, then it eventually must be absorbed. This absorption may correspond to a non-productive capture event, or it may induce a fission reaction--which would produce a new neutron generation. Schematically, we can represent these destinies as shown below:



To make this more formal, suppose we formally define the probabilities for each of these possible events as:

P_{NL} = probability that neutron won't leak out of system

P_{AF} = conditional probability that <u>if</u> neutron is absorbed, it will be absorbed in the fuel

P_f = conditional probability that <u>if</u> neutron is absorbed in fuel, it will induce a fission reaction

These latter two conditional probabilities are easily calculated. The conditional probability for absorption in the fuel, P_{AF}, can be expressed simply as the ratio of the macroscopic absorption cross sections for the fuel, Σ_a^F, and for the fuel plus the rest of the material in the core, [We will usually indicate with a superscript the material to which we are referring. The absence of the superscript will imply that the macroscopic cross section is the total for all of the materials in the system.]

$$P_{AF} = \frac{\Sigma_a^F}{\Sigma_a} \equiv f \equiv \quad \text{thermal utilization} \tag{3-8}$$

This quantity is known in reactor terminology as the "thermal utilization"-- a name whose meaning will only become apparent later in this chapter.

The conditional probability for inducing a fission reaction in the fuel can also be expressed in terms of the ratio of cross sections--in this case, corresponding to fission and absorption to fission and absorption in the fuel material:

$$P = \frac{\Sigma_f^F}{\Sigma_a^F} = \frac{\sigma_f^F}{\sigma_a^F} \tag{3-9}$$

Now suppose we have N_1 neutrons present in the reactor in a given generation. Then with the help of the above probabilities, we can compute the number of neutrons in the next generation (referring to our diagram) as

$$\begin{aligned} N_2 &= (P_{NL} P_{AF} P_f \nu) N_1 \\ &= P_{NL} f \eta N_1 . \end{aligned} \tag{3-10}$$

Here we have recalled that

$$\eta \equiv \frac{\nu \sigma_f^F}{\sigma_a^F} \equiv \text{number of fission neutrons produced per absorption in fuel} \tag{3-11}$$

Hence by our definition of the multiplication constant k, we find

$$k = \frac{N_2}{N_1} = \eta f P_{NL} \tag{3-12}$$

The non-leakage probability, P_{NL}, appearing in Eq. (3-12) and characterizing neutron leakage from the core, is much more difficult to compute.

It will require more elaborate mathematics (and in a realistic calculation, the use of a digital computer), and hence we will defer a discussion of it to later.

As a momentary detour, however, suppose our reactor were of infinite extent. Then since no neutrons could leak out, we immediately conclude that we must set P_{NL}, = 1. The corresponding multiplication factor is then known as the "infinite medium multiplication factor":

$$k_\infty = \eta f \tag{3-13}$$

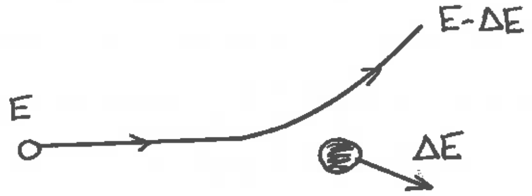
Now of course no reactor is of infinite size. Nevertheless, k_∞ is a useful parameter since it essentially characterizes the multiplication properties of the material in the reactor as distinct from the geometry of the reactor core. Of course, since $P_{NL} < 1$ more generally for a finite reactor, we must have

$$k_\infty < k \tag{3-14}$$

--that is, k_∞ must be greater than unity for us to have any chance of achieving a critical chain reaction.

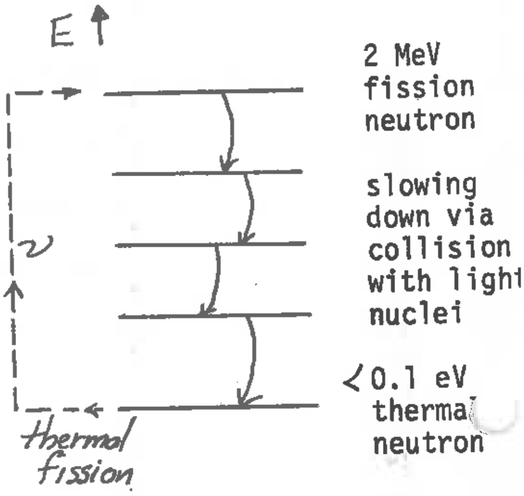
There are a couple of important modifications that must be introduced into this simple development in order to understand how the present generation of reactors works. We must account for the fact that the neutrons in a nuclear reactor have a distribution of energies. As we saw in Chapter 2, the fission neutrons are born at very high energies, roughly 2 MeV. But the fission cross section is largest at very low energies--

indeed, at those energies corresponding to neutrons in thermal equilibrium with the reactor core at a temperature T [e.g., T = 300°K $\Rightarrow$ E = 0.025 eV; T = 600°K $\Rightarrow$ E = 0.05 eV]. Hence it is obviously to our advantage to try to slow down (or, in the language of reactor physics, "moderate") the fast fission neutrons to take advantage of the fact that slow neutrons are more capable of inducing fission reactions. This can be accomplished rather easily, simply by letting the fast neutrons collide with light nuclei, thereby losing some of their kinetic energy in elastic scattering collisions (just as two billiard balls would collide).



The lighter the nucleus involved, the more effective the slowing down or moderation. In fact, the best nucleus to use is hydrogen--which is fortunately quite commonly available in the form H_2O. Hence just letting the fast neutrons rattle around in water for a bit will quickly slow them down to the desired thermal energy. In this sense, we refer to water as a neutron "moderator". [Numerous other materials can be used as moderators in nuclear reactors, and we will discuss these in more detail later.]

The presence of such "neutron moderation" in a reactor suggests a couple of new definitions to take account of the change in neutron energy as it slows down after being born in a fission reaction.



We first define a factor which takes account of the fact that, although most fissions will be induced in fissile material by thermal neutrons, some fissions will be induced in both fissile and fissionable material by fast neutrons

$$\epsilon \equiv \frac{\text{\# of fissions occurring in both fissile and fissionable material}}{\text{\# of fissions occurring in fissile material}}$$

$$\equiv \text{"fast fission factor"} \qquad (3\text{-}15)$$

We also must introduce a factor which describes the probability that a neutron can slow down from fission to thermal energies without being absorbed along the way. Since most absorptions which occur during the slowing down process correspond to resonance capture, we refer to this factor as the "resonance escape probability"

$$p \equiv \begin{array}{l}\text{fraction of neutrons which manage to slow}\\ \text{down fission to thermal energies without}\\ \text{being absorbed}\end{array} \equiv \begin{array}{l}\text{"resonance}\\ \text{escape}\\ \text{probability"}\end{array} \qquad (3\text{-}16)$$

Finally, it is useful to break up the non-leakage probability P_{NL} to specifically separate out neutron leakage during slowing down from that characterizing thermal neutrons:

$$P_{NL} = P_{NFL} \, P_{NTL} \,, \qquad (3\text{-}17)$$

where

P_{NFL} = probability that fast neutron will not leak out ,

P_{NTL} = probability that thermal neutron will not leak out .

If we now insert these new definitions into our earlier expressions, we find that the infinite medium multiplication factor becomes

$$k_\infty = \eta f p \epsilon \qquad \text{"4-factor formula"} \qquad (3\text{-}18)$$

and

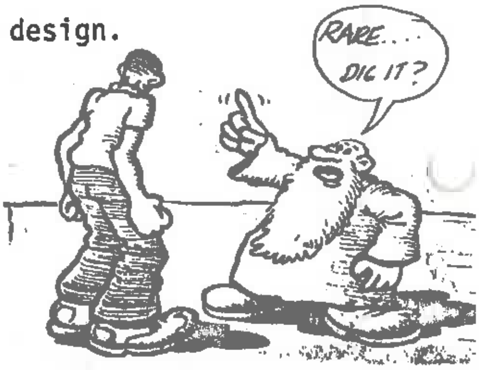
$$k = \eta f p \epsilon P_{NFL} P_{NTL} \qquad \text{"6-factor formula"} \qquad (3\text{-}19)$$

By way of example, for a typical thermal reactor:

$$\begin{array}{rl} \eta &= 1.65 \\ f &= 0.87 \\ \epsilon &= 1.02 \end{array} \qquad \left.\begin{array}{rl} p &= 0.87 \\ P_{NFL} &= 0.91 \\ P_{NTL} &= 0.86 \end{array}\right\} \Rightarrow \quad \begin{array}{rl} k_\infty &= 1.27 \\ k &= 1.00 \end{array}$$

Hence, provided we can calculate each of these factors, our criticality condition k = 1 can then be easily checked. Of course, the calculation of these factors is quite difficult in general. Indeed, one cannot really separate the various conditional probabilities as was done in these formulas. Instead, alternative schemes (usually iterative and numerical) must be used in practice to arrive at a criticality condition.

However, the 4-factor and 6-factor formulas are nevertheless quite useful because they provide insight into the various mechanisms involved in nuclear fission chain reactions--and, on rare occasions, such formulas can actually be used for crude estimates in nuclear design.



D. Conversion and Breeding

It is obvious that since $f < 1$ and $P_{NL} < 1$, we need $\eta > 1$ to achieve criticality. Fortunately, as we see from Figure 3-1, this condition is not only satisfied, but in fact for many energies, $\eta > 2$. Hence we in fact appear to have an extra neutron. This bonus neutron can be put to good use if we recall that certain isotopes ("fertile" nuclides) can be transmuted into fissile isotopes via neutron capture--e.g.,

$$U^{238}(n,\gamma)U^{239} \xrightarrow{\beta^-} Np^{239} \xrightarrow{\beta^-} Pu^{239} \tag{3-20}$$

or

$$Th^{232}(n,\gamma)Th^{233} \xrightarrow{\beta^-} Pa^{233} \xrightarrow{\beta^-} U^{233} \tag{3-21}$$

Hence if we load the core of a reactor with such fertile material, we can use the extra neutron to produce new fissile fuel material. This process is frequently referred to as "conversion", and reactors whose principal job is to produce Pu^{239} or U^{233} are called "converter" reactors. Actually, all power reactors are converter reactors in a sense, since they contain substantial amounts of U^{238} which will be transmuted into Pu^{239} via neutron capture during normal operation. For example, a light-water reactor will contain roughly 3% U^{235} and 97% U^{238} in a freshly loaded core. After a standard operating cycle, this core will contain roughly 1% U^{235} and 1% Pu^{239}, which can then be separated out of the spent fuel and refabricated into fresh fuel elements for reloading (so-called "plutonium recycling").

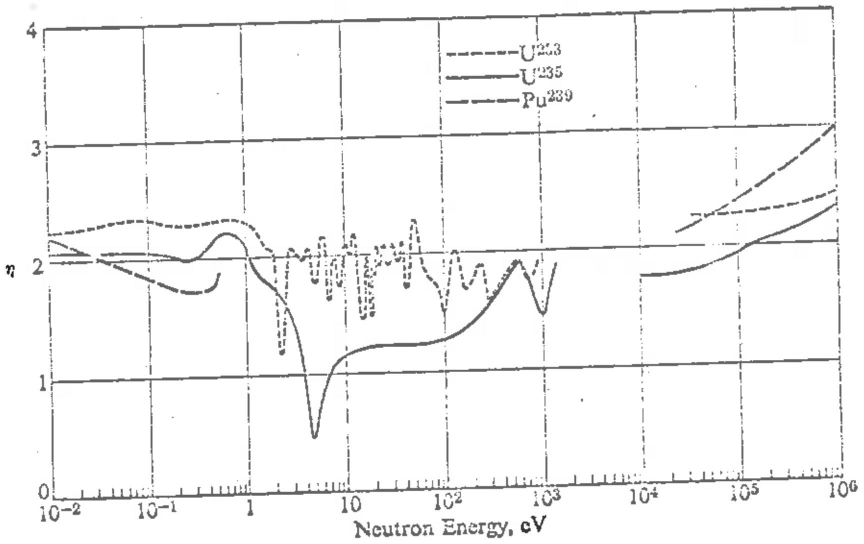


FIGURE 3-1: Variation of η with energy for U^{233}, U^{235}, and Pu^{239}

These considerations suggest that it might be possible, in fact, to fuel a reactor with Pu^{239} and U^{238} and then produce directly the fuel (Pu^{239}) needed for future operation. In fact, it might even be possible to produce more Pu^{239} than is burned--that is, to "breed" new fuel. This is the essential idea behind the "breeder" reactor.

To discuss this concept in more detail, it is useful to define the "conversion ratio"

$$C \equiv \frac{\text{average number of fissile atoms produced}}{\text{\# of fuel atoms consumed}} \equiv \text{"conversion" ratio} \tag{3-22}$$

(This is also referred to asthe "breeding ratio" if $C > 1$.) If we have conversion, then consuming N atoms of fuel during reactor operation will yield N C atoms of the new fissile isotope.

Now for breeding to occur, we require that the "breeding gain" G, defined by

$$\text{"breeding gain"} \equiv G \equiv C - 1 \tag{3-23}$$

be greater than zero. Of course, for this to happen, we need $\eta > 2$ since one neutron is needed to maintain the chain reaction, and one-plus neutrons are needed for breeding.

From Figure 3-1, we can see that the only attractive breeding cycle for low energy (thermal) neutrons would involve Th^{232}-U^{233}. To breed U^{238}-Pu^{239} requires that we use fast neutrons with energies greater than 100 keV. And, of course, this is the motivation behind the development of the fast breeder reactor.

At this point it is useful to digress a bit and discuss the average energy of the neutrons sustaining the chain reaction in various reactor types. As we have seen, the energies of neutrons in a reactor span an enormous range, from 10 MeV (usually the maximum energy of fission neutrons) down to as low as 0.01 eV after having suffered a number of scattering collisions with nuclei and slowing down. Furthermore, the neutron cross sections depend sensitively upon the neutron energy. As a general trend, cross sections decrease rapidly with increasing neutron energies (see the Figures in Chapter 2). This feature is particularly true of absorption cross sections such as capture or fission.

The fact that the fission cross section σ_f is largest at low energies implies that it is easiest to maintain a fission chain reaction using slow neutrons. Hence early nuclear reactors used light nuclei materials such as water or graphite to slow down or "moderate" the fast fission neutrons. Such moderating materials slowed the neutrons down to energies comparable to the thermal energies of the nuclei in the reactor core, e.g., to energies $E \sim kT = 0.25$ eV for $T = 300°K$. Reactors which are characterized by an average neutron energy $\langle E \rangle \sim$ thermal energy are referred to as "thermal" reactors. [A typical thermal reactor neutron energy spectrum is shown in Figure 3-2.] Such reactors require the minimum amount of fissile material for fueling, and are the simplest reactor types to build and operate. Most nuclear power plants in this country and abroad utilize thermal reactors.

However we have also seen that there is a very definite advantage in keeping the neutron energy high, since the number of neutrons emitted per neutron absorbed in the fuel, η, is largest for fast neutrons. Hence one can use the "extra" neutrons available in a fission chain reaction maintained by fast neutrons to convert or breed new fuel. But since σ_f

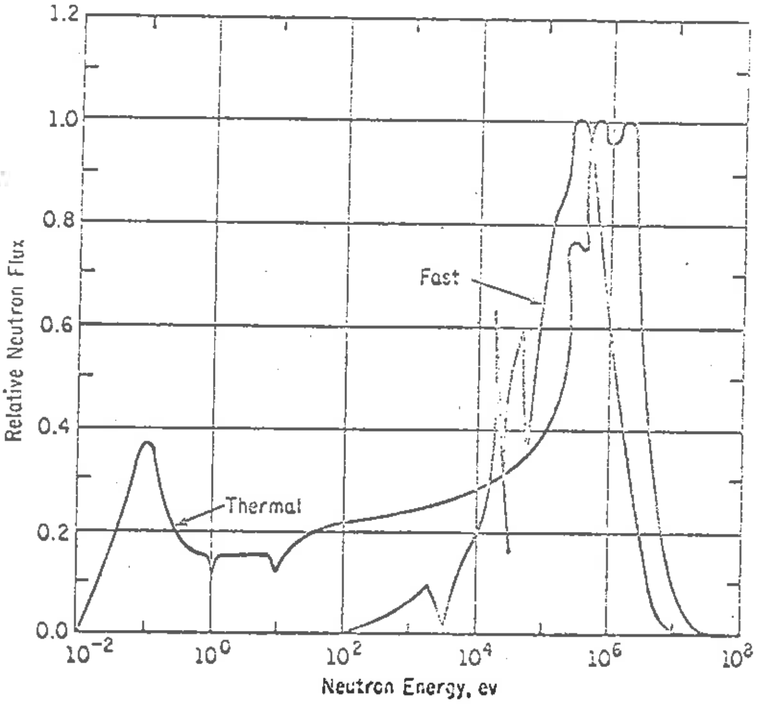
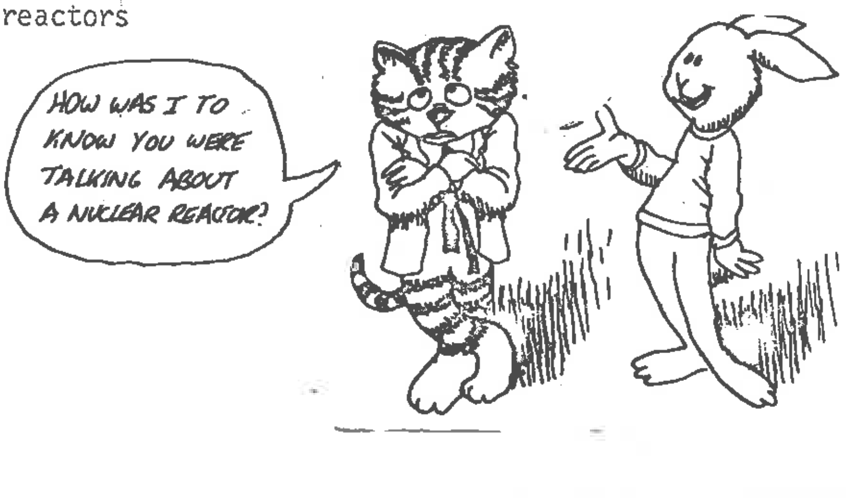


FIGURE 3-2: Typical neutron energy spectra in fast (LMFBR) and thermal (PWR) reactors



is smaller, one also needs much more fuel to sustain the chain reaction. Furthermore, to keep the neutron energy high, one wants to utilize only high mass number materials in the core to keep neutron slowing down to a minimum. Such reactors characterized by average neutron energies $\langle E \rangle >$ 100 keV are known as "fast" reactors. [A typical fast reactor neutron energy spectrum is shown in Figure 3-3.] It is generally felt that fast reactors will eventually replace the current generation of thermal power reactors because of their ability to breed fuel.

II. NUCLEAR REACTOR COMPONENTS

A. Nuclear Power Plants

A schematic of a typical large nuclear power plant is given in Figure 3-4. Such a diagram makes it apparent that the nuclear reactor itself is only one component of many in such a plant. Actually, aside from the nuclear reactor, such power plants are remarkable similar to large fossil fuel power plants. Only the source of the heat energy differs (nuclear vs. chemical combustion). Hence it is appropriate to begin with a brief description of the non-nuclear components of a large, central station power plant.

A very crude diagram of such a plant is given in Figure 3-5:

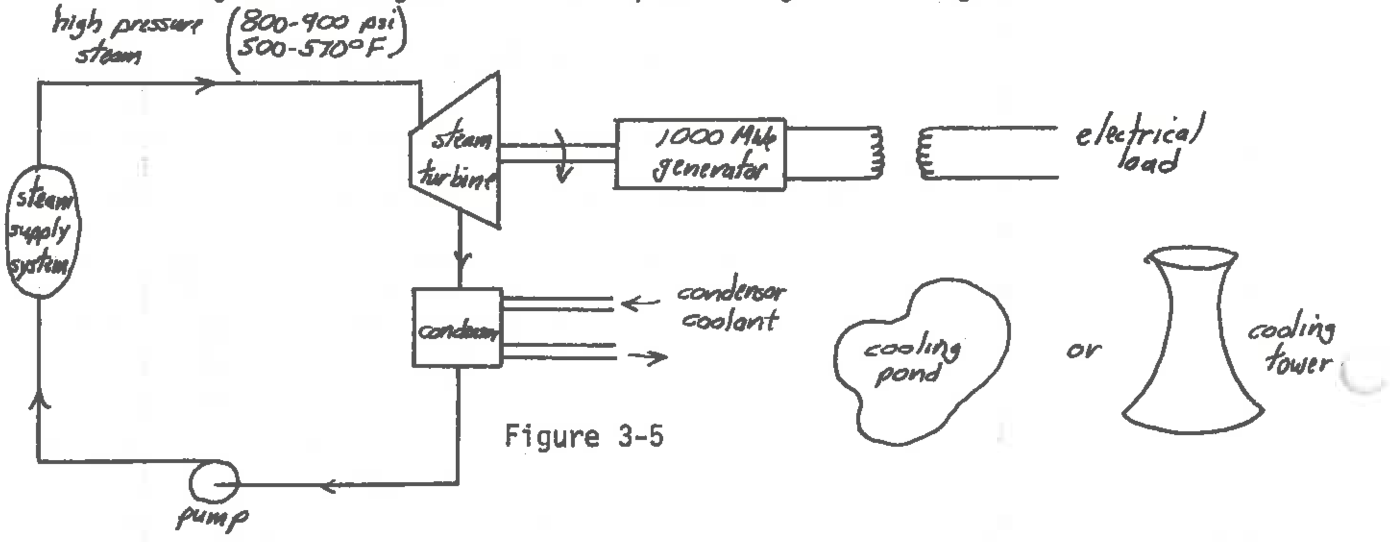


Figure 3-5

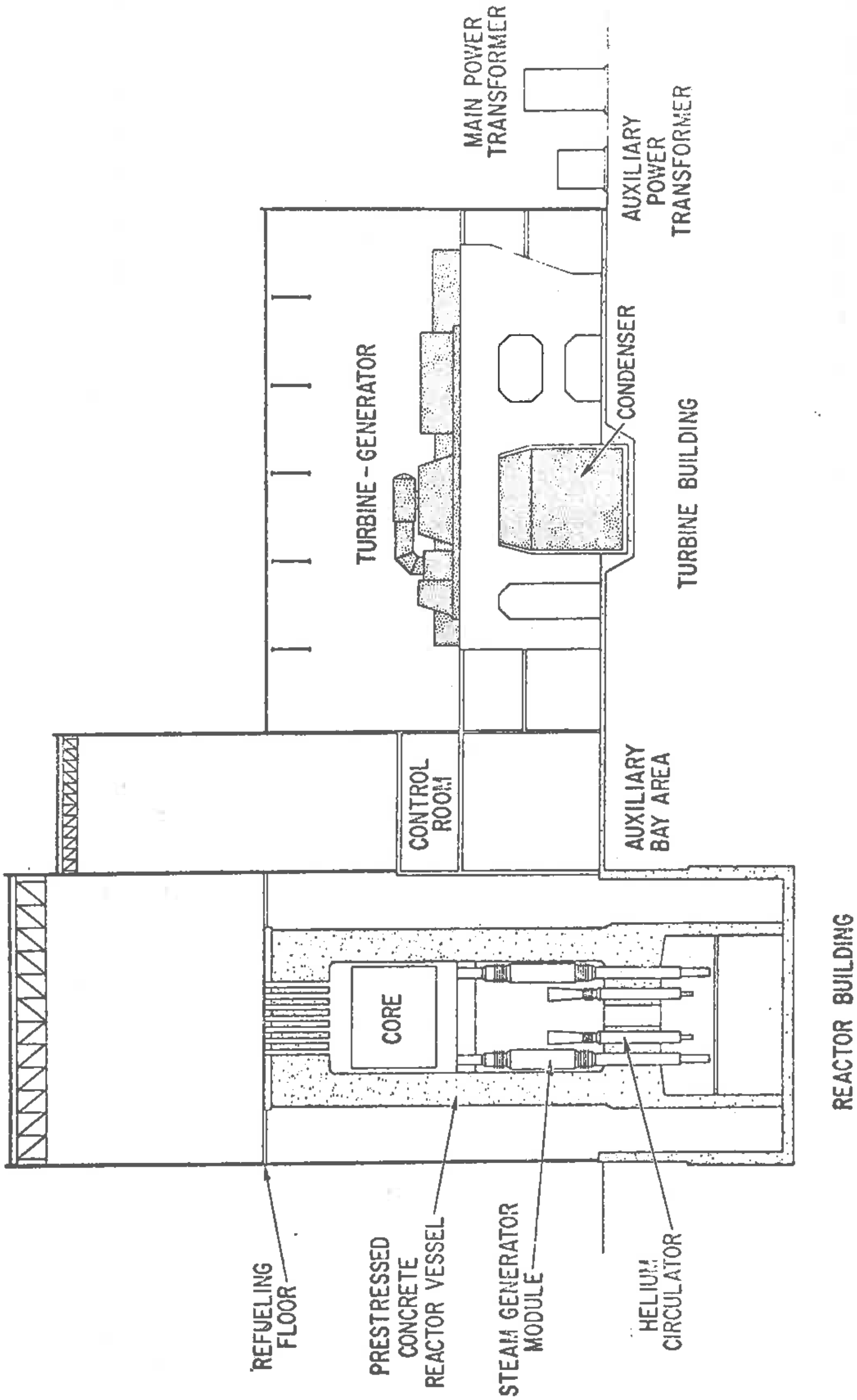


FIGURE 3-4: A typical nuclear plant (for variety, based upon an HTGR nuclear steam supply system)

As we have sketched it in this diagram, the steam supply system could be either a fossil-fueled boiler or a nuclear reactor and their associated coolant loops and steam generators. All large power plants today work on a steam cycle (a so-called Rankine cycle), in which the heat generated by combustion or nuclear fission is used to convert water into high pressure steam. This steam is then allowed to expand against the blades of a turbine, thereby converting the latent energy of the steam into mechanical work by turning the turbine rotor. This rotor is connected to a large electrical generator which converts the mechanical turbine energy into electrical energy which can then be distributed to the utilities' power grid. The low pressure steam leaving the turbine must then be re-condensed into water so that it can be pumped back to the steam supply system to complete the cycle. The condensor requires substantial amounts of water to re-condense the low pressure steam. This water is usually taken from a nearby river or lake (or in more recent designs, from an artificial cooling pond or cooling tower).

It should be noted that the details of this schematic are independent of whether the heat source used in the steam supply system is a coal-fired boiler or a nuclear reactor. Actually, as far as the steam cycle of the plant is concerned, the only real difference between the two types of steam supply systems is that the fossil-fueled system supplies slightly higher temperature steam (although certain reactor types such as the HTGR have overcome even this disadvantage).

At this point it is important to discuss another aspect of electrical power generation. This involves the unfortunate fact that it is impossible to convert heat energy into mechanical or electrical energy with a very high efficiency. Indeed, the laws of thermodynamics tell that the best efficiency we can possibly obtain (via a Carnot cycle) is

$$\text{efficiency} = 1 - \frac{T_{\text{condensor}}}{T_{\text{steam}}}$$

where T is the temperature (in degrees Kelvin or Rankine). Hence, since the condensor water temperature (the cooling pond or lake water) is usually at about 70°F, while the steam temperature is typically 500°F, we can see that the absolute maximum plant efficiency is around 40%. In any real system, there are numerous other inefficiencies (in pumping and pipe friction, heat exchangers, etc.) which reduce this efficiency to about 30% for an actual plant. That means if the plant is rated at 1000 Mwe (megawatts--electrical energy), the steam supply system must produce 3,333 Mw of thermal energy. The energy difference, in this case, 2,333 Mw, must be discharged as heat into the condensor coolant--and eventually to the environment.

It should be stressed that this thermal discharge is simply a consequence of fundamental laws of thermodynamics. It has nothing to do with whether a plant is fossil-fueled or nuclear--only with how high the steam temperature is. Only by going completely away from a steam cycle can one hope to improve significantly on this efficiency (e.g., by using gas turbines, magnetohydrodynamics, or direct conversion). But the development of such alternatives is many years down the road, so it looks like we are going to have to be content with dumping roughly 60% of our produced energy into the environment as waste heat for awhile.

Of course, this has been a very simple description of a very complex system. We will return later to discuss nuclear power plants in more detail in Chapter 14. At this point, we now focus our attention on the unique feature of a nuclear power plant, the nuclear steam supply system.

B. The Nuclear Steam Supply System

A NSSS consists essentially of three different components:

(i) a nuclear reactor which supplies the fission heat energy

(ii) the primary coolant loop (and primary coolant pump) which circulates a coolant through the nuclear reactor core to extract the fission heat energy

(iii) a heat exchanger (or steam generator) in which the heated primary coolant is used to turn water into steam.

A very simplified diagram of a NSSS is shown in Figure 3-6.

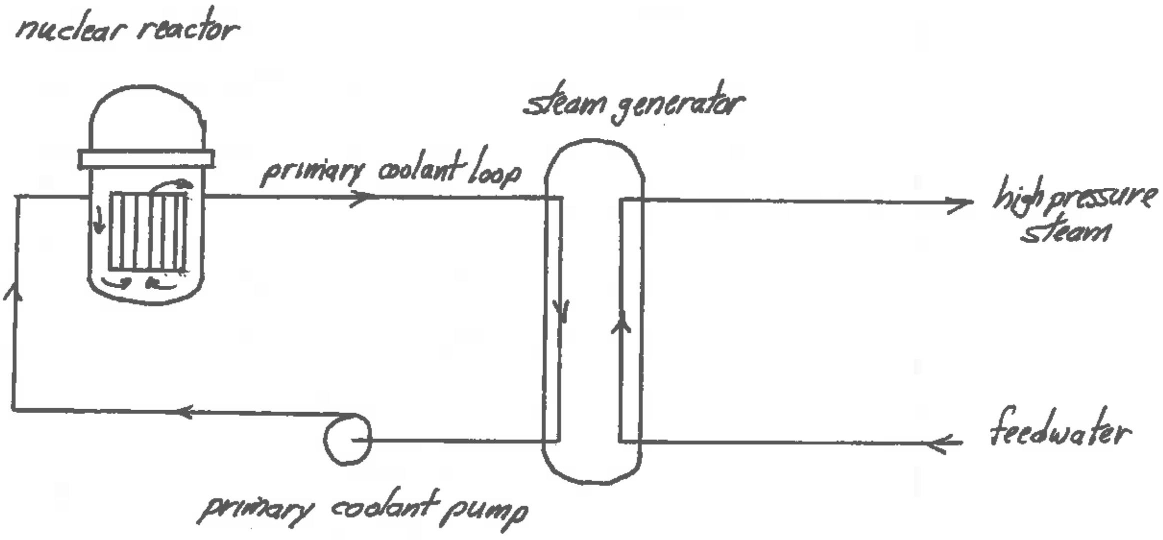


Figure 3-6

Of course, depending on the type of reactor, there will be additional components in the NSSS. There are a variety of possible coolants which can be used in the primary loop. The most common coolant is ordinary water, and most reactors being built in this country today are so-called light water reactors. There are two types of LWR's marketed in the United States today: pressurized water reactors (PWR's) and boiling water reactors (BWR's).

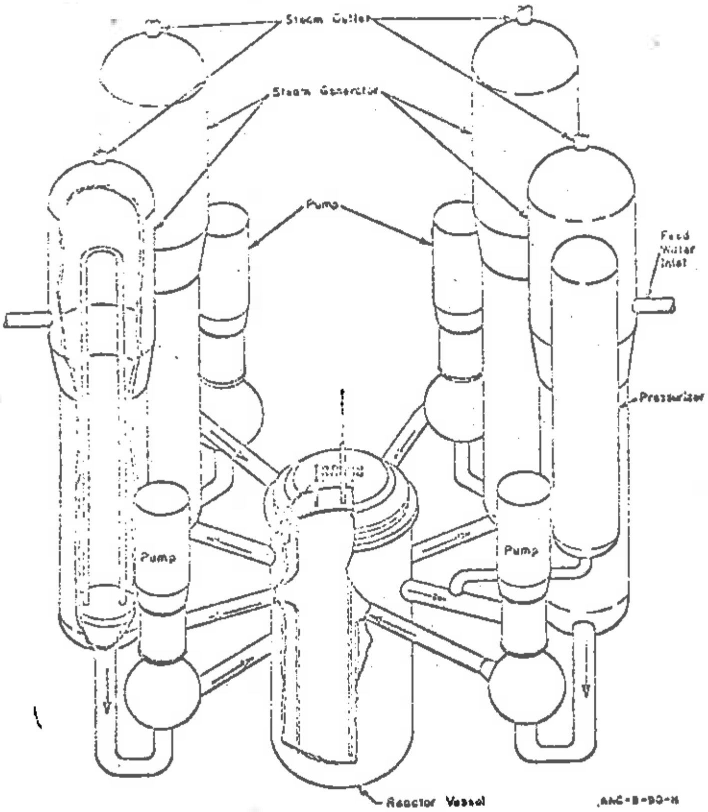
In a PWR, the primary coolant is water under high pressure (~2200 psia) to keep it from boiling as it passes through the reactor core. PWR's are manufactured by three firms in the U.S.: Westinghouse, Babcock & Wilcox, and Combustion Engineering. In Figures 3-7 we have shown the NSSS sold by each of these firms, and aside from the number of primary pumps and steam generators, the various NSSS are quite similar.

The principal competitor to the PWR is the boiling water reactor (BWR) produced by General Electric in which the water is allowed to boil in the reactor core itself. Hence in the BWR NSSS (see Figures 3-10), the steam generator and the reactor are combined together. The BWR is actually only a single loop system, since the high pressure steam is produced directly in the reactor core (eliminating the need for a separate steam generator). In this sense, the primary coolant loop feeds directly into the turbine. We will discuss the relative advantages and disadvantages of BWR's vs. PWR's later after we have learned more about the nuclear reactor core itself.

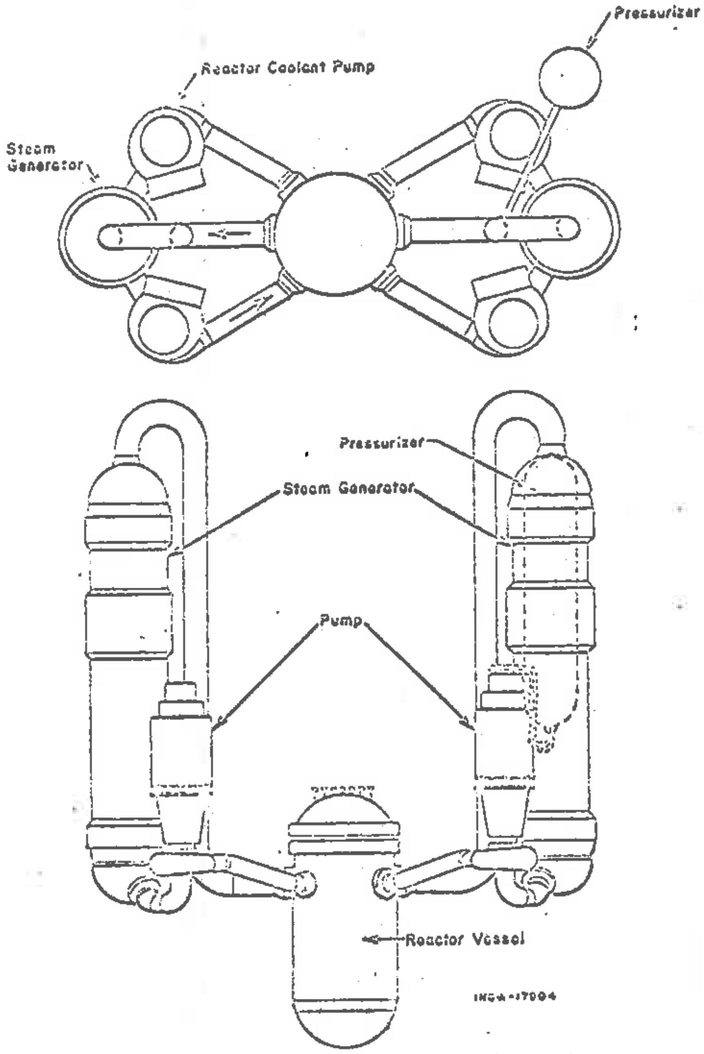
There has been considerable recent interest in an alternative coolant, high pressure helium. A number of such high temperature gas cooled reactors are being produced today--both by Gulf General Atomics in this country and in the United Kingdom. [See Figure 3-11.]

Yet another type of coolant is a liquid metal such as sodium. Such liquid metal coolant loops are most frequently considered for fast breeder reactors because the technical problems in working with extremely volatile

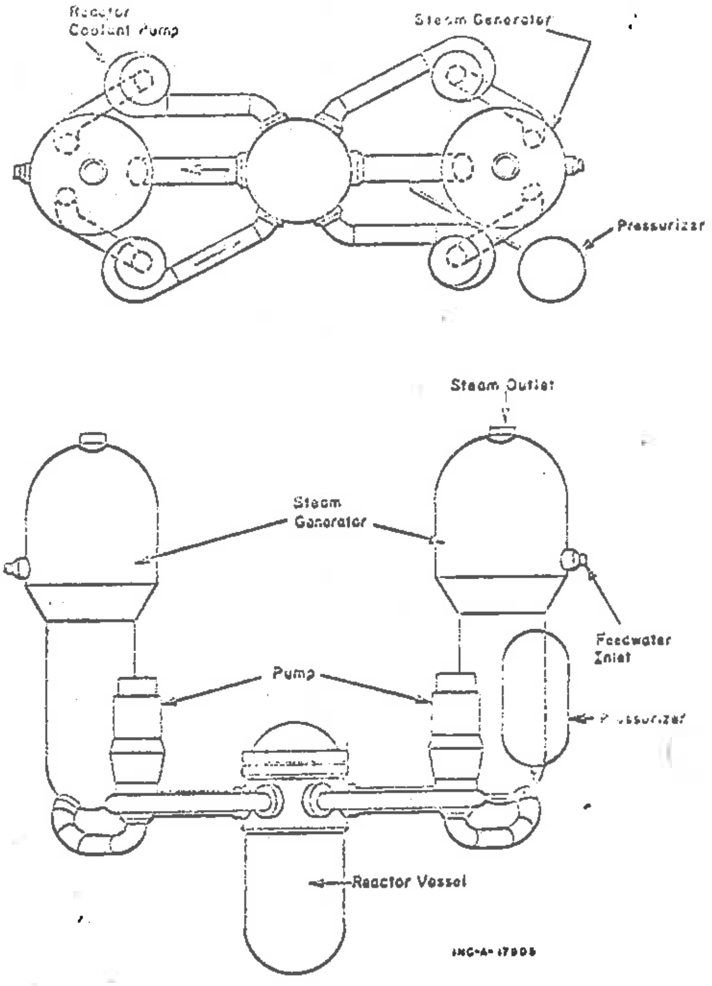
FIGURE 3-7: The various PWR NSSS manufactured in the United States



Typical Westinghouse Electric Corporation Four-Loop System.

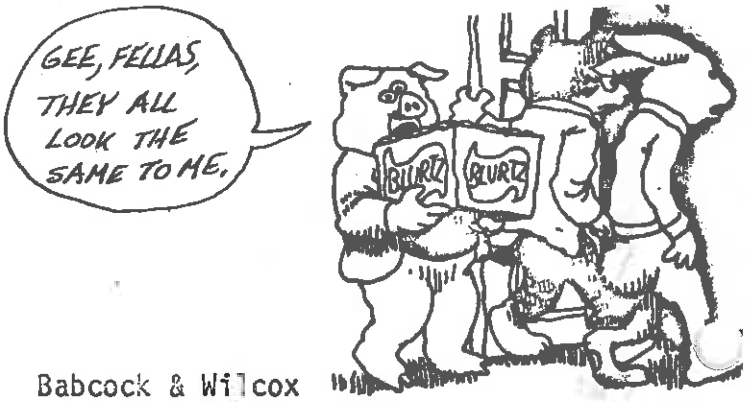


Davis-Besse Reactor Coolant System Arrangement (4).



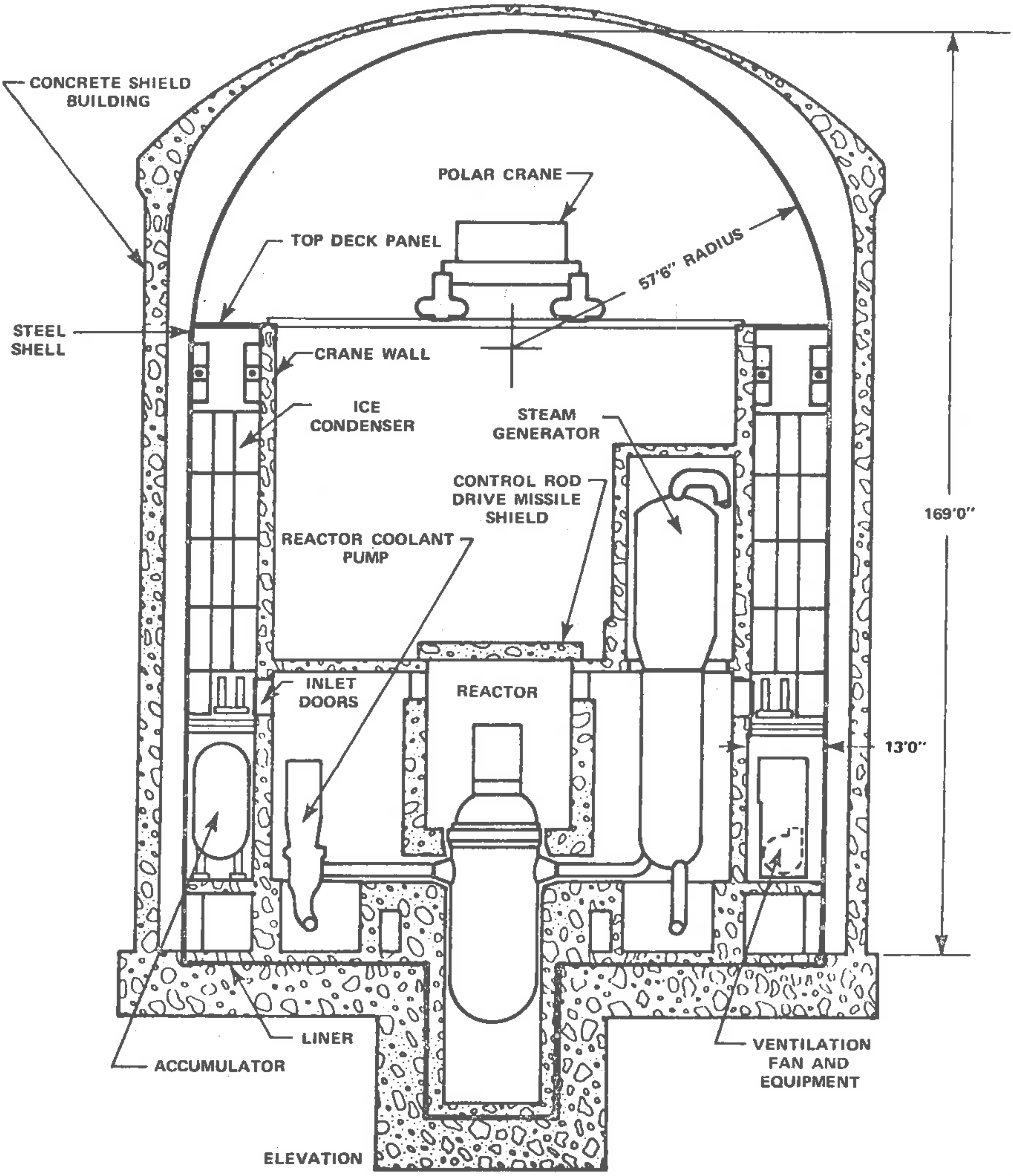
Forked River Reactor Coolant System Arrangement (4).

Combustion Engineering



Babcock & Wilcox

FIGURE 3-8: Cross section of the Westinghouse PWR nuclear steam supply system (inside of its containment structure)



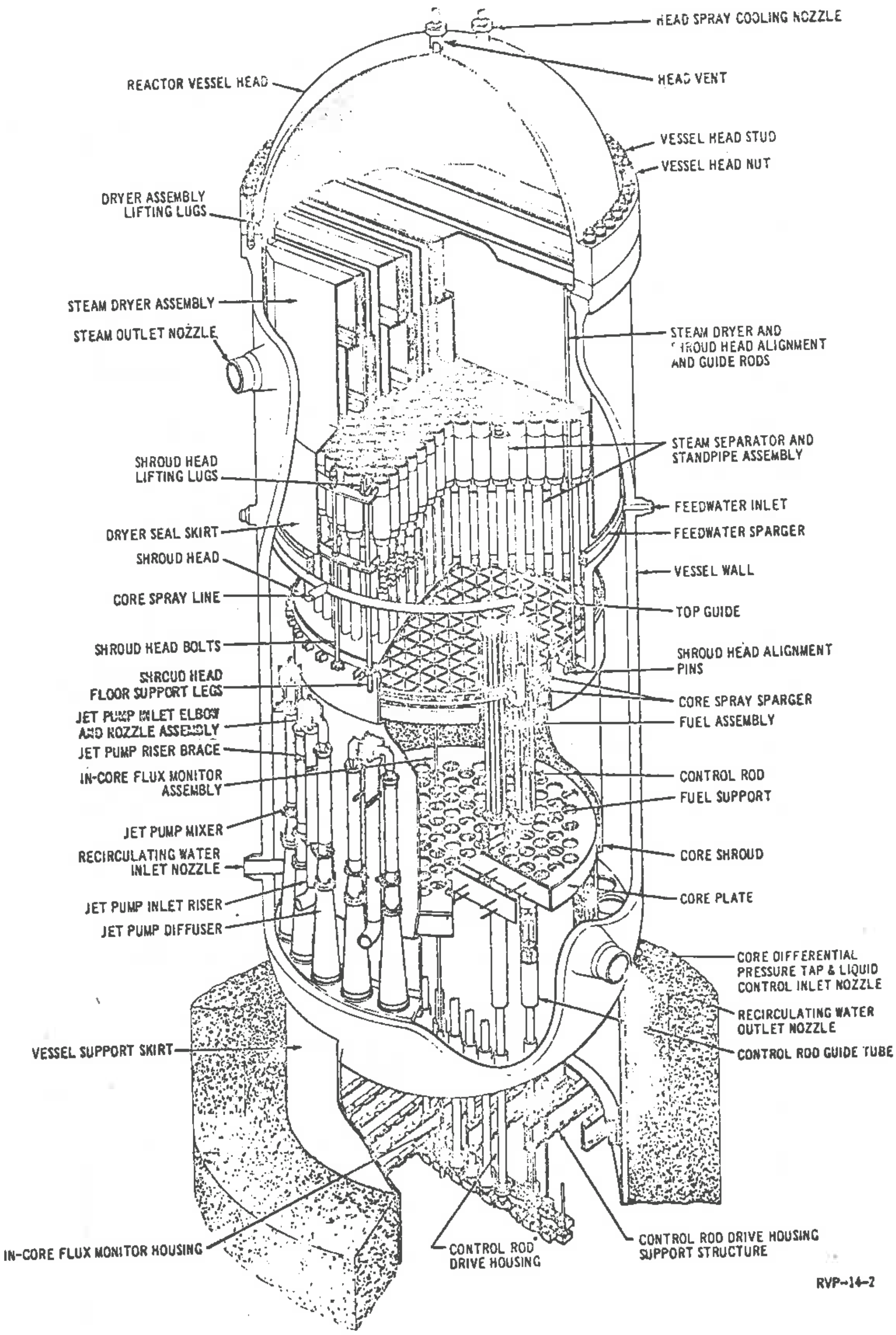


FIGURE 3-9: A Boiling Water Reactor (manufactured by General Electric)

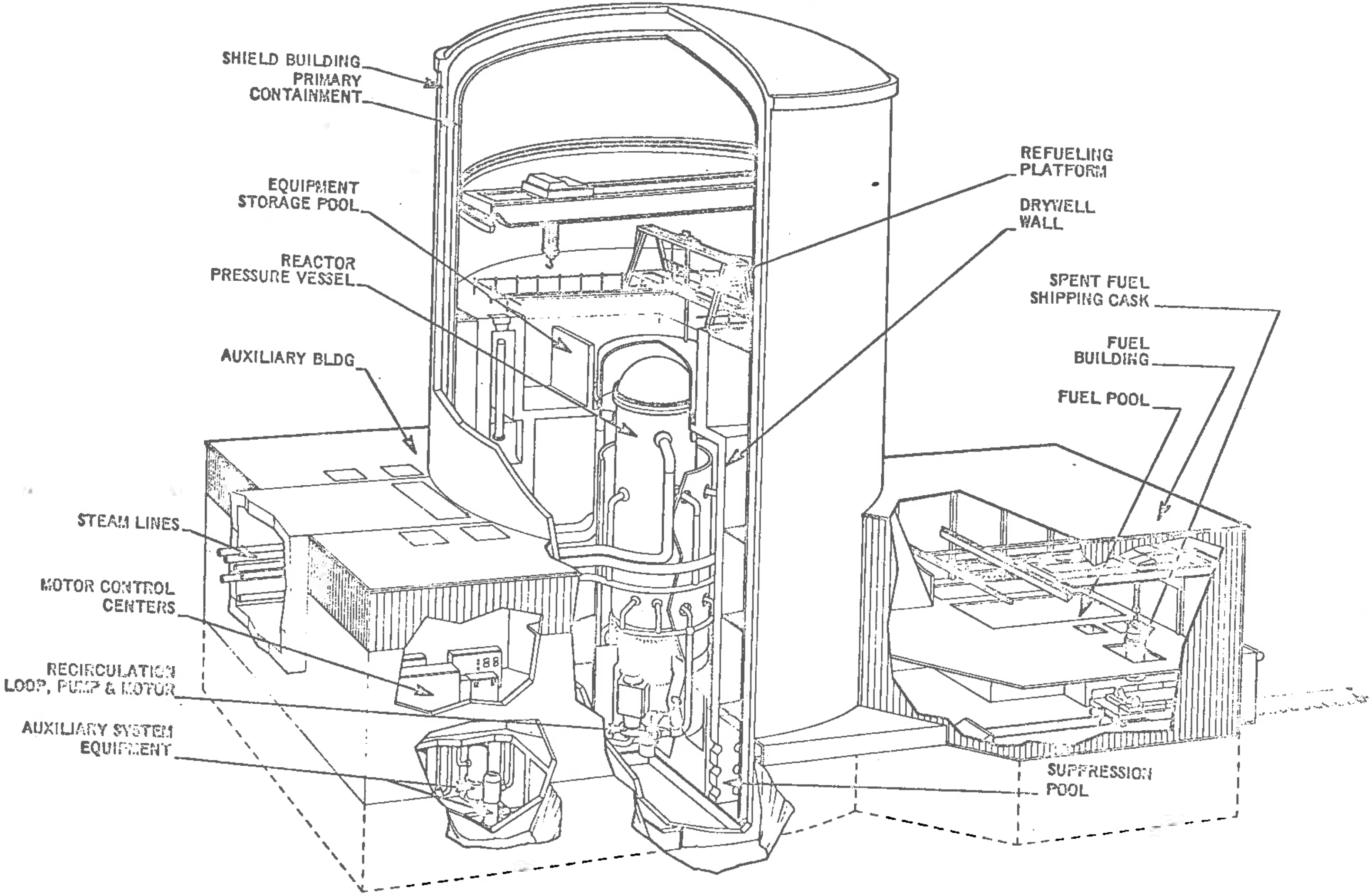
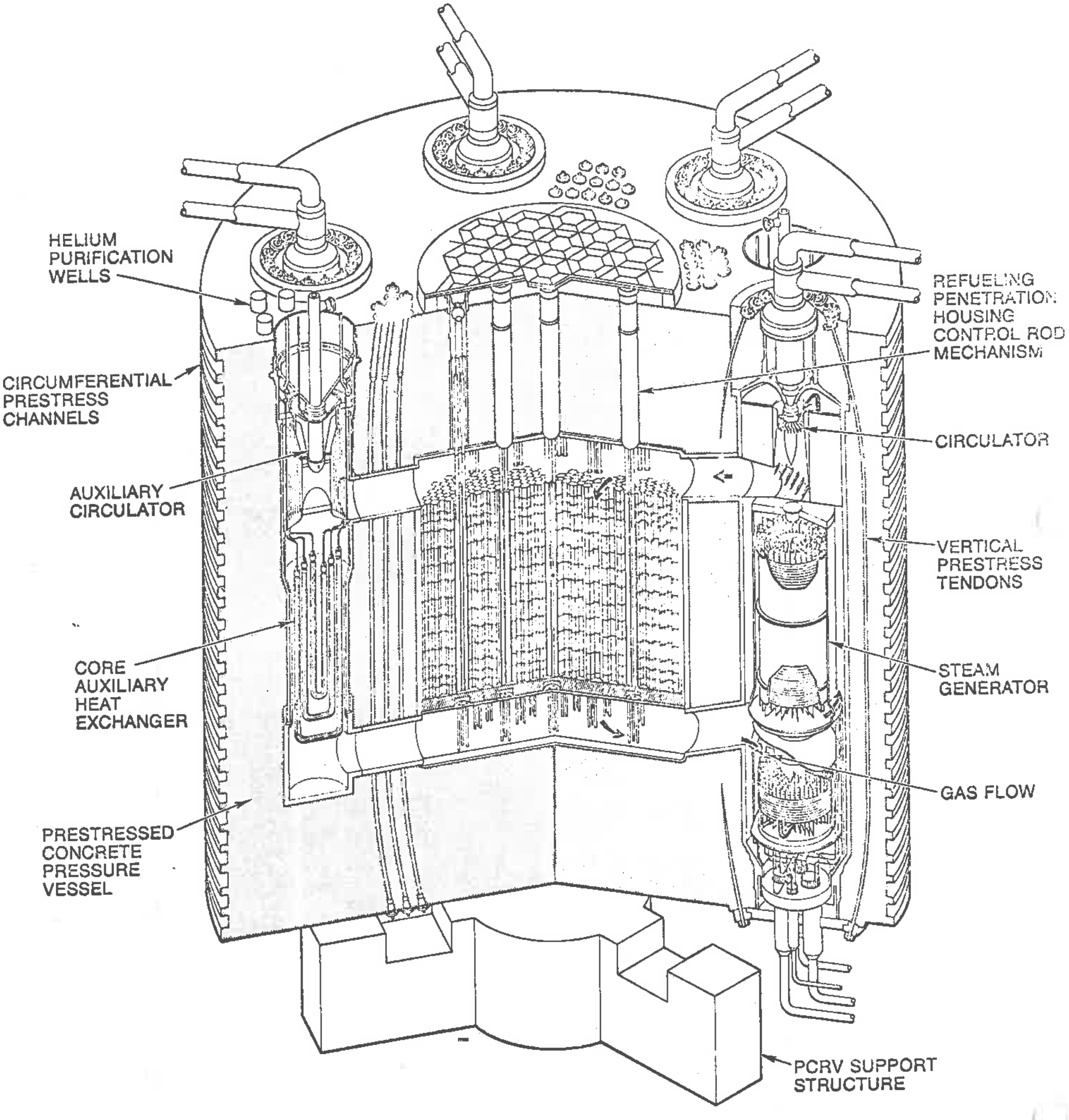


FIGURE 3-10: A BWR Nuclear Steam Supply System

FIGURE 3-11:: A High Temperature Gas Cooled Reactor



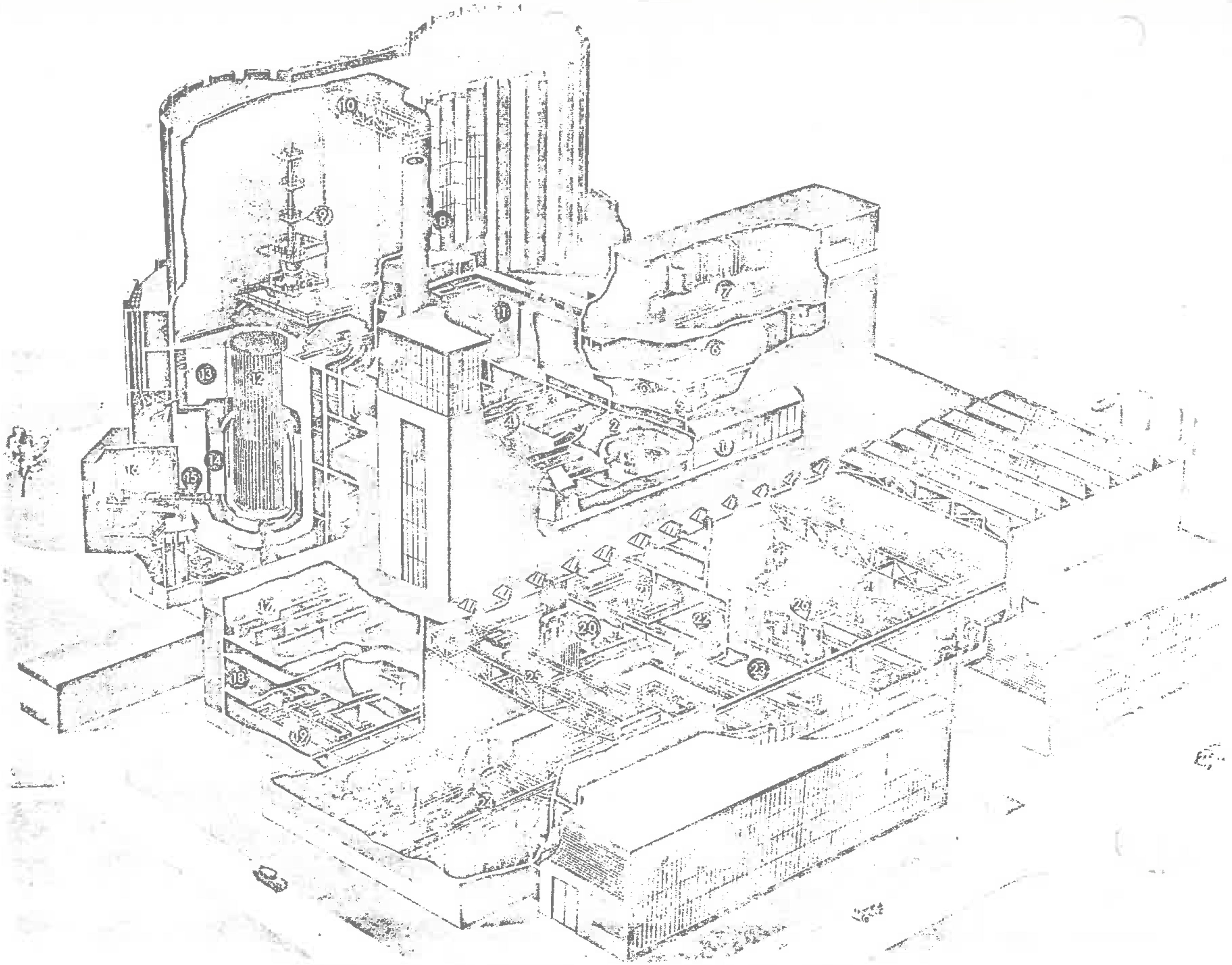


FIGURE 3-11: An Advanced Gas Cooled Reactor (AGR)

liquid metals is overcome by their superior heat transfer characteristics necessitated by fast reactor designs. [See Figure 3-12.]

C. The Nuclear Reactor

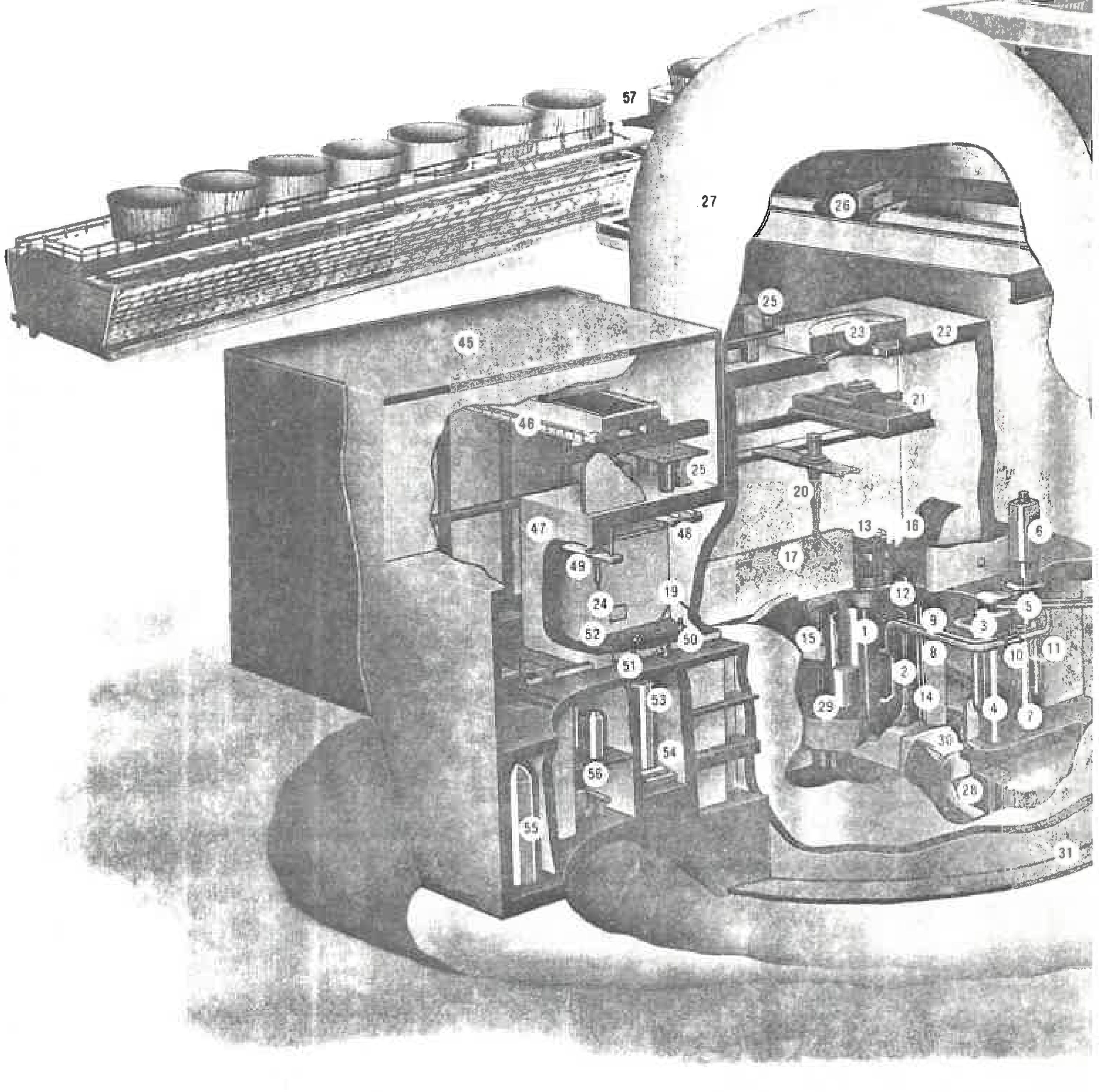
At the heart of the NSSS is the nuclear reactor itself. The cross section of a typical nuclear power reactor (in this case, a pressurized water reactor) is shown in Figure 3-13. At this time, merely notice that the core of the reactor consists of a cylindrically-shaped lattice (roughly 12 ft. in diameter by 12 ft. in height) of long fuel assemblies or bundles. These assemblies consist of a large number of long, narrow fuel rods or elements which are tubes made of a zirconium alloy which contain the nuclear fuel in the form of uranium dioxide (UO_2) pellets (see Figures 3-14, 3-15).

In the reactor core one induces and maintains the nuclear fission reactions which produce the desired heat. The core itself is contained in a much larger container, a pressure vessel, which is designed to withstand the enormous pressures of the coolant (up to 2200 psia) as well as to isolate the reactor core from the remainder of the NSSS. It should be admitted that most of our attention in this text will be directed at the nuclear analysis of the reactor core itself, since this is the principal activity of the nuclear engineer. However, as we have mentioned earlier, we will try to develop this nuclear analysis within the context of the other considerations influencing the design of the nuclear steam supply system.

D. Nuclear Reactor Components and Nomenclature

It is perhaps useful to make a formal list here of some of the various components one encounters in reactor analysis, as well as to introduce some standard nomenclature used in nuclear reactor engineering.

LMFBR Demonstratio



LMFBR: Keys to industrial success

by John H. Taylor and Nicholas A. Petrick

This year has seen a major step toward achieving the goal of fast breeder electrical power production with the decision to initiate the design and construction of a liquid metal fast breeder reactor demonstration power plant.

There are still major accomplishments, integral to the demonstration plant program and the Fast Flux Test Facility (FFTF) program, that must be made to fully achieve the goal of fast breeder electrical power production.

In the LMFBR development program to date, major attention has been centered on LMFBR research and development needs which involve unique technical features such as fuel and structural performance in the radiation and high-temperature environment, the properties of sodium and its compatibility with the materials of the system, and stability and control of the reactor. These should continue to receive attention, but there are other issues that are tied to the industrial success of the LMFBR. These issues have been emphasized recently as part of the FFTF program, and they must receive continuing emphasis in the demonstration plant program. These are:

- Adequate standards and design criteria must be defined that will assure reliability and safety in the high-temperature sodium environment of the LMFBR and that are practicable and cost-effective in their application.
- Licensability and environmental compatibility must be established with the regulatory agencies on the basis of definitive analyses and experimental data, and this technical position must be communicated to gain public acceptance.
- Industrial design competence and manufacturing capability must be developed to reliably and economically fabricate the unique reactor components and design and construct the LMFBR plants.
- The economics of the LMFBR must be established against vigorous competition with the light-water systems.

These are essential to LMFBR power generation because the utility industry will not buy LMFBR power plants unless:

1. They are convinced that it is a highly reliable power generator. The cost of unanticipated downtime (about $100,000 a day for a 1,000-MWe system in today's dollars), the difficulty in repairing a sodium-cooled system, and the role of the LMFBR as a high-capital-cost base-load generator make high reliability mandatory.

2. They are assured that the plant is licensable and can be licensed on a schedule on which they can depend. By the time the LMFBR is introduced, this problem will have been solved for the present-generation nuclear plants or there will be no nuclear industry whose expansion the LMFBR is to serve. No utility executive will therefore be willing to take licensing risks on the LMFBR unless he is confronted with a squeeze on fuel resources.

3. They ascertain that there are fully adequate and competent sources of supply for the equipment required and for construction of the plant and that the problems of procuring and contracting for this equipment and services are comparable to those for the present-generation nuclear power plants.

4. Their economic evaluation of the LMFBR as compared to other available nuclear power plant types show that its over-all energy cost will be less. After spending substantial funds in support of the LMFBR demonstration plant program, no utility executive will be interested in furthering the development of the LMFBR by putting commercial plants on his network which would impose a cost burden on his customers.

Each of these four requisites of the utility industry can be translated into detailed design, performance, and de-

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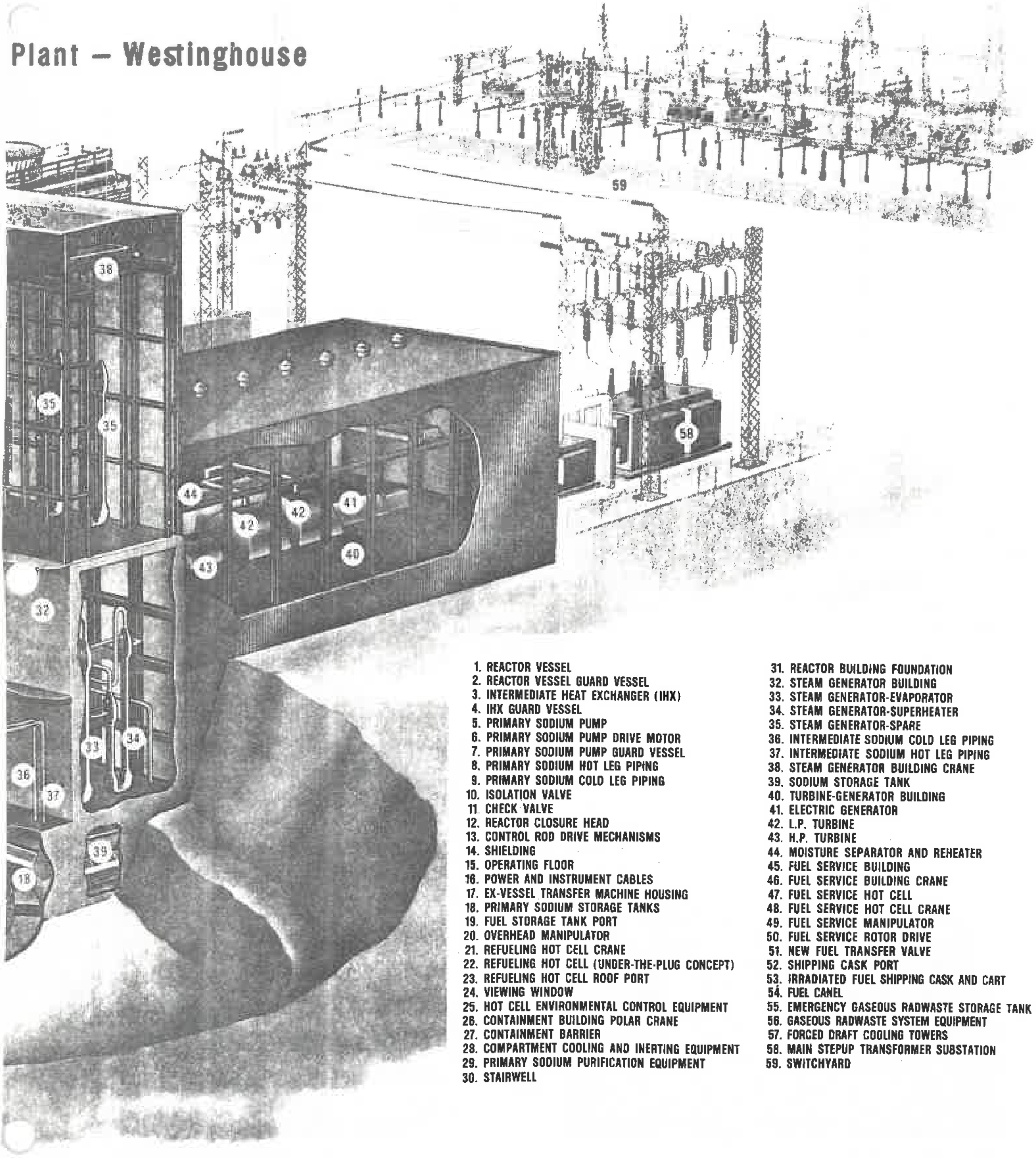
Mr. Taylor is general manager, Breeder Reactor Divisions, and Mr. Petrick, project manager, LMFBR Demo Plant, Advanced Reactors Division, Westinghouse Electric Corporation. This article is derived from their paper "Keys to Open the Door to Industrial Success of the Liquid Metal Fast Breeder Reactor," presented at the American Nuclear Society Topical Meeting on "Nuclear Power for Tomorrow," Atlantic City, N.J., August 23, 1972.

Plant — Westinghouse



1. REACTOR VESSEL
2. REACTOR VESSEL GUARD VESSEL
3. INTERMEDIATE HEAT EXCHANGER (IHX)
4. IHX GUARD VESSEL
5. PRIMARY SODIUM PUMP
6. PRIMARY SODIUM PUMP DRIVE MOTOR
7. PRIMARY SODIUM PUMP GUARD VESSEL
8. PRIMARY SODIUM HOT LEG PIPING
9. PRIMARY SODIUM COLD LEG PIPING
10. ISOLATION VALVE
11. CHECK VALVE
12. REACTOR CLOSURE HEAD
13. CONTROL ROD DRIVE MECHANISMS
14. SHIELDING
15. OPERATING FLOOR
16. POWER AND INSTRUMENT CABLES
17. EX-VESSEL TRANSFER MACHINE HOUSING
18. PRIMARY SODIUM STORAGE TANKS
19. FUEL STORAGE TANK PORT
20. OVERHEAD MANIPULATOR
21. REFUELING HOT CELL CRANE
22. REFUELING HOT CELL (UNDER-THE-PLUG CONCEPT)
23. REFUELING HOT CELL ROOF PORT
24. VIEWING WINDOW
25. HOT CELL ENVIRONMENTAL CONTROL EQUIPMENT
26. CONTAINMENT BUILDING POLAR CRANE
27. CONTAINMENT BARRIER
28. COMPARTMENT COOLING AND INERTING EQUIPMENT
29. PRIMARY SODIUM PURIFICATION EQUIPMENT
30. STAIRWELL
31. REACTOR BUILDING FOUNDATION
32. STEAM GENERATOR BUILDING
33. STEAM GENERATOR-EVAPORATOR
34. STEAM GENERATOR-SUPERHEATER
35. STEAM GENERATOR-SPARE
36. INTERMEDIATE SODIUM COLD LEG PIPING
37. INTERMEDIATE SODIUM HOT LEG PIPING
38. STEAM GENERATOR BUILDING CRANE
39. SODIUM STORAGE TANK
40. TURBINE-GENERATOR BUILDING
41. ELECTRIC GENERATOR
42. L.P. TURBINE
43. H.P. TURBINE
44. MOISTURE SEPARATOR AND REHEATER
45. FUEL SERVICE BUILDING
46. FUEL SERVICE BUILDING CRANE
47. FUEL SERVICE HOT CELL
48. FUEL SERVICE HOT CELL CRANE
49. FUEL SERVICE MANIPULATOR
50. FUEL SERVICE ROTOR DRIVE
51. NEW FUEL TRANSFER VALVE
52. SHIPPING CASK PORT
53. IRRADIATED FUEL SHIPPING CASK AND CART
54. FUEL CANEL
55. EMERGENCY GASEOUS RADWASTE STORAGE TANK
56. GASEOUS RADWASTE SYSTEM EQUIPMENT
57. FORCED DRAFT COOLING TOWERS
58. MAIN STEPUP TRANSFORMER SUBSTATION
59. SWITCHYARD

velopment requirements that must guide the demonstration plant program, the FFTF program, and all supporting LMFBR technology efforts.

Standards and design criteria

The AEC has been spearheading development of standards for the LMFBR under the RDT standards program using its contractor organizations to prepare the standards. This work is being implemented with strong industry participation. The standards deal primarily with operation; instrumentation and controls; equipment, mechanical and fluid; programs, procedures and methods; materials; and electrical systems and equipment.

There is a continuing need to modify and improve these RDT standards as experience is gained in their application. There are two main motivations for such improvement: to better define requirements where gaps are detected and to be more practical and less costly in achieving the reliability desired. For example, the welding standards originally specified for FFTF components required inert gas welds. Subsequent development demonstrated acceptability of high-production, automatic submerged-arc processes, which have resulted in excellent welds with extremely low defect ratios. A better product on a better schedule and at a lower cost has resulted. In another example, the RDT standards proved to be sufficiently rigorous: The initial standards for castings for the FFTF pump proved to be unacceptable for the highly stressed components. More demanding non-destructive test requirements had to be imposed.

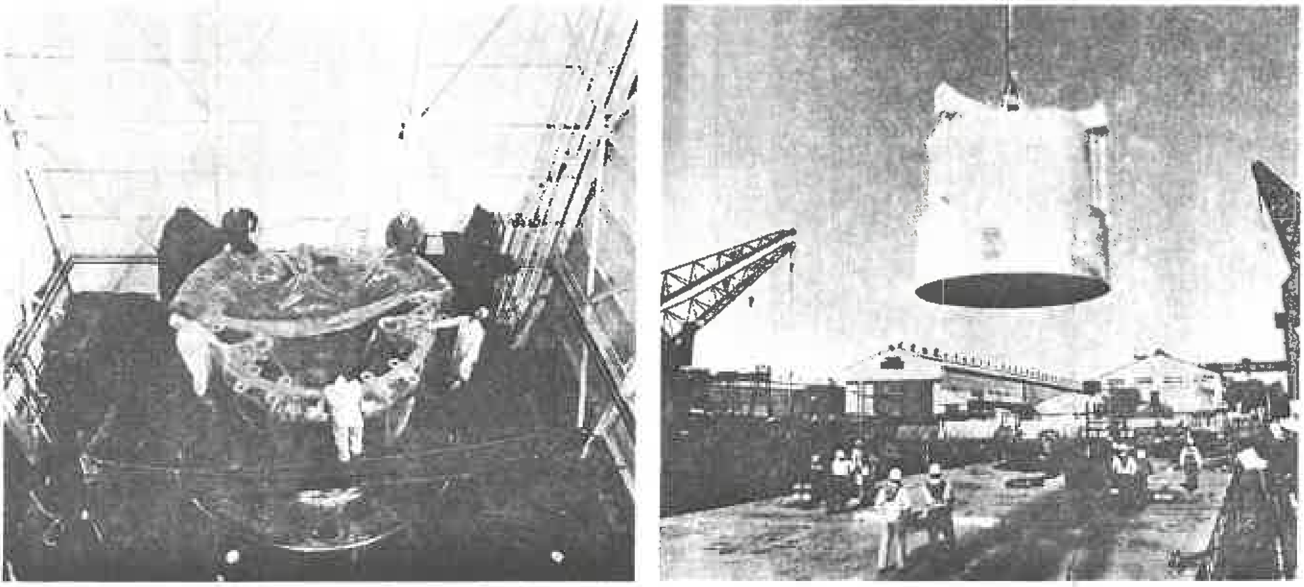
An important portion of the new standards work stems from the need to design and fabricate a highly reliable product to operate at the high temperature and large temperature differentials inherent in LMFBR components. Design criteria and fabrication standards must be incorporated into codes, usable by the designers and fabricators, which will assure reliability and safety in the high-temperature environment. Such definition also implies the availability and practical utilization of analytical methods and materials properties data which makes such criteria and codes sufficiently quantitative to fulfill their purpose.

Progress made to date on defining adequate high-temperature standards and design criteria has included the issuance of an interim high-temperature design criteria document, FRA-152 ("Interim Supplementary Structural Design Criteria for Elevated Temperatures," Revision 3 as of November 6, 1970), which is presently being incorporated as supplemental criteria to Code Case 1331-4 of the ASME 1331 Code on Elevated Temperature Design. Full utilization of FRA-152 requires considerable facility in in-elastic (elastic-plastic-creep) analysis and predictions of creep behavior, capability for which is still limited. However, we are not yet satisfied that either the criteria are well enough defined or that the underlying analytical methods or materials properties data are sufficiently well developed.

Experience with application of the RDT standards to component procurements has ranged from complete acceptance by some qualified nuclear contractors familiar with similar high-quality nuclear standards to reluctance from firms not previously familiar with them. In most instances, we have been successful in demonstrating that application of many of the practices involved can improve product quality, reduce rejects and need for reworking, and up-grade record-keeping and inventory control. The RDT and related standards utilize to a heavy degree existing ASME codes and other practices that are familiar to qualified nuclear contractors. Application of these standards has involved higher costs to date, which we judge to be caused primarily by first-of-a-kind application problems. With continued effort we hope to bring these costs down to a level which the reduction in rework clearly pays for.

Another important standards effort is an industry-spearheaded activity to develop LMFBR general and principal design criteria under the aegis of the American Nuclear Society, with the participation of utility, manufacturer, and AEC personnel. The goal of this activity is to specify a complete set of LMFBR general and principal design criteria, compliance with which will ensure a safe, readily licensable plant.

The success of the LMFBR is contingent on system designs that lead to high reliability, high operating availability, and low cost. An important method of achieving this objective has



THE CORE SUPPORT STRUCTURE for the Fast Flux Test Facility (FFTF) is wrapped in plastic (left) before installation in its container. The 215,000-pound, 18-foot high, all-stainless-steel structure was built by Newport News Shipbuilding & Dry Dock Company under contract to the Westinghouse Advanced Reactors Division. Inside the container, the structure is lowered onto a barge (right) for shipment to Combustion Engineering for installation in the FFTF reactor vessel.

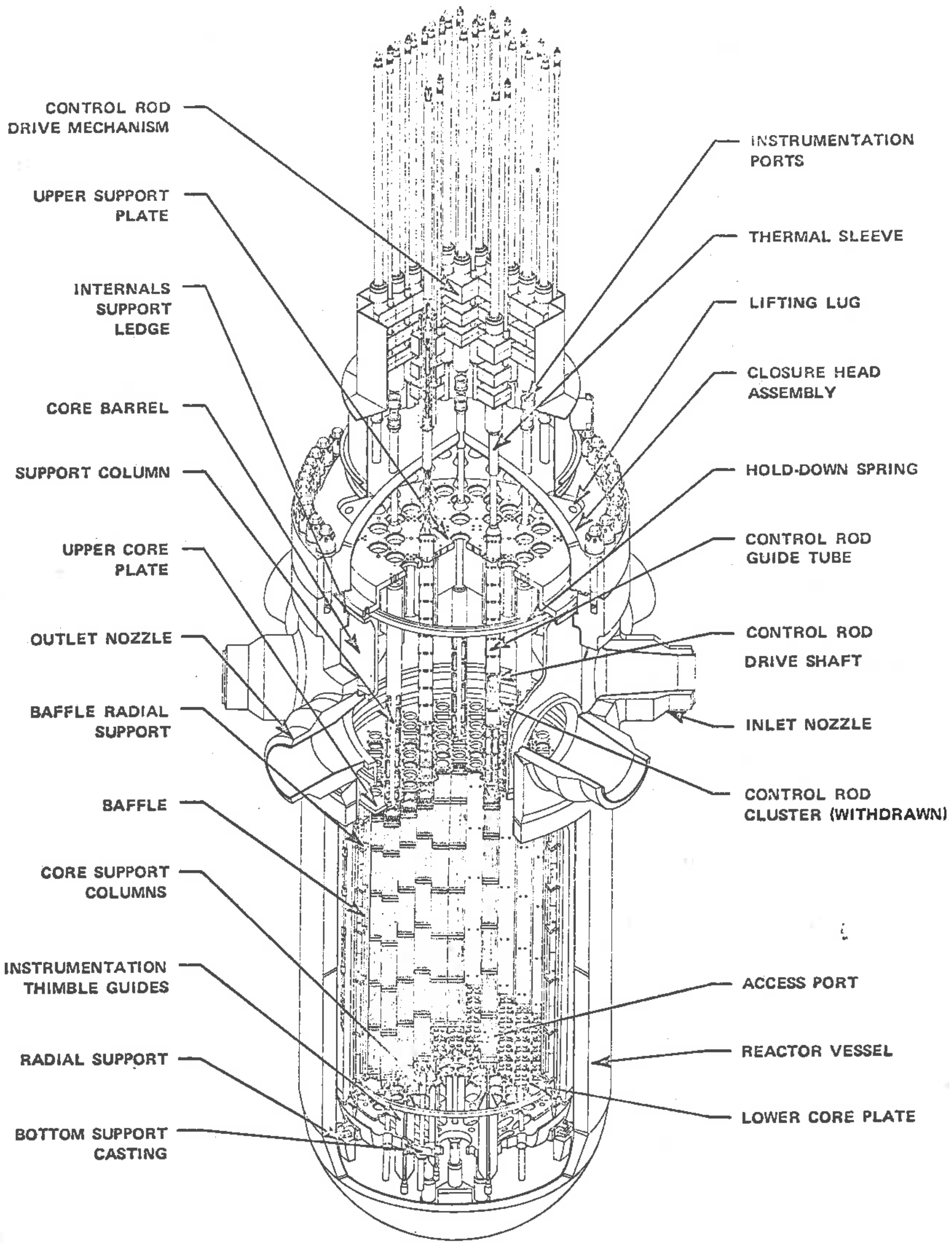
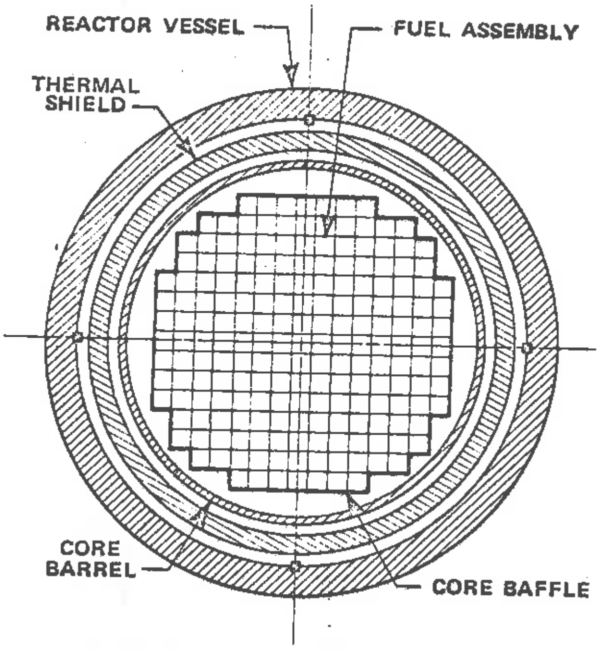


FIGURE 3-13: A pressurized water reactor

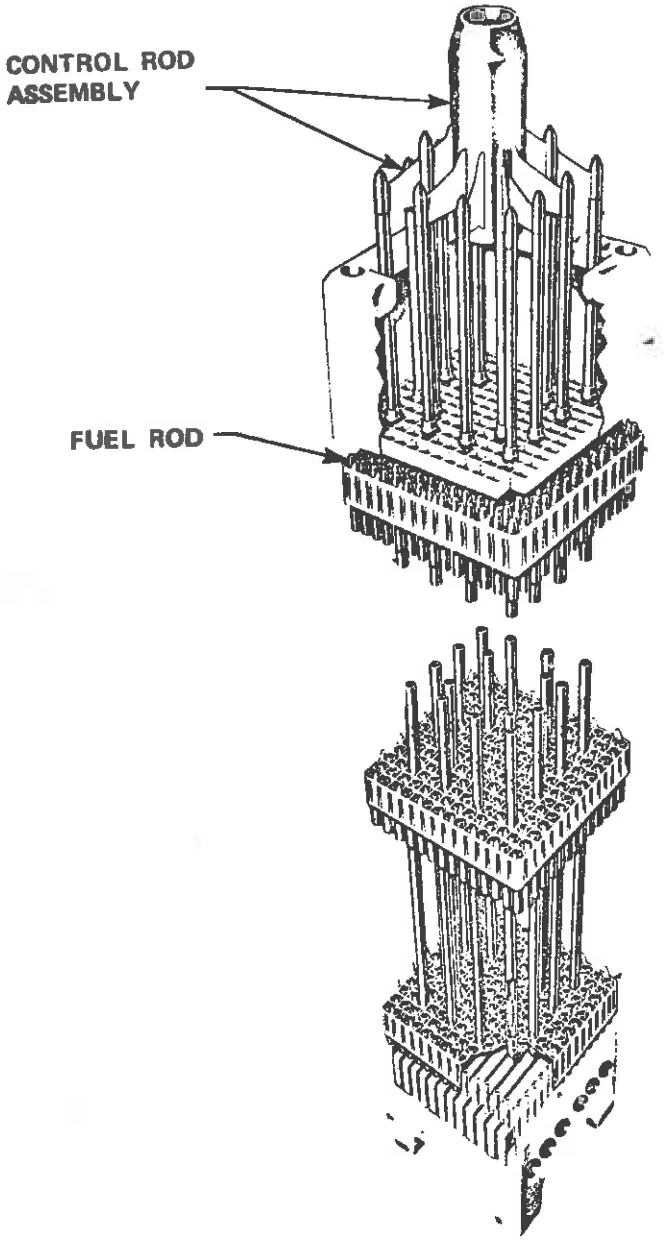


Cross Section of Typical Four-Loop Core (193 Fuel Assemblies)

TYPICAL FOUR-LOOP REACTOR CORE PARAMETERS

Total heat output	~3250-3411 MWt
Heat generated in fuel	97.4%
Nominal system pressure	2250 psia
Total coolant flow rate	~138.4×10^6 lb per hr
Coolant temperature	
Nominal inlet	557.5°F
Average rise in vessel	61.0°F
Outlet from vessel	618.5°F
Equivalent core diameter	11.06 ft
Core length, between fuel ends	12.0 ft
Fuel weight, uranium (first core)	86,270 kg
Number of fuel assemblies	193

FIGURE 3-14 : Cross section and parameters of a typical PWR core



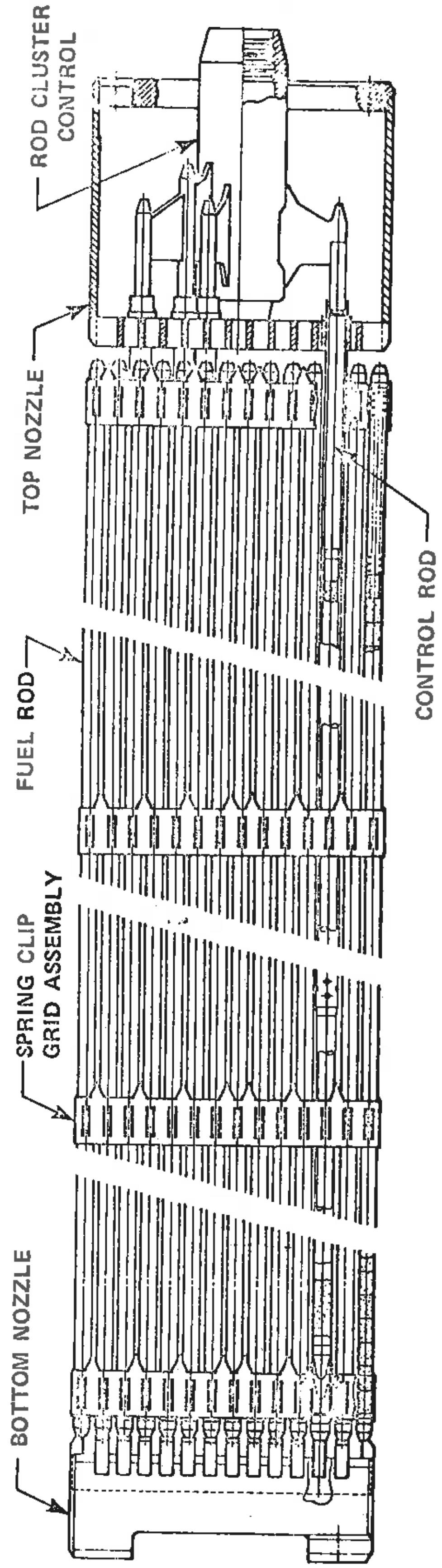


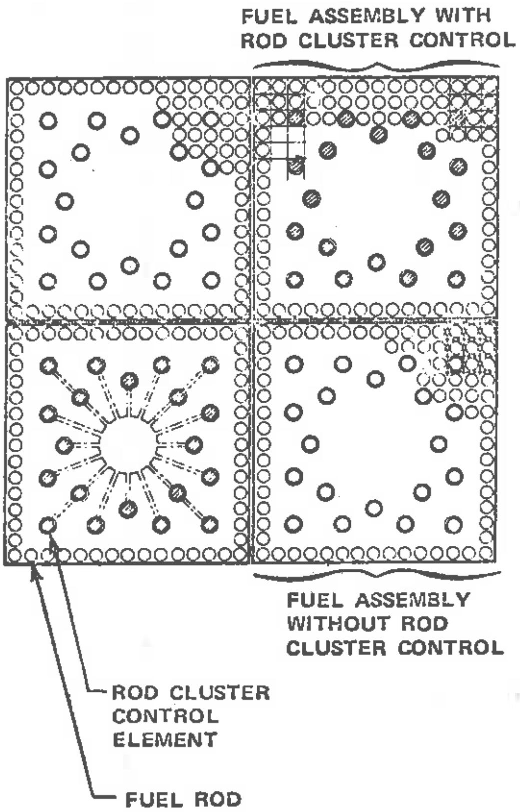
FIGURE 3-15: Cross section of a PWR fuel bundle (with rod cluster control assembly)

FIGURE 3-16: PWR fuel assembly components and parameters

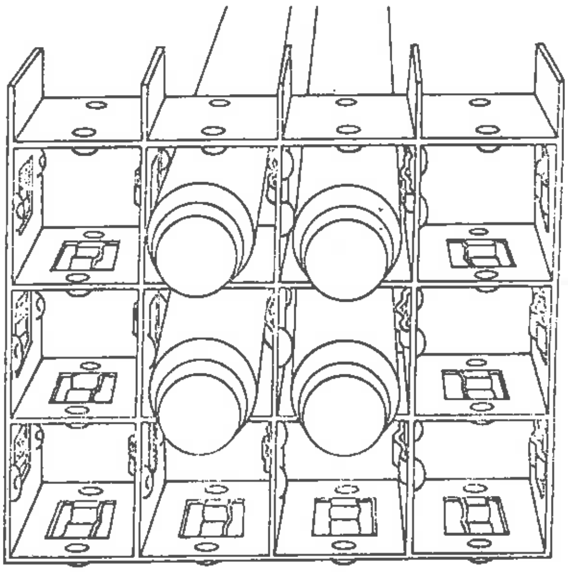
Fuel Pellets

FUEL ROD PARAMETERS

Outside diameter	0.422 in.
Cladding thickness	0.0243 in.
Diametral gap (first and second region/other regions)	0.0075/0.0085 in.
Pellet diameter (first and second region/other regions)	0.3659/0.3649 in.
Pitch	0.563 in.
Rods array in assembly	15 x 15
Rods in assembly	204
Total number of fuel rods in core	39,372



Cross Section of Fuel Assemblies with and without Rod Cluster Control



Portion of Spring Clip Grid Assembly

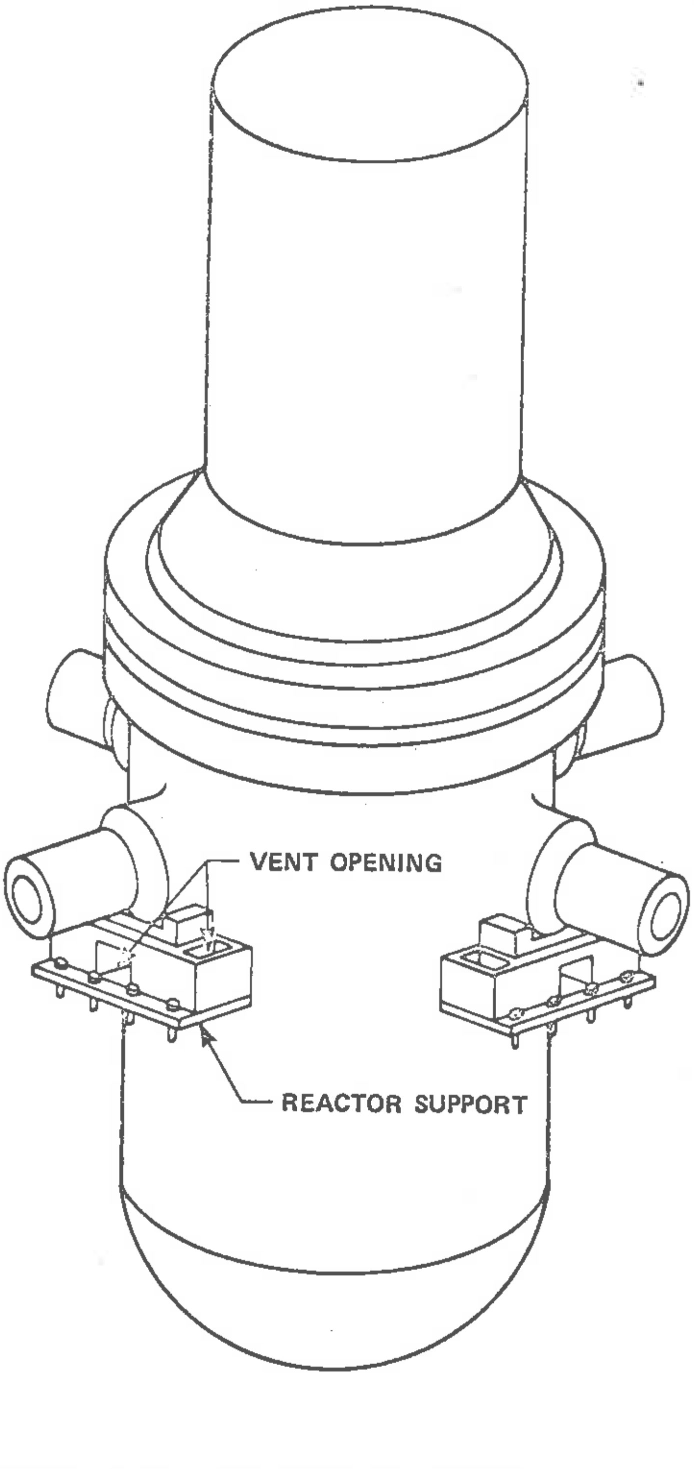
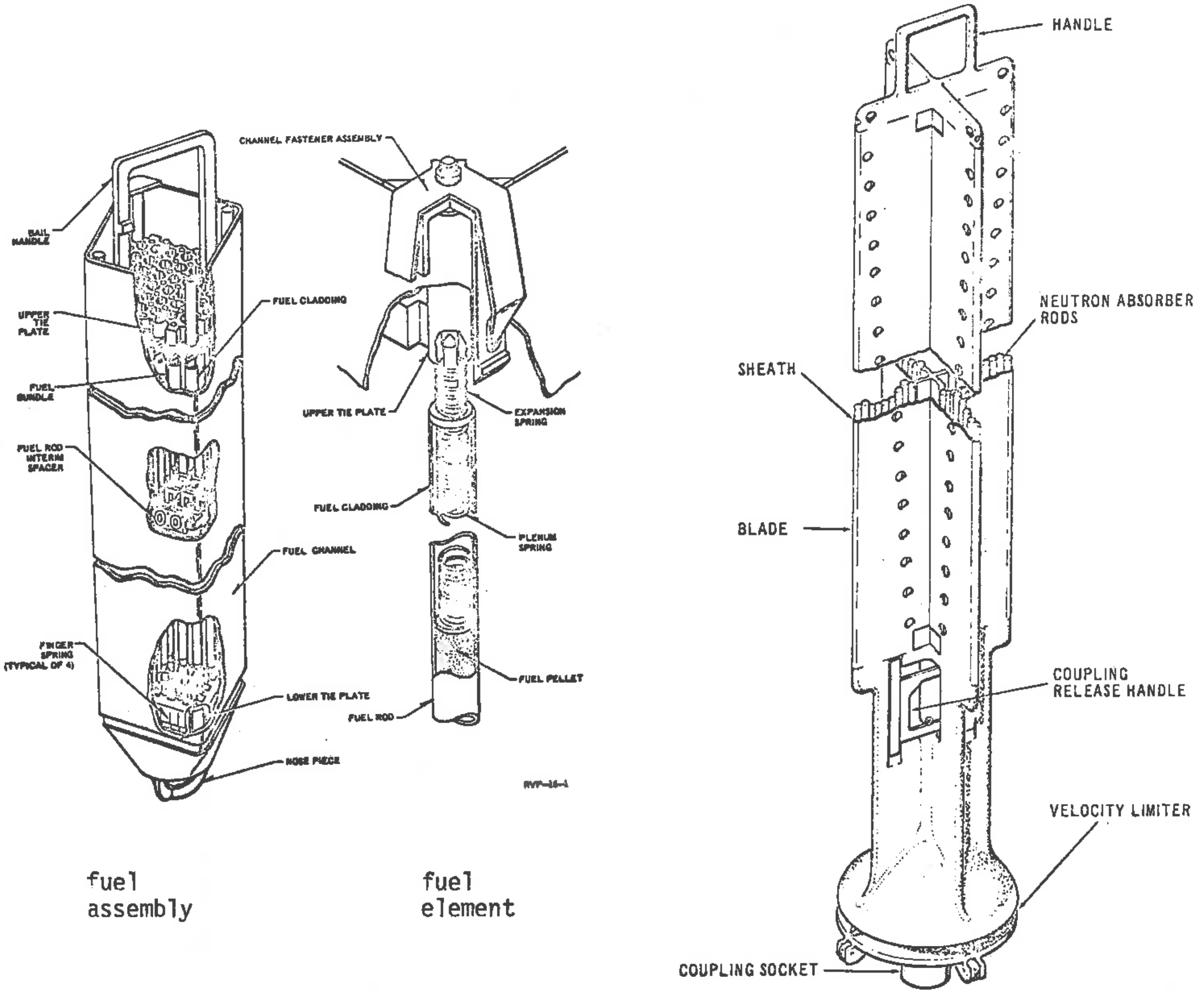


FIGURE 3-17 : PWR pressure vessel

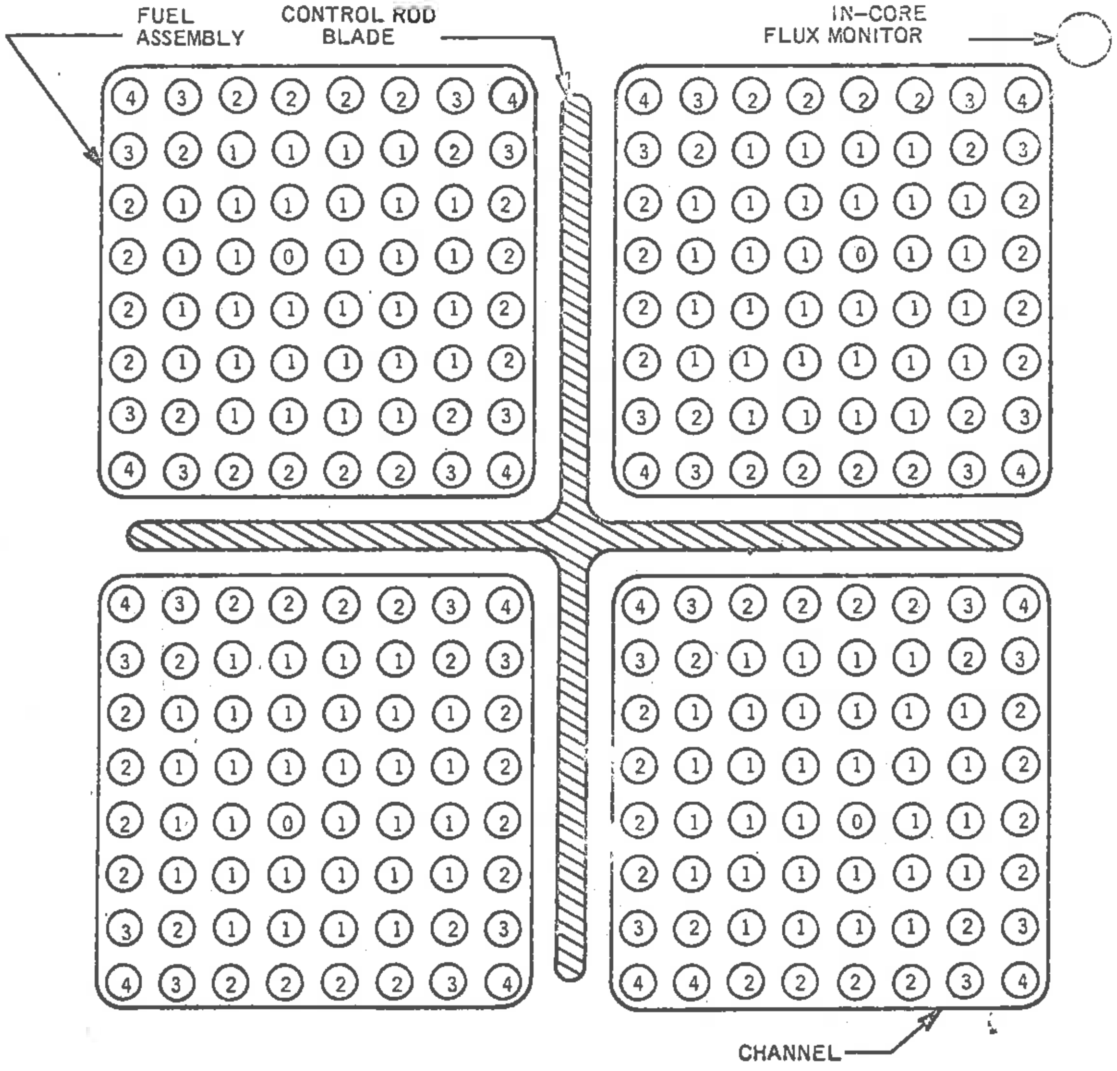


fuel assembly

fuel element

CONTROL ROD

FIGURE 3-18: BWR fuel assembly and control rod



NOTE: 1, 2, 3, & 4 INDICATE LOCATION OF FOUR DIFFERENT ROD ENRICHMENTS IN FUEL ASSEMBLY 0 INDICATES A WATER ROD.

FIGURE 3-19: Arrangement of BWR fuel assemblies and control elements

(a) Fuel - Fissionable material which produces neutrons and thermal energy. This can be either fissile material (fissionable at all neutron energies) such as U^{233}, U^{235}, Pu^{239} or fertile materials such as Th^{232}, U^{238}, Pu^{240} which are fissionable only with high energy neutrons.

(b) Moderator - All except fast spectrum reactors contain material which consists of light elements to reduce neutron energy (moderation). Typical moderators are H_2O, D_2O, Graphite, Beryllium, etc.

(c) Coolant - All power reactors require a fluid to remove heat produced by fission. This can be liquid (H_2O, Na) or gas (He, CO_2, steam). Moderator and coolant can be common material, such as in light water reactors.

(d) Structure - All reactors utilize some sort of structure to maintain the geometry of fuel, coolant, and moderator or to separate elements which are not chemically compatible. Structure and moderator may be common material (e.g., the graphite in HTGR fuel pellets)

(e) Control Material - The chain reaction in a nuclear reactor is usually controlled by inserting some material which will soak up or absorb neutrons, hence "poisoning" the chain reaction. Common neutron absorbers are boron, hafnium, cadmium, rare earth elements, and silver-cadmium-indium ($A_gC_dI_n$)

(f) Fuel Element - This is usually the smallest sealed unit of fuel. In water reactors it is the fuel rod or the tube containing ceramic fuel. (Fuel pin and fuel slug are also used). In an experimental reactor it may be the fuel plate - fuel alloy meat with cladding.

(g) Fuel Assembly - Although usage varies from one reactor type to another, the smallest unit which combines fuel elements is usually termed an assembly. Sub-assembly and bundle are also commonly used for the smallest unit of fuel elements.

(h) Control Rod - The smallest unit of neutron absorber is termed a control rod. Control element is also used.

(i) Reactor Core - Total array of fuel and control elements.

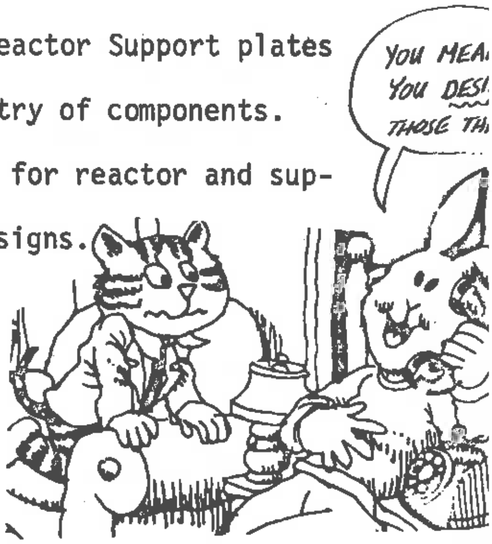
(j) Reactor Blanket - In a breeder or high conversion reactor there is usually a region surrounding the core which contains natural or depleted uranium to improve neutron economy.

(k) Reflector - Most reactors are surrounded by a region which serves to reduce neutron leakage by reflecting some neutrons back into the reactor.

(l) Shielding - Shielding attenuates both neutron and gamma radiation. Thermal shielding attenuates to radiation levels which do not result in significant heat generation. Biological shielding reduces radiation to acceptalbe levels for personal access.

(m) Support Structure - Upper and Lower Reactor Support plates and other structure which serves to maintain geometry of components.

(n) Reactor Vessel - Provides containment for reactor and support structure in water reactors and some LMFBR designs.



III. NUCLEAR REACTOR DESIGN

A. General Design Functions

The design of a large nuclear power plant is an enormously complex task, and involves the coordination of a remarkably diverse range of disciplines. Typical design topics include: core neutronics, fuel performance, It is also useful to introduce at this point several terms which are used to characterize reactor performance:

Reactor thermal power ≡ total heat produced in the reactor core [usually denoted in units of megawatts—thermal or MW_{th}]

Plant electric output ≡ total net electrical power generated by the plant [denoted in units of megawatts—electric or MWe]

Net plant efficiency ≡ $\dfrac{\text{Plant electrical output}}{\text{Reactor thermal power}}$

Core power density ≡ $\dfrac{\text{Reactor thermal power}}{\text{Total core volume (including moderator, control rods, etc.)}}$ (Kw/liter)

Linear power density ≡ thermal heat generated per unit length of coolant channel (Kw/ft)

Specific power ≡ $\dfrac{\text{Reactor thermal power}}{\text{Fissionable fuel loading (gm of metal)}}$ (Kw/kg)

Fuel loading ≡ total mass of fissionable material (Kg)

Fuel enrichment ≡ $\dfrac{\text{Mass of fissile material}}{\text{Mass of fissile and fertile material}}$

Plant capacity factor ≡ $\dfrac{\text{energy generated over time period}}{\text{(plant rating) x (time)}}$

Load factor ≡ $\dfrac{\text{average power level}}{\text{peak power level}}$

Fuel burnup ≡ $\dfrac{\text{energy generated in fuel during residence}}{\text{total mass of fuel}}$

$$\left(\frac{\text{megawatt-days}}{\text{metric ton}} = \text{MWD/tonne}\right)^{*}$$

Fuel residence time ≡ $\dfrac{\text{Fuel burnup}}{\text{(Specific power) x (capacity factor)}}$

---

* 1 tonne = 1000 kg = 1 MTU (metric ton uranium)

heat transfer from core, coolant loop design, steam generator design, pressure vessel and containment, shielding, turbogenerator design, and so on. Essentially all of our concern in this course will be with core design, but of course this cannot be studied completely independently from the other topics above which characterize more general power plant design.

The criteria for a design effort are also varied, encompassing considerations of performance, reliability, economics, and safety. These criteria are frequently contradictory in nature, and hence optimization is necessary. To optimize a nuclear reactor design, one must build a computer model of the reactor which can be used in parameter studies. Perhaps the central functions of nuclear reactor theory is to develop such models which adequately describe a nuclear reactor. There are many types of such design models with which a nuclear engineer must be familiar, including those used in nuclear design (neutronics and shielding), thermal-hydraulic design, mechanical design, fuel performance and management, and, of course, nuclear power economics. Before discussing the details of such models, it is useful to consider a typical nuclear reactor design sequence, ignoring other aspects of the power plant design for the present.

B. A Typical Sequence of Steps in Nuclear Reactor Design

Step 1: Determine the desired electrical capacity of the plant. This is a decision which must be made by the utility, based on their needs for new generating capacity, and the characteristics of their existing power generation and distribution equipment. [For example, a utility would be reluctant to build a single new unit with more than 10% of their existing generation capacity.] Since the capital cost per unit of generation capacity decreases with increasing plant size, there is strong incentive to build as large a unit as possible. Today's "canonical" nuclear unit is roughly 1150 Mwe.

Step 2: Determine the maximum allowable linear power density in the fuel elements. The thermal out put of a nuclear power plant is limited by the maximum operating conditions imposed by the materials or components of the reactor. These take the form of temperature limitations on fuel, structure, or coolant, as well as limits on heat flux. For example, in power reactors which utilize ceramic fuel material (oxide, carbide, etc.), a maximum fuel temperature is usually established so as to avoid either melting of the ceramic material or some constituent of the fuel if it is in a mixture. The centerline temperature limit for UO_2 fueled reactors is usually expressed in terms of linear power density (kw/ft). Similar limitations must be placed on clad and structural temperatures, as well as on coolant temperatures (so that bulk boiling does not occur in certain classes of reactors.)

Step 3: Next, one determines the maximum to average power density ratio. This depends upon the arrangement of the fuel, and the detailed mechanical design of the core.

Step 4: Determine the fuel rod size and pitch (spacing between fuel rods). This determination is essentially an optimization problem, involving consideration of nuclear behavior, thermal-hydraulic design, and fuel economics (e.g., fabrication).

Step 5: Establish the thermal efficiency of the plant. Here, one must consider the thermodynamic cycle efficiency of the plant, as well as the internal power requirements (e.g., pumps).

Step 6: Establish the core volume. Knowing the desired electrical power output, the thermal efficiency, and the maximum and average power densities, one can now determine the required core volume. It should be noted that this is essentially determined by thermal considerations.

Step 7: Determine the excess core multiplication requirements and the desired fuel enrichment. At this point, the actual nuclear design takes over, by determining the detailed fuel composition and arrangement that can guarantee proper reactor operation (startup, rated power operation, shutdown).

Step 8: Optimization. The design must finally be refined to optimize the economic cost of the power generated while satisfying constraints imposed by safety and environmental considerations. This involves parametric studies over broad ranges of plant variables using simple models, trade-off studies in the vicinity of the optimum design, and finally detailed evaluations of the reference design.

Of course this is an extremely simple-minded example of a reactor design sequence, and it was only included at this point to illustrate some of the considerations which arise in reactor analysis. It should be pointed out that the principal limitation in this design sequence is not the nuclear design of the core, but rather the thermal constraints imposed by temperature limitations. We will later find that the principal limitations on the economic operation of the plant are usually imposed by materials limitations. For example, the length of time which a given fuel element can remain in the core is usually not determined by the depletion of fissile isotopes, but rather by the degree to which the element can withstand radiation damage in the intense radiation environment of the reactor core without experiencing failure (e.g., rupturing its clad). Hence both thermal and mechanical considerations weigh heavily in any realistic power reactor core design.

C. Nuclear Reactor Design Codes

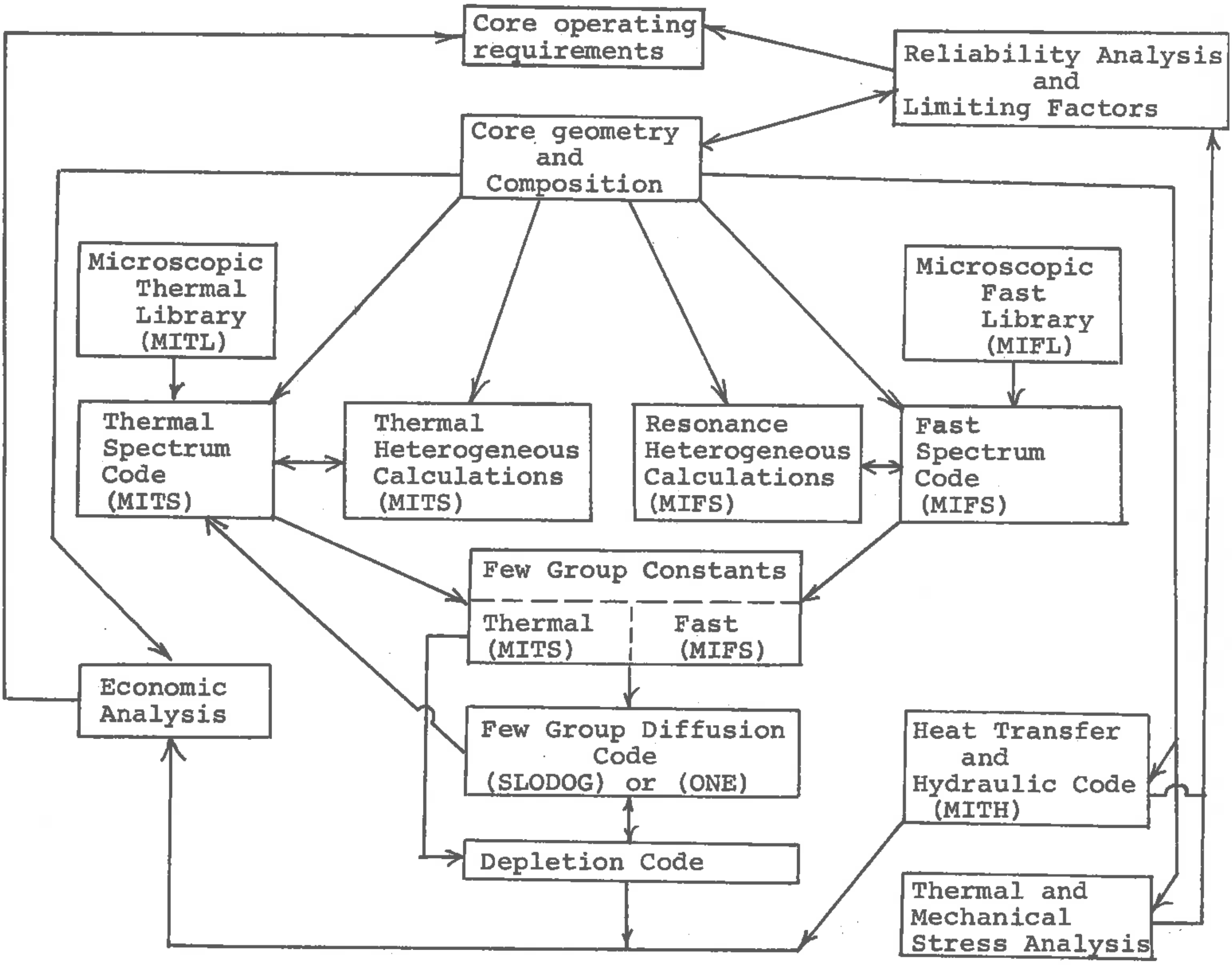
The above procedure makes apparent the importance of adequate models of a nuclear reactor in order to carry out the required parameter and optimization studies. These models must be realistic, since nuclear reactors are far too expensive to be built without detailed and accurate design information. Unfortunately, any calculation which is sufficiently realistic to be of use in reactor design is far too complex to be carried out by hand. Hence the digital computer plays a key role in reactor design.

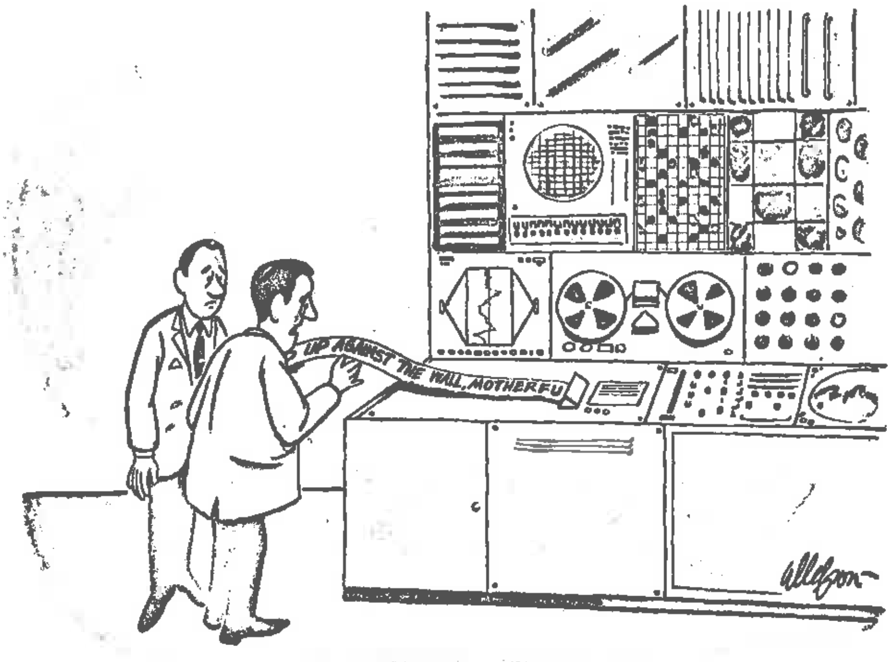
A key task of the nuclear reactor engineer is to develop models of nuclear reactors which can then be solved on the computer. Such models result in large computer programs or "codes" which can then be used by other nuclear engineers in reactor design. Most of our emphasis in this text will be on learning how to synthesize such approximate models and then adapt them to a form suitable for reactor design. In later courses, one is more concerned with learning how to use (and occasionally modify) existing computer codes in design applications.

The Nuclear Engineering Department has an extensive library of such reactor codes on file (or tape) on M.T.S. for the use of students. A brief list of some of the more popular codes is given in Table 3-3. It should be apparent that these codes cover a variety of areas, from neutron physics to thermal-hydraulics to fuel management to cost analysis. We will have occasion to use several of these codes later in this course, as well as to write similar codes "from scratch".

TABLE 3-3

Reactor Calculational Model





"Uh-oh!"

The intimate relation between computers and reactor design cannot be overstressed. It is essentially impossible for the present day nuclear engineer to function without a reasonable background in computer applications (programming and numerical analysis).

D. Some Concluding Remarks

After these very brief comments on some simple ideas concerned with nuclear fission chain reactions, and then a brief overview of nuclear reactor systems and design, we now turn our attention to a development of the theory underlying the nuclear analysis of fission reactors. We have seen that the neutron plays the central role as the chain carrier which perpetuates the chain reaction. The key problem of reactor theory, then, is to determine the distribution of neutrons in a reactor core. This will not only allow one to study the chain reaction, but since the neutron density is proportional to the rate at which fission reactions occur, and hence proportional to the power density, the neutron density is also the key to the subsequent thermal and mechanical analysis of the reactor.

As we have mentioned, there are two aspects to this problem:

(1) One must study the interaction of neutrons with matter (more specifically, with the nuclei which make up the matter). This amounts to either an experimental or theoretical determination of the probabilities that various neutron-nuclear interactions will occur--that is, a determination of the appropriate neutron-nuclear cross sections. This, however, is not the principal concern of the theory we will develop in this text. Hence we will tend to take microscopic cross section data as given (in a form to be discussed later), and turn our attention instead to how this data is utilized in nuclear reactor analysis.

(2) To study the transport (diffusion) of neutrons within a nuclear reactor core--as they stream around inside the core, suffering collisions with nuclei, occasionally being absorbed, inducing fission reactions, or leaking out through the surface of the core. It is this latter study which will allow us to develop models for calculating the distribution of neutrons in the reactor core.

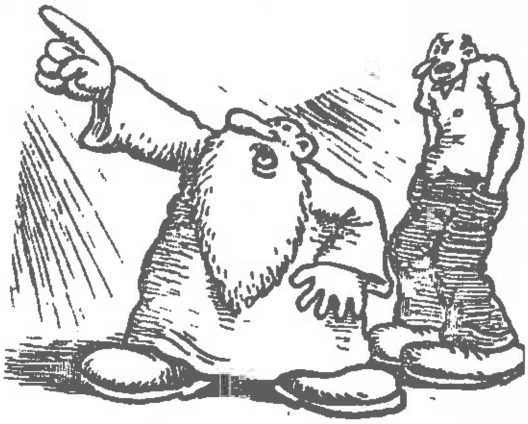
Our theoretical approach will be to begin with an essentially exact description of the neutron density in the reactor based upon the so-called neutron transport equation. This equation, while relatively easy to derive, is extremely difficult to solve, and hence we will be concerned with developing various approximations to it which lend themselves more readily to practical application. We will begin our actual study of nuclear reactor theory by using the simplest such approximation, that in which the neutron energy dependence is neglected (all neutrons will be assumed to have one speed), and their transport from point to point in the core is described as a simple diffusion process. This very simple model suffices to develop most of the concepts, as well as to illustrate most of the practical computational techniques, used in more detailed reactor analysis.

We will next develop a more sophisticated model of the neutron density behavior based upon breaking the range of neutron energies up into intervals or groups and then describing the diffusion of neutrons in each of these groups separately, accounting for transfer of neutrons between groups. Such multi-group diffusion models are the principal tools used in modern reactor analysis, and we will consider them in some detail.

In the final portion of the book, we will illustrate these models by applying them to analyze several typical problems encountered in nuclear reactor analysis.


NOW, LOOK HERE! IF YOU'RE GOING TO MAKE ME TYPE THESE NOTES, THEN YOU'RE GOING TO HAVE TO ENDURE MY SENSE OF HUMOR!

CHAPTER 4: NEUTRON TRANSPORT

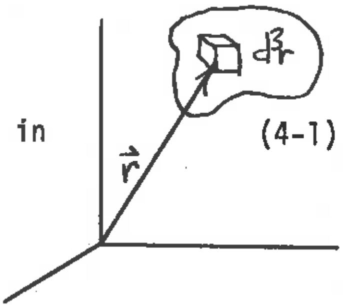


I. INTRODUCTORY CONCEPTS

A. Neutron Density and Flux

Our ultimate goal is to determine the distribution of neutrons in a nuclear reactor core. This requires accounting for the neutron motion about the core, and their interactions with nuclei in the core. We will begin by defining the neutron density, $N(\vec{r},t)$, at any point $\vec{r}$ in the reactor core by:

$$N(\vec{r},t)\, d^3r \equiv \text{expected number of neutrons in } d^3r \text{ about } \vec{r} \text{ at a time } t \tag{4-1}$$



The word "expected" has been inserted into this definition to indicate that this will be a statistical theory in which only mean values are actually calculated. (The actual neutron density will fluctuate about this mean value, of course.) The neutron density $N(\vec{r},t)$ is of interest because it allows us to calculate the rate at which nuclear reactions are occurring at any point in the reactor. To see this, suppose for convenience, that all the neutrons in the reactor have the same speed v. Now recall that one can express the frequency with which a neutron will experience a given neutron-nuclear reaction in terms of the macroscopic cross section characterizing that reaction, say Σ , and the neutron speed, v, as

$$v\Sigma = \left[\frac{cm}{sec}\right]\left[\frac{1}{cm}\right] = \text{"interaction frequency"} \tag{4-2}$$

Hence we can define the reaction rate density, $R(\vec{r},t)$, at any point in the system by merely multiplying the neutron density $N(\vec{r},t)$ by the interaction frequency $v\Sigma$:

$$R(\vec{r},t)d^3r \equiv v\Sigma N(\vec{r},t)d^3r \equiv \text{expected rate at which interactions are occurring in } d^3r \text{ about } \vec{r} \text{ at time } t \tag{4-3}$$

This discussion can be easily generalized to the case in which the neutron density is different for various neutron energies by defining

$$N(\vec{r},E,t)d^3r\,dE \equiv \text{expected number of neutrons in } d^3r \text{ about } \vec{r}\text{, energies in } dE \text{ about } E\text{, at time } t \tag{4-4}$$

(Notice that the "density" is now defined with respect to both space and energy.) Similarly, we can define

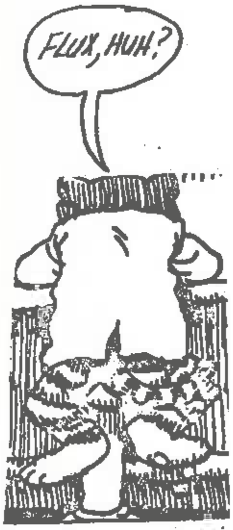
$$R(\vec{r},E,t)\,d^3r\,dE = v\Sigma(E)N(\vec{r},E,t)\,d^3r \tag{4-5}$$

where we recall

$$v = \sqrt{2E/m} \tag{4-6}$$

(Here we could have also used v as the independent variable instead of E. However in most reactor applications, it is more convenient to use the energy variable E, or in some cases, as we will see later, its natural logarithm, $u = \ln E$.)

The quantity v $N(\vec{r},t)$ occurs very frequently in reactor theory, and hence it is given a special name:



$$\Phi(\vec{r},t) \equiv v N(\vec{r},t) \quad \equiv \quad \text{"neutron flux"} \tag{4-7}$$

$$\left[\frac{cm}{sec}\right]\left[\frac{\#}{cm^3}\right] = \left[\frac{1}{sec\text{-}cm^2}\right]$$

The name "flux" is actually very misleading, however. $\Phi(\vec{r},t)$ is not at all like the fluxes encountered in electromagnetic theory or heat conduction, since these latter fluxes are vector quantities, whereas $\Phi(\vec{r},t)$ is a scalar quantity. Actually, the "neutron current", $\vec{J}(\vec{r},t)$, which we shall introduce momentarily corresponds more closely to the conventional interpretation of a "flux". Note that to compute a reaction rate density, one need only multiply the flux by the appropriate macroscopic cross section--e.g.,

$$R(\vec{r},E,t) = \Sigma(E)\, \Phi(\vec{r},E,t) \tag{4-8}$$

B. Angular Densities and Currents

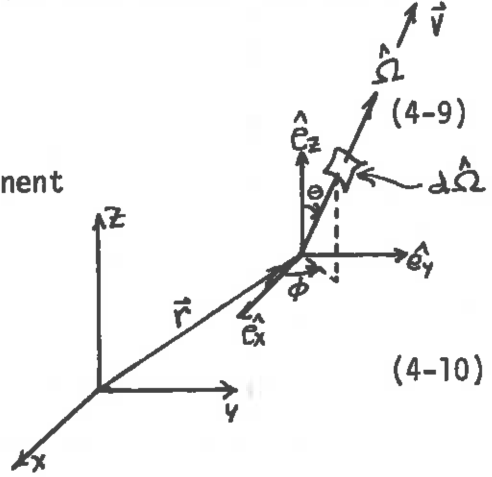
The significance of the neutron density $N(\vec{r},t)$ or flux $\Phi(\vec{r},t)$ in determining nuclear reaction rates leads us to search for an equation which describes these quantities. Unfortunately, there is no exact equation which is satisfied by $N(\vec{r},t)$ or $\Phi(\vec{r},t)$--only approximate equations. To understand why, we must generalize the concept of the neutron density somewhat.

First, let us determine just what variables characterize the state of an individual neutron. Certainly these include:

$\vec{r}$	position
E	energy (or speed $v = \sqrt{2\ E/m}$)
t	time at which neutron is observed

But notice that to specify the state of the neutron, we must also give its direction of motion, characterized by the unit vector $\hat{\Omega}$ where

$$\hat{\Omega} = \vec{v}/|\vec{v}| \qquad (4\text{-}9)$$



where $\vec{v}$ is the neutron velocity. In component form, we can write

$$\hat{\Omega} = \hat{e}_x \cos\phi \sin\theta + \hat{e}_y \sin\phi \sin\theta + \hat{e}_z \cos\theta. \qquad (4\text{-}10)$$

Let us now generalize the concept of density by defining the angular neutron density which depends upon all of these variables

$n(\vec{r},E,\hat{\Omega},t)d^3r\,dE\,d\hat{\Omega} \equiv$ expected number of neutrons in d^3r about $\vec{r}$, energy dE about E, moving in direction $\hat{\Omega}$ in solid angle $d\hat{\Omega}$, at time t

The term "angular" arises from the fact that $n(\vec{r},E,\hat{\Omega},t)$ depends on the angles θ and ϕ which specify the neutron direction $\hat{\Omega}$. This is the most general neutron density function we need to define. (Actually, one could also worry about specifying quantities such as the neutron spin, but for reactor calculations, the above quantities, $\vec{r}$, E, $\hat{\Omega}$, t, are sufficient.) Fortunately, it so happens that there is an exact equation for the angular neutron density: the neutron transport equation.

But before deriving this equation, let's introduce a couple of other definitions:

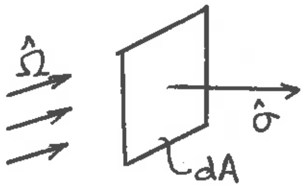
$$\text{angular flux} \equiv \phi(\vec{r},E,\hat{\Omega},t) \equiv v\, n(\vec{r},E,\hat{\Omega},t) \qquad (4\text{-}11)$$

$$\text{angular current density} \equiv \vec{j}(\vec{r},E,\hat{\Omega},t) = v\hat{\Omega}\, n(\vec{r},E,\hat{\Omega},t) \qquad (4\text{-}12)$$
$$= \hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t)$$

In particular, note that if we consider a small area dA at a point $\vec{r}$ with surface normal $\hat{\sigma}$, then

$$\hat{\sigma}\cdot\vec{j}(\vec{r},E,\hat{\Omega},t)\,dA\,dE\,d\hat{\Omega} \equiv$$

expected number of neutrons passing through an area dA per unit time with energy E in dE, direction $\hat{\Omega}$ in $d\hat{\Omega}$ at time t



(4-13)

One can also define an angular interaction rate

$$R(\vec{r},E,\hat{\Omega},t) = v\Sigma(\vec{r},E)\, n(\vec{r},E,\hat{\Omega},t) = \Sigma(\vec{r},E)\, \phi(\vec{r},E,\hat{\Omega},t). \qquad (4\text{-}14)$$

We can relate all of these angle-dependent quantities to our earlier definitions in section 4-A by integration over the angular variables. For example:

$$N(\vec{r},E,t) = \int_{4\pi} d\hat{\Omega}\, n(\vec{r},E,\hat{\Omega},t) \qquad (4\text{-}15)$$

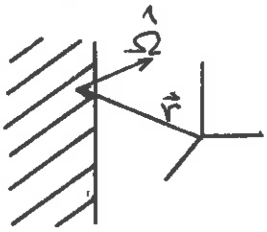
$$N(\vec{r},t) = \int_0^\infty dE\, N(\vec{r},E,t) = \int_0^\infty dE \int_{4\pi} d\hat{\Omega}\, n(\vec{r},E,\hat{\Omega},t) \qquad (4\text{-}16)$$

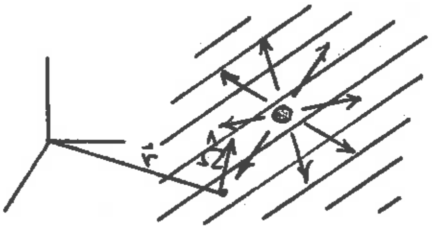
Sometimes quantities such as $N(\vec{r},t)$ and $\Phi(\vec{r},t)$ which do not depend on $\hat{\Omega}$ are referred to as scalar or total densities and fluxes, to distinguish them from $n(\vec{r},E,\hat{\Omega},t)$ and $\phi(\vec{r},E,\hat{\Omega},t)$. We find this nomenclature cumbersome and will avoid it in our development.

Notice that if the angular density is independent of $\hat{\Omega}$ (i.e., it is "isotropic"), then we find that (4-15) demands the presence of a 4π normalization factor

$$n(\vec{r},E,\hat{\Omega},t) = \frac{1}{4\pi} N(\vec{r},E,t) \tag{4-17}$$

More generally, however, $n(\vec{r},E,\hat{\Omega},t)$ will have a directional dependence--particularly if we are near a boundary or a source of neutrons, as a little geometrical reasoning should quickly convince you:





In a similar fashion, we find

$$\Phi(\vec{r},E,t) = \int_{4\pi} d\hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t) \tag{4-18}$$

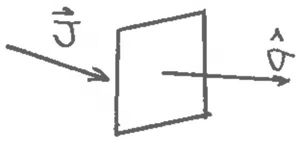
$$\Phi(\vec{r},t) = \int_0^\infty dE\, \Phi(\vec{r},E,t) = \int_0^\infty dE \int_{4\pi} d\hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t) \tag{4-19}$$

Finally, we can define the neutron current density, $\vec{J}(\vec{r},E,t)$, in terms of the angular current density, $\vec{j}(\vec{r},E,\hat{\Omega},t)$ as

$$\vec{J}(\vec{r},E,t) \equiv \int_{4\pi} d\hat{\Omega}\; \vec{j}(\vec{r},E,\hat{\Omega},t) \tag{4-20}$$

$$\vec{J}(\vec{r},t) \equiv \int_0^\infty dE\; \vec{J}(\vec{r},E,t) = \int_0^\infty dE \int_{4\pi} d\hat{\Omega}\; \vec{j}(\vec{r},E,\hat{\Omega},t) \tag{4-21}$$

Notice that $\vec{J}(\vec{r},t)$ is actually what would be called the "flux" in other fields, since



$$\hat{\sigma}\cdot\vec{J}(\vec{r},t)\,dA = \text{net rate at which neutrons pass through a surface area } dA \text{ normal to } \hat{\sigma} \tag{4-22}$$

We can also define partial current densities, $J_\pm(\vec{r},t)$ corresponding to the rates at which neutrons flow through a unit area from left to right (J_+) or from right to left (J_-) by simply integrating $\vec{j}(\vec{r},E,\hat{\Omega},t)$ only over half the directions:

$$J_\pm(\vec{r},t) \equiv \int_0^\infty dE \int_{2\pi^\pm} d\hat{\Omega}\; \hat{\sigma}\cdot\vec{j}(\vec{r},E,\hat{\Omega},t)\,. \tag{4-23}$$

It is obvious from this definition that

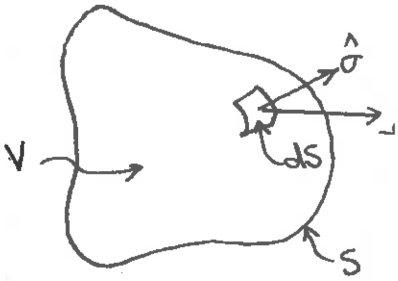
$$\hat{\sigma}\cdot\vec{J}(\vec{r},t) = J_+(\vec{r},t) - J_-(\vec{r},t) \tag{4-24}$$

hence, $\vec{J}$ is sometimes referred to as the net current density.

The neutron current $\vec{J}(\vec{r},t)$ is a very useful concept, but frequently appears rather confusing when confronted for the first time. We will rely upon examples and problems to illustrate the concept in more detail.

II. THE NEUTRON TRANSPORT EQUATION

We will now derive an exact equation for the angular neutron density in a system by simply balancing gain and loss mechanisms in an arbitrary volume V within the system. That is, we will consider mechanisms which will change the number of neutrons in this volume which have a specific energy E and are traveling in a specific direction $\hat{\Omega}$. It is convenient to use a bit of vector calculus here, but hopefully this will not obscure the simple physics behind this equation (which is just a mathematical expression of the "count-the-neutrons game".)



To this end, consider any old arbitrary volume V. The number of neutrons in V with energy E in dE and traveling in a direction $\hat{\Omega}$ in $d\hat{\Omega}$ is just

$$\left[\int_V n(\vec{r},E,\hat{\Omega},t)\,d^3r\right] dE\, d\hat{\Omega} \,. \qquad (4-25)$$

(Since $n(\vec{r},E,\hat{\Omega},t,)$ is a "density" in E and $\hat{\Omega}$ space, we must multiply it by dE and $d\hat{\Omega}$ in order to get a number.) The time rate of change of this number, then, is given by a balance relation

$$\frac{\partial}{\partial t}\left[\int_V n(\vec{r},E,\hat{\Omega},t)\,d^3r\right] dE\, d\hat{\Omega} \equiv \text{gain in V} - \text{loss from V} \,. \qquad (4-26)$$

If we note that the arbitrary volume V is chosen not to be dependent upon time, then we can bring the time differentiation inside the spatial integration

$$\frac{\partial}{\partial t}\left[\int_V n(\vec{r},E,\hat{\Omega},t)\,d^3r\right] dE\, d\hat{\Omega} = \left[\int_V \frac{\partial n}{\partial t}\, d^3r\right] dE\, d\hat{\Omega} \,. \qquad (4-27)$$

We can now classify the various ways that neutrons can appear or disappear from V, and then we will try to write mathematical expressions for each of these mechanisms in terms of the angular density $n(\vec{r},E,\hat{\Omega},t)$.

Gain mechanisms:

① Any neutron sources in V (e.g., fissions)

② Neutrons streaming into V through the surface S

③ Neutrons of different E', $\hat{\Omega}'$ which suffer a scattering collision in V which changes E', $\hat{\Omega}'$ into the E, $\hat{\Omega}$ of interest

Loss mechanisms:

④ Neutrons leaking out through the surface S

⑤ Neutrons in V which suffer a collision (That an absorption interaction removes a neutron from V is obvious. And since by definition, a scattering collision changes E, $\hat{\Omega}$, and we are only keeping track of neutrons in V with these specific energies and direction, a scattering collision also amounts to a loss of neutrons.)

We can now write down a mathematical expression for each of these contributions. We'll work from the easiest first to the more difficult:

① Source terms: If we define

$$s(\vec{r},E,\hat{\Omega},t)\,d^3r\,dE\,d\hat{\Omega} \equiv \begin{array}{l}\text{rate of source neutrons appearing}\\ \text{in } d^3r \text{ about } \vec{r},\ dE \text{ about } E\text{, and}\\ d\hat{\Omega} \text{ about } \hat{\Omega}\end{array} \qquad (4\text{-}28)$$

then obviously

$$\textcircled{1} = \left[\int_V s(\vec{r},E,\hat{\Omega},t)\,d^3r\right]dE\,d\hat{\Omega} \qquad (4\text{-}29)$$

[This term was really easy--we only needed to define a source density.]

② Loss due to collisions in V: The rate at which neutrons suffer collisions at a point $\vec{r}$ is

$$\mathcal{R}_t(\vec{r},E,\hat{\Omega},t) = v\Sigma_t(\vec{r},E)\,n(\vec{r},E,\hat{\Omega},t)\,. \qquad (4\text{-}30)$$

Hence integrating this collision rate over the volume V,

$$\textcircled{5} = \left[\int_V v\Sigma_t(\vec{r},E)\, n(\vec{r},E,\hat{\Omega},t)\, d^3r \right] dE\, d\hat{\Omega} \tag{4-31}$$

③ Gain due to neutrons scattering into dE about E, d$\hat{\Omega}$ about $\hat{\Omega}$ from other energies E' and directions $\hat{\Omega}'$: If we recall from section 2-II-C that the probability of scattering from E', $\hat{\Omega}'$ to E, $\hat{\Omega}$ is given by the double differential scattering cross section, then the rate at which neutrons scatter from E', $\hat{\Omega}'$ to E, $\hat{\Omega}$ is

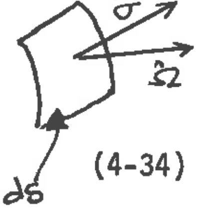
$$\left[\int_V v'\Sigma_s(E'\rightarrow E,\hat{\Omega}'\rightarrow\hat{\Omega})\, n(\vec{r},E',\hat{\Omega}',t)\, d^3r \right] dE\, d\hat{\Omega} \tag{4-32}$$

But we must consider contributions from any E', $\hat{\Omega}'$. Hence

$$\textcircled{3} = \left[\int_V d^3r \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, v'\Sigma_s(E'\rightarrow E,\hat{\Omega}'\rightarrow\hat{\Omega})\, n(\vec{r},E',\hat{\Omega}',t) \right] dE\, d\hat{\Omega} \tag{4-33}$$

②, ④ Leakage into or from the volume V: We will combine these terms together and calculate the net leakage through the surface S. If we use the concept of the angular current density, $\vec{j}(\vec{r},E,\hat{\Omega},t)$, then we can write the rate at which neutrons of E, $\hat{\Omega}$ leak out of a piece of the surface, dS, as

$$\hat{\sigma}\cdot\vec{j}(\vec{r},E,\hat{\Omega},t)\, dS = v(\hat{\sigma}\cdot\hat{\Omega})\, n(\vec{r},E,\hat{\Omega},t)\, dS \tag{4-34}$$



Hence the leakage contribution over the entire surface area S is

$$\textcircled{4} - \textcircled{2} = \int_S dS\ \hat{\sigma}\cdot v\hat{\Omega}\, n(\vec{r},E,\hat{\Omega},t) \tag{4-35}$$

We can rewrite this in terms of a volume integral if we use Gauss's theorem

$$\int_S dS\,\hat{\sigma}\cdot\vec{A}(\vec{r}) = \int_V d^3r\,\nabla\cdot\vec{A}(\vec{r}) \tag{4-36}$$

to find

$$\begin{aligned}\left[\int_S dS\,\hat{\sigma}\cdot v\hat{\Omega}\,n(\vec{r},E,\hat{\Omega},t)\right]dE\,d\hat{\Omega} &= \left[\int_V d^3r\,\nabla\cdot v\hat{\Omega}\,n(\vec{r},E,\hat{\Omega},t)\right]dE\,d\hat{\Omega}\\ &= \left[\int_V d^3r\,v\hat{\Omega}\cdot\nabla n(\vec{r},E,\hat{\Omega},t)\right]dE\,d\hat{\Omega}\end{aligned} \tag{4-37}$$

[Here we have noted that $\nabla\cdot v\hat{\Omega} = v\hat{\Omega}\cdot\nabla$ (4-38)
since $\hat{\Omega}$ does not depend on $\vec{r}$]

If we now combine all of these terms such that

$$\text{rate of change of number of neutrons in } V = ① + ② + ③ - ④ - ⑤ \tag{4-39}$$

then we find

$$\int_V d^3r\left[\frac{\partial n}{\partial t} + v\hat{\Omega}\cdot\nabla n + v\Sigma_t n - \int_{4\pi} d\hat{\Omega}'\int_0^\infty dE'\,v'\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega})\,n(\vec{r},E',\hat{\Omega}',t) - S\right]dE\,d\hat{\Omega} = 0 \tag{4-40}$$

But we now use the fact that the volume V was quite arbitrarily chosen. Hence the only way for the integral to vanish for any V is for its integrand to be identically zero--that is

$$\int_{\text{any } V} d^3r\,f(\vec{r}) = 0 \quad\Rightarrow\quad f(\vec{r}) \equiv 0 \tag{4-41}$$

Hence we arrive at a balance relation

$$\frac{\partial n}{\partial t} + v\hat{\Omega}\cdot\nabla n + v\Sigma_t n(\vec{r},E,\hat{\Omega},t)$$
$$= \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, v'\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega})\, n(\vec{r},E',\hat{\Omega}',t) + s(\vec{r},E,\hat{\Omega},t) . \quad (4\text{-}42)$$

This equation is known as the "neutron transport equation".

There are several features of this equation which should be noted:

(i) It is a linear, integro-differential equation in seven variables, $\vec{r}$, E, $\hat{\Omega}$, and t.

(ii) It is essentially exact.

(iii) One can easily modify the equation to include fission sources by including in the source term

$$s_f(\vec{r},E,\hat{\Omega},t) = \frac{\chi(E)}{4\pi}\int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \nu(E')\, v'\Sigma_f(E')\, n(\vec{r},E',\hat{\Omega}',t) \quad (4\text{-}43)$$

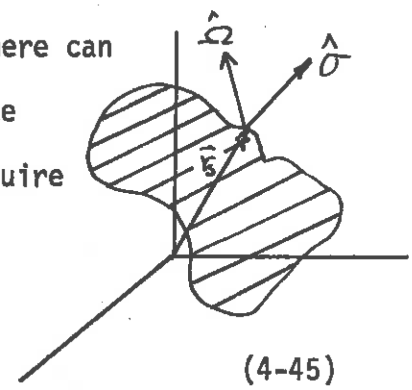
where we have ascribed an energy dependence to the average number of neutrons emitted in a fission while $\chi(E)$ is the fission neutron energy spectrum.

(iv) Since this equation has derivatives in space and time, we must include appropriate boundary and initial conditions on the angular density to complete the specification of the problem. The initial condition is easy:

$$n(\vec{r},E,\hat{\Omega},0) = n_0(\vec{r},E,\hat{\Omega}) \quad \text{all } \vec{r}\in V \quad (4\text{-}44)$$

--that is, we must specify the angular density in the volume at the initial time t = 0.

To determine the appropriate boundary condition on the surface of the system, we first assume there is only a vacuum surrounding the system. Hence there can be no neutrons entering the system from the outside. Expressed mathematically, we require that



$$n(\vec{r}_s,E,\hat{\Omega},t)=0 \quad \text{if} \quad \hat{\Omega}\cdot\hat{\sigma}<0, \quad \text{for all } \vec{r}_s \text{ on } S. \tag{4-45}$$

where $\vec{r}$ denotes a point on the surface S. There are other possible boundary conditions but we will discuss these later.

(v) Oh yes, one additional feature--it is a real sonofabitch to solve. We will not even attempt a solution in this text--but will instead use the transport equation to develop simple approximate descriptions of neutron transport. We will frequently rewrite the neutron transport equation and its initial and boundary conditions in terms of the angular flux.

$$\frac{1}{v}\frac{\partial\phi}{\partial t}+\hat{\Omega}\cdot\nabla\phi+\Sigma_t(\vec{r},E)\phi(\vec{r},E,\hat{\Omega},t) \tag{4-46}$$
$$=\int_{4\pi}d\hat{\Omega}'\int_0^\infty dE'\,\Sigma_s(E'\rightarrow E,\hat{\Omega}'\rightarrow\hat{\Omega})\phi(\vec{r},E',\hat{\Omega}',t)+s(\vec{r},E,\hat{\Omega},t)$$

initial condition: $\phi(\vec{r},E,\hat{\Omega},0)=\phi_0(\vec{r},E,\hat{\Omega})$

(4-47)

boundary condition: $\phi(\vec{r}_s,E,\hat{\Omega},t)=0$ if $\hat{\Omega}\cdot\hat{\sigma}<0$ for all $\vec{r}_s$ on S

This equation, then, will give the neutron flux distribution in a reactor, which, in turn, contains essentially all the information we require (considerably more information than we require, in fact.) All we have to do is solve this equation. But note:

(i) seven independent variables: $x, y, z, E, \theta, \phi, t$

(ii) The dependence on $\vec{r}$ is bound to be complicated because of the complicated, nonuniform structure of a reactor core.

(iii) And, as we have seen in Chapter 2, the cross section dependence upon energy, $\Sigma_t(E)$, is as complicated as hell (resonances and such.)

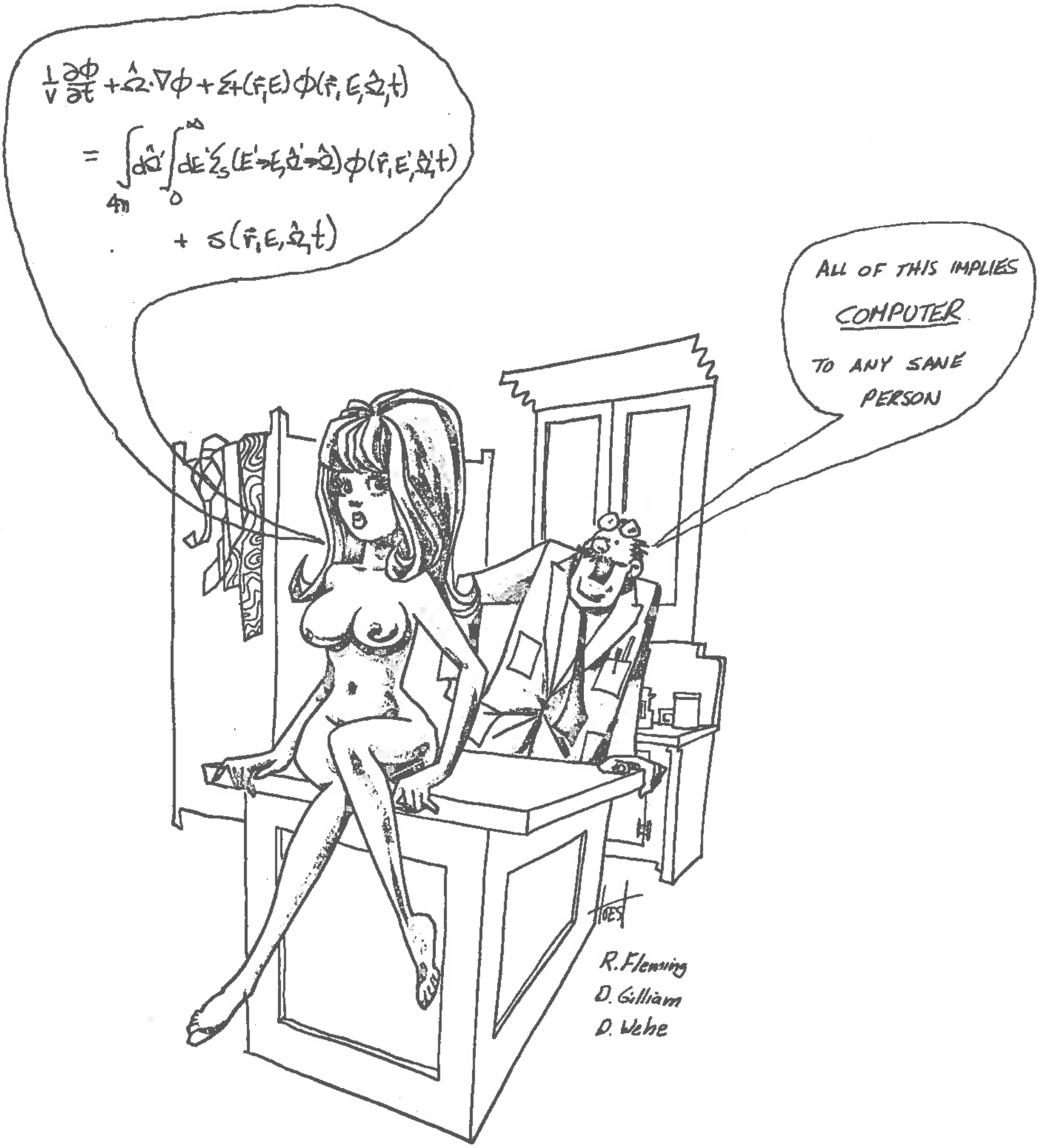
All of this implies COMPUTER to any sane person. Unfortunately, no computer is big enough (yet) to solve this equation in the general form in which we have derived it. This second fact implies that the major task of nuclear reactor analysis will be to introduce suitable approximations to the neutron transport equation which will allow us to solve it (at least on a computer), and yet still preserve enough reality so that we get a useful description of the nuclear reactor.

III. APPROXIMATIONS TO THE TRANSPORT EQUATION--A QUALITATIVE DESCRIPTION

A. The Neutron Continuity Equation

For most reactor calculations, the details of the angular dependence of the flux are not necessary, and we really only need to calculate the angle integrated flux:

$$\Phi(\vec{r},E,t) = \int_{4\pi} d\hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t) \tag{4-48}$$



R. Fleming
D. Gilliam
D. Wehe

in order to calculate nuclear reaction rates and hence study the chain reaction (e.g., by calculating the multiplication factor k).

But we surely can get an equation for $\Phi(\vec{r},E,t)$ by simply integrating the transport equation over angle. Let's try it and see what happens:

$$\underset{\textcircled{1}}{\int_{4\pi} d\hat{\Omega}\,\frac{1}{v}\frac{\partial\phi}{\partial t}} + \underset{\textcircled{2}}{\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\cdot\nabla\phi} + \underset{\textcircled{3}}{\int_{4\pi} d\hat{\Omega}\,\Sigma_t\phi}$$

$$= \underset{\textcircled{4}}{\int_{4\pi} d\hat{\Omega}\int_{4\pi} d\hat{\Omega}'\int_0^{\infty} dE'\,\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega})\,\phi(\vec{r},E',\hat{\Omega}',t)} + \underset{\textcircled{5}}{\int_{4\pi} d\hat{\Omega}\,s(\vec{r},E,\hat{\Omega},t)} \tag{4-49}$$

If we consider each of these terms

$$\textcircled{1} = \int_{4\pi} d\hat{\Omega}\,\frac{1}{v}\frac{\partial\phi}{\partial t} = \frac{1}{v}\frac{\partial}{\partial t}\int_{4\pi} d\hat{\Omega}\,\phi = \frac{1}{v}\frac{\partial\Phi}{\partial t} \tag{4-50}$$

$$\textcircled{3} = \int_{4\pi} d\hat{\Omega}\,\Sigma_t\phi = \Sigma_t\int_{4\pi} d\hat{\Omega}\,\phi = \Sigma_t\Phi \tag{4-51}$$

$$\textcircled{5} = \int_{4\pi} d\hat{\Omega}\,s(\vec{r},E,\hat{\Omega},t) = S(\vec{r},E,t) \tag{4-52}$$

To evaluate ④, we first recall that $\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega})$ usually depends only upon the scattering angle $\theta = \cos^{-1}(\hat{\Omega}'\cdot\hat{\Omega})$. This implies that

$$\int_{4\pi} d\hat{\Omega}\,\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega}) = \Sigma_s(E'\to E) \tag{4-53}$$

where $\Sigma_s(E'\to E)$ is just the "single" differential scattering cross section. Hence we can write

$$④ = \int_{4\pi} d\hat{\Omega} \int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE' \, \Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega}) \phi(\vec{r},E',\hat{\Omega}',t) = \int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE' \underbrace{\left[\int_{4\pi} d\hat{\Omega} \, \Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega})\right]}_{\Sigma_s(E' \to E)} \phi(\vec{r},E',\hat{\Omega}',$$

$$= \int_0^{\infty} dE' \, \Sigma_s(E' \to E) \underbrace{\int_{4\pi} d\hat{\Omega}' \phi(\vec{r},E',\hat{\Omega}',t)}_{\Phi(\vec{r},E',t)} = \int_0^{\infty} dE' \, \Sigma_s(E' \to E) \Phi(\vec{r},E',t) \qquad (4\text{-}54)$$

So far everything is straightforward. But unfortunately, the last term ② cannot be evaluated in terms of $\Phi(\vec{r},E,t)$. In fact, we find ② must be evaluated in terms of the neutron current:

$$② = \int_{4\pi} d\hat{\Omega} \, \hat{\Omega} \cdot \nabla \phi = \nabla \cdot \underbrace{\int_{4\pi} d\hat{\Omega} \, \hat{\Omega} \, \phi(\vec{r},E,\hat{\Omega},t)}_{\vec{J}(\vec{r},E,t)}$$

$$= \nabla \cdot \vec{J}(\vec{r},E,t) \qquad (4\text{-}55)$$

If we now rewrite Eq. (4-33), it takes the form

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} + \nabla \cdot \vec{J}(\vec{r},E,t) + \Sigma_t(\vec{r},E)\, \Phi(\vec{r},E,t)$$

$$= \int_0^{\infty} dE' \, \Sigma_s(E' \to E) \Phi(\vec{r},E',t) + S(\vec{r},E,t) \quad . \qquad (4\text{-}56)$$

This is known as the "neutron continuity equation", since it is just the mathematical statement of neutron balance.

It is important to note that this equation contains two unknowns, $\Phi(\vec{r},E,t)$ and $\vec{J}(\vec{r},E,t)$, unlike the neutron transport equation which only contained one unknown, the angular flux $\phi(\vec{r},E,\hat{\Omega},t)$. Hence by removing the angular dependence, we have in the process introduced another unknown,

$\vec{J}(\vec{r},E,t)$ and hence now have an incomplete equation (i.e., one equation in two unknowns). The moral of this story is that you don't get something for nothing--that is, merely integrating out the angular dependence doesn't remove the complexities of the angular variation. It just shifts them by demanding that one obtain yet another equation relating $\Phi(\vec{r},E,t)$ and $\vec{J}(\vec{r},E,t)$.

It is impossible to express $\vec{J}(\vec{r},E,t)$ in terms of $\Phi(\vec{r},E,t)$ in an exact manner. This is more apparent if we recall the definitions:

$$\Phi(\vec{r},E,t) = \int_{4\pi} d\hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t) \tag{4-57}$$

$$\vec{J}(\vec{r},E,t) = \int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\, \phi(\vec{r},E,\hat{\Omega},t) \tag{4-58}$$

It is obvious that these two quantities are entirely different functions, although they can both be expressed in terms of an angular integral of the angular flux $\phi(\vec{r},E,\hat{\Omega},t)$. Hence there is no reason why one would expect these functions to be simply related.

To proceed further, one must introduce approximations into the neutron conservation equation to eliminate $\vec{J}(\vec{r},E,t)$ in terms of $\Phi(\vec{r},E,t)$, and then simplify the resultant equation.

B. Neutron Diffusion Theory

In this section we will introduce the most popular scheme for obtaining an approximate equation for the neutron flux $\Phi(\vec{r},E,t)$. This scheme which is known as neutron diffusion theory consists of the following sequence of approximations:

(i) The Diffusion Approximation (sometimes called "Fick's Law)

One begins by assuming that the neutron current is proportional to the gradient of the neutron flux

$$\vec{J}(\vec{r},E,t) \cong -D(E)\,\nabla\Phi(\vec{r},E,t). \tag{4-59}$$

The proportionality factor D is known as the "diffusion coefficient", while Eq. (4-43) is known as the "diffusion approximation". We will see in the next chapter that this relation arises from assuming that the angular flux $\phi(\vec{r},E,\hat{\Omega},t)$ is only weakly dependent upon angle $\hat{\Omega}$, and in the process of deriving Eq. (4-43) we will also determine an expression for the diffusion coefficient D. Its physical implication is simply that neutrons tend to diffuse from regions of high neutron density to regions of low neutron density.

If we now substitute the diffusion approximation (4-43) into the conservation equation (4-40), we arrive at a closed equation for the neutron flux:

$$\begin{aligned}\frac{1}{v}\frac{\partial\Phi}{\partial t} - \nabla\cdot D(\vec{r},E)\nabla\Phi + \Sigma_t(\vec{r},E)\,\Phi(\vec{r},E,t)\\ = \int_0^\infty dE'\,\Sigma_s(E'\to E)\,\Phi(\vec{r},E',t) + S(\vec{r},E,t).\end{aligned} \tag{4-60}$$

This equation is known as the "energy-dependent neutron diffusion equation".

(ii) The One-Speed Approximation

We can simplify this equation even further by assuming that the neutron energy does not change during a collision--that is,

$$\Sigma_s(E' \to E) = \Sigma_s(E)\,\delta(E-E') \tag{4-61}$$

where $\delta(E - E')$ is the Dirac δ-function, defined by

$$\int dx'\, f(x')\,\delta(x-x') = f(x) \qquad \text{for any } f(x) \tag{4-62}$$

[See Appendix C for more discussion of animals such as the δ-function.]

Using this definition,

$$\begin{aligned}\int_0^\infty dE'\,\Sigma_s(E' \to E)\,\Phi(\vec{r},E',t) &= \Sigma_s(E)\int_0^\infty dE'\,\delta(E-E')\,\Phi(\vec{r},E',t) \\ &= \Sigma_s(E)\,\Phi(\vec{r},E,t)\,.\end{aligned} \tag{4-63}$$

Then Eq. (4-44] becomes

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - \nabla\cdot D\nabla\Phi + \Sigma_t\Phi = \Sigma_s\Phi + S \tag{4-64}$$

If we recall, $\Sigma_t = \Sigma_s + \Sigma_a$, then we arrive at

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - \nabla\cdot D(\vec{r})\nabla\Phi(\vec{r},t) + \Sigma_a(\vec{r})\Phi(\vec{r},t) = S(\vec{r},t) \tag{4-65}$$

where the energy variable has not been explicitly written, since all neutrons considered in this approximation are characterized by the same speed or energy. Eq. (4-49) is known as the "one-speed diffusion equation". We will derive it in more detail in the next chapter and then use it to study the theory of nuclear reactors.

(iii) Uniform Media

We can specialize even further to the case of uniform media in which the cross sections do not depend upon position. Then Eq. (4-49) becomes

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a\Phi(\vec{r},t) = S(\vec{r},t) \quad . \tag{4-66}$$

This equation is now sufficiently simple that is can be solved using standard techniques for partial differential equations and boundary value problems. We will return to consider it in exhaustive detail later.

C. Numerical Approximations

Neutron diffusion theory, although certainly the most popular, is only one of a variety of approximations one can make to the neutron transport equation. Before developing diffusion theory in detail, it is useful to discuss some of these alternative types of approximations.

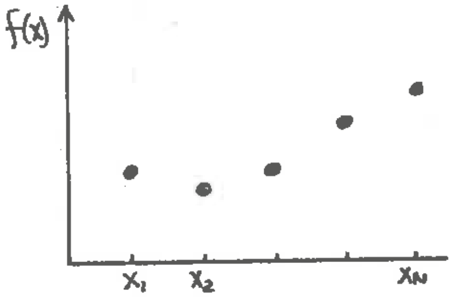
The principal class of approximations we will discuss attempt to reduce the complicated differential equations to a set of algebraic equations more suitable for solution on a digital computer by replacing each function by a discrete set of points. This can be accomplished in two ways: by using discrete ordinates methods or polynomial expansions. To illustrate these two approaches, consider an arbitrary function f(x). Then we can approximate f(x) by a discrete set of points by:

(i) discrete ordinates methods: Represent f(x) only by its values at a discrete set of points x_j:

$f(x) \longrightarrow f(x_j) \equiv f_j$, $j = 1,\dots,N$

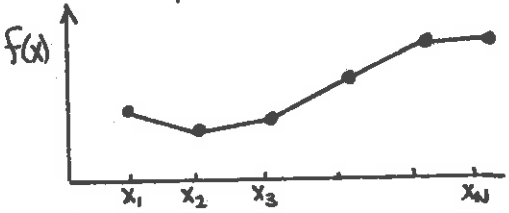
That is, we replace the function f(x) by a vector of numbers

$\underline{f} = (f_1, f_2, \dots, f_N)$



[Example: $f(x) = x^2 \longrightarrow \underline{f} = (1, 4, 9, 16)$ at x = 1, 2, 3, 4]

Now to reconstruct f(x) from $\underline{f}$, we must somehow interpolate between the points f_i -- e.g., by straight lines or polynomials



We can now replace the various operations in a differential equation for f by their discretized counterparts, numerical quadrature and finite differences:

$$\int_a^b dx\, f(x) \cong \sum_{i=1}^{N} w_i f(x_i) = \sum_{i=1}^{N} w_i f_i \tag{4-67}$$

$$\left.\frac{df}{dx}\right|_{x=x_i} \cong \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{f_i - f_{i-1}}{x_i - x_{i-1}} \tag{4-68}$$

Such a scheme then leads to a set of coupled algebraic equations for the f_i.

(ii) polynomial expansions: An alternative way to represent f(x) by a discrete set of values is to write it as an expansion in a finite number of polynomials (or other suitable expansion functions). If we call these polynomials $P_\ell(x)$, then we write

$$f(x) \cong \sum_{\ell=1}^{N} b_\ell P_\ell(x) \tag{4-69}$$

Once again we find the function f(x) is represented by a vector

$$f(x) \rightarrow (b_1, b_2, \cdots b_N) \equiv \underline{b} \tag{4-70}$$

In this case, we can easily reconstruct f(x) from a knowledge of $\underline{b}$ by merely using Eq. (4-55).

[Example:

$$\phi(\cos\theta) \cong \sum_{\ell=1}^{N} \phi_\ell P_\ell(\cos\theta) \tag{4-71}$$

where $P_\ell(\cos\theta)$ are the Legendre polynomials

$$P_0(\cos\theta) = 1, \quad P_1(\cos\theta) = \cos\theta, \quad P_2(\cos\theta) = \frac{1}{2}(3-\cos^2\theta), \cdots \tag{4-72}$$

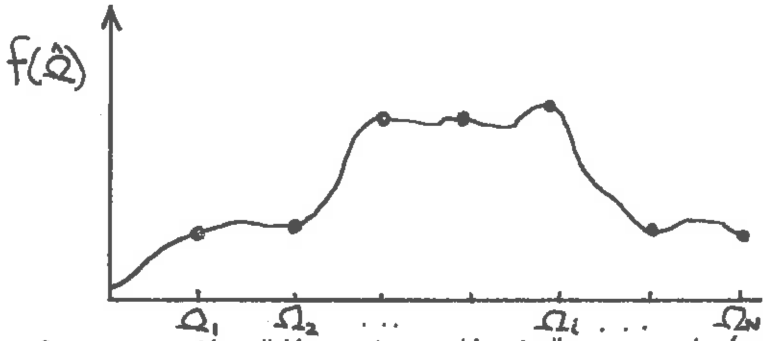
Upon substituting this expansion into the original equation for f(x), then multiplying by $P_\ell(x)$, integrating over x, and then using properties of the $P_\ell(x)$ [such as the property of "orthogonality" which we will discuss later], one again arrives at a set of algebraic equations for the b_i. These are the two principal schemes used in approximating the transport equation.

D. Approximations of the Angular Dependence

To be more precise, consider some of these ideas applied to the angular variation. That is, consider a function of the angle variable $\hat{\Omega}$, say $f(\hat{\Omega})$. Perhaps the simplest scheme for approximating this function is to represent it by a discrete set of points*

$$f(\hat{\Omega}) \rightarrow f(\hat{\Omega}_i) \equiv f_i \quad \text{for} \quad i = 1, \ldots, N \tag{4-73}$$

That is, we discretize the independent variable $\hat{\Omega}$ by replacing it by a discrete set of points $\hat{\Omega}_i$, and then only attempt to calculate the function $f(\hat{\Omega})$ at each of these points



This is, of course, the "discrete ordinate" approach (sometimes known as the "S_N" approach when applied to the angular variable). In such a discrete representation, an integral over $\hat{\Omega}$ becomes a sum

$$\int_{4\pi} d\hat{\Omega}\, f(\hat{\Omega}) \cong \sum_{i=1}^{N} w_i f_i \tag{4-74}$$

where the w_i are the "quadrature weights" of the numerical integration scheme. In this scheme, the transport equation reduces to a coupled set of N equations of the form:

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*In much of this discussion we will treat $\hat{\Omega}$ as if it were a scalar variable for convenience, when of course it should actually be regarded as a two-component vector $\hat{\Omega} = (\theta, \phi)$.

$$\frac{1}{v}\frac{\partial \phi_j}{\partial t} + \hat{\Omega}_j \cdot \nabla \phi_j + \Sigma_t \phi_j(\vec{r},E,t)$$

$$= \sum_{i=1}^{N} w_i \int_0^\infty dE' \, \Sigma_s(E' \to E, \hat{\Omega}_i \to \hat{\Omega}_j) \phi_i(\vec{r},E',t) + S_j \qquad (4\text{-}75)$$

$$j = 1, \dots, N$$

where

$$\phi_j(\vec{r},E,t) \equiv \phi(\vec{r},E,\hat{\Omega}_j,t) \qquad (4\text{-}76)$$

The set of equations (4-61) is known as the discrete ordinate or S_N equations.

There is another common approach to approximating the angular dependence by a discrete set of numbers, and this consists of expanding the function $f(\hat{\Omega})$ in a finite series of known functions of $\hat{\Omega}$

$$f(\hat{\Omega}) \cong \sum_{i=1}^{N} f_i \, p_i(\hat{\Omega}) \qquad (4\text{-}77)$$

where $p_i(\hat{\Omega})$ is a known function of $\hat{\Omega}$ (frequently a polynomial). The functions of most use here are the spherical harmonics $Y_{lm}(\hat{\Omega}) = Y_{lm}(\theta,\phi)$ familiar from quantum mechanics. Then (4-63) becomes

$$f(\hat{\Omega}) \cong \sum_{l,m}^{N} f_{lm} Y_{lm}(\hat{\Omega}) \qquad (4\text{-}78)$$

Here the f_{lm} play the same role that the $f_i = f(\hat{\Omega}_i)$ did in the discrete ordinates method. This expansion scheme is known as the "P_N-method".

since in one-dimensional geometries the spherical harmonics reduce to Legendre polynomials which are usually denoted by $P_n(x)$.

In the particular case of N = 1, the P_N expansion for the flux is just

$$\phi(\vec{r},E,\hat{\Omega},t) \cong \frac{1}{4\pi}\Phi(\vec{r},E,t) + \frac{3}{4\pi}\vec{J}(\vec{r},E,t)\cdot\hat{\Omega} \tag{4-79}$$

We will find in the next section that this "P_1 approximation" can be used to derive the neutron diffusion equation.

E. Energy Approximations

Similar approximate treatments can be given of the energy variable. Here, the discrete ordinate approach is far more common and is referred to as the "multigroup" method. One replaces

$$\phi(E) \to \phi(E_g) \equiv \phi^g \quad , \quad g=1,\dots,G \tag{4-80}$$

In a similar manner,

$$\int_0^\infty dE'\,\Sigma_s(E'\to E)\phi(E') \cong \sum_{g'=1}^{G} w_{g'}\,\Sigma_s^{g'g}\phi^{g'} \tag{4-81}$$

where $w_{g'}$ are the energy "quadrature weights", while

$$\Sigma_s^{g'g} \equiv \Sigma_s(E_{g'}\to E_g). \tag{4-82}$$

[Actually the multigroup equations are more commonly derived by integration over an energy interval or group. This approach will be developed in Chapter 7.]

For example, the multigroup-S_N equations are

$$\frac{1}{v^g}\frac{\partial}{\partial t}\phi_j^g + \hat{\Omega}_j\cdot\nabla\phi_j^g + \Sigma_t^g\phi_j^g$$

$$= \sum_{i=1}^{N}\sum_{g'=1}^{G} w_i w_{g'}\,\Sigma_{s_{ij}}^{g'g}\,\phi_i^{g'} + S_i^g \qquad (4\text{-}83)$$

$$i = 1, \cdots, N$$
$$g = 1, \cdots, G$$

F. Space and Time Approximations

One usually uses a discrete ordinate approximation of the space and time variable by choosing a discrete space "mesh"

$$\vec{r} \longrightarrow x_1, y_1, z_1\,;\ x_2, y_2, z_2\,;\ \cdots\ ;\ x_N, y_N, z_N$$

and discrete time "steps"

$$t \rightarrow t_0, t_1, \cdots$$

One then replaces all of the derivatives in space and time by appropriate difference formulas--e.g.,

$$\frac{df}{dt} \cong \frac{f(t_{m+1}) - f(t_m)}{t_{m+1} - t_m}\ , \quad \frac{df}{dx} \cong \frac{f(x_{n+1}) - f(x_n)}{x_{n+1} - x_n} \qquad (4\text{-}84)$$

$$\frac{d^2f}{dx^2} \cong \frac{f(x_{n+1}) - 2f(x_n) + f(x_{n-1})}{(x_{n+1} - x_n)(x_n - x_{n-1})} \qquad (4\text{-}85)$$

and so on.

When all of these discretization steps have been inserted, the integro-differential transport equation is reduced to a set of algebraic equations for each of the discretized fluxes

$$\phi(x_\ell, y_m, z_n, E_g, \hat{\Omega}_i, t_m) .$$

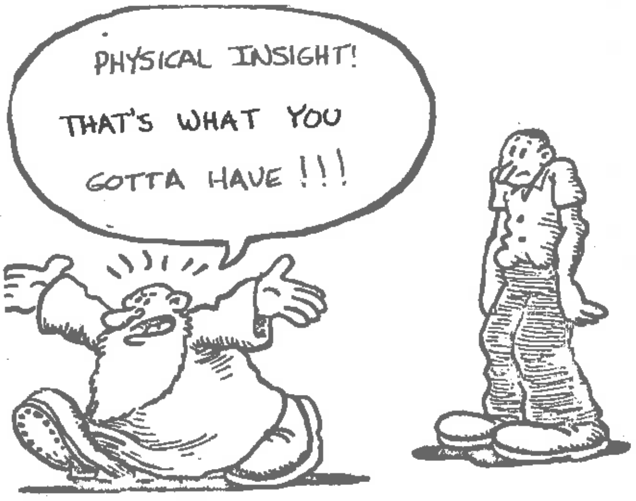
Such algebraic equations can then be solved using routine methods on a digital computer.

Unfortunately, such a calculation becomes an immense undertaking if only a "brute force" discretization of the transport equation is applied. Consider "typical" mesh sizes of

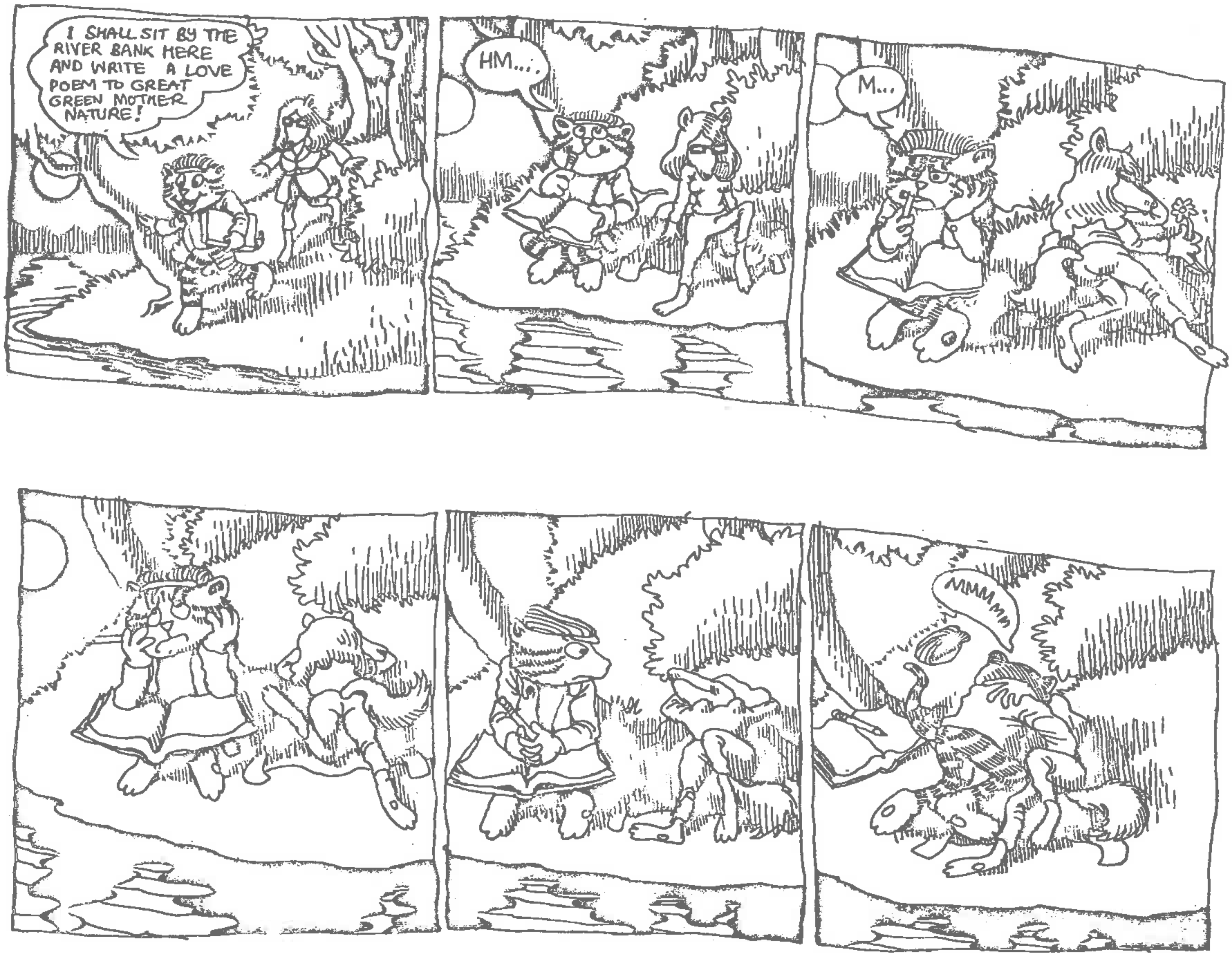
100 x 100 x 100	space points
10	energy groups
10	angle points

Then for each time step we wish to calculate, we must solve 10^8 simultaneous algebraic equations--a rather formidable task, even on a computer.

Hence the nuclear engineer cannot blindly depend upon the computer to solve his problem, but rather he must first rely upon physical insight (rather than brute force mathematics) to reduce the transport equation to more manageable form. Perhaps the most useful approximation to this end is the diffusion approximation. Hence we begin our detailed study of nuclear reactor theory by first developing neutron diffusion theory.



" AN EXERCISE IN PHYSICAL INSIGHT "



PART II

THE ONE-SPEED DIFFUSION MODEL
OF A
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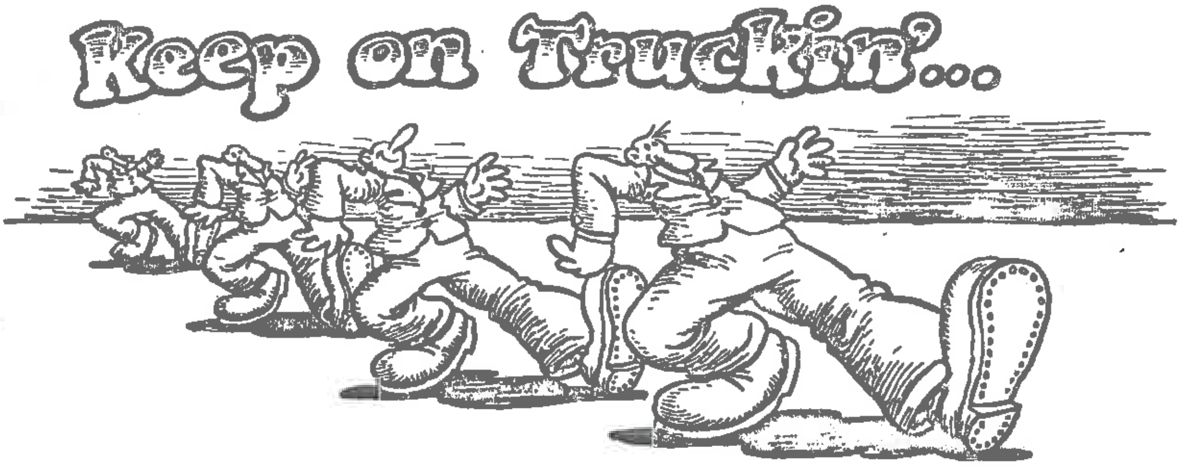


CHAPTER 5: THE ONE-SPEED DIFFUSION THEORY MODEL

In this chapter we will develop the one-speed diffusion model of neutron transport. This model plays an extremely important role in reactor theory, since not only is it sufficiently simple to allow detailed calculations, but at the same time it is sufficiently realistic to allow us to study many of the more important concepts arising in nuclear reactor analysis. The one-speed diffusion model is in fact capable of yielding quantitative information about nuclear reactor behavior and can be used to provide preliminary design estimates. Moreover, many of the mathematical techniques we will use to solve and analyze this model are in fact identical to those applied to the more sophisticated models (e.g., multigroup diffusion theory) used today in actual nuclear reactor design.

I. THE ONE-SPEED DIFFUSION APPROXIMATION

A. Derivation of the Diffusion Equation

To make the model as simple as possible, we will introduce three initial assumptions:

(i) Only a single neutron speed will be considered--i.e., we assume there is no energy change in a collision

$$\Sigma_s(E'\to E,\hat{\Omega}'\to\hat{\Omega}) = \Sigma_s(\hat{\Omega}'\to\hat{\Omega})\,\delta(E'-E) \qquad (5\text{-}1)$$

and that all the neutrons are characterized by one speed.

(ii) We assume that scattering is isotropic in the LAB system

$$\Sigma_s(\hat{\Omega}'\to\hat{\Omega}) = \frac{\Sigma_s}{4\pi} \tag{5-2}$$

and that the source is isotropic as well,

$$S(\vec{r},\hat{\Omega},t) = \frac{1}{4\pi} S(\vec{r},t) \tag{5-3}$$

[Recall that the $\frac{1}{4\pi}$ factors are necessary for normalization.]

(iii) We will assume that the neutrons are diffusing in a homogeneous, uniform medium--i.e., that the atomic number density does not depend upon position $\vec{r}$, hence implying that the macroscopic cross sections Σ are also independent of $\vec{r}$.

We will discuss later how each of these assumptions can be removed, if desired.

The neutron transport equation (4-31) then simplifies to

$$\frac{1}{v}\frac{\partial\phi}{\partial t} + \hat{\Omega}\cdot\nabla\phi + \Sigma_t\phi(\vec{r},\hat{\Omega},t) = \frac{\Sigma_s}{4\pi}\int_{4\pi} d\hat{\Omega}'\phi(\vec{r},\hat{\Omega}',t) + \frac{S(\vec{r},t)}{4\pi} \tag{5-4}$$

We now describe the sequence of steps needed to "derive" the neutron diffusion model from this equation:

STEP 1: Begin by integrating the transport equation (5-4) over angle to obtain the neutron continuity equation:

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} + \nabla\cdot\vec{J}(\vec{r},t) + \Sigma_t\Phi(\vec{r},t) = \Sigma_s\Phi(\vec{r},t) + S(\vec{r},t) \tag{5-5}$$

where we recall

$$\Phi(\vec{r},t) \equiv \int_{4\pi} d\hat{\Omega}\, \phi(\vec{r},\hat{\Omega},t) \tag{5-6}$$

$$\vec{J}(\vec{r},t) \equiv \int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\, \phi(\vec{r},\hat{\Omega},t)\,. \tag{5-7}$$

<u>STEP 2</u>: Next, multiply the transport equation by $\hat{\Omega}$ and integrate once again over angle. Actually, since the direction $\hat{\Omega}$ is a vector,

$$\hat{\Omega} = \hat{e}_x \underbrace{\sin\theta\cos\phi}_{\Omega_x} + \hat{e}_y \underbrace{\sin\theta\sin\phi}_{\Omega_y} + \hat{e}_z \underbrace{\cos\theta}_{\Omega_z} \tag{5-8}$$

we should multiply by each component separately and integrate. For example, the Ω_x component yields

$$\underset{①}{\int_{4\pi} d\hat{\Omega}\, \Omega_x \frac{1}{v}\frac{\partial \phi}{\partial t}} + \underset{②}{\int_{4\pi} d\hat{\Omega}\, \Omega_x \hat{\Omega}\cdot\nabla\phi} + \underset{③}{\int_{4\pi} d\hat{\Omega}\, \Omega_x \Sigma_t \phi}$$

$$= \underset{④}{\int_{4\pi} d\hat{\Omega}\, \Omega_x \frac{\Sigma_s}{4\pi} \int_{4\pi} d\hat{\Omega}'\, \phi(\vec{r},\hat{\Omega}',t)} + \underset{⑤}{\int_{4\pi} d\hat{\Omega}\, \Omega_x \frac{S(\vec{r},t)}{4\pi}}\,. \tag{5-9}$$

Each of these terms can be simplified:

$$① = \frac{1}{v}\frac{\partial}{\partial t} \underbrace{\int_{4\pi} d\hat{\Omega}\, \Omega_x \phi(\vec{r},\hat{\Omega},t)}_{J_x(\vec{r},t)} = \frac{1}{v}\frac{\partial J_x}{\partial t}\,, \tag{5-10}$$

$$② = \nabla\cdot \int_{4\pi} d\hat{\Omega}\, \Omega_x \hat{\Omega}\, \phi(\vec{r},\hat{\Omega},t)\,, \tag{5-11}$$

$$③ = \Sigma_t \int_{4\pi} d\hat{\Omega}\, \Omega_x \phi(\vec{r},\hat{\Omega},t) = \Sigma_t J_x(\vec{r},t)\,. \tag{5-12}$$

The last two terms are particularly simple if we note

$$\int_{4\pi} d\hat{\Omega}\,\Omega_x = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, [\sin\theta\cos\phi] = 0. \tag{5-13}$$

[In a similar fashion, $\int_{4\pi} d\hat{\Omega}\,\Omega_y = \int_{4\pi} d\hat{\Omega}\,\Omega_z = 0$.]

Hence

$$④ = \left[\int_{4\pi} d\hat{\Omega}\,\Omega_x\right] \frac{\Sigma_s}{4\pi} \int_{4\pi} d\hat{\Omega}'\,\phi(\vec{r},\hat{\Omega}',t) = 0 , \tag{5-14}$$

$$⑤ = \frac{S(\vec{r},t)}{4\pi} \int_{4\pi} d\hat{\Omega}\,\Omega_x = 0 . \tag{5-15}$$

Thus we can combine these results to rewrite (5-9), including the Ω_y and Ω_z components, as

$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} + \nabla\cdot \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) + \Sigma_t \vec{J}(\vec{r},t) = 0. \tag{5-16}$$

Notice that just as in the case of the neutron conservation equation (5-5), we find that integrating over $\hat{\Omega}$ yields one equation (5-16)--but two unknowns, $\vec{J}(\vec{r},t)$ and

$$\overleftrightarrow{\Pi}(\vec{r},t) \equiv \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) . \tag{5-17}$$

It should be evident that we can get a new equation for $\overleftrightarrow{\Pi}(\vec{r},t)$ by multiplying the transport equation (5-4) by $\hat{\Omega}\hat{\Omega}$ and integrating; but this new equation will contain yet another unknown,

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t)$$

Hence all we are doing by multiplying by $[\hat{\Omega}]^n$ and integrating is generating an infinite set of coupled equations (which we can't solve). [Incidently, it should be apparent that the culprit is the "streaming" or "leakage" term

$$\hat{\Omega}\cdot\nabla\phi$$

which contains a factor of $\hat{\Omega}$ and hence generates the new unknowns in each equation.]

The only way to cut off this chain of coupled equations is to introduce an approximation. We shall now do this by assuming the angular flux is only <u>weakly dependent upon angle</u>.

<u>STEP 3</u>: To be more specific, we will expand the angular flux in angle as

$$\phi(\vec{r},\hat{\Omega},t)=\phi_0(\vec{r},t)+\phi_{1x}(\vec{r},t)\Omega_x+\phi_{1y}(\vec{r},t)\Omega_y+\phi_{1z}(\vec{r},t)\Omega_z+\cdots \tag{5-18}$$

and neglect all terms of higher than linear order in $\hat{\Omega}$. Actually, a slightly different notation for the unknown functions $\phi_0, \phi_{1x}, \phi_{1y}, \phi_{1z}$ is useful. Write (5-18) as

$$\begin{aligned}\phi(\vec{r},\hat{\Omega},t) &\cong \frac{1}{4\pi}\Phi(\vec{r},t)+\frac{3}{4\pi}\left[J_x(\vec{r},t)\Omega_x+J_y(\vec{r},t)\Omega_y+J_z(\vec{r},t)\Omega_z\right] \\ &\cong \frac{1}{4\pi}\Phi(\vec{r},t)+\frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega}\end{aligned} \tag{5-19}$$

Notice that we have labeled the unknown expansion coefficients as the flux and current. That this notation is perfectly consistent can be seen by noting from (5-19) that

$$\int_{4\pi} d\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) = \Phi(\vec{r},t)\,\underbrace{\frac{1}{4\pi}\int_{4\pi} d\hat{\Omega}}_{\overset{\shortparallel}{1}} + \frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\underbrace{\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}}_{\overset{\shortparallel}{0}} \tag{5-20}$$

$$= \Phi(\vec{r},t)\,,$$

and

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) = \Phi(\vec{r},t)\frac{1}{4\pi}\int_{4\pi} d\hat{\Omega}\,\hat{\Omega} + \frac{3}{4\pi}\Big[J_x(\vec{r},t)\int_{4\pi} d\hat{\Omega}\,\Omega_x\hat{\Omega} + J_y(\vec{r},t)\int_{4\pi} d\hat{\Omega}\,\Omega_y\hat{\Omega} + J_z(\vec{r},t)\int_{4\pi} d\hat{\Omega}\,\Omega_z\hat{\Omega}\Big] \tag{5-21}$$

But

$$\int_{4\pi} d\hat{\Omega}\,\Omega_i\Omega_j = \begin{cases} \frac{4\pi}{3} & i=j \\ 0 & i\neq j \end{cases} \qquad i,j=x,y,z \tag{5-22}$$

Hence

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) = \vec{J}(\vec{r},t)\,. \tag{5-23}$$

Of course (5-20) and (5-23) are identical to our original definitions of the flux and current in Chapter 4.

If we now insert the approximate form (5-19) into the term (5-11), we find

$$② = \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega}\left[\frac{1}{4\pi}\Phi(\vec{r},t) + \frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega}\right]\,. \tag{5-24}$$

Now note that

$$\int_{4\pi} d\hat{\Omega}\,[\hat{\Omega}]^{n} = 0 \qquad \text{for any } \underline{\text{odd}} \text{ power } n\,. \tag{5-25}$$

If we also use Eq. (5-22), then we find

$$\textcircled{2} = \left\{ \left[\hat{e}_x \int_{4\pi} d\hat{\Omega}\,\Omega_x\Omega_x \frac{\partial}{\partial x}\right] + \left[\hat{e}_y \int_{4\pi} d\hat{\Omega}\,\Omega_y\Omega_y \frac{\partial}{\partial y}\right] + \left[\hat{e}_z \int_{4\pi} d\hat{\Omega}\,\Omega_z\Omega_z \frac{\partial}{\partial z}\right]\right\} \frac{\Phi(\vec{r},t)}{4\pi} + \nabla\cdot \underbrace{\left[\int_{4\pi} d\hat{\Omega}\,(\hat{\Omega})^{3}\right]}_{0} \frac{3}{4\pi}\vec{J}(\vec{r},t) \tag{5-26}$$

or

$$\textcircled{2} = \frac{1}{3}\left[\hat{e}_x\frac{\partial}{\partial x} + \hat{e}_y\frac{\partial}{\partial y} + \hat{e}_z\frac{\partial}{\partial z}\right]\Phi(\vec{r},t) = \frac{1}{3}\nabla\Phi(\vec{r},t)\,. \tag{5-27}$$

Hence we find that (5-16) becomes

$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} + \frac{1}{3}\nabla\Phi + \Sigma_t \vec{J}(\vec{r},t) = 0\,. \tag{5-28}$$

We could stop at this point because equations (5-28) and (5-5) form a set of two equations and two unknowns, $\Phi(\vec{r},t)$ and $\vec{J}(\vec{r},t)$. However it is useful to make one additional approximation.

STEP 4: We will assume that we can neglect the term $\frac{1}{v}\frac{\partial \vec{J}}{\partial t}$ in comparison with the remaining terms in (5-28). This assumption implies, for example, that

$$\frac{1}{|\vec{J}|}\frac{\partial |\vec{J}|}{\partial t} << v\Sigma_t\,.$$

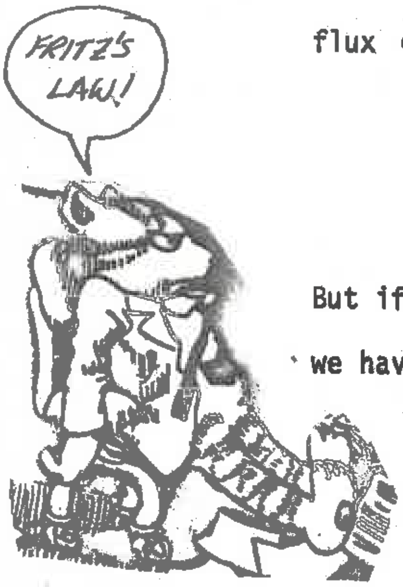
But since $v\Sigma_t$ is typically of order 10^5 sec^{-1}, only an extremely rapid time variation of the current (on a scale of 10^{-5} sec) would invalidate this assumption. We will later find that such rapid changes are very rarely encountered in reactor dynamics. Hence we are justified in rewriting Eq. (5-28) as

$$\frac{1}{3}\nabla\Phi(\vec{r},t) + \Sigma_t\vec{J}(\vec{r},t) = 0. \tag{5-29}$$

We can solve Eq. (5-29) for the current $\vec{J}(\vec{r},t)$ in terms of the flux $\Phi(\vec{r},t)$

$$\vec{J}(\vec{r},t) = -\frac{1}{3\Sigma_t}\nabla\Phi(\vec{r},t). \tag{5-30}$$

But if we compare this with Eq. (4-43) from Chapter 4, we find that we have just derived Fick's law:



$$\vec{J}(\vec{r},t) = -D\nabla\Phi(\vec{r},t), \tag{5-31}$$

where the diffusion coefficient is defined now as

$$D \equiv \frac{1}{3\Sigma_t} \tag{5-32}$$

If we return to the conservation equation (5-5) and substitute (5-31) in for $\vec{J}(\vec{r},t)$, we find

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a\Phi(\vec{r},t) = S(\vec{r},t), \tag{5-33}$$

which is known as the "one-speed diffusion equation".

B. Validity of Diffusion Theory

Remember the two approximations required to obtain the diffusion equation:

(i) The angular flux is only weakly dependent upon angle

$$\phi(\vec{r},\hat{\Omega},t) \cong \frac{1}{4\pi}\Phi(\vec{r},t) + \frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega}\,. \qquad (5\text{-}19)$$

(ii) The flux and current change in time slowing compared to the mean collision time, $(v\Sigma_t)^{-1}$ or

$$\frac{1}{J_i}\frac{\partial J_i}{\partial t} << v\Sigma_t\,. \qquad (5\text{-}34)$$

Actually, only the first of these approximations is really crucial. The second can easily be relaxed (see the problem set). The assumption of only linear angle dependence (sometimes referred to as "linear anisotropy") is occasionally referred to as "the diffusion approximation", since it essentially implies Fick's law Eq. (5-31).

It is natural to ask when the flux is sufficiently weakly dependent upon angle so that the diffusion approximation is valid. More detailed studies of the transport equation itself indicate that the assumption of weak angular dependence is violated

(i) near boundaries

(ii) near sources

(iii) in strongly absorbing media

In fact, strong angular dependence can be associated with fluxes which change rapidly in space. Usually if one is over several mean free paths from any sources of boundaries in a weakly absorbing media, the flux is slowly varying in space, and diffusion theory is valid.

C. Generalizations

1. Non-Uniform Media

The extension of these results to nonuniform media in which the cross sections depend upon position is straightforward and merely involves noting that the diffusion coefficient D is now $\vec{r}$-dependent:

$$\vec{J}(\vec{r},t) = -\frac{1}{3\Sigma_t(\vec{r})}\nabla\Phi(\vec{r},t) = -D(\vec{r})\nabla\Phi(\vec{r},t) \qquad (5\text{-}35)$$

so that the one-speed diffusion equation must be written as

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - \nabla\cdot D(\vec{r})\nabla\Phi + \Sigma_a(\vec{r})\Phi(\vec{r},t) = S(\vec{r},t). \qquad (5\text{-}36)$$

2. Energy Dependence

We can <u>formally</u> generalize to include energy dependence by writing

$$\vec{J}(\vec{r},E,t) = -\frac{1}{3\Sigma_t(E)}\nabla\Phi(\vec{r},E,t) = -D(E)\nabla\Phi(\vec{r},E,t). \qquad (5\text{-}37)$$

Hence the energy-dependent diffusion equation is just

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D(E)\nabla^2\Phi + \Sigma_t(E)\Phi(\vec{r},E,t) = \int_0^\infty dE'\,\Sigma_s(E'\to E)\Phi(\vec{r},E',t) + S(\vec{r},E,t). \qquad (5\text{-}38)$$

We will use this equation in Chapter 7 to derive the principal tool of reactor analysis, multigroup diffusion theory.

In practice, however, the derivation of the energy dependent diffusion equation is by no means a trivial extension of our earlier development, and requires several additional approximations. We will avoid a consideration of this topic, however, and refer the interested reader to more advanced treatises for further discussion.

3. Anisotropic Scattering

We now relax the assumption of isotropic scattering and allow a differential scattering cross section which depends upon the scattering angle

$$\Sigma_s(\hat{\Omega}'\to\hat{\Omega}) = \Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}). \tag{5-39}$$

Return to the two conservation equations in which the more general scattering cross section (5-39) has been used:

$$\frac{1}{v}\frac{\partial\Phi}{\partial t}+\nabla\cdot\vec{J}+\Sigma_t\Phi(\vec{r},t) = \int_{4\pi} d\hat{\Omega}'\left[\int_{4\pi} d\hat{\Omega}\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\right]\phi(\vec{r},\hat{\Omega}',t)+S(\vec{r},t) \tag{5-40}$$

$$\frac{1}{v}\frac{\partial\vec{J}}{\partial t}+\nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\phi(\vec{r},\hat{\Omega},t)+\Sigma_t\vec{J}(\vec{r},t) = \int_{4\pi} d\hat{\Omega}'\left[\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\right]\phi(\vec{r},\hat{\Omega}',t) \tag{5-41}$$

We first note that $\int_{4\pi} d\hat{\Omega}\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) = \Sigma_s$ so that (5-40) is identical to our earlier conservation (5-5).

We now introduce the diffusion approximation as before

$$\phi(\vec{r},\hat{\Omega},t) \cong \frac{1}{4\pi}\Phi(\vec{r},t)+\frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega} \tag{5-19}$$

Once again, we find

$$\nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\phi(\vec{r},\hat{\Omega},t) \cong \frac{1}{3}\nabla\Phi(\vec{r},t) \tag{5-27}$$

To evaluate the "inscattering" term, substitute (5-19) for ϕ to find

$$\int_{4\pi} d\hat{\Omega}'\left[\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\Sigma_s(\hat{\Omega}'\to\hat{\Omega})\right]\phi(\vec{r},\hat{\Omega}',t) = \frac{1}{4\pi}\Phi(\vec{r},t)\underbrace{\int_{4\pi} d\hat{\Omega}'\left[\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\right]}_{①}$$

$$+\frac{3}{4\pi}\underbrace{\left[\int_{4\pi} d\hat{\Omega}'\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega}'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\right]}_{②}\cdot\vec{J}(\vec{r},t) \qquad (5\text{-}42)$$

Now

$$① = \frac{1}{4\pi}\Phi(\vec{r},t)\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\left[\int_{4\pi} d\hat{\Omega}'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\right] = \frac{1}{4\pi}\Phi(\vec{r},t)\underbrace{\left[\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\right]}_{\overset{\shortparallel}{0}}\Sigma_s = 0 \qquad (5\text{-}43)$$

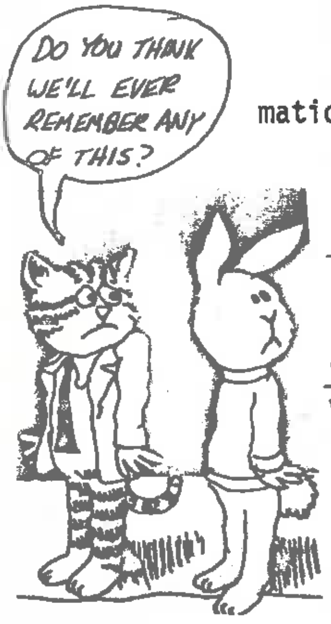
$$② = \frac{3}{4\pi}\Big[\int_{4\pi} d\hat{\Omega}'\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\cdot\hat{\Omega}'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\vec{J}(\vec{r},t) = \Sigma_s\bar{\mu}_0\,\vec{J}(\vec{r},t) \qquad (5\text{-}44)$$

where we have identified the average scattering angle cosine

$$\bar{\mu}_0 \equiv \langle\hat{\Omega}'\cdot\hat{\Omega}\rangle = \frac{3}{4\pi}\frac{1}{\Sigma_s}\int_{4\pi} d\hat{\Omega}\int_{4\pi} d\hat{\Omega}'\,\hat{\Omega}\cdot\hat{\Omega}'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) \ . \qquad (5\text{-}45)$$

[This quantity can be readily calculated for elastic scattering, and we shall do so when we consider neutron slowing down in Chapter 8. For now, however, we will merely assume $\bar{\mu}_0$ is known.]

Hence we can now write (5-40) and (5-41) after the "diffusion approximation" (5-19) as



$$\begin{aligned}\frac{1}{v}\frac{\partial\Phi}{\partial t} + \nabla\cdot\vec{J} + \Sigma_a\Phi(\vec{r},t) &= S(\vec{r},t)\\ \frac{1}{v}\frac{\partial\vec{J}}{\partial t} + \frac{1}{3}\nabla\Phi + \Sigma_t\vec{J}(\vec{r},t) &= \bar{\mu}_0\Sigma_s\vec{J}(\vec{r},t)\end{aligned} \qquad (5\text{-}46)$$

[Incidently, this coupled set of equations is known as the "P_1 equations", since the assumption ofonly a linearly anisotropic angular flux

$$\phi(\vec{r},\hat{\Omega},t) \cong \frac{1}{4\pi}\Phi(\vec{r},t) + \frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega} \qquad (5\text{-}19)$$

is equivalent to expanding the flux in spherical harmonics and retaining only the $\ell = 0$ and $\ell = 1$ terms

$$\phi(\vec{r},\hat{\Omega},t) \cong \Phi(\vec{r},t)\,Y_{0,0}(\hat{\Omega}) + J_x(\vec{r},t)Y_{1,1}(\hat{\Omega}) + J_y(\vec{r},t)Y_{1,-1}(\hat{\Omega}) + J_z(\vec{r},t)Y_{1,0}(\hat{\Omega}) \qquad (5\text{-}47)$$

In one dimensional geometries, this is equivalent to an expansion in Legendre polynomials P_ℓ $(\cos\theta)$

$$\phi(x,\cos\theta,t) \cong \Phi(x,t)P_0(\cos\theta) + J(x,t)P_1(\cos\theta) \qquad (5\text{-}48)$$

--hence the name "P_1 approximation". Notice that this could be easily generalized to obtain the "P_N approximation".]

If we now continue on and assume the current changes sufficiently slowly in time that $\frac{1}{v}\frac{\partial\vec{J}}{\partial t}$ can be neglected, then the second of equations (5-46) can be solved for

$$\vec{J}(\vec{r},t) = -\left[\frac{1}{3(\Sigma_t - \bar{\mu}_0\Sigma_s)}\right]\nabla\Phi(\vec{r},t)\,. \qquad (5\text{-}49)$$

Hence, when anisotropic scattering is included, one still finds the diffusion approximation yields Fick's Law

$$\vec{J}(\vec{r},t) = -D\nabla\Phi(\vec{r},t) \qquad (5\text{-}50)$$

except that the definition of the diffusion coefficient is now modified to

$$D \equiv \frac{1}{3(\Sigma_t - \bar{\mu}_0 \Sigma_s)} \quad . \qquad (5\text{-}51)$$

Occasionally one runs into the notation of a "transport cross section"

$$\Sigma_{tr} \equiv \Sigma_t - \bar{\mu}_0 \Sigma_s \qquad (5\text{-}52)$$

such that

$$D = \frac{1}{3\Sigma_{tr}} = \frac{\lambda_{tr}}{3} \qquad (5\text{-}53)$$

where $\lambda_{tr} \equiv 1/\Sigma_{tr}$ is the "transport mean free path". Notice that the transport cross section adjusts the scattering cross section to account for forward (anisotropic) scattering. If forward scattering is large, $\bar{\mu}_0$ is appreciable and $\Sigma_{tr} < \Sigma_t$. By setting $\bar{\mu}_0 = 0$, we return to our earlier results for isotropic scattering. Henceforth, we shall take D to be given by the more general expression (5-53).

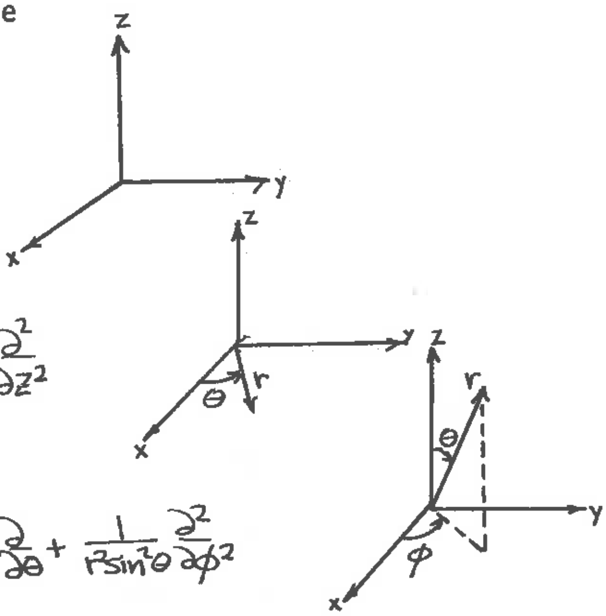
D. Boundary Conditions

Consider now the situation in which the neutrons are diffusing in a uniform material (such that cross sections are not position-dependent). Then the one-speed neutron diffusion equation is

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a \Phi(\vec{r},t) = S(\vec{r},t) \quad . \qquad (5\text{-}54)$$

This is a "parabolic" partial differential equation (PDE) which has been "beaten-to-death" by mathematicians over the years, since it also describes processes like heat conduction, gas diffusion, and even a wave function (note if we stick an "i" in front of $\partial/\partial t$, we have essentially just the Schrödinger equation). We will later review some of the more popular ways to solve such PDE's.

It is useful to note the forms taken by the "Laplacian" ∇^2 in the various coordinate systems we will use



(i) rectangular:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

(ii) cylindrical:

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}$$

(iii) spherical;

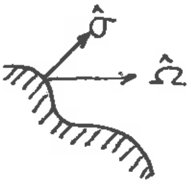
$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\sin\theta\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

We will usually consider situations in which the flux is not a function of time. Then (5-54) becomes

$$-D\nabla^2\Phi(\vec{r}) + \Sigma_a\Phi(\vec{r}) = S(\vec{r}) . \tag{5-56}$$

This equation is known as the "Helmholtz equation" and is also a very familiar beast in mathematical physics.

However before we dive into the mathematics of solving the diffusion equation, we must return to physics for a moment. Since Eq. (5-54) has derivatives in space and time, we know the equation is incomplete until we specify boundary and initial conditions. We are guided in our choice of conditions by the transport theory conditions discussed earlier (p. 105);



initial condition: $\phi(\vec{r},\hat{\Omega},0)=\phi_0(\vec{r},\hat{\Omega})$ (5-57)

boundary condition: $\phi(\vec{r}_s,\hat{\Omega},t)=0$ for $\hat{\Omega}\cdot\hat{\sigma}<0$ all $\vec{r}_s$ on S (5-58)

We can obtain the appropriate initial condition for the diffusion equation by merely integrating the transport condition over angle to obtain

initial condition $\Phi(\vec{r},0)=\Phi_0(\vec{r})$ (5-59)

The boundary conditions are a bit harder to come by. Actually, we will need three different types of boundary conditions to handle

(i) boundaries at infinity

(ii) boundaries at interfaces

(iii) vacuum boundaries

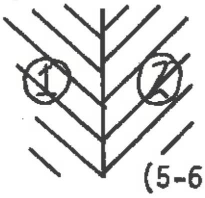
The transport boundary condition we have mentioned above is only for a vacuum boundary. Consider each of the above boundaries in turn:

(i) <u>boundaries at infinity</u>: This boundary condition is easy to determine, since clearly we must demand that the flux be finite

$$\lim_{r\to\infty}\Phi(\vec{r},t)<\infty \qquad (5\text{-}60)$$

provided we do not allow sources of infinite magnitude at infinity. [Sometimes this latter pathological case is of interest, such as in the "Milne problem" in which one studies the behavior of the flux near a vacuum boundary which is fed by a source at infinity. But we will avoid a consideration of such problems here.]

(ii) <u>boundaries at interfaces</u>: Consider an interface between two regions of differing cross sections. Now clearly the correct transport boundary condition is that



$$\phi_1(\vec{r}_s,\hat{\Omega},t)=\phi_2(\vec{r}_s,\hat{\Omega},t) \qquad \text{for all } \hat{\Omega} \tag{5-61}$$

where ϕ_1 is the angular flux in region 1, while ϕ_2 is the angular flux in region 2. This condition insures conservation of neutrons across the boundary.

Unfortunately, we cannot satisfy this boundary condition exactly using diffusion theory. At best, we can only insure that angular moments of (5-61) are satisfied. And since diffusion theory yields only the first two moments of the angular flux:

$$\Phi(\vec{r},t)=\int_{4\pi} d\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) \quad \text{and} \quad \vec{J}(\vec{r},t)=\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t)$$

at best we can demand

$$\int_{4\pi} d\hat{\Omega}\,\phi_1(\vec{r}_s,\hat{\Omega},t)=\int_{4\pi} d\hat{\Omega}\,\phi_2(\vec{r}_s,\hat{\Omega},t) \Rightarrow \Phi_1(\vec{r}_s,t)=\Phi_2(\vec{r}_s,t) \tag{5-62}$$

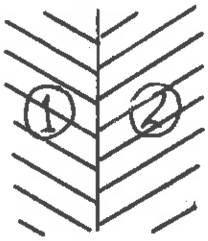
and

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\phi_1(\vec{r}_s,\hat{\Omega},t)=\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\phi_2(\vec{r}_s,\hat{\Omega},t) \Rightarrow \vec{J}_1(\vec{r}_s,t)=\vec{J}_2(\vec{r}_s,t) \tag{5-63}$$

Hence the interface diffusion theory boundary conditions are

$$\Phi_1(\vec{r}_s,t) = \Phi_2(\vec{r}_s,t)$$

$$-D_1\nabla\Phi_1(\vec{r}_s,t) = -D_2\nabla\Phi_2(\vec{r}_s,t) \qquad (5\text{-}64)$$



[We will occasionally find it mathematically expedient to imagine an infinitestimally thin source of neutrons S at an interface boundary. Then the interface boundary conditions are modified to read:

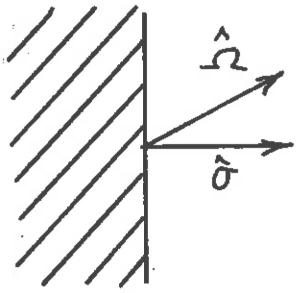
$$\Phi_1(\vec{r}_s,t) = \Phi_2(\vec{r}_s,t)$$

$$\hat{\sigma}\cdot\vec{J}_2(\vec{r}_s,t) - \hat{\sigma}\cdot\vec{J}_1(\vec{r}_s,t) = S(t) \qquad (5\text{-}65)$$

where $\hat{\sigma}$ is the unit normal to the surface.]

(iii) Vacuum boundary: Recall our transport theory boundary condition implying no incoming neutrons was

$$\phi(\vec{r}_s,\hat{\Omega},t) = 0 \quad \text{for } \hat{\Omega}\cdot\hat{\sigma} < 0$$
$$\vec{r}_s \in S$$



Once again, diffusion theory will only be able to approximate this boundary condition. Notice that the boundary condition is given over half of the solid angle (corresponding to incoming neutrons). Hence suppose we again seek to satisfy the transport condition in an "integral" sense by demanding

$$\int_{\substack{2\pi \\ \hat{\sigma}\cdot\hat{\Omega}<0}} d\hat{\Omega}\,\phi(\vec{r}_s,\hat{\Omega},t) = 0 \qquad (5\text{-}67)$$

But in diffusion theory we know

$$\phi(\vec{r},\hat{\Omega},t) \cong \frac{1}{4\pi}\Phi(\vec{r},t) + \frac{3}{4\pi}\vec{J}(\vec{r},t)\cdot\hat{\Omega} \qquad (5\text{-}68)$$

If we integrate this over the solid angle corresponding to incoming neutrons, we find

$$\int_{\substack{2\pi \\ \hat{\sigma}\cdot\hat{\Omega}<0}} d\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) = \frac{1}{4}\Phi(\vec{r},t) - \frac{1}{2}\hat{\sigma}\cdot\vec{J}(\vec{r},t) \equiv J_-(\vec{r},t) \qquad (5\text{-}69)$$

Similarly for outgoing neutrons,

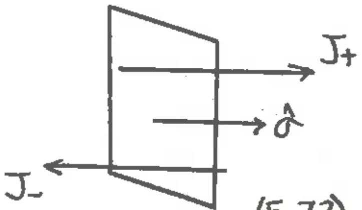
$$\int_{\substack{2\pi \\ \hat{\sigma}\cdot\hat{\Omega}>0}} d\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},t) = \frac{1}{4}\Phi(\vec{r},t) + \frac{1}{2}\hat{\sigma}\cdot\vec{J}(\vec{r},t) \equiv J_+(\vec{r},t) \qquad (5\text{-}70)$$

Here we have defined the partial currents $J_{\pm}(\underline{r},t)$

$$J_{\pm}(\vec{r},t) = \frac{1}{4}\Phi(\vec{r},t) \mp \frac{D}{2}\hat{\sigma}\cdot\nabla\Phi(\vec{r},t) \qquad (5\text{-}71)$$

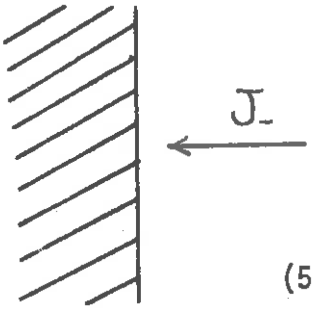
which denote the number of neutrons/sec passing through a unit area normal to $\hat{\sigma}$ from left to right and from right to left, respectively. Note that the net current is just

$$\hat{\sigma}\cdot\vec{J}(\vec{r},t) = J_+(\vec{r},t) - J_-(\vec{r},t)$$



(5-72)

Hence we can see that the integral condition (5-67) is equivalent to the requirement that the inwardly directed partial current $J_-(\vec{r},t)$ vanish on the boundary

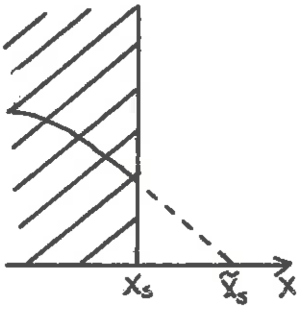


$$J_-(\vec{r}_s,t)=0$$

or

$$\frac{1}{4}\Phi(\vec{r}_s,t)+\frac{D}{2}\hat{\sigma}\cdot\nabla\Phi(\vec{r}_s,t)=0 \tag{5-73}$$

For convenience, consider this boundary condition applied to a one-dimensional geometry with the boundary at $x = x_s$



$$J_-(x_s)=\frac{1}{4}\Phi(x_s)+\frac{D}{2}\frac{d\Phi}{dx}\bigg|_{x_s}=0$$

or

$$\frac{1}{\Phi(x_s)}\frac{d\Phi}{dx}\bigg|_{x_s}=-\frac{1}{2D} \tag{5-74}$$

Notice that this relation implies that if we "extrapolated" the flux linearly beyond the boundary, it would vanish at a point

$$\tilde{x}_s\equiv x_s+2D=x_s+\frac{2}{3}\lambda_{tr} \tag{5-75}$$

For this reason, one frequently replaces the vacuum boundary condition

$$J_-(x_s)=0 \tag{5-76}$$

by the slightly simpler condition

$$\Phi(\tilde{x}_s) = 0 \tag{5-77}$$

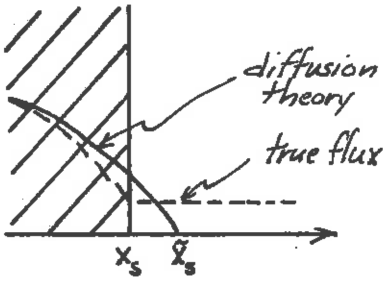
where x_s is referred to as the "extrapolated" boundary. More advanced transport theory calculations of the extrapolated boundary indicate that one should choose

$$\tilde{x}_s = x_s + z_o \tag{5-78}$$

where the "extrapolation length" z_0 is given (for plane geometries) by

$$z_o = 0.7104\ \lambda_{tr} \tag{5-79}$$

It should be remembered that the true flux does <u>not</u> vanish even outside the boundary. The diffusion theory flux is a poor representation of the true flux near the boundary (as we saw earlier, diffusion theory is not valid near a boundary). The boundary conditions we have derived are intended to yield the proper flux only in the <u>interior</u> of the reactor.



E. Summary of the One-Speed Diffusion Model

In summary then, we will describe the neutron flux $\Phi(\vec{r},t)$ by

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a\Phi(\vec{r},t) = S(\vec{r},t) \tag{5-80}$$

with

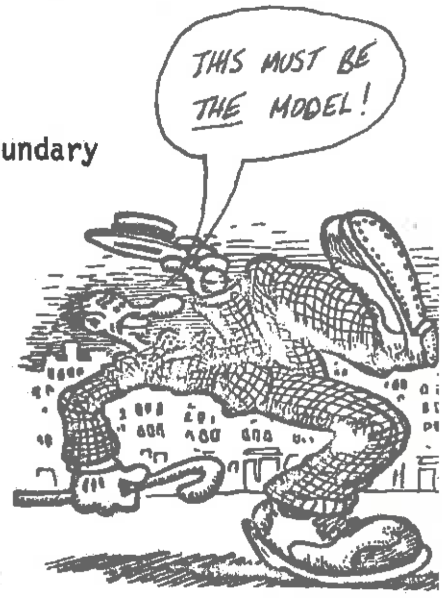
initial conditions: $\Phi(\vec{r},0) = \Phi_o(\vec{r})$

boundary conditions:

(i) infinity: $\Phi(\vec{r},t) < \infty$

(ii) interface: Φ and $\vec{J}$ continuous across boundary

(iii) vacuum: $\Phi(\tilde{r}_s) = 0$ [or $J_-(\vec{r}_s) = 0$]



where

$$D = \lambda_{tr}/3$$

$$\tilde{x}_s = x_s + .7104\ \lambda_{tr}$$

$$\lambda_{tr} = (\Sigma_t - \bar{\mu}_o \Sigma_s)^{-1} \equiv 1/\Sigma_{tr}\ .$$

We now turn our attention to the application of this model to some important problems in nuclear reactor theory. We will first study neutron diffusion in "nonmultiplying" media--i.e., media containing no fissile material. Then we will turn to the study of the neutron flux in fissile material and begin our investigation of nuclear reactor core physics.

II. NEUTRON DIFFUSION IN NON-MULTIPLYING MEDIA

Since we have not yet explicitly included the possibility of fission in our transport or diffusion equations, we will begin by studying the diffusion of neutrons in a nonmultiplying media from a steady-state source:

$$-D\nabla^2\Phi(\vec{r}) + \Sigma_a \Phi(\vec{r}) = S(\vec{r})\ . \tag{5-82}$$

It is useful to divide by -D to rewrite Eq. (5-82) as

$$\nabla^2\Phi(\vec{r}) - \frac{1}{L^2}\Phi(\vec{r}) = -\frac{S(\vec{r})}{D} \tag{5-83}$$

where we have defined

$$L \equiv \sqrt{\frac{D}{\Sigma_a}} \equiv \qquad \text{"neutron diffusion length"}$$

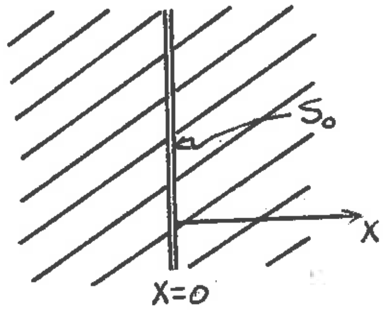
We will later find that L is a measure of how far the neutrons diffuse before they are absorbed.

We will now apply this equation to study neutron diffusion in a variety of different geometries. All of the mathematical techniques we will use are standard schemes used to solve partial differential equation (PDE) boundary value problems and can be found discussed in any text on mathematical physics or applied mathematics.

A. Elementary Solutions of the Diffusion Equation

1. Infinite Planar Source

Consider an infinitely long plane source of neutrons located at the origin plane of an infinite medium emitting S_0 neutrons per second per unit area. In this case, our diffusion equation reduces to the one-dimensional form



$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = -\frac{S(x)}{D} \tag{5-84}$$

where we can mathematically model the source by

$$S(x) = S_o\,\delta(x) \tag{5-85}$$

Hence we just have an inhomogeneous ordinary differential equation (ODE) to solve with a slightly weird source. If one recalls the properites of the Dirac δ-function (see Appendix C), then it becomes clear that if we restrict $x \neq 0$, the source term disappears from (5-84)

$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = 0, \qquad x \neq 0 \tag{5-86}$$

Our approach will be to solve this homogeneous equation for $x \neq 0$ and then use a boundary condition at x = 0 to "fix up these solutions".

To determine this boundary condition, suppose we integrate (5-84) from $0 - \epsilon$ to $0 + \epsilon$ across the source

$$\int_{-\epsilon}^{+\epsilon} dx\, \frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\int_{-\epsilon}^{+\epsilon} dx\,\Phi(x) = -\frac{S_o}{D}\int_{-\epsilon}^{+\epsilon} dx\,\delta(x) \tag{5-87}$$

or

$$\left.\frac{d\Phi}{dx}\right|_{-\epsilon} - \left.\frac{d\Phi}{dx}\right|_{+\epsilon} - 2\epsilon\,\Phi(0) = -\frac{S_o}{D} \tag{5-88}$$

or letting $\epsilon \to 0$,

$$\left.\frac{d\Phi}{dx}\right|_{-\epsilon} - \left.\frac{d\Phi}{dx}\right|_{+\epsilon} = -\frac{S_o}{D} \tag{5-89}$$

If we now recall that $J(x) = -D\, d\Phi/dx$, then we can rewrite this boundary condttion as

$$J(0^+) - J(0^-) = S_0 \tag{5-90}$$

Note that this is the same form we suggested for a source located at an interface on p. 126.

We can use the symmetry of the geometry to simplify this further by noting

$$J(0^+) = -J(0^-) \equiv J(0) \tag{5-91}$$

Hence our boundary condition at the source is just

$$\lim_{x \to 0^+} J(x) = S_0/2 \tag{5-92}$$

This source boundary condition makes sense physically, since it merely says that the net neutron current at the origin on either side must be just 1/2 of the source strength.

We are not through with boundary conditions yet. Since we have a second order derivative, d^2/dx^2, we need another boundary condition. We will use the boundary condition of finite flux as $x \to \infty$.

Hence the mathematical problem to be solved is

$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = 0$$

b.c.: (i) $\lim_{x \to 0^+} -D\frac{d\Phi}{dx} = \frac{S_0}{2}$ (5-93)

(ii) $\lim_{x \to \infty} \Phi(x) < \infty$.

[We will then use symmetry to infer the solution for $x < 0$.]

To solve this equation, we note the general solution

$$\Phi(x) = Ae^{-x/L} + Be^{+x/L} \tag{5-94}$$

Applying the boundary conditions,

$$\text{(ii)} \Rightarrow B = 0$$

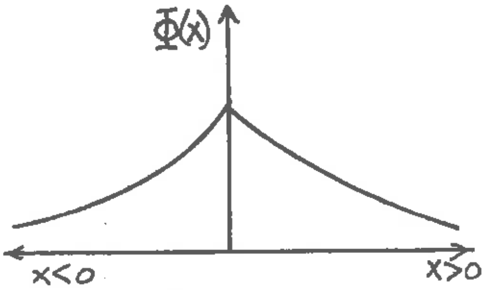
$$\text{(i)} \Rightarrow \lim_{x \to 0} -D\left(-\frac{A}{L}e^{-x/L}\right) = \frac{AD}{L} = \frac{S_0}{2}$$

$$\text{or} \qquad A = \frac{S_0 L}{2D}$$

Hence our solution is

$$\Phi(x) = \frac{S_0 L}{2D} e^{-x/L} \qquad x > 0 \tag{5-95}$$

$$= \frac{S_0 L}{2D} e^{+x/L} \qquad x < 0 \qquad \text{(by symmetry)}$$



Hence the neutron flux falls off exponentially as one moves away from the source plane, with a characteristic decay length of L. As one might expect, the larger L (i.e., the smaller Σ_a), the less the neutron flux is attenuated as we move into the medium.

Notice something rather important here: By integrating the original equation (5-84) over the δ-function source, we have managed to convert our original inhomogeneous equation into a homogeneous equation with a boundary condition at the source. This trick usually works for δ-function sources and vastly simplifies their solution.

The general approach to this problem should also be noted, because we will use it time and time again in solving diffusion theory problems:

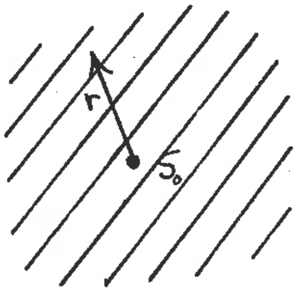
A) Physical Modeling

  1. Write down diffusion equation appropriate for problem.
  2. Figure out boundary conditions.

B) Mathematical solution

  1. Obtain general solution.
  2. Apply boundary conditions.

2. Point Source in an Infinite Medium



Consider an isotropic point source at the origin of an infinite medium emitting S_0 neutrons/sec. Symmetry removes the angular variables and leaves the radial diffusion equation

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\Phi}{dr} - \frac{1}{L^2}\Phi(r) = 0 \qquad r>0 \qquad (5\text{-}96)$$

We will use our previous problem as a guide and seek solutions such that the boundary conditions are

(i) $\lim_{r\to 0} 4\pi r^2 J(r) = S_o$

(ii) $\lim_{r\to\infty} \Phi(r) < \infty$

To determine the general solution, make a variable transformation by letting

$$w(r) \equiv r\Phi(r)$$

Then substituting in

$$\frac{d^2W}{dr^2} - \frac{1}{L^2}w(r) = 0 \Rightarrow w(r) \sim e^{-r/L}, e^{+r/L}$$

Hence the general solution to (5-96) is

$$\Phi(r) = A\frac{e^{-r/L}}{r} + B\frac{e^{+r/L}}{r} . \tag{5-97}$$

Applying the boundary conditions:

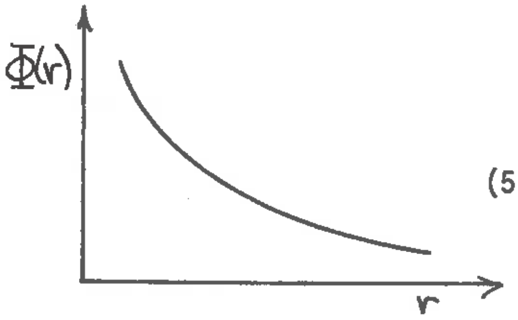
(ii) $\Rightarrow B = 0$

(i) $\Rightarrow \lim\limits_{r\to 0} 4\pi r^2(-DA)\left[-\frac{1}{L}\frac{e^{-r/L}}{r} - \frac{e^{r/L}}{r^2}\right] = S_0$

$$\Rightarrow A = S/4\pi D .$$

Hence the solution is

$$\Phi(r) = \frac{S_0 e^{-r/L}}{4\pi r D} . \tag{5-98}$$



An interesting application of this result is to calculate the mean square distance to absorption in a diffusing media. Note the number of neutrons absorbed between r and r + dr is just

$$\left(\frac{S_0 e^{-r/L}}{4\pi r D}\right)(4\pi r^2 dr)(\Sigma_a) . \tag{5-99}$$

Hence the probabilility that the neutron is absorbed in dr is just

$$p(r)\,dr = \frac{r}{L^2}e^{-r/L}\,dr . \tag{5-100}$$

Thus we can calculate

$$\langle r^2 \rangle = \int_0^\infty dr\, r^2 p(r) = 6L^2 \tag{5-101}$$

Hence, L has the interesting physical interpretation as

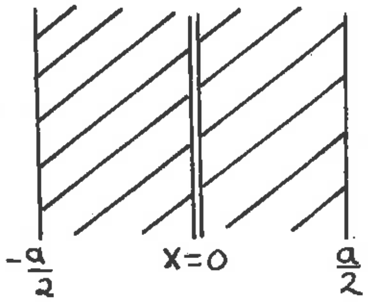
$$L^2 = \frac{1}{6}\langle r^2 \rangle \tag{5-102}$$

--$1/\sqrt{6}$ the rms distance to absorption--that is, it measures how far the neutron will diffuse (on the average) away from the source before it is absorbed.

The cylindrical geometry problem of a line source at the origin of an infinite medium can be worked out in a very similar way. It will be left as an exercise in the problem sets.

3. Finite Plane Geometries

Consider a slab of width a with a plane source at the origin and bounded on both sides by a vacuum. Working from our earlier problems, we know we must solve



$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = 0 \qquad x \neq 0 \tag{5-103}$$

$$\text{(i)} \quad \lim_{x \to 0^\pm} -D\frac{d\Phi}{dx} = \frac{S_0}{2}$$

$$\text{(ii)} \quad \Phi\left(\pm\frac{\tilde{a}}{2}\right) = 0$$

But now we have replaced the boundary condition at infinity by the vacuum boundary condition--in this case, using an extrapolated boundary $\frac{\tilde{a}}{2} = \frac{a}{2} + Z_0$.

Again our general solution is

$$\Phi(x) = Ae^{-x/L} + Be^{x/L} \tag{5-104}$$

Applying b.c. (ii):

$$\Phi\left(\frac{\tilde{a}}{2}\right) = 0 = Ae^{-\tilde{a}/2L} + Be^{+\tilde{a}/2L}$$

$$\Rightarrow B = -Ae^{-\tilde{a}/L}$$

Hence

$$\Phi(x) = A\left[e^{-x/L} - e^{-(\tilde{a}-x)/L}\right].$$

Then b.c. (i) ⇒

$$A = \frac{SL}{2D}\left[1 + e^{-\tilde{a}/L}\right]^{-1}.$$

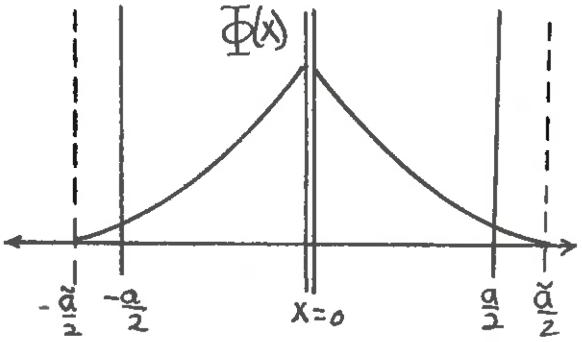
Our final solution is therefore

$$\Phi(x) = \frac{SL}{2D}\,\frac{e^{-x/L} - e^{-(\tilde{a}-x)/L}}{1 + e^{-\tilde{a}/L}} = \frac{SL}{2D}\,\frac{\sinh[(\tilde{a}-2x)/2L]}{\cosh(\tilde{a}/2L)} \tag{5-105}$$

where we have recalled

$$\sinh x = \frac{e^{x} - e^{-x}}{2}$$

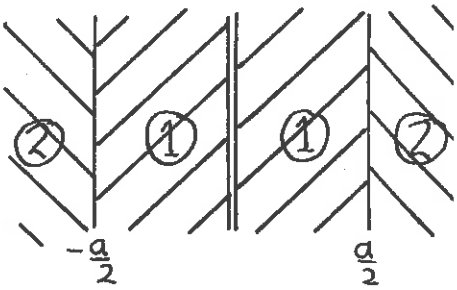
$$\cosh x = \frac{e^{x} + e^{-x}}{2}$$



As a rule of thumb, for finite geometry problems in nonmultiplying media, it is easier to write the general solution directly in terms of hyperbolic functions--e.g.

$$\Phi(x) = A\cosh x/L + B\sinh x/L \tag{5-106}$$

A variant on the above problem is a multi-region problem. Now we must solve a different diffusion equation in each region



$$\frac{d^2\Phi_1}{dx^2} - \frac{1}{L_1^2}\Phi_1(x) = 0, \qquad 0<x<\frac{a}{2}$$

$$\frac{d^2\Phi_2}{dx^2} - \frac{1}{L_2^2}\Phi_2(x) = 0, \qquad \frac{a}{2}<x<\infty. \tag{5-107}$$

We need lots of boundary conditions now. We can use our earlier ones:

(i) $\lim_{x\to 0^+} J_1(x) = S_0/2$

(ii) $\Phi_2(x) < \infty$ as $x \to \infty$

In addition, we now need the interface conditions

(iii) $\Phi_1(\frac{a}{2}) = \Phi_2(\frac{a}{2})$

(iv) $D_1 \left.\frac{d\Phi_1}{dx}\right|_{\frac{a}{2}} = D_2 \left.\frac{d\Phi_2}{dx}\right|_{\frac{a}{2}}$

Using our earlier work as a guide, we seek the general solutions as

$$\Phi_1(x) = A_1\cosh x/L_1 + B_1\sinh x/L_1 \qquad \text{in region ①}$$

$$\Phi_2(x) = A_2 e^{-x/L_2} + B_2 e^{+x/L_2} \qquad \text{in region ②} \tag{5-108}$$

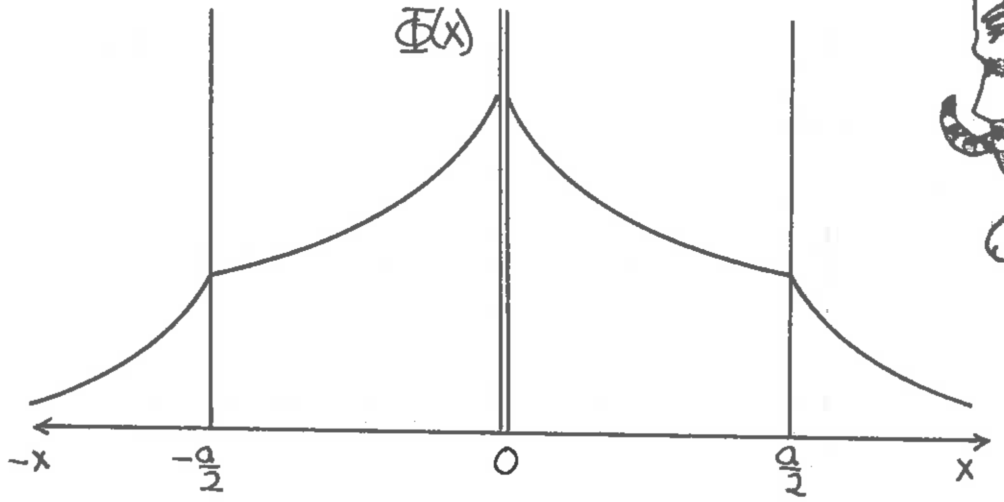
and apply the boundary conditions to find (after a bit of algebra)

$$B_2 = 0, \quad B_1 = -SL_1/2D_1$$

$$A_1 = \frac{SL_1}{2D_1}\,\frac{D_1L_2\cosh(a/2L_1) + D_2L_1\sinh(a/2L_1)}{D_2L_1\cosh(a/2L_2) + D_1L_2\sinh(a/2L_1)}$$

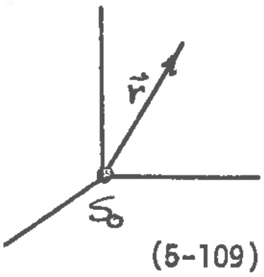
$$A_2 = \frac{SL_1L_2}{2}\,\frac{e^{a/2L_2}}{D_2L_1\cosh(a/2L_2) + D_1L_2\sinh(a/2L_1)}$$

The form of this solution is sketched below:



One can continue this game of solving the diffusion equation in various geometries indefinitely. As we mentioned before, it is just an exercise in partial differential equations (sometimes even ordinary differential equations) with very little in the way of novel physics arising from problem to problem. Hence we will bypass further examples in favor of moving directly to more general problems.

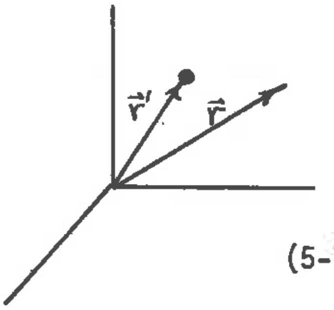
4. General Diffusion Problems



Recall that the neutron flux resulting from an isotropic point source of strength S_0 located at the origin was found to be

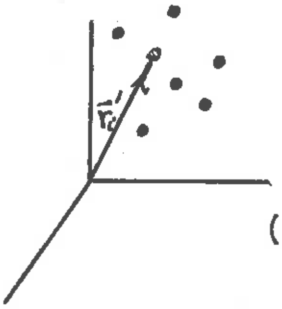
$$\Phi(\vec{r}) = \frac{S_0 e^{-r/L}}{4\pi D r} \qquad (5\text{-}109)$$

Suppose this source was located at the point $\vec{r}'$ instead. Then the flux would be



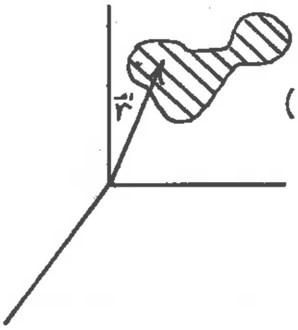
$$\Phi(\vec{r}) = S_0 \frac{e^{-|\vec{r}-\vec{r}'|/L}}{4\pi D|\vec{r}-\vec{r}'|} . \tag{5-110}$$

Now suppose we have several point sources at positions $\vec{r}_i'$, each of strength S_i. Then



$$\Phi(\vec{r}) = \sum_i \frac{S_i e^{-|\vec{r}-\vec{r}_i'|/L}}{4\pi D|\vec{r}-\vec{r}_i'|} . \tag{5-111}$$

Finally, suppose we have an arbitrary distribution of sources of strength $S(\vec{r}')\, d^3r'$. Then the flux resulting from this distributed source is just



$$\Phi(\vec{r}) = \int d^3r' \frac{e^{-|\vec{r}-\vec{r}'|/L}}{4\pi D|\vec{r}-\vec{r}'|} S(\vec{r}') . \tag{5-112}$$

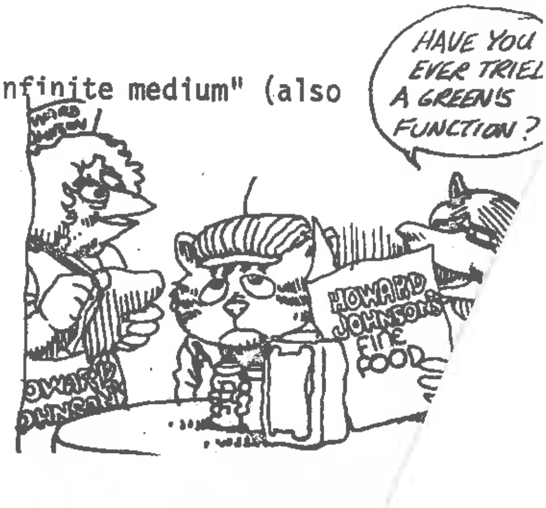
This is frequently rewritten as

$$\Phi(\vec{r}) = \int d^3r' \, G_{pt}(\vec{r},\vec{r}') \, S(\vec{r}') \tag{5-113}$$

where

$$G_{pt}(\vec{r},\vec{r}') \equiv \frac{e^{-|\vec{r}-\vec{r}'|/L}}{4\pi D|\vec{r}-\vec{r}'|} . \tag{5-114}$$

is known as the "point diffusion kernel for an infinite medium" (also called the "infinite medium Green's function").



[Note: A function K(x,x') in an integral

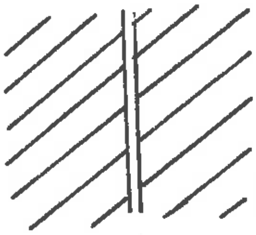
$$\int dx'\, K(x,x')\, f(x') \tag{5-115}$$

is known as a "kernel". As an example, $\Sigma_s(E'\rightarrow E, \hat{\Omega}'\rightarrow\hat{\Omega})$ in

$$\int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \Sigma_s(E'\rightarrow E, \hat{\Omega}'\rightarrow\hat{\Omega})\, \phi(\vec{r}, E', \hat{\Omega}', t) \tag{5-116}$$

is known as the "scattering kernel".]

As a second example of such kernels, consider the flux resulting from a plane source at the origin



$$\Phi(x) = \frac{SL}{2D}\, e^{-|x|/L} \,. \tag{5-117}$$

If this had been located at x',

$$\Phi(x) = \frac{SL}{2D}\, e^{-|x-x'|/L} \tag{5-118}$$

Hence in general, for S → S(x') dx', we find

$$\begin{aligned} \Phi(x) &= \int_{-\infty}^{\infty} dx' \left[\frac{L}{2D}\, e^{-|x-x'|/L}\right] S(x') \\ &= \int_{-\infty}^{\infty} dx'\, G_{pl}(x,x')\, S(x') \end{aligned} \tag{5-119}$$

where we have identified the "plane source kernel"

$$G_{pl}(x,x') = \frac{L}{2D}\, e^{-|x-x'|/L} \tag{5-120}$$

A Brief Digression on the Subject of Inhomogeneous Equations:

Consider a general inhomogeneous equation of the form

$$M\phi(x) = f(x) \tag{5-121}$$

where M is a differential operator--e.g.

$$M = \frac{d^2}{dx^2} - \frac{1}{L^2} \tag{5-122}$$

There are several standard ways to solve such an equation:

a.) Green's function methods: In this technique we first construct the solution to

$$M\phi_g(x) = \delta(x-x') \tag{5-123}$$

Then if we call $\phi_g(x) = G(x,x')$ the "Green's function" for the operator M, we find that the general solution to (5-121) is just

$$\phi(x) = \int dx'\, G(x,x')\, f(x') \tag{5-124}$$

[Proof:

$$M\phi = \int dx' \underbrace{MG(x,x')}_{\delta(x-x')} f(x') = f(x) \quad]$$

Example:

$$M\phi = \left(\frac{d^2}{dx^2} - \frac{1}{L^2}\right)\phi(x) = -\frac{S(x)}{D} \tag{5-125}$$

Now define G by

$$\frac{d^2G}{dx^2} - \frac{1}{L^2}G(x,x') = -\frac{\delta(x-x')}{D} \qquad (5\text{-}126)$$

But we have just solved this for

$$G(x,x') = G_{p\ell}(x,x') = \frac{L}{2D}e^{-|x-x'|/L} \qquad (5\text{-}127)$$

Hence the plane source kernel is just the Green's function for this operator, and we find

$$\phi(x) = \int_{-\infty}^{\infty} dx'\, G_{p\ell}(x,x')\, S(x') \qquad (5\text{-}128)$$

b.) Consider again $M\phi(x) = f(x)$.

Now suppose we can find a "homogeneous" solution

$$M\phi_{homo}(x) = 0 \qquad (5\text{-}129)$$

and a "particular" solution

$$M\phi_{part.}(x) = f(x) \qquad (5\text{-}130)$$

(which doesn't have to satsify the boundary conditions, incidently). Then we seek a general solution

$$\phi(x) = \phi_{homo}(x) + \phi_{part.}(x) \qquad (5\text{-}131)$$

and apply boundary conditions to determine the unknown coefficients in $\phi_{homo}(x)$. Usually for this approach to be of use, one must be able to guess $\phi_{part}(x)$ "by inspection". Otherwise the Green's function technique or the method described below in (c) are more convenient.

Example: Consider a constant source $S(x) = S_o$. Then

$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = -\frac{S_o}{D}$$

$$\text{b.c.} \quad (i) \lim_{x\to 0} J(x) = 0 \tag{5-132}$$

$$(ii) \lim_{x\to\infty} \Phi(x) < \infty$$

The homogeneous solution is

$$\Phi_{homo}(x) = Ae^{-x/L} + Be^{x/L} \tag{5-133}$$

The particular solution is

$$\Phi_{part}(x) = \frac{SL^2}{D} \tag{5-134}$$

Hence we will seek a general solution

$$\Phi(x) = Ae^{-x/L} + Be^{x/L} + SL^2/D \tag{5-135}$$

Now applying the b.c.:

(ii) $\Phi < \infty \Rightarrow B = 0$

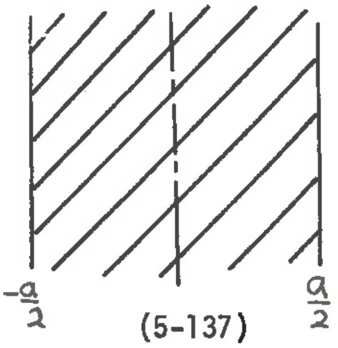
(i) $J(0) = 0 \Rightarrow A = 0$

Hence

$$\Phi(x) = \frac{SL^2}{D} \tag{5-136}$$

c.) Eigenfunction Expansion Method: We now consider the eigenfunction expansion method of solving inhomogeneous problems. We will introduce this scheme by considering an example:

Example: Consider a symmetric, distributed source in a finite slab:



$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = -\frac{S(x)}{D} \qquad (5\text{-}137)$$

We will take our usual vacuum boundary conditions

(i) $\Phi(\tilde{a}/2) = 0$

(ii) $\Phi(-\tilde{a}/2) = 0$

The symmetry, S(x) = S(-x), is chosen for convenience. Otherwise S(x) will be assumed to be arbitrary.

Our approach to solving this problem may at first seem a bit irrelevant. We begin by considering a homogeneous problem very similar to the above:

$$\frac{d^2\varphi}{dx^2} + B^2\varphi(x) = 0$$

$$\varphi\left(\frac{\tilde{a}}{2}\right) = 0 = \varphi\left(-\frac{\tilde{a}}{2}\right), \quad \varphi(x) \text{ even in } x \qquad (5\text{-}138)$$

Here, B^2 is arbitrary for the moment. Now let's solve this associated homogeneous problem by noting the general solution

$$\varphi(x) = A\cos Bx + C\sin Bx. \qquad (5\text{-}139)$$

If we want symmetric solutions, we can immediately set C = 0. Hence

$$\varphi(x) = A\cos Bx. \qquad (5\text{-}140)$$

Now applying the b.c. demands

$$\varphi\left(\pm\frac{\tilde{a}}{2}\right) = A\cos\left(\frac{B\tilde{a}}{2}\right) = 0 \qquad (5\text{-}141)$$

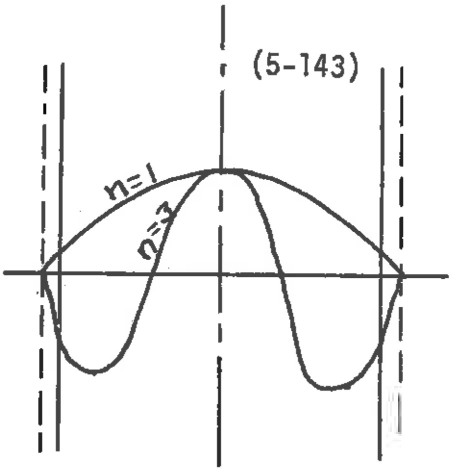
But how? Certainly A ≠ 0 since then we would have the "trivial" solution $\varphi(x) \equiv 0$. Instead we must fix B. But lots of values of B will work--indeed, any

$$B = B_n \equiv \frac{n\pi}{\tilde{a}} \qquad \text{for any odd } n = 1,3,5,\ldots \qquad (5\text{-}142)$$

Hence our homogeneous problem can be solved only for certain values of the parameter B. One refers to these as

$$B_n = \frac{n\pi}{\tilde{a}},\ n=1,3,5,\ldots \qquad \text{"eigenvalues"}$$

$$\varphi_n(x) = A_n \cos\frac{n\pi x}{\tilde{a}} \qquad \text{"eigenfunctions"} \qquad (5\text{-}143)$$



In acoustics, these are called the "normal modes" or harmonics of the system, and this terminology is frequently carried over to reactor analysis. Notice that the A_n are still undetermined. These can be fixed in a number of ways. For now we will just set them all equal to unity for convenience.

So now this auxiliary problem has given us an infinite set of solutions, $\varphi_n(x)$. What good are they? Well, they have a couple of very useful properties:

Orthogonality: Note that

$$\int_{-\tilde{a}/2}^{\tilde{a}/2} \varphi_m(x)\varphi_n(x)\,dx = \int_{-\tilde{a}/2}^{\tilde{a}/2} \cos\frac{m\pi x}{\tilde{a}} \cos\frac{n\pi x}{\tilde{a}}\,dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{\tilde{a}}{2} & \text{if } m = n \end{cases} \tag{5-144}$$

This property is known as "orthogonality" and proves to be of very considerable usefulness, as we will see in a moment.

Completeness: The eigenfunctions $\varphi_n(x)$ form a "complete set" in the sense that any "well-behaved" symmetric function can be expanded in terms of the $\varphi_n(x)$

$$f(x) = \sum_{n \text{ odd}} c_n \varphi_n(x)\,. \tag{5-145}$$

But what are the c_n? Here is where we use orthogonality. Multiply (5-145) by $\varphi_m(x)$ and integrate over x:

$$\begin{aligned} \int_{\tilde{a}/2}^{-\tilde{a}/2} dx\,\varphi_m(x) f(x) &= \sum_{\substack{n=1 \\ \text{odd}}}^{\infty} c_n \int_{-\tilde{a}/2}^{\tilde{a}/2} dx\,\varphi_m(x)\varphi_n(x) = c_m \int_{-\tilde{a}/2}^{\tilde{a}/2} dx\,\varphi_m^2(x) \\ &= c_m \int_{-\tilde{a}/2}^{\tilde{a}/2} dx \cos^2\frac{m\pi x}{\tilde{a}} = c_m\left(\frac{\tilde{a}}{2}\right) \end{aligned} \tag{5-146}$$

Hence we find

$$c_m = \frac{2}{\tilde{a}} \int_{-\tilde{a}/2}^{\tilde{a}/2} dx\, f(x) \cos\frac{m\pi x}{\tilde{a}} \tag{5-147}$$

[It might be noted that this particular example of eigenfunctions corresponds to a Fourier series expansion.]

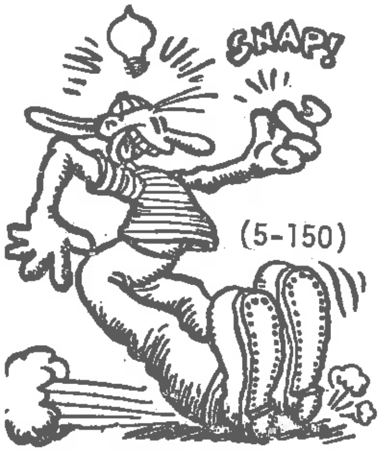
So much for the auxiliary problem. We will now use these eigenfunctions to solve our original problem (5-137). Expand

$$\Phi(x) = \sum_n A_n \varphi_n(x)$$

$$S(x) = \sum_n \Delta_n \varphi_n(x) \tag{5-148}$$

Notice that since S(x) is given, we can use (5-147) to evaluate the Δ_n; but of course, $\Phi(x)$ is unknown, so (5-147) is useless in determining A_n. But that is just what we can use the original equation (5-137) to do. Substitute (5-148) into (5-137) to find

$$\sum_n A_n \left[\frac{d^2\varphi_n}{dx^2} - \frac{1}{L^2}\varphi_n\right] = -\frac{1}{D}\sum_n \Delta_n \varphi_n \tag{5-149}$$



But from Eq. (5-138) we know

$$\frac{d^2\varphi_n}{dx^2} = -B_n^2 \varphi_n(x) \tag{5-150}$$

Hence

$$\sum_n A_n \left(B_n^2 + \frac{1}{L^2}\right)\varphi_n = \frac{1}{D}\sum_n \Delta_n \varphi_n \tag{5-151}$$

Now multiply by $\varphi_m(x)$ and integrate, using orthogonality to find

$$A_n = \frac{S_n/D}{B_n^2 + 1/L^2} = \frac{S_n/\Sigma_a}{1 + L^2 B_n^2} \tag{5-152}$$

Thus we find

$$\Phi(x) = \frac{1}{\Sigma_a}\sum_n \frac{\Delta_n}{1 + L^2 B_n^2}\cos\frac{n\pi x}{a} \tag{5-153}$$

where

$$\Delta_n = \frac{2}{\tilde{a}}\int_{-\tilde{a}/2}^{\tilde{a}/2} dx\, f(x)\, \cos\frac{n\pi x}{\tilde{a}} \qquad (5\text{-}154)$$

Now notice something: If we substituted Δ_n into our solution and rearrange it a bit, we find

$$\begin{aligned}\Phi(x) &= \int_{-\tilde{a}/2}^{\tilde{a}/2} dx' \left[\frac{2}{\tilde{a}\Sigma_a}\sum_{n}\frac{\phi_n(x)\phi_n(x')}{1+L^2B_n^2}\right] S(x') \\ &= \int_{-\tilde{a}/2}^{\tilde{a}/2} dx'\, G_{pl}(x,x')\, S(x').\end{aligned} \qquad (5\text{-}155)$$

Hence we have found a representation of the Green's function in terms of an eigenfunction expansion:

$$G_{pl}(x,x') = \frac{2}{\tilde{a}\Sigma_a}\sum_{\substack{n \\ \text{odd}}}\frac{\phi_n(x)\phi_n(x')}{1+L^2B_n^2}\,. \qquad (5\text{-}156)$$

This intimate relationship between Green's functions and eigenfunction expansions in a very general result, as we have demonstrated in Appendix E.

B. Numerical Methods

1. Introduction

Thus far we have confined our attention to neutron diffusion in homogeneous, uniform media, since in this case the one-speed diffusion equation could be solved analytically. However in any realistic reactor calculation, the heterogeneous nature of the core (including fuel, clad, moderator, structure, control, and so on) must be taken into account. This complexity immediately forces one to discard analytical methods in favor of a direct numerical solution of the diffusion equation. The procedure is to rewrite the differential diffusion equation in finite difference form, and then to solve the resulting system of difference equations on a computer.

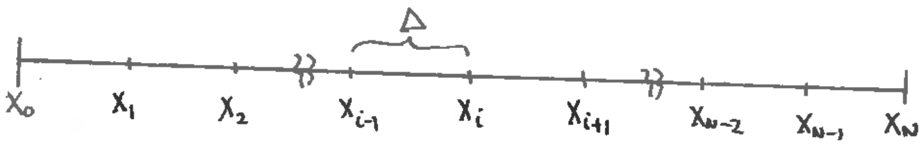
It is perhaps easiest to illustrate this approach by a very simple example (one sufficiently simple, in fact, that it could be solved analytically): Suppose we wish to solve

$$-D\frac{d^2\Phi}{dx^2} + \Sigma_a \Phi(x) = S(x) \qquad (5\text{-}157)$$

subject to the usual boundary conditions:

$$\Phi(0) = \Phi(a) = 0$$

We first discretize the spatial variable x by choosing a set of N+1 discrete points (equally spaced a distance Δ apart for convenience)



We now want to rewrite Eq. (5-157) at each of these discrete points x_i. But to do so, we need an approximation for $\frac{d^2\Phi}{dx^2}$. Suppose we Taylor expand:

$$\Phi_{i+1} \equiv \Phi(x_{i+1}) = \Phi_i + \Delta \left.\frac{d\Phi}{dx}\right|_i + \frac{\Delta^2}{2} \left.\frac{d^2\Phi}{dx^2}\right|_i + \cdots$$

$$\Phi_{i-1} \equiv \Phi(x_{i-1}) = \Phi_i - \Delta \left.\frac{d\Phi}{dx}\right|_i + \frac{\Delta^2}{2} \left.\frac{d^2\Phi}{dx^2}\right|_i - \cdots \tag{5-158}$$

If we add these expressions, we find

$$\left.\frac{d^2\Phi}{dx^2}\right|_i \cong \frac{\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}}{\Delta^2} \tag{5-159}$$

to within order Δ^2. Hence, if Δ is chosen sufficiently small, this "3 point central difference formula" should be a reasonable approximation to the value of $\frac{d^2\Phi}{dx^2}$ at the point x_i.

If we now use this difference formula to write Eq. (5-157) at any "mesh point" x_i, we find

$$-D\left(\frac{\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}}{\Delta^2}\right) + \Sigma_a \Phi_i = S_i, \quad i = 1, 2, \cdots \tag{5-160}$$

where again we have defined $S_i \equiv S(x_i)$. We can rearrange this "difference" equation to rewrite it as

$$\underbrace{-\frac{D}{\Delta^2}}_{a_{i,i-1}} \Phi_{i-1} + \underbrace{\left(\frac{2D}{\Delta^2} + \Sigma_a\right)}_{a_{i,i}} \Phi_i \underbrace{- \frac{D}{\Delta^2}}_{a_{i,i+1}} \Phi_{i+1} = S_i \tag{5-161}$$

or

$$a_{i,i-1}\Phi_i + a_{i,i}\Phi_i + a_{i,i+1}\Phi_{i+1} = S_i \qquad (5\text{-}162)$$

$$i = 1, \ldots, N-1$$

Hence we now have reduced Eq. (5-157) to a set of N-1 algebraic equations for N+1 unknowns $(\Phi_0, \Phi_1, \cdots, \Phi_N)$. If we add on the boundary conditions at either end, say $\Phi_0 = 0,\ \Phi_N = 0$, we can now imagine solving (or imagine the computer solving) this set of algebraic equations.

This very simple example illustrates the two essential tasks involved in the numerical solution of the diffusion equation: first, the derivation of the corresponding difference equations, and second, the formulation of a suitable algorithm for solving these equations on a digital computer. The methods used will vary from problem to problem. For example, whereas a direct solution of the difference equations (e.g., Eq. (5-162) is possible for one-dimensional problems, iterative methods are required for two- and three-dimensional problems. Furthermore, one generally desires to work with non-uniform meshes in reactor calculations, to take account of the fact that the neutron flux may very much more rapidly in certain regions than in others.

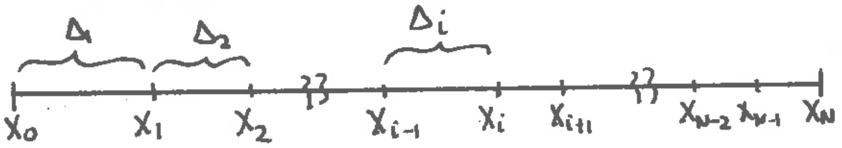
In this section, we will illustrate several of the techniques that are commonly applied in reactor analysis to the derivation and solution of difference equations. However, just as in our earlier study of analytical techniques, we do not intend this presentation to be a detailed presentation of numerical methods in nuclear reactor calculations--but instead we refer the interested reader to the existing literature on this topic.

2. Derivation of Difference Equations for One-Dimensional Diffusion Problems

We will now consider the general one-dimensional diffusion equation

$$-\frac{d}{dx}D(x)\frac{d\Phi}{dx}+\Sigma_a(x)\Phi(x)=S(x) \tag{5-163}$$

subject to boundary or interface conditions which we will leave arbitrary for the present. Once again we will set up our discrete spatial "mesh"



where x_0, x_1, . . .are the "mesh points", while the distance between mesh points--the "mesh spacing" is

$$\Delta_i \equiv x_i - x_{i-1} \tag{5-164}$$

[Notice we have now generalized our notation to allow for a non-uniform mesh spacing Δ_i.]

There are a variety of schemes which can be used to generate difference equations. These include

(i) Taylor series methods: We have already seen an example of this scheme when we derived our earlier central difference formula for $\frac{d^2\Phi}{dx^2}$.

(ii) Integration over the mesh interval: The essential idea here is to integrate the original differential equation (5-163) over an arbitrary mesh interval, and then to suitably approximate these integrals using finite difference formulas (occasionally after integrating by parts).

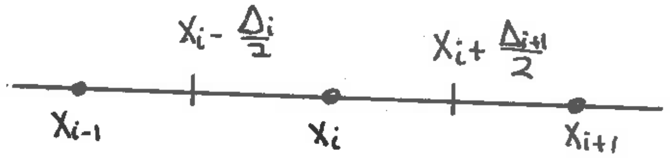
(iii) Variational methods: A variational functional can be used to determine difference equations by choosing appropriate trial functions for the flux (say, as a set of disjoint step functions), and then determining the stationary point of the resulting reduced functional.

(iv) Asymmetrical finite difference network method: This method uses geometrical definitions of the finite difference coefficients to derive formulas for either regular or irregular mesh networks.

All of these schemes lead to a finite difference representation of the derivative term of the general form:

$$\frac{d}{dx}D(x)\frac{d\Phi}{dx}\Big|_i \cong \left(\frac{D_i+D_{i-1}}{2\Delta_i}\right)\Phi_{i-1} - \left(\frac{D_{i+1}+D_i}{2\Delta_{i+1}} + \frac{D_i+D_{i-1}}{2\Delta_i}\right)\Phi_i + \left(\frac{D_{i+1}+D_i}{2\Delta_i}\right)\Phi_{i+1} \qquad (5\text{-}165)$$

For example, consider the integration over mesh interval scheme. Here we want to integrate each term in Eq. (5-163) over the mesh interval $x_i - \frac{\Delta_i}{2} < x < x_i + \frac{\Delta_i}{2}$



For example, we can approximate the simple integrals by midpoint values

$$\int_{x_i-\frac{\Delta_i}{2}}^{x_i+\frac{\Delta_{i+1}}{2}} dx\, \Sigma_a(x)\,\Phi(x) \cong \left(\frac{\Delta_i+\Delta_{i+1}}{2}\right)\underbrace{\Sigma_a(x_i)\,\Phi(x_i)}_{\Sigma_{a_i}\,\Phi_i}, \qquad (5\text{-}166)$$

and similarly

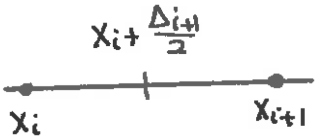
$$\int_{x_i-\frac{\Delta_i}{2}}^{x_i+\frac{\Delta_{i+1}}{2}} dx\, S(x) \cong \left(\frac{\Delta_i+\Delta_{i+1}}{2}\right)\underbrace{S(x_i)}_{S_i} \qquad (5\text{-}167)$$

The derivative term is a bit more complex

$$\int_{x_i-\frac{\Delta_i}{2}}^{x_i+\frac{\Delta_{i+1}}{2}} dx\, \frac{d}{dx} D(x)\frac{d\Phi}{dx} = D(x)\frac{d\Phi}{dx}\Bigg|_{x_i-\frac{\Delta_i}{2}}^{x_i+\frac{\Delta_{i+1}}{2}} \qquad (5\text{-}168)$$

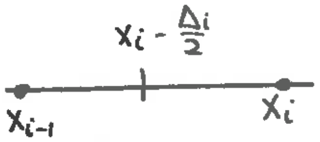
Now to handle $\frac{d\Phi}{dx}$, we can use a simple two-point difference formula (which can be derived by subtracting Eqs. (5-158):

$$\frac{d\Phi}{dx}\bigg|_{x_i+\frac{\Delta_{i+1}}{2}} \cong \frac{\Phi_{i+1}-\Phi_i}{\Delta_{i+1}}$$



(5-169)

$$\frac{d\Phi}{dx}\bigg|_{x_i-\frac{\Delta_i}{2}} \cong \frac{\Phi_i-\Phi_{i-1}}{\Delta_i}$$



Furthermore, we will use a centered average for D:

$$D\left(x_i+\frac{\Delta_{i+1}}{2}\right) = \frac{D_{i+1}+D_i}{2}, \quad D\left(x_i-\frac{\Delta_i}{2}\right) = \frac{D_{i-1}+D_i}{2} \qquad (5\text{-}170)$$

Then we find, using Eqs. (5-168 - 170):

$$\int_{x_i-\frac{\Delta_i}{2}}^{x_i+\frac{\Delta_{i+1}}{2}} dx\, \frac{d}{dx} D(x)\frac{d\Phi}{dx} \cong \left(\frac{D_i+D_{i-1}}{2\Delta_i}\right)\Phi_{i-1} - \left(\frac{D_{i+1}+D_i}{2\Delta_{i+1}} + \frac{D_{i-1}+D_i}{2\Delta_i}\right)\Phi_i + \left(\frac{D_i+D_{i+1}}{2\Delta_{i+1}}\right)\Phi_{i+1} \qquad (5\text{-}171)$$

If we now combine Eqs. (5-166), (5-167) and (5-179), we arrive at a set of difference equations very similar to our earlier results

$$a_{i,i-1}\Phi_{i-1} + a_{i,i}\Phi_i + a_{i,i-1}\Phi_{i-1} = S_i \tag{5-172}$$

wheee

$$\begin{aligned} a_{i,i-1} &= -\left(\frac{D_i + D_{i-1}}{\Delta_i}\right)\frac{1}{\Delta_i + \Delta_{i+1}} \ , \\ a_{i,i} &= \Sigma_{a_i} + \left(\frac{D_{i+1}+D_i}{\Delta_{i+1}} + \frac{D_{i-1}+D_i}{\Delta_i}\right)\frac{1}{\Delta_i + \Delta_{i+1}} \ , \\ a_{i,i+1} &= -\left(\frac{D_{i+1}+D_i}{\Delta_i}\right)\frac{1}{\Delta_i + \Delta_{i+1}} \ . \end{aligned} \tag{5-173}$$

Hence we once again have arrived at a set of N-1 three-point difference equations for the unknown discretized fluxes, $\Phi_o, \Phi_1, \cdots \Phi_N$. In the particular case in which the mesh size Δ_i is constant, say Δ, and the coefficients D(x) and $\Sigma_a(x)$ do not depend upon x, we return to our earlier results derived via a Taylor series expansion.

Our final task is to append to these equations two additional equations taking into account the boundary conditions. Of course, we could just simply use the vacuum extrapolated boundary conditions, $\Phi_o = 0 = \Phi_N$ as before (taking care to place the mesh points x_0 and x_N on these extrapolated boundaries). More general boundary conditions (such as nonreentrant current or such) can be developed by taking the final two difference equations in the set as

$$a_{0,0}\Phi_0 + a_{0,1}\Phi_1 = S_0$$

and

$$a_{N,N-1}\Phi_{N-1} + a_{N,N}\Phi_N = S_N \ . \tag{5-174}$$

Such sets of three-point difference equations are characteristic of one-dimensional diffusion problems (indeed, of any ordinary differential equation of second order). The coefficients a_{ij} will depend upon the scheme used to derive the difference equations. Fortunately, if the mesh spacing Δ is small, these differences will be insignificant in actual calculations. As a rule of thumb, one generally choses the mesh spacing to be comparable to a neutron mean free path (unless the flux is known to be very slowly varying within a region, in which case a coarser mesh can be used.)

Similar three-point differences equations will also arise in curvilinear geometries with one-dimensional symmetry. For example, in cylindrical coördinates, the diffusion equation becomes

$$-D\left[\frac{d^2\Phi}{dr^2} + \frac{1}{r}\frac{d\Phi}{dr}\right] + \Sigma_a \Phi = S \tag{5-175}$$

while in spherical coordinates, we find

$$-D\left[\frac{d^2\Phi}{dr^2} + \frac{2}{r}\frac{d\Phi}{dr}\right] + \Sigma_a \Phi = S \tag{5-176}$$

Hence, we can derive difference equations corresponding to these geometries, using either of the earlier techniques, to find for uniform mesh spacing

$$a_{i,i-1}\Phi_{i-1} + a_{i,i}\Phi_i + a_{i,i+1}\Phi_{i+1} = S_i \tag{5-177}$$

where now

$$a_{i,i-1} = -\frac{D}{\Delta^2}\left[1 - \frac{C}{2i-1}\right]$$

$$a_{i,i} = \frac{2D}{\Delta^2} + \Sigma_a \qquad (5\text{-}178)$$

$$a_{i,i+1} = -\frac{D}{\Delta^2}\left[1 + \frac{C}{2i+1}\right]$$

where

$$C = \begin{cases} 0 & \text{plane geometry} \\ 1 & \text{cylindrical geometry} \\ 2 & \text{spherical geometry} \end{cases}$$

The extension to non-uniform media and mesh intervals is left as an exercise for the reader.

3. Solution of Three-Point Difference Equations

Suppose we have devloped an appropriate set of difference equations similar to Eq. (5-162). Our next task is to solve this set for the discretized fluxes, Φ_i . To be more explicit, let's first write out the equations in detail:

$$\begin{aligned}
a_{00}\Phi_0 + a_{01}\Phi_1 \qquad\qquad\qquad\qquad &= S_0 \\
a_{10}\Phi_0 + a_{11}\Phi_1 + a_{12}\Phi_2 \qquad\qquad &= S_1 \qquad (5\text{-}179) \\
a_{21}\Phi_1 + a_{22}\Phi_2 + a_{23}\Phi_3 &= S_2 \\
&\vdots \\
a_{N,N-1}\Phi_{N-1} + a_{NN}\Phi_N &= S_N
\end{aligned}$$

How do we solve such a set of equations? Easy. First solve for

$$\Phi_0 = -\frac{a_{01}}{a_{00}}\Phi_1 + S_0 \tag{5-180}$$

Now plug this in the second equation

$$a_{10}\left[-\frac{a_{01}}{a_{00}}\Phi_1 + S_0\right] + a_{11}\Phi_1 + a_{12}\Phi_2 = S_1 \tag{5-181}$$

and solve for

$$\Phi_1 = \frac{-a_{12}\Phi_2 + S_1 - a_{10}S_0}{a_{11} - \dfrac{a_{10}a_{01}}{a_{00}}} \tag{5-182}$$

Next, plug this into the third equation to eliminate Φ_1 in terms of Φ_2 --and so on, until we work down to

$$a_{N,N-1}\Phi_{N-1} + a_{N,N}\Phi_N = S_N \tag{5-183}$$

At this point we have Φ_{N-1} in terms of Φ_N. Hence we can solve for Φ_N. Then we can work back up the set to find $\Phi_{N-1}, \Phi_{N-2}, \dots \Phi_0$.

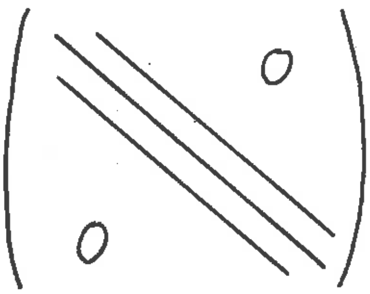
This systematic scheme for solving algebraic equations is called "Gaussian elimination". We can formalize this scheme a bit if we rewrite the difference equations in matrix form

$$\begin{pmatrix} a_{00} & a_{01} & 0 & 0 & \cdots & \\ a_{10} & a_{11} & a_{12} & 0 & \cdots & \\ 0 & a_{21} & a_{22} & a_{23} & \cdots & \\ \vdots & \vdots & \vdots & \vdots & & \\ & & & & a_{N,N-1} & a_{N,N} \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{pmatrix} = \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ \vdots \\ S_N \end{pmatrix} \qquad (5\text{-}184)$$

or

$$\underline{\underline{A}}\,\underline{\Phi} = \underline{S} \qquad (5\text{-}185)$$

Hence the solution of this set of equations corresponds to inverting the matrix $\underline{\underline{A}}$. Fortunately, for one-dimensional problems this matrix is particularly simple--tridiagonal. It can be directly inverted using Gaussian elimination--just the sequence of steps we followed on the previous pages.



[As we will see, Gaussian elimination proves impractical for more complicated matrices because of the storage requirements it places upon the computer.]

To see how this works in matrix form, first divide the first row by a_{00}

$$\begin{pmatrix} 1 & \frac{a_{01}}{a_{00}} & 0 & 0 & \cdots \\ a_{10} & a_{11} & a_{12} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} S_0/a_{00} \\ S_1 \\ \vdots \end{pmatrix} \qquad (5\text{-}186)$$

Next, multiply the first row by $-a_{10}$ and add it to the second row

$$\begin{pmatrix} 1 & \frac{a_{01}}{a_{00}} & 0 & \cdots \\ 0 & \left(a_{11} - \frac{a_{10}a_{01}}{a_{00}}\right) & a_{12} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} \frac{S_0}{a_{00}} \\ S_1 - \frac{a_{10}}{a_{00}} S_0 \\ \vdots \end{pmatrix} \qquad (5\text{-}187)$$

Now divide the second row by the diagonal element

$$\begin{pmatrix} 1 & \frac{a_{01}}{a_{00}} & 0 & \cdots \\ 0 & 1 & \dfrac{a_{12}}{a_{11} - \frac{a_{10}a_{01}}{a_{00}}} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} \frac{S_0}{a_{00}} \\ \dfrac{S_1 - \frac{a_{10}}{a_{00}} S_0}{a_{11} - \frac{a_{10}a_{01}}{a_{00}}} \\ \vdots \end{pmatrix} \qquad (5\text{-}188)$$

If we continue on in this fashion, we "sweep" forward through the matrix to find

$$\begin{pmatrix} 1 & A_0 & 0 & 0 & \cdots \\ 0 & 1 & A_1 & 0 & \cdots \\ 0 & 0 & 1 & A_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} \qquad (5\text{-}189)$$

where

$$A_n = \frac{a_{n,n+1}}{a_{n,n} - a_{n,n-1} A_{n-1}} \,, \qquad A_0 = \frac{a_{01}}{a_{00}}$$

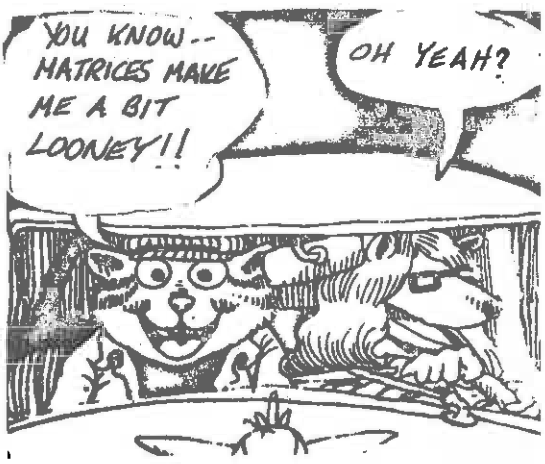
$$\alpha_n = \frac{S_n - \dfrac{a_{n,n-1}}{a_{n-1,n-1}} S_{n-1}}{a_{n,n} - \dfrac{a_{n,n-1}\, a_{n-1,n}}{a_{n-1,n-1}}} \,, \qquad \alpha_0 = \frac{S_0}{a_{00}} \qquad (5\text{-}190)$$

Now we can substitute back up the matrix to find

$$\Phi_N = \alpha_N \,, \qquad \Phi_{N-1} = -A_{N-1}\Phi_N + \alpha_{N-1} \,, \quad \ldots \qquad (5\text{-}191)$$

$$= -A_{N-1}\alpha_N + \alpha_{N-1}$$

and so on.



Example: Consider the simple equation

$$\frac{d^2\Phi}{dx^2} - \frac{1}{L^2}\Phi(x) = -\frac{S(x)}{D} \tag{5-192}$$

$$\Phi(0) = \Phi(a) = 0$$

Then our difference equation for a uniform mesh spacing Δ is

$$-\frac{1}{\Delta^2}\Phi_{i-1} + \left[\frac{2}{\Delta^2} + \frac{1}{L^2}\right]\Phi_i - \frac{1}{\Delta^2}\Phi_{i+1} = \frac{S_i}{D} \tag{5-193}$$

or

$$-C\Phi_{i-1} + B\Phi_i - C\Phi_{i+1} = s_i$$

or using our b.c., $\Phi_0 = \Phi_N = 0$

$$\begin{pmatrix} B & -C & 0 & 0 & \cdots \\ -C & B & -C & 0 & \cdots \\ 0 & -C & B & -C & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ \vdots \end{pmatrix} \tag{5-194}$$

If we now apply Gaussian elimination, the forward sweep generates

$$\begin{pmatrix} 1 & A_1 & 0 & 0 \\ 0 & 1 & A_2 & 0 \\ 0 & 0 & 1 & A_3 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \end{pmatrix} \tag{5-195}$$

where

$$A_i = -\frac{C}{B - CA_{i-1}}, \quad A_i = -C/B$$

$$\alpha_i = \frac{\delta_i + C\alpha_{i-1}}{B + CA_{i-1}}, \quad \alpha_1 = \delta_i/B \qquad (5\text{-}196)$$

Then backward substitution yields

$$\begin{aligned} \Phi_{N-1} &= \alpha_{N-1}, \\ \Phi_{N-2} &= \alpha_{N-2} - A_{N-2}\Phi_{N-1}, \\ &\vdots \\ \Phi_i &= \alpha_i - A_i\Phi_{i+1}, \qquad 1 \le i \le N-2 \end{aligned} \qquad (5\text{-}197)$$

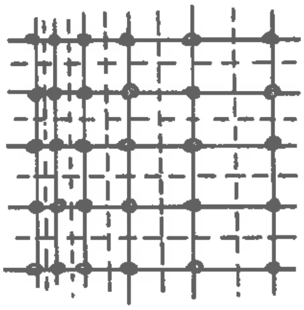
This algorithm for solving such sets of 3-term equations (i.e., inverting tridiagonal matrices) is easily programmed and executed on a digital computer. The algorithm would also formally work for solving difference equations characterizing 2 or 3-dimensional diffusion problems, however it then encounters some severe computing limitations. To see this more clearly, we will now briefly comment upon the numerical solution of multi-dimensional diffusion equations.

4. Derivation of Multidimensional Difference Equations

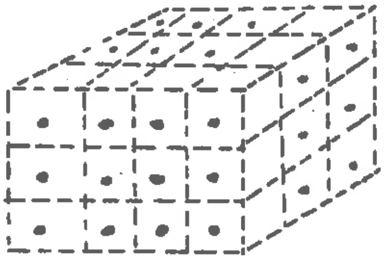
Most detailed neutron diffusion calculations characterizing nuclear reactors require either two or three dimensional treatments. Such details are particularly important in studying power profiles in large reactors as they operate over several core lifetimes. Hence we now must consider the numerical solution of the more general diffusion equation

$$-\nabla \cdot D(\vec{r}) \nabla \Phi(\vec{r}) + \Sigma_a(\vec{r}) \Phi(\vec{r}) = S(\vec{r}) \qquad (5\text{-}198)$$

Once again the geometry of interest is discretized into a mesh of cells--rectangular grids are illustrated below:



Two dimensions



Three dimensions

Perhaps the most straightforward way to derive difference equations for the mesh is to integrate the diffusion equation (5-198) over the spatial volume of a cell, using this to define the spatially averaged cell properties--for example,

$$\frac{1}{V_i} \int_{V_i^{th}\text{cell}} \Phi(\vec{r})\, d^3r = \Phi_i \qquad (5\text{-}199)$$

$$\frac{1}{V_i} \int_{V_i^{th}\text{cell}} \Sigma_a(\vec{r}) \Phi(\vec{r})\, d^3r = \Sigma_{ai} \Phi_i \qquad (5\text{-}200)$$

$$\frac{1}{V_i} \int_{V_i^{th}\text{cell}} \left[-\nabla \cdot D(\vec{r}) \nabla \Phi\right] d^3r = L_i \Phi_i - \sum_{\substack{\text{adjacent}\\ \text{mesh point}\\ \text{neighbors } j}}^{J} l_{ij} \Phi_j \qquad (5\text{-}201)$$

where $J = \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}$ in $\begin{bmatrix} \text{one} \\ \text{two} \\ \text{three} \end{bmatrix}$ dimensional rectangular geometries.

Here one finds in cartesian coordinate geometry

$$L_i = \sum_j^J l_{ij}\,, \quad l_{ij} = \frac{D_{ij}}{\Delta_{ij}^2}\,, \quad D_{ij} = \frac{D_i + D_j}{2} \tag{5-202}$$

$\Delta_{ij} \equiv$ distance between mesh points i and j

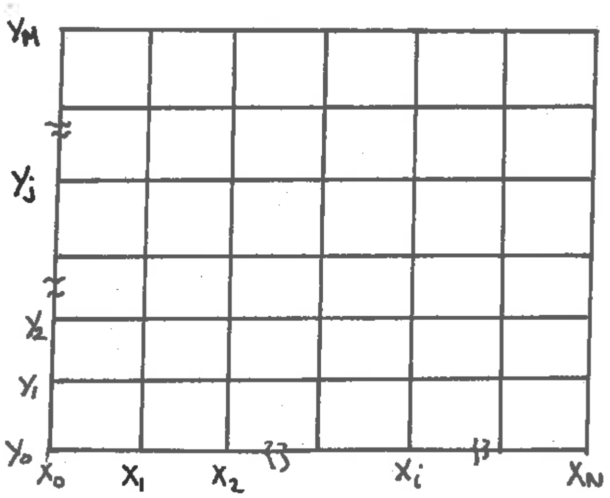
The difference equations then take the form

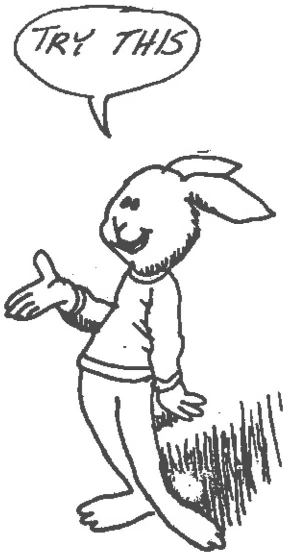
$$\Sigma_{a_i}\Phi_i + \left[\sum_j^J \frac{D_{ij}}{\Delta_{ij}^2}\right]\Phi_i - \sum_j^J \frac{D_{ij}}{\Delta_{ij}^2}\Phi_j = S_i \tag{5-203}$$

Example: Let's derive the difference equations characterizing the 2-dimensional diffusion equations for a uniform medium with a uniform mesh in rectangular geometry

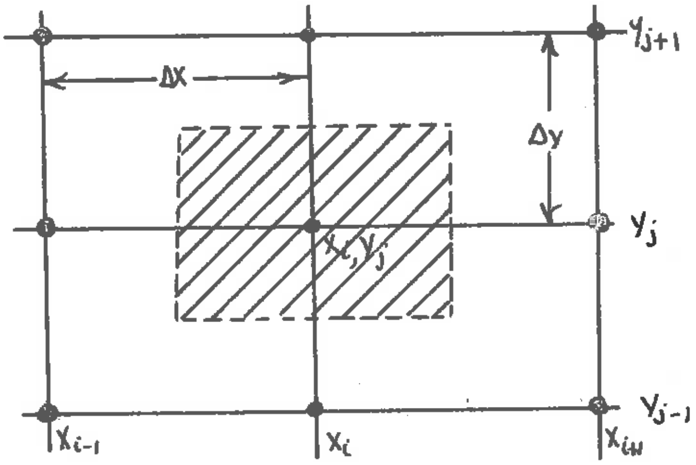
$$-D\frac{\partial^2\Phi}{\partial x^2} - D\frac{\partial^2\Phi}{\partial y^2} + \Sigma_a\Phi = S \tag{5-204}$$

We will label our mesh as shown below:





Now integrate the diffusion equations over the cell shown below centered at x_i, y_j



$$-D\int_{y_j-\frac{\Delta y}{2}}^{y_j+\frac{\Delta y}{2}} dy\ \frac{\partial\Phi}{\partial x}\Bigg|_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} - D\int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} dx\ \frac{\partial\Phi}{\partial y}\Bigg|_{y_j-\frac{\Delta y}{2}}^{y_j+\frac{\Delta y}{2}}$$

$$+\Sigma_a\int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} dx\int_{y_j-\frac{\Delta y}{2}}^{y_j+\frac{\Delta y}{2}} dy\ \Phi = \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} dx\int_{y_j-\frac{\Delta y}{2}}^{y_j+\frac{\Delta y}{2}} dy\ S \qquad (5\text{-}205)$$

Here we use as before

$$\frac{\partial\Phi}{\partial x}\Bigg|_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \cong \frac{\Phi_{i+1,j}-\Phi_{i,j}}{\Delta x} - \frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}$$

$$= \frac{\Phi_{i+1,j}-2\Phi_{i,j}+\Phi_{i-1,j}}{\Delta x} \qquad (5\text{-}206)$$

while

$$\int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} dx \int_{y_j-\frac{\Delta y}{2}}^{y_j+\frac{\Delta y}{2}} dy \; \Phi(x,y) = \underbrace{\Phi(x_i,y_j)}_{\Phi_{ij}} \Delta x \Delta y \qquad (5\text{-}207)$$

to find

$$-D\frac{\Delta y}{\Delta x}\left[\Phi_{i+1,j} - 2\Phi_{i,j} + \Phi_{i-1,j}\right] - D\frac{\Delta x}{\Delta y}\left[\Phi_{i,j+1} - 2\Phi_{i,j} + \Phi_{i,j-1}\right]$$
$$+ \Sigma_a \Delta x \Delta y\, \Phi_{i,j} = \Delta x\, \Delta y\, S_{i,j} \qquad (5\text{-}208)$$

or

$$-\frac{D}{(\Delta x)^2}\left[\Phi_{i+1,j} + \Phi_{i-1,j}\right] - \frac{D}{(\Delta y)^2}\left[\Phi_{i,j+1} + \Phi_{i,j-1}\right]$$
$$+ \left[\Sigma_a + 2D\left(\frac{1}{(\Delta y)^2} + \frac{1}{(\Delta x)^2}\right)\right]\Phi_{i,j} = S_{i,j} \qquad (5\text{-}209)$$

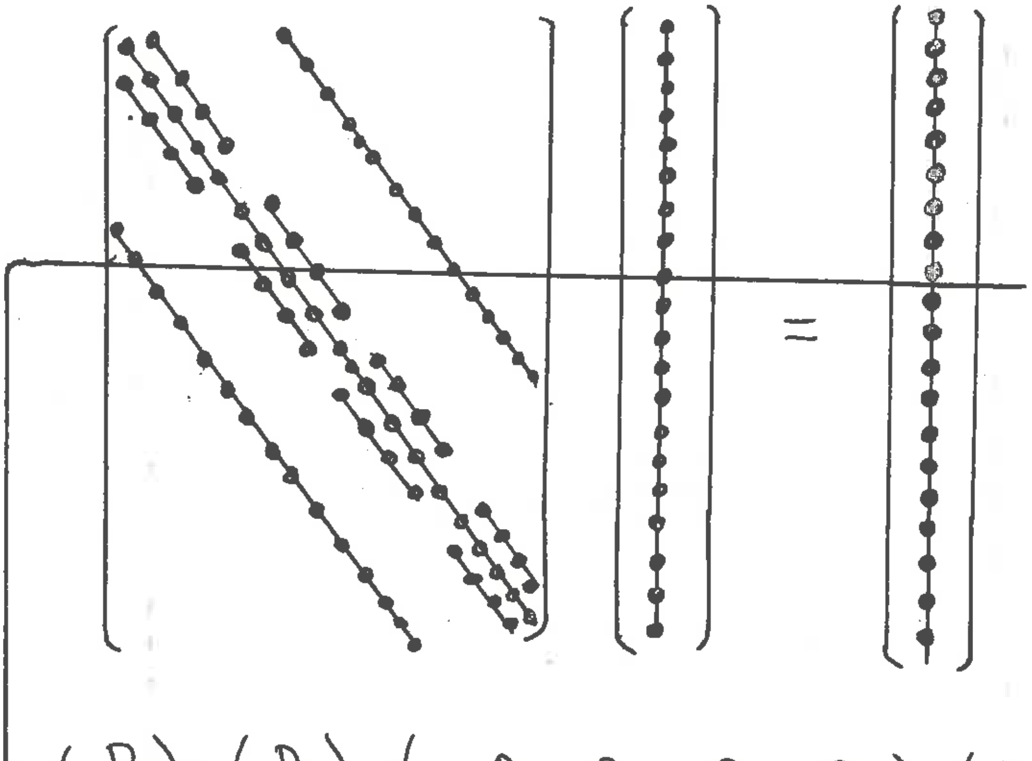
Very similar techniques could be used to derive more general difference characterizing inhomogeneous 2 or 3-dimensional geometries with non-uniform mesh structures.

5. Iterative Solution of Multidimensional Difference Equations

We now turn our attention to the solution of these difference equations. Our first task is to cast the set of equations into matrix form. This requires first assigning a single index to each mesh point. For example, in a 2-dimensional mesh we would probably label the mesh points as

i,j	(0,0),	(1,0),	(2,0),	....	(N,0),	(0,1),	(1,1),	..(N,1)
i	0	1	2		N	N+1	N+2	2N+1

For a two dimensional problem, the matrix structure takes the following form--in this case, for a 5 x 4 mesh point array

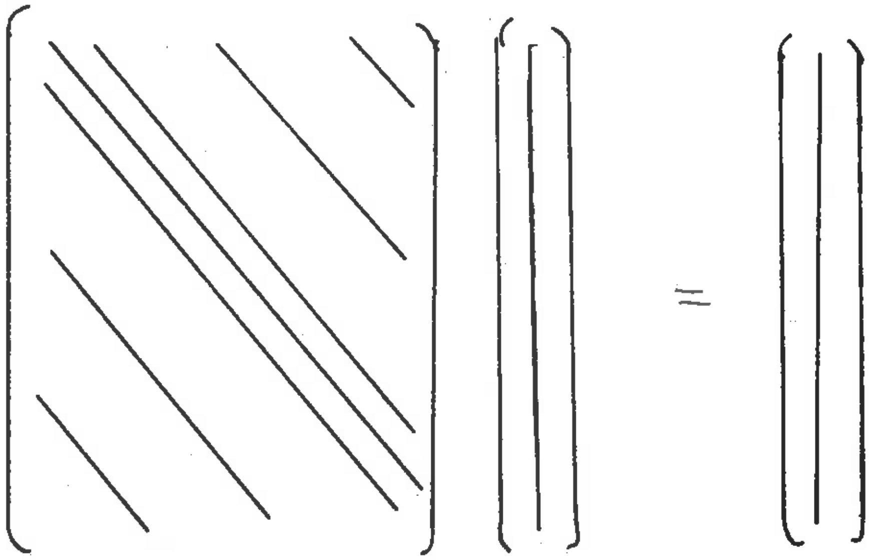


(5-210)

$$\left(-\frac{D_{7,2}}{(\Delta_{7,2})^2}\right)-\left(-\frac{D_{7,6}}{(\Delta_{7,6})^2}\right)-\left(\Sigma_{a7}+\frac{D_{7,2}}{(\Delta_{7,2})^2}+\frac{D_{7,6}}{(\Delta_{7,6})^2}+\frac{D_{7,8}}{(\Delta_{7,8})^2}+\frac{D_{7,12}}{(\Delta_{7,12})^2}\right)-\left(-\frac{D_{7,8}}{(\Delta_{7,8})^2}\right)-\left(-\frac{D_{7,12}}{(\Delta_{7,12})^2}\right)-\left(\Phi_7\right)-($$

Notice that the tridiagonal form we encountered in the one-dimensional case has now been augmented by two additional side-band diagonals--as we might have expected, since upon closer examination we find the 2-dimensional case yields a 5-point difference equation.

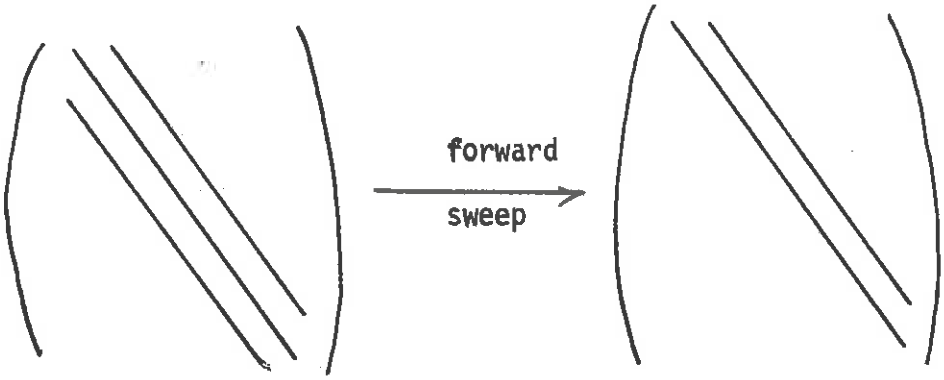
Similarly, assigning a single index to each mesh point of a 3-dimensional problem yields the matrix structure



(5-211)

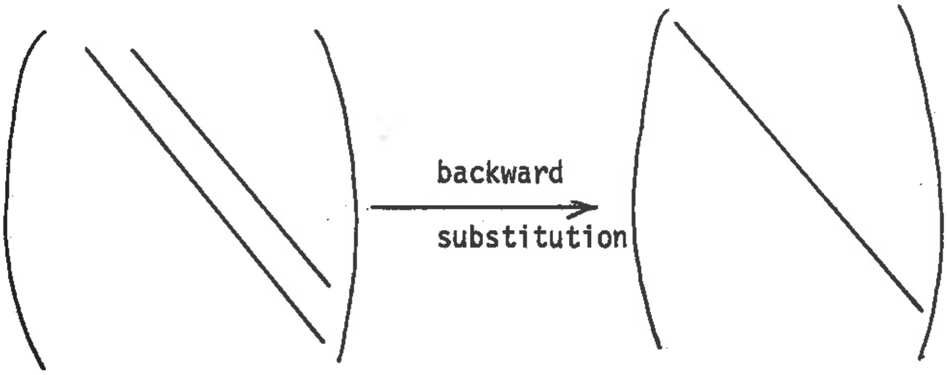
which corresponds to a 7-point difference equation.

Now let's consider how we might solve such systems--i.e., invert such matrices. First let's see what happens if we try Gauss reduction. Recall that the forward Gauss sweep reduced a tridiagonal matrix to a form with only two diagonals



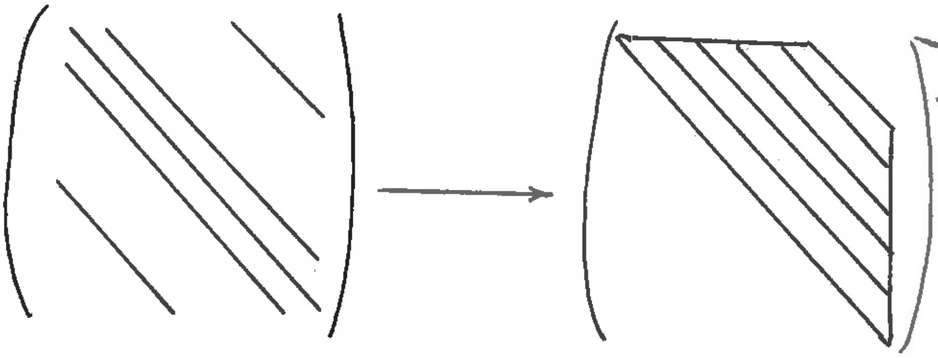
(5-212)

The backward substitution step then completed the inversion:



(5-213)

After a bit of examination, one can quickly convince oneself that when a similar forward sweep is conducted on the 5-diagonal matrix characterizing 2-dimensional problems, the result is to fill in all of the zero entries between the outer diagonals:



(5-214)

This implies that one will require a considerably larger computer memory to allow such a direct inversion of the matrix. Such a direct algorithm is also rather complicated to program and leads to problems resulting from computer round off error. For these reasons, it is far more efficient to use an iterative procedure to invert such matrices when N is large (> 20).

Let's illustrate the basic idea with a simple example: Suppose we wish to invert a matrix $\underline{\underline{A}}$--that is, we wish to solve

$$\underline{\underline{A}}\,\underline{\Phi} = \underline{S} \qquad (5\text{-}215)$$

Suppose we first decompose $\underline{\underline{A}}$ into its diagonal and off diagonal pieces

$$\underline{\underline{A}} = \underline{\underline{D}} - \underline{\underline{B}}$$

(5-216)

Now $\underline{\underline{D}}$ can be easily inverted:

$$\underline{\underline{D}}^{-1} = \begin{pmatrix} D_{11}^{-1} & & 0 \\ & D_{22}^{-1} & \\ 0 & & D_{33}^{-1} \\ & & & \ddots \end{pmatrix} \tag{5-217}$$

Hence suppose we use (5-216) to rewrite (5-215) first as

$$\underline{\underline{D}}\,\underline{\Phi} = \underline{\underline{B}}\,\underline{\Phi} + \underline{S} \tag{5-218}$$

and then invert $\underline{\underline{D}}$ to find

$$\underline{\Phi} = \underline{\underline{D}}^{-1}\left[\underline{\underline{B}}\,\underline{\Phi}\right] + \underline{\underline{D}}^{-1}\underline{S}\,. \tag{5-219}$$

Now is where the iterative philosophy comes in: Suppose we guess $\underline{\Phi}$ on the right hand side--call the guess $\underline{\Phi}^{(0)}$ --and then use it to calculate a new guess, $\underline{\Phi}^{(1)}$ as

$$\underline{\Phi}^{(1)} = \underline{\underline{D}}^{-1}\underline{\underline{B}}\,\underline{\Phi}^{(0)} + \underline{\underline{D}}^{-1}\underline{S}\,. \tag{5-220}$$

We can continue this iteration, calculating the i+1 guess as

$$\underline{\Phi}^{(i+1)} = \underline{\underline{D}}^{-1}\underline{\underline{B}}\,\underline{\Phi}^{(i)} + \underline{\underline{D}}^{-1}\underline{S}\,. \tag{5-221}$$

Hopefully, then, as i becomes large, we converge to the true solution

$$\underline{\Phi}^{(i)} \longrightarrow \underline{\Phi}$$

This scheme is known as the Jacobi-Richardson or Point-Jacobi method, and although very simple, it has the drawback that it converges very slowly (requiring many iterations). The slow convergence arises because information about the next flux iterate is not used until the next iteration, and no extrapolation of the flux iterate to approach the solution quicker is performed.

Successive relaxation or Gauss-Seidel Method: A substantially more efficient iterative scheme begins by decomposing $\underline{\underline{A}}$ into the sum of a lower and upper triangular matrix

$$\underline{\underline{A}} = \underline{\underline{L}} - \underline{\underline{U}}$$

(5-223)

Here $\underline{\underline{L}}$ contains elements of the main diagonal and below it, while $\underline{\underline{U}}$ contains elements above the main diagonal. We next write

$$\underline{\underline{L}}\,\underline{\Phi} = \underline{\underline{U}}\,\underline{\Phi} + \underline{S} \tag{5-224}$$

Now $\underline{\underline{L}}$ can be easily inverted using forward subsitution--stepping row by row down the matrix. Hence our iterative scheme is

$$\underline{\Phi}^{(i+1)} = \underline{\underline{L}}^{-1}\,\underline{\underline{U}}\,\underline{\Phi}^{(i)} + \underline{\underline{L}}^{-1}\,\underline{S}\,. \tag{5-225}$$

Unlike the Point-Jacobi Method, this scheme uses the latest iterate elements of $\underline{\Phi}^{i+1}$ when solving <u>successive</u> equations (i.e., inverting $\underline{\underline{L}}$ by forward substitution)--hence it exhibits a factor of two better in error reduction per iteration than the Point-Jacobi Method.

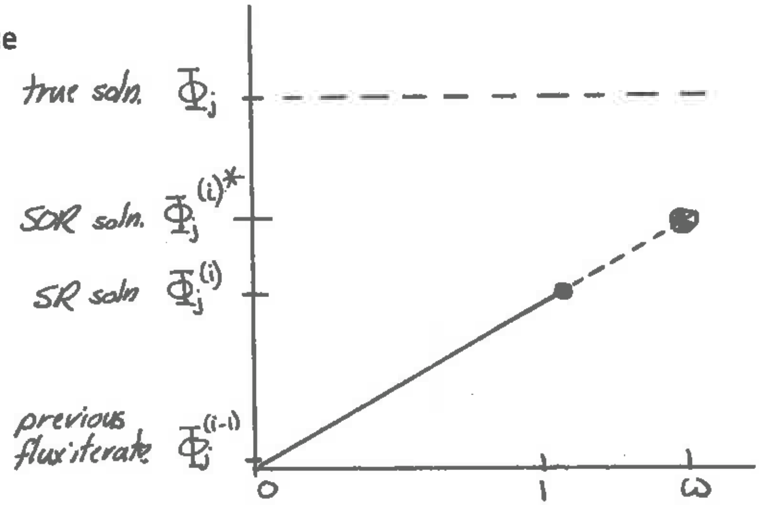
<u>Successive Overrelaxation (SOR)</u>: This method is very similar to Successive Relaxation, except that the change in each flux element since the last iteration gets multiplied by an extrapolation parameter, ω. (where $1<\omega<2$), before adding it to the previous flux iterate element to give the present flux iterate element

$$\Phi_j^{(i)} = \Phi_j^{(i)} + \omega\left(\Phi_j^{(i+1)} - \Phi_j^{(i)}\right) \qquad (5\text{-}226)$$

as determined by SOR

as would be determined by suceessive relaxation

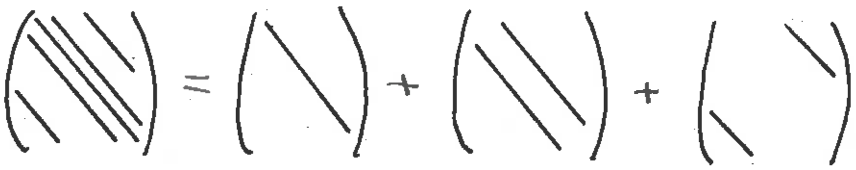
A quatitative sketch illustrates how flux extrapolation can enhance the rate of convergence to the true pointwise solution:



Successive Overrelaxation (SOR) reduces to Successive Relaxation (SR) when $\omega = 1$ is used (no extrapolation). The optimum value of ω which gives the maximum rate of convergence can be related to characteristics of the original matrix, and an accurate estimate of ω can strongly affect the convergence rate of this method.

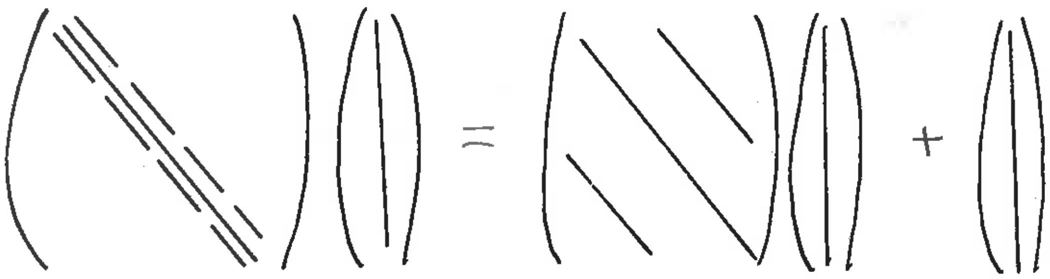
Alternating Direction Implicit Method (ADI); In this scheme, one decomposes

$$\underline{\underline{A}} = \underline{\underline{D}} + \underline{\underline{H}} + \underline{\underline{V}} \tag{5-227}$$



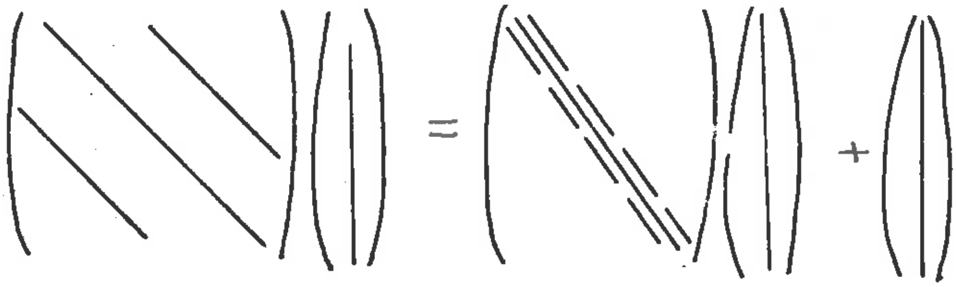
where $\underline{\underline{D}}$ contains the main diagonal elements, $\underline{\underline{H}}$ contains the elements of the adjacent two off-diagonals, and $\underline{\underline{V}}$ contains elements of the outer two off-diagonals. The matrix equation is then manipulated into two matrix equations that are solved in sequence, representing one iteration:

$$\left[\underline{\underline{D}} + \underline{\underline{H}} + \alpha\,\underline{\underline{I}}\right] \underline{\Phi}^{(i-\frac{1}{2})} = \left[-\underline{\underline{V}} - \alpha\,\underline{\underline{I}}\right] \underline{\Phi}^{(i-1)} + \underline{S} \tag{5-228}$$



and

$$[\underline{\underline{D}} + \underline{\underline{V}} + \alpha \underline{\underline{I}}] \cdot \underline{\Phi}^{(i)} = [-\underline{\underline{H}} - \alpha \underline{\underline{I}}] \cdot \underline{\Phi}^{(i-\frac{1}{2})} + \underline{S} \qquad (5\text{-}229)$$



The diagonal matrix $\alpha \underline{\underline{I}}$ is introduced to accelerate convergence of the iterative procedure. α is one of a set of acceleration parameters that are applied cyclically. Note that solving for each unknown flux vector, $\underline{\Phi}^{(i-\frac{1}{2})}$ and $\underline{\Phi}^{(i)}$, involves solving each matrix equation using Gauss elimination.

In practice, one frequently finds that the ADI method is a great deal more efficient that either the Point Jacobi or SOR method--provided the geometry being studied is reasonably homogeneous. For problems in which large changes in regional properties occur, the ADI method may converge very slowly--or not at all!

Such iterative algorithms for the solution of the finite difference equations characterizing 2 or 3-dimensional diffusion problems are frequently referred to as "inner iterations". This nomenclature arises from the fact that in a nuclear reactor criticality study, the solution of the diffusion equation is itself imbedded in a iterative scheme--the so-called "outer" or "source" iterations--necessary to handle the presence of a fission term. We will study this latter scheme in section (5-IV).

We will leave numerical methods for solving diffusion equations at this point, but we will return later when we must generalize these methods to account for fission processes and energy dependence. The above discussion has been an admittedly curse description of numerical methods for solving differential equations. There is a vast literature on this subject which provides the details of the methods we have so briefly outlined. And perhaps the most valid argument for presenting only a brief sketch of such numerical methods lies in the recognition that such topics are of such vital importance to the practicing nuclear engineer, that he almost certainly will have had or will take further courses on numerical analysis in any event.

III. THE ONE-SPEED DIFFUSION MODEL OF A NUCLEAR REACTOR

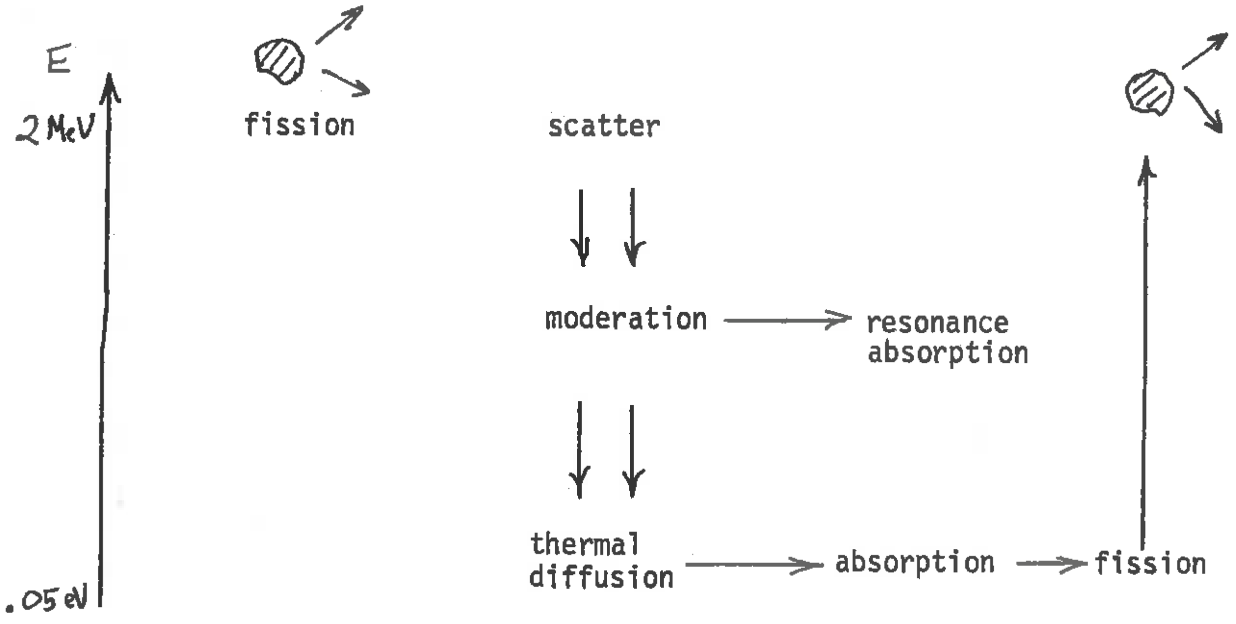
A. Introduction

Thus far we have studied the diffusion of neutrons in non-multiplying media as described by the one-speed diffusion equation

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a \Phi(\vec{r},t) = S(\vec{r},t) \qquad (5\text{-}230)$$

[More precisely, we have studied time-independent neutron diffusion for which $\frac{\partial \Phi}{\partial t} \equiv 0$]. We now wish to apply this equation to the study of nuclear reactors in which fissile material is present. Hence we must figure out how to include nuclear fission in the above diffusion equation.

Recall the sequence of events in a thermal nuclear reactor* as depicted in the sketch below:



Here, several fast (~2MeV) neutrons are born in a fission reaction. These neutrons are then either absorbed, leak out, or are scattered to lower energies. As neutrons are moderated to lower energies by elastic scattering collisions, they pass through energies comparable to the absorption resonances in heavy nuclei such as U^{238}, and hence experience an appreciable probability of being absorbed while slowing down. If they make it to thermal energies, they then diffuse through the reactor core until they either leak out or are absorbed. If they are absorbed in the fuel, then they may induce a new fission, hence repeating the cycle.

---

*This treatment holds also for fast reactors of course. However for historical reasons, we shall first develop the theory in the conventional notation introduced for thermal reactor analysis.

It should be evident that the various processes which occur during this sequence are strongly energy dependent--as manifested in the energy dependence of the cross sections. We will continue to use the one-speed model to study such processes, however, for awhile. Why?

(i) Because this is the easiest model with which to understand a reactor.

(ii) It even gives reasonable quantitative estimates for

(a) very fast reactors

(b) very thermal reactors

--provided one uses the correct values for D, Σ_a, and Σ_f. (We'll discuss how to choose these values when we re-derive the one-speed or "one-group" equation within the more general framework of multigroup diffusion theory.)

B. The Fission Source Term

We now direct our attention towards determining a way to include fission in the one-speed diffusion equation. We will assume that diffusion, absorption, and fission all occur at the same energy. Then a term to represent fissions can easily be derived by noting

$$\text{rate at which fissions occur/cm}^3 \equiv \Sigma_f \Phi(\vec{r},t) . \tag{5-231}$$

Hence the rate at which fission neutrons appear in the reactor--that is, the "fission source" is given by

$$S(\vec{r},t) = \nu \Sigma_f \Phi(\vec{r},t) \tag{5-232}$$

If this is the only source of neutrons in the reactor*, then the appropriate diffusion equation becomes

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a\Phi(\hat{r},t) = \nu\Sigma_f\Phi(\hat{r},t) \qquad (5\text{-}233)$$

[Note here that

$$\Sigma_a = \Sigma_a^{\text{Moderator}} + \Sigma_a^{\text{Structure}} + \Sigma_a^{\text{Fuel}}$$

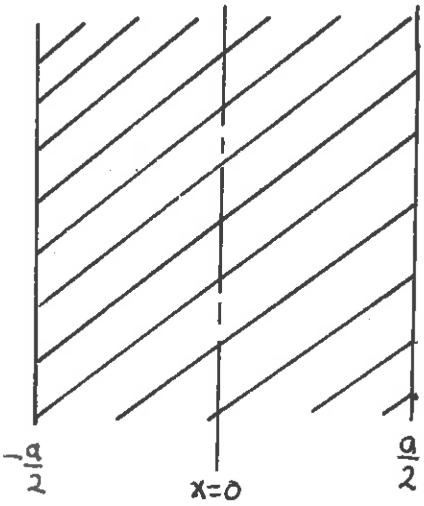
and

$$\Sigma_a^{\text{Fuel}} = \Sigma_\gamma^{\text{Fuel}} + \Sigma_f^{\text{Fuel}} \;] \qquad (5\text{-}234)$$

This is the basic equation we will apply to analyze nuclear reactors.

C. The Time-Dependent "Slab" Reactor

1. General Solution



We will now consider a uniform infinite slab of fissionable material of width a characterized by cross sections Σ_a, Σ_s, and Σ_f. This unrealistic appearing "slab reactor" is chosen to introduce many of the concepts of reactor analysis for convenience, since its one dimensional geometry makes the detailed solution of the one-speed diffusion equation

---

*Actually we should hedge here a bit. Eq. (5-233) actually represents only "prompt" neutrons, i.e., those born instantaneously in fission. The "delayed" neutrons arising from fission product decay require a slightly different treatment. We will defer this until Chapter 6.

very easy*. The appropriate mathematical description of the neutron flux in such a reactor is

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\frac{\partial^2\Phi}{\partial x^2} + \Sigma_a\Phi(x,t) = \nu\Sigma_f\Phi(x,t) \tag{5-235}$$

with initial condition: $\Phi(x,0) = \Phi_0(x)$ (symmetric)

boundary conditions: $\Phi(\frac{\tilde{a}}{2},t) = \Phi(-\frac{\tilde{a}}{2},t) = 0$.

Unlike our earlier studies of time-independent neutron diffusion, we are now faced with a partial differential equation to solve. There are a number of ways to attack this problem, but perhaps the simplest is to use separation of variables by seeking a solution of the form

$$\Phi(x,t) = \varphi(x)\,T(t). \tag{5-236}$$

If we now substitute this form into (5-209) and divide by $\varphi(x)\,T(t)$, we find

$$\frac{1}{T}\frac{dT}{dt} = \frac{v}{\varphi}\left[D\frac{d^2\varphi}{dx^2} + (\nu\Sigma_f - \Sigma_a)\varphi(x)\right] = \text{constant} \equiv -\lambda \tag{5-237}$$

---

*In this sense it is somewhat akin to the "vibrating string" or "simple harmonic oscillator" problems in physics which also get beat to death since they contain most of the interesting physics--and are easy to solve.

Here we have noted that since we have a function only of x set equal to a function only of t, both terms must in fact be equal to a constant. We have named this constant-λ . [Note, however, that λ is as yet unknown.]

Hence we have two ordinary differential equations to solve

$$\frac{dT}{dt} = -\lambda T(t)$$

$$D\frac{d^2\phi}{dx^2} + (\nu\Sigma_f - \Sigma_a)\phi(x) = -\frac{\lambda}{V}\phi(x) \qquad (5\text{-}238)$$

We can easily solve the time-dependent equation

$$T(t) = T(0)e^{-\lambda t} \qquad (5\text{-}239)$$

To solve the space-dependent equation, we must tack on the boundary conditions

$$D\frac{d^2\phi}{dx^2} + \left(\frac{\lambda}{V} + \nu\Sigma_f - \Sigma_a\right)\phi(x) = 0$$

$$\text{b.c.} \quad \phi\left(\frac{\tilde{a}}{2}\right) = \phi\left(\frac{-\tilde{a}}{2}\right) = 0 \qquad (5\text{-}240)$$

Here λ is still to be determined. But we recall the eigenvalue problem

$$\frac{d^2\phi_n}{dx^2} + B_n^2\phi_n(x) = 0$$

$$\phi_n\left(\frac{\tilde{a}}{2}\right) = \phi_n\left(-\frac{\tilde{a}}{2}\right) = 0 \qquad (5\text{-}241)$$

has symmetric solutions (we are only interested in symmetric solutions since $\Phi_o(x)$ is symmetric):

$$\text{eigenfunctions:} \quad \varphi_n(x) = \cos B_n x$$

$$\text{eigenvalues:} \quad B_n = \frac{n\pi}{a}, \quad n = 1, 3, 5, \ldots \tag{5-242}$$

If we identify (5-214) as the same problem, then it is apparent that we must choose

$$\frac{\lambda}{vD} + \frac{\nu\Sigma_f - \Sigma_a}{D} = B_n^2 \tag{5-243}$$

or

$$\lambda = v\Sigma_a + vDB_n^2 - v\nu\Sigma_f \equiv \lambda_n$$

$$= v\Sigma_a\left[1 + L^2B_n^2 - \nu\Sigma_f/\Sigma_a\right]$$

or

$$\lambda_n = v\Sigma_a(1 + L^2B_n^2)\left[1 - \frac{\nu\Sigma_f/\Sigma_a}{1 + L^2B_n^2}\right], \quad n = 1, 3, 5, \ldots \tag{5-244}$$

These values of λ_n are known as the "time eigenvalues" of the equation, since they characterize the time decay in Eq. (5-213). The general solution to (5-209) must therefore be of the form

$$\Phi(x,t) = \sum_{\substack{n \\ \text{odd}}} A_n e^{-\lambda_n t} \varphi_n(x)$$

$$= \sum_{\substack{n \\ \text{odd}}} A_n e^{-\lambda_n t} \cos \frac{n\pi x}{a} \tag{5-245}$$

This solution automatically satifies the boundary condition. To determine the A_n, we use the initial condition

$$\text{i.c.} \quad \Phi(x,0) = \Phi_0(x) = \sum_{\substack{n \\ \text{odd}}} A_n \cos\frac{n\pi x}{\tilde{a}} \tag{5-246}$$

Uisng orthogonality, we find

$$A_n = \frac{2}{\tilde{a}} \int_{-\tilde{a}/2}^{\tilde{a}/2} dx \, \Phi_0(x) \cos\frac{n\pi x}{\tilde{a}} \quad . \tag{5-247}$$

Thus we have found that the flux (for any symmetric initial distribution) is

$$\Phi(x,t) = \sum_{\substack{n \\ \text{odd}}} \left[\frac{2}{\tilde{a}} \int_{-\tilde{a}/2}^{\tilde{a}/2} dx' \, \Phi_0(x') \cos B_n x' \right] e^{-\lambda_n t} \cos B_n x \tag{5-248}$$

where the time eigenvalues λ_n are given by

$$\lambda_n = v\Sigma_a + vDB_n^2 - v\nu\Sigma_f \, , \quad B_n = \frac{n\pi}{\tilde{a}} \tag{5-249}$$

2. Long Time Behavior

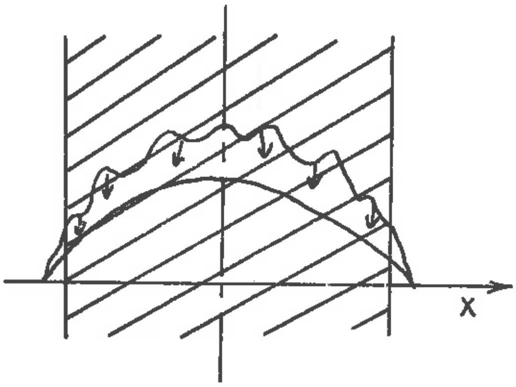
Now notice that $B_1 < B_3 < B_5 \; \cdots\cdot$

Hence $-\lambda_1 > -\lambda_3 > -\lambda_5 \cdots$

This means that the "modes" corresponding to larger n decay out more rapidly in time. If we wait long enough, then only the "fundamental mode" remains:

$$\Phi(x,t) \sim A_1 e^{-\lambda_1 t} \cos B_1 x \quad \text{as } t \to \infty. \tag{5-250}$$

This implies that regardless of what the initial shape $\Phi_o(x)$ is (at least, provided $A_1 \neq 0$), the flux will decay into the fundamental mode shape.



Actually, for sufficiently large $\nu\Sigma_f$, $\nu\Sigma_f - \lambda_n$ may be positive corresponding to an exponentially <u>growing</u> flux. However the same argument will hold since

$$-\lambda_1 > -\lambda_2 > \cdots$$

Hence regardless of whether the flux grows or decays, it will eventually approach a "persistent" or fundamental cosine distribution.

It is customary to refer to the value of B_n^2 characterizing this mode as

$$B_1^2 = \left(\frac{\pi}{\tilde{a}}\right)^2 \equiv B_g^2 \qquad \text{"geometric buckling"} \tag{5-251}$$

[This nomenclature is used since B_n^2 is a measure of the curvature of the mode shape

$$B_n^2 = -\frac{1}{\phi_n}\frac{d^2\phi_n}{dx^2} \ . \tag{5-252}$$

Hence the mode with the least curvature persists in time the longest.]

3. The Criticality Condition

Let us now see what is required to make the flux distribution in the reactor time-independent--that is, to make the fission chain reaction steady-state. We will define this situation to be that of reactor <u>criticality</u>.

criticality $\equiv$ when a time-independent neutron flux can be sustained in the reactor in the absence of sources (other than fission)

If we write out the general solution for the flux

$$\Phi(x,t) = A_1 e^{-\lambda_1 t} \cos B_1 x + \sum_{n=3}^{\infty} A_n e^{-\lambda_n t} \cos B_n x, \qquad (5\text{-}253)$$

it is evident that the requirement for a time-independent flux is just

$$\lambda_1 = 0 = v(\Sigma_a - \nu\Sigma_f) + vDB_1^2 \qquad (5\text{-}254)$$

since then the higher modes will all be negative and decay out in time, leaving just

$$\Phi(x,t) \rightarrow A_1 \cos B_1 x \neq \text{function of time} \qquad (5\text{-}255)$$

If we rewrite this "criticality condition" using the notation $B_1^2 = B_g^2$, then we find we must require

$$\frac{\nu\Sigma_f - \Sigma_a}{D} = B_g^2 \qquad (5\text{-}256)$$

It has become customary to refer to

$$\frac{\nu\Sigma_f - \Sigma_a}{D} \equiv B_m^2 \equiv \text{"material buckling"} \qquad (5\text{-}257)$$

since it depends only upon the material composition of the reactor core (whereas B_g^2 depends only upon the core geometry). Hence our criticality condition can be written very concisely as

$$\text{(material composition)} \quad B_m^{\ 2} = B_g^{\ 2} \quad \text{(core geometry)} \tag{5-258}$$

Thus, to achieve a critical reactor, we must either adjust the size ($B_g^{\ 2}$) or the core composition ($B_m^{\ 2}$) such that $B_m^{\ 2} = B_g^{\ 2}$. We also note

$$\begin{array}{llll} B_m^2 > B_g^2 & \Rightarrow \lambda_1 < 0 & \Rightarrow & \text{supercritical} \\ B_m^2 = B_g^2 & \Rightarrow \lambda_1 = 0 & \Rightarrow & \text{critical} \\ B_m^2 < B_g^2 & \Rightarrow \lambda_1 > 0 & \Rightarrow & \text{subcritical} \end{array} \tag{5-259}$$

But recall that in Chapter 3 we expressed the criticality condition in terms of the multiplication factor k. We can make the connection between these two criteria if we write

$$\lambda_1 = v\Sigma_a(1+L^2B_g^2)\left[1 - \frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_g^2}\right] \tag{5-260}$$

Now recall that $\frac{1}{v\Sigma}$ is the mean lifetime for a given neutron-nuclear reaction to occur. Hence

$$\frac{1}{v\Sigma_a} \equiv \text{mean lifetime of neutron to absorption} \tag{5-261}$$

Furthermore, if we recall our work in Chapter 3,

$$\frac{\nu\Sigma_f}{\Sigma_a} = \frac{\nu\Sigma_f^{\text{Fuel}}}{\Sigma_a^{\text{Fuel}}}\,\frac{\Sigma_a^{\text{Fuel}}}{\Sigma_a} = \eta f = k_\infty \tag{5-262}$$

Now the only remaining task is to identify $(1+L^2B_g^{\ 2})^{-1}$. Recall that

$$\textit{rate of neutron leakage} = -D\nabla^2\Phi \tag{5-263}$$

Hence

$$\frac{\text{rate of neutron absorption}}{\text{rate of neutron absorption + leakage}} = \frac{\Sigma_a \Phi}{\Sigma_a \Phi - D\nabla^2\Phi}$$

$$= \frac{\Sigma_a \Phi}{\Sigma_a \Phi + D B_g^2 \Phi} = \frac{1}{1+L^2B_g^2} \tag{5-264}$$

Hence

$$\frac{1}{1+L^2B_g^2} \equiv \begin{array}{c}\text{non-leakage probability}\\ \text{for thermal neutrons}\end{array} \equiv P_{NL} \tag{5-265}$$

We can now identify

$$\frac{1}{(v\Sigma_a)(1+L^2B_g^2)} = P_{NL}\left(\frac{1}{v\Sigma_a}\right) \equiv \ell \equiv \begin{array}{l}\text{neutron lifetime}\\ \text{in finite reactor}\end{array} \tag{5-266}$$

while

$$\frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_g^2} = \eta f P_{NL} = k \equiv \begin{array}{c}\text{multiplication}\\ \text{factor}\end{array} \tag{5-267}$$

Thus

$$-\lambda_1 = \frac{k-1}{\ell} \doteq \frac{1}{T} \tag{5-268}$$

where T is the reactor period. Now it is evident that

$$B_m^2 = B_g^2 \quad \Longleftrightarrow \quad k = 1, \tag{5-269}$$

hence our two criticality conditions are actually identical.

Thus we see that by using the one-speed diffusion equation we have been able to evaluate the non-leakage probability for a slab reactor.

Example: It is useful at this point to give an illustration of how such an analysis can be used. Suppose the composition of the slab is given (Σ_f, Σ_a, and D), and we wish to determine the critical size. Then all we need do is first calculate

$$B_m^2 = \frac{\nu\Sigma_f - \Sigma_a}{D} = \frac{\nu\Sigma_f/\Sigma_a - 1}{L^2} . \tag{5-270}$$

Then the critical extrapolated width is given by

$$\left(\frac{\pi}{\tilde{a}}\right)^2 = B_g^2 = B_m^2 \tag{5-271}$$

or

$$\tilde{a} = \frac{\pi}{B_m} \tag{5-272}$$

Hence the true width is just

$$a = \frac{\pi}{B_m} - 2z_0 = \frac{\pi L}{\sqrt{\frac{\nu\Sigma_f}{\Sigma_a} - 1}} - 2(.7104\,\lambda_{tr}) \tag{5-273}$$

in particular note that if $\frac{\nu\Sigma_f}{\Sigma_a} = k_\infty \leq 1$, no width a exists such that the reactor will be critical. [One must have $k_\infty > 1$ to achieve a critical system.]

Example: Suppose now that the dimensions of the reactor are specified, and we wish to calculate the necessary fuel loading (i.e., the "critical mass").

We first calculate

$$B_g^2 = \left(\frac{\pi}{\tilde{a}}\right)^2 \tag{5-274}$$

and equate

$$\frac{\nu\Sigma_f/\Sigma_a - 1}{L^2} = B_g^2 \tag{5-275}$$

Let F = fuel, M = moderator. Then

$$\Sigma_a = \Sigma_f + \Sigma_c^F + \Sigma_c^M$$

$$L^2 = D/\Sigma_a = 1/3\Sigma_{tr}\Sigma_a = \left[3\underbrace{(\Sigma_{tr}^M + \Sigma_{tr}^F)}_{\sim \Sigma_{tr}^M}(\Sigma_a^M + \Sigma_a^F)\right] \tag{5-276}$$

$$= \frac{(3\Sigma_{tr}^M\Sigma_a^M)^{-1}}{1 + \Sigma_a^F/\Sigma_a^M} = \frac{L_M^2}{1 + (\Sigma_a^F/\Sigma_a^M)}$$

Then

$$\frac{\nu\Sigma_f}{\Sigma_a} = \frac{\nu\Sigma_f}{\Sigma_a}\frac{\Sigma_a^F}{\Sigma_a^F + \Sigma_a^M} = \eta\frac{(\Sigma_a^F/\Sigma_a^M)}{1 + (\Sigma_a^F/\Sigma_a^M)} \tag{5-277}$$

Hence our criticality condition becomes

$$\frac{(\eta - 1)\left[\left(\frac{\Sigma_a^F}{\Sigma_a^M}\right) - 1\right]}{L_M^2} = \left(\frac{\pi}{\tilde{a}}\right)^2 \tag{5-278}$$

Now $\frac{\Sigma_a^F}{\Sigma_a^M} = \frac{N_F}{N_M}\frac{\sigma_a^F}{\sigma_a^M}$, so we can solve directly for the critical density and hence the critical mass.

4. Extension to More General Geometries

Note that the only quantity characteristic of the size or geometry of the reactor which appears in k or P_{NL} is the geometric buckling B_g^2. For a slab reactor of width a, we found

$$B_g^2 = \left(\frac{\pi}{a}\right)^2 \tag{5-279}$$

Hence to compute k or P_{NL} for more general geometries, we need only compute the geometric buckling for the geometry.

In general, B_g^2 is defined as the smallest eigenvalue B^2 of the Helmholtz equation

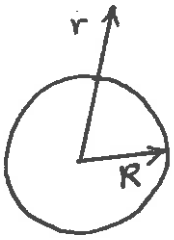
$$\nabla^2\Phi + B^2\Phi(\vec{r}) = 0 \tag{5-280}$$

subject to boundary conditions that $\Phi(\vec{r})$ vanish on the extrapolated boundary $\vec{R}$ of the reactor. To see how we compute B_g^2, we will consider several examples:

Example: Sphere

Now the Helmholtz equation becomes

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\Phi}{dr} + B^2\Phi(r) = 0 \tag{5-281}$$



with boundary conditions:

(i) $\Phi(\tilde{R}) = 0$

(ii) $\Phi(r) < \infty$

A general solution to this equation is

$$\Phi(r) = A\frac{\sin Br}{r} + C\frac{\cos Br}{r} \tag{5-282}$$

Applying b.c. (ii) $\Rightarrow C = 0$

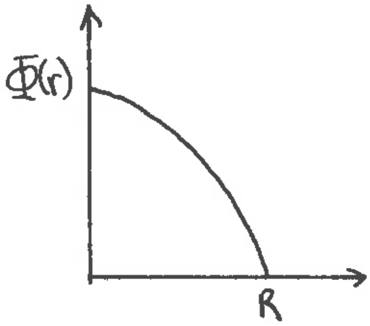
b.c. (i) $\Rightarrow A\sin B\tilde{R} = 0$

$\Rightarrow B\tilde{R} = n\pi$

$$\text{or} \quad B = \frac{n\pi}{\tilde{R}}, \quad n = 1, 2, \cdots \tag{5-283}$$

Hence we find that the geometric buckling is just the smallest of these values

$$B_g^2 = \left(\frac{\pi}{\tilde{R}}\right)^2 \tag{5-284}$$



The corresponding critical flux is

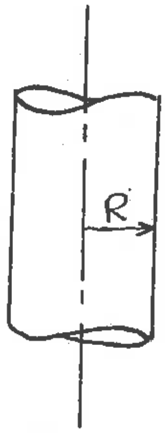
$$\Phi(r) = A\frac{\sin(\pi r/R)}{r} \tag{5-285}$$

Notice that this analysis says nothing about the magnitude A of the flux. This is related to the power level of the reactor and must be adjusted by varying the cross sections (using control rods) to make the reactor slightly supercritical until the flux grows to the desired power level, and then leveling it off by making the reactor critical. The subject of reactor startup and control will be discussed in Chapter 6.

Example: Infinite Cylinder

Now we must solve

$$\begin{aligned} &\frac{1}{r}\frac{d}{dr} r \frac{d\Phi}{dr} + B^2\Phi(r) = 0 \\ &(i)\ \Phi(\tilde{R}) = 0 \\ &(ii)\ \Phi(r) < \infty \end{aligned} \tag{5-286}$$



The general solution of this equation is given in terms of Bessel functions as

$$\Phi(r) = A J_0(Br) + C Y_0(Br) \tag{5-287}$$

Note that $Y_0(Br) \rightarrow \infty$ as r 0. Hence b.c. (ii) $\Rightarrow$ C = 0. Applying b.c. (i), we find

$$\Phi(\tilde{R}) = A J_0(B\tilde{R}) = 0 \tag{5-288}$$

If we define the zeros of $J_0(x)$ as

$$J_0(\nu_n) = 0 \tag{5-289}$$

then (5-261) demands we choose B such that

$$B\tilde{R} = \nu_n \quad \text{or} \quad B = \frac{\nu_n}{\tilde{R}} \tag{5-290}$$

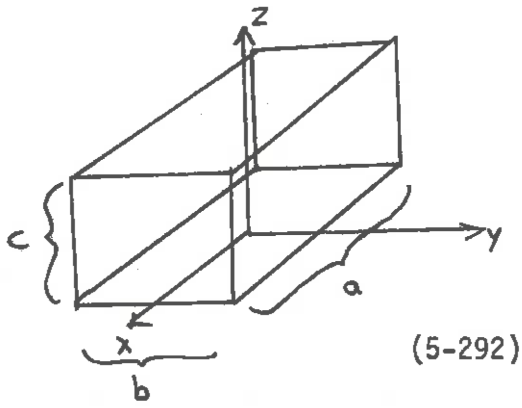
Now the smallest zero of J_0 is $\nu_0 = 2.405$ [kind of like π to a Bessel function]. Thus

$$B_g^2 = \left(\frac{\nu_0}{\tilde{R}}\right)^2 \qquad (5\text{-}291)$$

while $$\Phi(r) = A\,J_0\left(\frac{\nu_0 r}{\tilde{R}}\right)$$

Example: Rectangular Parallelpiped

Now we consider



$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2} + B^2\Phi(x,y,z) = 0 \qquad (5\text{-}292)$$

b.c:

$$\Phi\left(\pm\frac{\tilde{a}}{2}, y, z\right) = \Phi\left(x, \frac{\tilde{b}}{2}, z\right) = \Phi\left(x, y, \frac{\tilde{c}}{2}\right) = 0$$

Since this is a PDE, we will use separation of variables

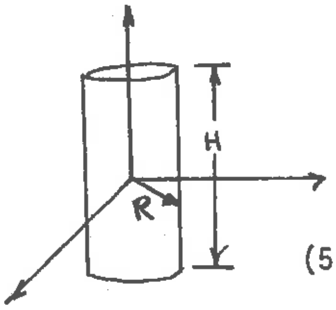
$$\Phi(x,y,z) = X(x)\,Y(y)\,Z(z) \qquad (5\text{-}293)$$

to find a solution

$$\Phi(x,y,z) = A\cos\left(\frac{\pi x}{\tilde{a}}\right)\cos\left(\frac{\pi y}{\tilde{b}}\right)\cos\left(\frac{\pi z}{\tilde{c}}\right) \qquad (5\text{-}294)$$

with $$B_g^2 = \left(\frac{\pi}{\tilde{a}}\right)^2 + \left(\frac{\pi}{\tilde{b}}\right)^2 + \left(\frac{\pi}{\tilde{c}}\right)^2$$

Example: Finite Cylinder



$$\frac{1}{r}\frac{\partial}{\partial r} r\frac{\partial\Phi}{\partial r} + \frac{\partial^2\Phi}{\partial z^2} + B^2\Phi(r,z) = 0 \qquad (5\text{-}295)$$

b.c: $$\Phi(\tilde{R}, z) = \Phi\left(r, \pm\frac{\tilde{H}}{2}\right) = 0$$

Now one finds

$$\Phi(r,z) = A\,J_0\left(\frac{\nu_0 r}{\tilde{R}}\right)\cos\left(\frac{\pi z}{\tilde{H}}\right) \tag{5-296}$$

$$B_g^2 = \left(\frac{\nu_0}{\tilde{R}}\right)^2 + \left(\frac{\pi}{\tilde{H}}\right)^2 \tag{5-297}$$

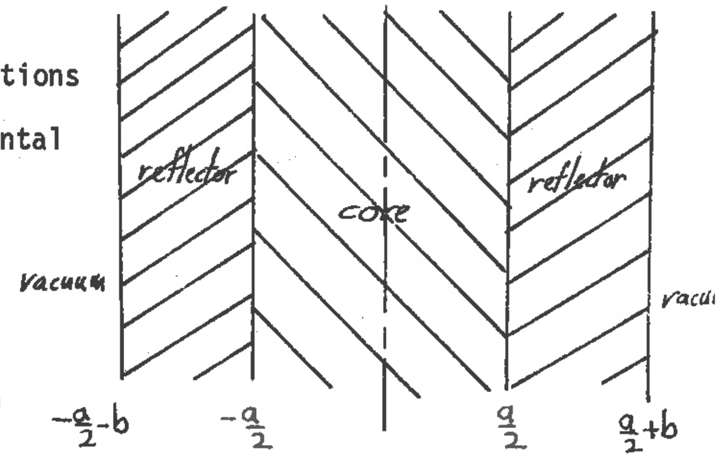
Thus far our analysis has considered only simple reactor geometries of a uniform composition. Such reactors are referred to as "bare" in con trast to "reflected" reactors in which one wraps nonmultiplying material around the reactor core to reflect back in some of the neutrons which leak out. As we will see, our simple expressions for P_{NL} and k which were derived for bare reactors are no longer valid for reflected geometries.

5. Reflected Reactors

Let's now see how the analysis goes if we slap some scattering material on either side of our slab reactor to reflect back in some of the leaking neutrons. The appropriate set of time-independent diffusion equations which must be satisfied by the fundamental mode flux shape are

core: $-D^c \dfrac{d^2\Phi_c}{dx^2} + (\Sigma_a^c - \nu\Sigma_f^c)\Phi_c(x) = 0$

reflector: $-D^R \dfrac{d^2\Phi_R}{dx^2} + \Sigma_a^R \Phi_R(x) = 0$



subject to b.c.

(i) $\Phi_c\left(\pm\frac{a}{2}\right) = \Phi_R\left(\pm\frac{a}{2}\right)$
(ii) $J_c\left(\pm\frac{a}{2}\right) = J_R\left(\pm\frac{a}{2}\right)$
(iii) $\Phi_R\left(\pm\left(\frac{a}{2}+b\right)\right) = 0$

[Note we have assumed the reflector contains no fissile material.] The general approach, as always, is to determine the general solutions in the core and in the reflector, and then use the boundary conditions to determine the unknown coefficients. In the core, the general solution is

$$\Phi_c(x) = A \cos B_m^c x + C \sin B_m^c x \tag{5-299}$$

where

$$B_m^{c\,2} \equiv \frac{\nu\Sigma_f^c - \Sigma_a^c}{D^c}$$

while in the reflector, we seek (using (iii))

$$\Phi_R(x) = A' \sinh\left[\frac{a/2 + \tilde{b} - |x|}{L_R}\right] \tag{5-300}$$

where

$$L_R^2 = \frac{\Sigma_a^R}{D^R}$$

Uisng the b.c. (i) and (ii) implies

$$\begin{gathered} A \cos\left(\frac{B_m^c a}{2}\right) = A' \sinh(\tilde{b}/L_R) \\ D^c B_m^c A \sin\left(\frac{B_m^c a}{2}\right) = \frac{D^R}{L_R} A' \cosh \frac{b}{L_R} \end{gathered} \tag{5-301}$$

Dividing, we can cancel A and A' to find

$$D^c B_m^c \tan\left(\frac{B_m^c a}{2}\right) = \frac{D^R}{L_R} \coth\left(\frac{\tilde{b}}{L_R}\right) \tag{5-302}$$

This is our criticality condition on composition and size. [Note how it doesn't look anything like the condition

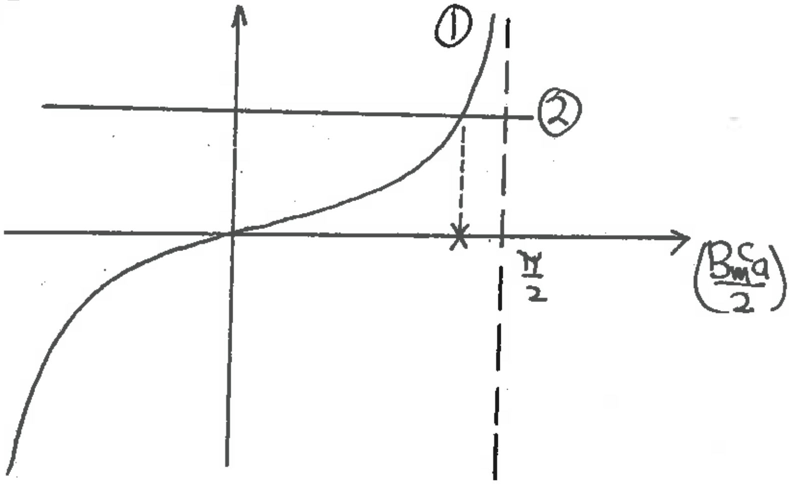
$$B_m^2 = B_g^2$$

we obtained for bare reactors.]

To see what is going on, rewrite this equation as

$$\underbrace{\frac{B_m^c a}{2} \tan\left(\frac{B_m^c a}{2}\right)}_{①} = \underbrace{\frac{D^R a}{2D^c L_R} \coth \tilde{b}/L_R}_{②} \tag{5-303}$$

If we plot ① vs. $B\,m_c\,a/2$, we can then determine the solution of this transcendental equation graphically by noting where it intersects the value of ② :



Notice that the critical value of B_m^c must be such that

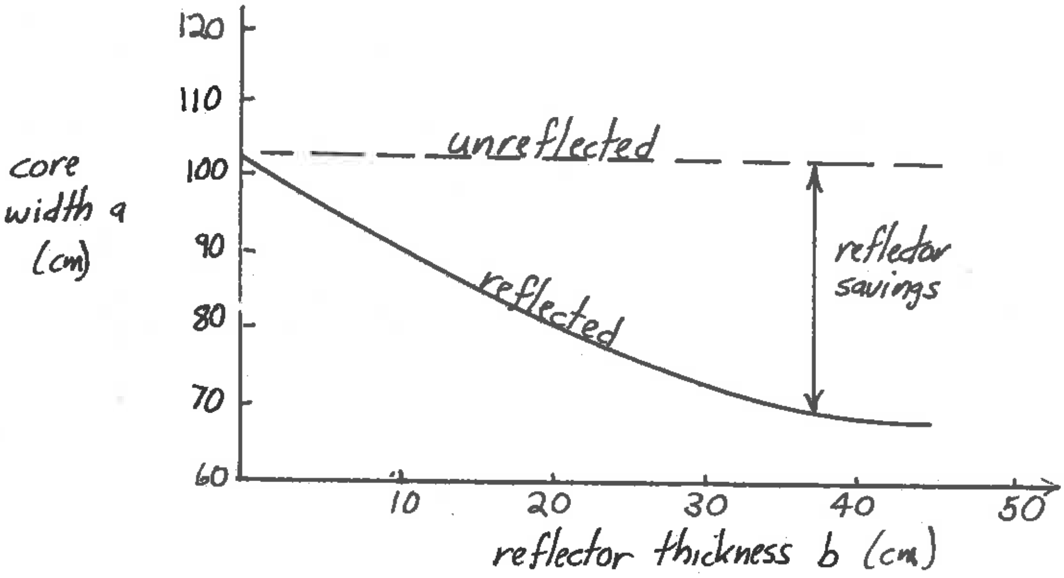
$$\frac{B_m^c a}{2} < \frac{\pi}{2} \quad \text{or} \quad B_m^{c2} < \left(\frac{\pi}{a}\right)^2 \tag{5-304}$$

In contrast to the unreflected (bare) core in which

$$B_m^{c2} = \left(\frac{\pi}{a}\right)^2 \tag{5-305}$$

Hence for the same condition, we can get by with a smaller core if we add a reflector:

Example:

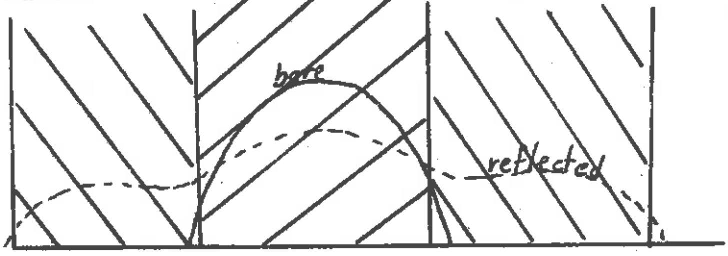


We can define the

$$\text{"reflector savings"} \equiv a\ (\text{bare}) - a\ (\text{reflected}) \qquad (5\text{-}306)$$

Hence one big advantage of a reflector is to diminish the leakage and hence allow a smaller core.

Another important function is to flatten the flux profile and hence the power distribution



We will see that this latter effect is much more dramatic when we include energy dependence.

IV. REACTOR CRITICALITY CALCULATIONS

A. Introduction

Let us now turn to the very important question of just how one determines the composition or size of a reactor which will guarantee criticality. It should be apparent after the last example that in most practical reactor designs one cannot simply determine the geometric buckling for a core geometry and then use $B_m^2 = B_g^2$ to arrive at criticality.

One "brute force" procedure would be to determine the lowest time eigenvalue of

$$-\nabla\cdot D\nabla\Phi + (\Sigma_a - \nu\Sigma_f)\Phi(\vec{r}) = \frac{\lambda}{v}\Phi(\vec{r}) \tag{5-307}$$

and then keep adjusting things until $\lambda = 0$. But this is tough (and introduces errors in an unnatural way). Let's try something else. Suppose we write our diffusion equation as

$$-\nabla\cdot D\nabla\Phi + \Sigma_a\Phi(\vec{r}) = \nu\Sigma_f\Phi(\vec{r}) \tag{5-308}$$

$$\text{b.c.}\quad \Phi(\tilde{R}_s) = 0$$

(which, of course, is the steady-state equation we solved analytically in the earlier simple examples). Unfortunately this equation has <u>no</u> solution in general--unless we just happen to hit on the exact combination of core composition and geometry such that the reactor is critical (a highly unlikely possibility on a computer).

What one must do is introduce an artificial free parameter "k" into

$$-\nabla\cdot D\nabla\Phi + \Sigma_a\Phi(\vec{r}) = \frac{1}{k}\nu\Sigma_f\Phi(\vec{r}). \qquad (5\text{-}309)$$

Then for some value of k, this equation will always have a solution. The idea then is to pick a core size and composition, solve the above equation while determining k. If k should happen to be unity, we have chosen the critical size and composition. If k ≠ 1, however, we must choose a new size and composition and repeat the calculation. As one might expect, k turns out to indeed be the multiplication factor we defined earlier in Chapter 3, as we will demonstrate later.

Sometimes a slightly different formulation is used in which one pretends that ν, the number of neutrons emitted per fission, is in fact a variable. [Of course, it isn't, but it is a useful device to regard it as adjustable for the moment.] Now physically, we know that there must be some value of ν, call it ν_c, which will yield a nontrivial solution to

$$-\nabla\cdot D\nabla\Phi + \Sigma_a\Phi = \nu_c\Sigma_f\Phi \qquad (5\text{-}310)$$

--regardless of what composition or geometry we have chosen. Hence the idea is to determine this ν_c, then readjust composition and geometry until we have forced

$$\nu_c \rightarrow \nu_{actual} = \nu \tag{5-311}$$

If we compare this approach to our earlier scheme in which we calculate k, it is evident that

$$k = \frac{\nu}{\nu_c} \tag{5-312}$$

From a mathematical point of view, each of these approaches introduces a new parameter into the steady-state diffusion equation, either k or ν_c, which can then be regarded as an <u>eigenvalue</u> in a subsequent analysis. Once this eigenvalue has been calculated, one can return and readjust composition and geometry in an effort to force this eigenvalue to a desired value (e.g., $k \rightarrow 1$ or $\nu_c \rightarrow \nu$). Hence the criticality calculation is converted into a sequence of eigenvalue problems.

Before discussing this scheme in detail, however, it is useful to make a few more general remarks about criticality calculations. In reactor design calculations, one refers to a "criticality search" as the procedure in which one guesses a geometry and composition in an iterative fashion to force k to unity. Actually, however, reactors are designed with $k > 1$ to compensate for

(i) fuel burnup
(ii) fission product poisoning
(iii) control

The excess reactivity must be "held down" with control rods or "burnable poisons", i.e., absorbers which gradually disappear over the life of the core.

Many factors must be taken into account in criticality calculations, including control margins, fuel loading history, temperature effects, and so on. Hence a criticality search, although certainly a very central problem in reactor design, must in addition be closely coupled to other facets of the design.

B. Numerical Criticality Searches

We have seen how one can obtain a criticality condition for a bare, uniform reactor. Let's now see how the criticality search is conducted in a practical reactor calculations in which numerical methods must be used to solve the one-speed diffusion equation

$$\begin{gathered} -\nabla\cdot D(\vec{r})\nabla\Phi(\vec{r}) + \Sigma_a(\vec{r})\Phi(\vec{r}) = \nu\Sigma_f(\vec{r})\Phi(\vec{r}) \\ \text{b.c.} \quad \Phi(\vec{R}_s)=0 \end{gathered} \tag{5-313}$$

Let's rewrite this symbolically as

$$A\Phi = S \tag{5-314}$$

where

$$A = -\nabla\cdot D\nabla + \Sigma_a$$

$$S = \nu\Sigma_f\Phi \equiv F\Phi \tag{5-315}$$

Now notice that if we assume that the "source" term S is <u>known</u>, then (5-283) is just the diffusion problem for a source S in a nonmultiplying medium--which we know how to solve. [E.g., we can difference this equation to write it in matrix form as

$$\underline{\underline{A}}\,\underline{\Phi} = \underline{S} \tag{5-316}$$

and then invert A to find $\underline{\Phi} = \underline{\underline{A}}^{-1}\underline{S}$.]

But, of course, we do not know S since it involves Φ itself. Hence we do the next best thing and try to guess it--that is, we guess a "fission source"

$$S(\vec{r}) \cong S^{(0)}(\vec{r}) . \qquad (5\text{-}317)$$

Now we solve for the flux from this guessed source

$$-\nabla\cdot D\nabla\Phi^{(1)} + \Sigma_a\Phi^{(1)} = S^{(0)} \qquad (5\text{-}318)$$

$$\left[\text{e.g.,}\quad \underline{\Phi}^{(1)} = \underline{\underline{A}}^{-1}\underline{S}^{(0)}\right]$$

With this solution, we can now explicitly calculate the fission source and use this as a second guess

$$S^{(1)} = \nu\Sigma_f\Phi^{(1)} \qquad (5\text{-}319)$$

[Notice that this is actually just the number of neutrons in the first fission operation.] Now we can solve again for the flux

$$-\nabla\cdot D\nabla\Phi^{(2)} + \Sigma_a\Phi^{(2)} = S^{(1)} \qquad (5\text{-}320)$$

We can continue on this way in an iterative fashion

$$-\nabla\cdot D\nabla\Phi^{(n)} + \Sigma_a\Phi^{(n)} = S^{(n-1)} \qquad (5\text{-}321)$$

$$S^{(n)} = \nu\Sigma_f\Phi^{(n)}$$

Now notice something:

$s^{(n)}$ is the number of neutrons in d^3r about $\vec{r}$ in the nth fission generation

Hence for large n, we expect the flux to approach the fundamental mode

$$\Phi^{(n)}(\vec{r}) \longrightarrow \Phi(\vec{r})$$

which satisfies

$$-\nabla\cdot D\nabla\Phi(\vec{r}) + \Sigma_a\Phi(\vec{r}) = \frac{1}{k}\nu\Sigma_f\Phi(\vec{r}) \tag{5-322}$$

In practice, a couple of minor changes are made in this iterative scheme:

(i) Guess $S(\underline{r}) = s^{(0)}(\underline{r})$ and $k = k^{(0)}$ (5-323)

(ii) Now solve

$$-\nabla\cdot D\nabla\Phi^{(1)} + \Sigma_a\Phi^{(1)} = \frac{1}{k^{(0)}}S^{(0)}(\vec{r}) \tag{5-324}$$

for $\Phi^{(1)}(\vec{r})$.

(iii) Calculate a new value of the source

$$S^{(1)}(\vec{r}) = \nu\Sigma_f\Phi^{(1)}(\vec{r}) \tag{5-325}$$

and a new value of k

$$k^{(1)} = \frac{\int d^3r\, S^{(1)}(\vec{r})}{\frac{1}{k^{(0)}}\int d^3r\, S^{(0)}(\vec{r})} \tag{5-326}$$

(iv) Iterate this scheme:

$$-\nabla\cdot D\nabla\Phi^{(n+1)}+\Sigma_a\Phi^{(n+1)}(\vec{r})=\frac{1}{k^{(n)}}S^{(n)}(\vec{r})$$

$$S^{(n+1)}(\vec{r})=\nu\Sigma_f\,\Phi^{(n+1)}(\vec{r}) \tag{5-327}$$

$$k^{(n+1)}=\frac{\int d^3r\,S^{(n+1)}(\vec{r})}{\frac{1}{k^{(n)}}\int d^3r\,S^{(n)}(\vec{r})}$$

(v) We continue iterating until the error in k and/or S decreases below some specified amount:

$$\left|\frac{k^{(n)}-k^{(n-1)}}{k^{(n)}}\right|<\epsilon_1 \quad \text{and/or} \quad \left|\frac{S^{(n)}-S^{(n-1)}}{S^{(n)}}\right|<\epsilon_2 \tag{5-328}$$

for all $\vec{r}$.

This iterative scheme to determine the multiplication factor k and the corresponding flux is known as the "power iteration" or "source iteration" method. The iterations themselves are known as "outer" or "source" iterations.

Thus far, we have given only a simple physical description of the source iteration method. In actual fact, however, we have merely given a physical motivation for the most common method of computing the largest eigenvalue of a matrix, the "power" method. To see this more clearly, first rewrite our criticality eigenvalue problem as

$$\underline{\underline{A}}\,\underline{\Phi}=\frac{1}{k}\underline{\underline{F}}\,\underline{\Phi} \tag{5-329}$$

where we have inserted the eigenvalue $^1/_k$. Now to correspond more clearly with our earlier discussion, let

$$\underline{S} = \underline{\underline{F}}\,\underline{\Phi} \qquad \text{or} \qquad \underline{\Phi} = \underline{\underline{F}}^{-1}\underline{S}\,. \tag{5-330}$$

Then we can rewrite (5-329) as

$$\underline{\underline{A}}\,\underline{\underline{F}}^{-1}\underline{S} = \frac{1}{k}\underline{S} \tag{5-331}$$

This is now in the usual matrix eigenvalue problem form $\underline{\underline{M}}\underline{x} = \lambda\,\underline{x}$ if we identify

$$\underline{\underline{M}} \equiv \underline{\underline{A}}\,\underline{\underline{F}}^{-1} \tag{5-332}$$

Now suppose we define $\underline{x}_j$ and λ_j as the eigenvectors and eigenvalues of $\underline{\underline{M}}$. Then since these eigenvectors form a complete set, any initial guess we make of the fission source, say $\underline{S}^{(0)}$ must be expandable as a linear combination of the x_j--i.e.,

$$\underline{S}^{(0)} = \sum_j a_j \underline{x}_j \tag{5-333}$$

Now suppose we operate on this initial guess n times with $\underline{M} = \underline{\underline{A}}\underline{\underline{F}}^{-1}$ (of course this is just what our source iterations are doing); then

$$\underline{S}^{(n)} \equiv \underline{\underline{M}}^n \underline{S}^{(0)} = \sum_j a_j \lambda_j^n \underline{x}_j \tag{5-334}$$

Call λ_1, the largest eigenvalue of $\underline{\underline{M}}$. Then it is apparent that as n becomes very large, $\lambda_1^n >> \lambda_j^n$ for $j > 1$ and hence

$$\underline{S}^{(n)} \longrightarrow a_1 \lambda_1^n \underline{x}_1 \tag{5-335}$$

To properly scale these iterations, we need only take the ratio of various fission source components--say pointwise--to find

$$\frac{S_i^{(n+1)}}{S_i^{(n)}} \rightarrow \frac{\lambda_1^{n+1}}{\lambda_1^{n}} = \lambda_1 = \frac{1}{k} \qquad (5\text{-}336)$$

while, to within a normalization factor, $\underline{S}^n \rightarrow \underline{S}$ where $\underline{S}$ satisfies

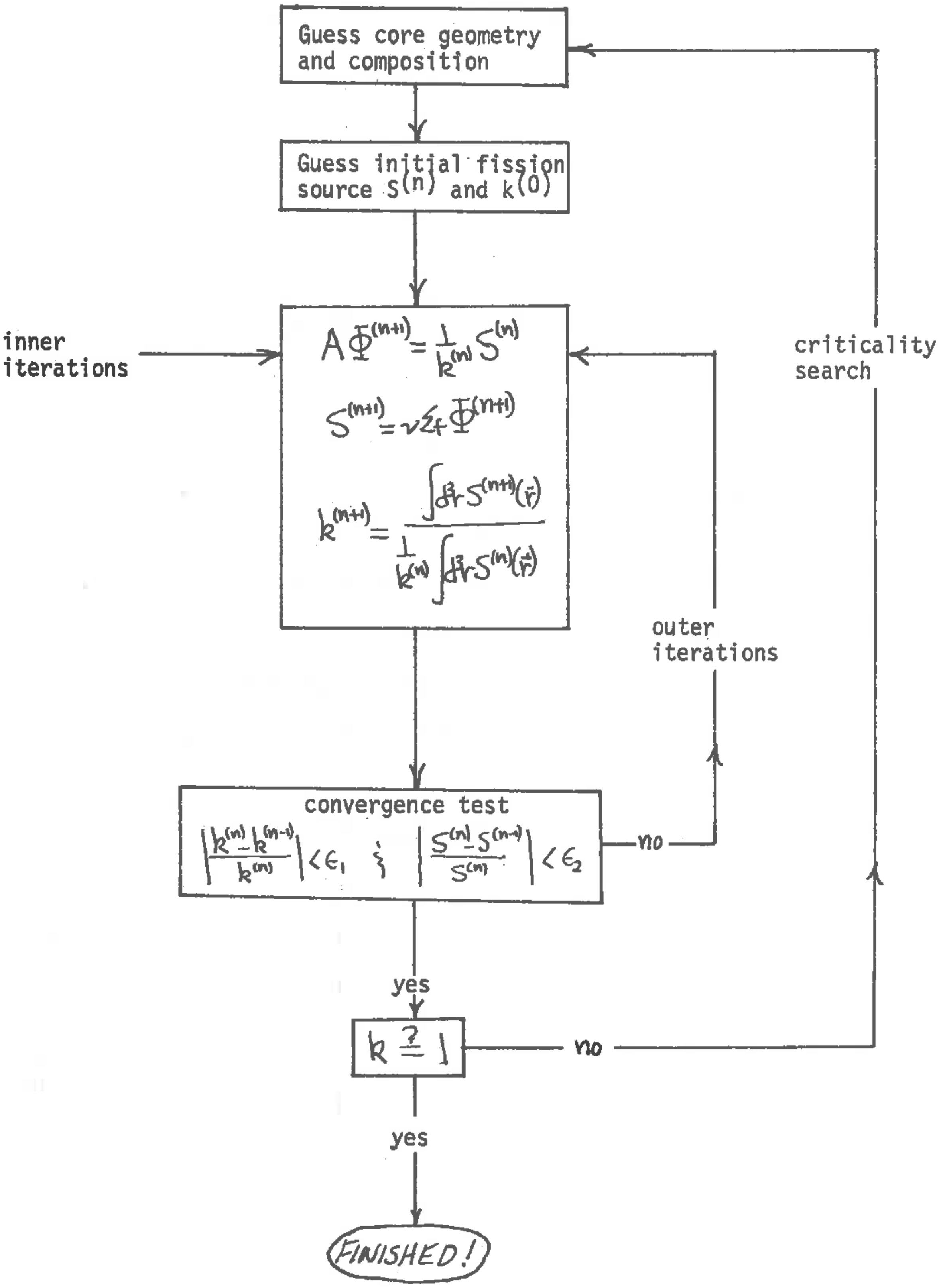
$$\underline{\underline{A}}\,\underline{F}^{-1}\underline{\underline{S}} = \frac{1}{k}\underline{S} \qquad (5\text{-}337)$$

This demonstrates that the "power" method indeed converges to the smallest value of k which will yield a nontrivial solution of the eigenvalue problem (5-331).

In addition to such outer or source iterations, one will also be required to perform "inner iterations" to solve the diffusion problem

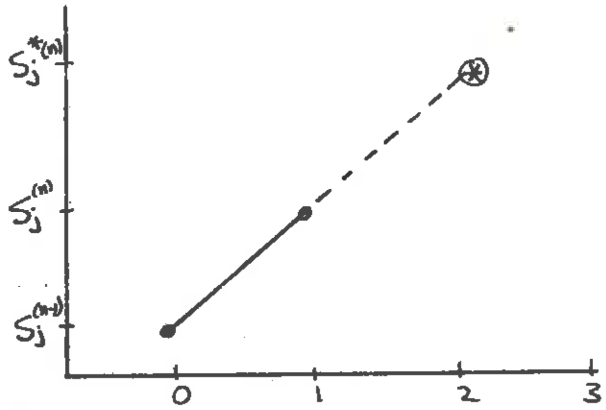
$$A\,\Phi^{(n+1)} = \frac{1}{k^{(n)}}S^{(n)} \qquad (5\text{-}338)$$

when 2 or 3-dimensional calculations are necessary. The general strategy then takes the form sketched below:


Guess core geometry and composition
Guess initial fission source $S^{(n)}$ and $k^{(0)}$
inner iterations
$A\Phi^{(n+1)} = \frac{1}{k^{(n)}} S^{(n)}$
$S^{(n+1)} = \nu\Sigma_f \Phi^{(n+1)}$
$k^{(n+1)} = \frac{\int d^3r\, S^{(n+1)}(\vec{r})}{\frac{1}{k^{(n)}} \int d^3r\, S^{(n)}(\vec{r})}$
outer iterations
criticality search
convergence test
$\left|\frac{k^{(n)} - k^{(n-1)}}{k^{(n)}}\right| < \epsilon_1$; $\left|\frac{S^{(n)} - S^{(n-1)}}{S^{(n)}}\right| < \epsilon_2$
no
yes
$k \overset{?}{=} 1$
no
yes
FINISHED!

D. Source Extrapolation

Needless to say, there is strong incentive to perform as few iterations as possible in converging to the desired accuracy. For that reason, one usually attempts to accelerate the source iteration convergence by extrapolating ahead to a new source guess. This is accomplished by introducing an extrapolation parameter (much as is used in relaxation methods). For example, in a one parameter extrapolation, one would use as the source definition



$$\underline{S}^{(n)} = \underline{\underline{F}}\left[\frac{1}{k^{(n)}}\underline{\Phi}^{(n)} + \alpha\left\{\frac{1}{k^{(n)}}\underline{\Phi}^{(n)} - \underline{S}^{(n-1)}\right\}\right] \qquad (5\text{-}339)$$

A two parameter extrapolation takes the form

$$\underline{S}^{(n)} = \underline{\underline{F}}\left[\frac{1}{k^{(n)}}\underline{\Phi}^{(n)} + \alpha\left\{\frac{1}{k^{(n)}}\underline{\Phi}^{(n)} - \underline{S}^{(n-1)}\right\} + \beta\left\{\underline{S}^{(n-1)} - \underline{S}^{(n-2)}\right\}\right] \qquad (5\text{-}340)$$

The extrapolation parameters α and β range between 0 and 1, and can be chosen either based upon prior experience or more detailed investigations of $\underline{\underline{A}}$ and $\underline{\underline{F}}$.

"Some of you may be wondering what application any of this could possibly have to the real world of drugs."

CHAPTER 6: NUCLEAR REACTOR KINETICS

We now turn our attention to an investigation of the time behavior of the neutron population in a nuclear reactor. The study of the time dependence of the neutron flux is usually referred to as nuclear reactor kinetics, in contrast to nuclear reactor dynamics which considers not only the neutronic behavior of the core, but as well those factors such as heat transfer and fluid flow which are responsible for this temporal behavior. [Although we will briefly discuss such "feedback" mechanisms in this chapter, our more detailed discussion of the dynamics of a NSSS will be deferred to Chapter 14.] One can roughly distinguish between short term changes in the neutron population such as might occur due to normal power level changes (e.g., startup or shutdown) or in an accident analysis, and longer term changes such as are induced by fission product buildup or fuel depletion. The former usually occur on a time scale of minutes or less, while the latter occur over periods of days or months. Needless to say, the analysis for each class of time behavior is quite different.

Fortunately, the one-speed diffusion model which was developed in the last chapter is capable of describing qualitatively the time behavior of a nuclear reactor--provided we make one very important modification by explicitly including the presence of delayed neutrons. Once again, such a model also illustrates the computational techniques utilized in more sophisticated models.

We begin our study of nuclear reactor kinetics by reviewing our earlier time-dependent diffusion model which assumed that all fission neutrons were emitted promptly at the time of fission in order to illustrate the importance of delayed neutrons in reactor kinetics.

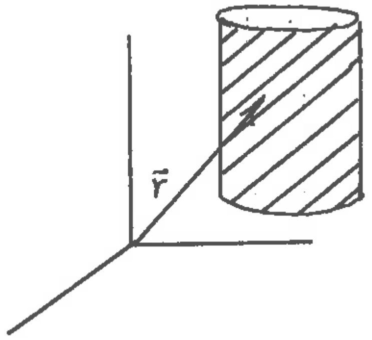
I. REACTOR KINETICS IN THE ABSENCE OF DELAYED NEUTRONS

Consider a bare, uniform reactor as described by the one-speed diffusion theory developed in Chapter 5:

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a\Phi(\vec{r},t) = \nu\Sigma_f\Phi(\vec{r},t)$$

$$\text{i.c.:}\quad \Phi(\vec{r},0) = \Phi_0(\vec{r})$$

$$\text{b.c.:}\quad \Phi(\tilde{R}_s,t) = 0 \tag{6-1}$$



Here we assume for convenience

(i) constant cross sections (uniform media)

(ii) only sources are due to fission

(iii) only "prompt" neutrons (instantaneously appear with fission)

The last assumption implies that this model is capable of only describing the prompt neutron kinetics of the reactor--a very serious limitation for most applications, as we will see momentarily.

Now recall that the solution to this initial value problem can be written in terms of an eigenfunction expansion as:

$$\Phi(\vec{r},t) = \sum_n A_n e^{-\lambda_n t}\varphi_n(\vec{r}) \tag{6-2}$$

where the eigenfunctions $\varphi_n(\vec{r})$ are defined by the eigenvalue problem:

$$\nabla^2\varphi_n + B_n^2\varphi_n(\vec{r}) = 0$$

$$\text{b.c:}\quad \varphi_n(\tilde{R}_s) = 0 \tag{6-3}$$

while the time eigenvalues λ_n are given by

$$\lambda_n = vDB_n^2 + v\Sigma_a - v\nu\Sigma_f$$

$$= v\Sigma_a(1+L^2B_n^2)\left[1 - \frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_n^2}\right] \tag{6-4}$$

Recall also that the eigenvalues are ordered as $-\lambda_1 > -\lambda_2 > \cdots\cdots$.

Hence for long times:

$$\Phi(\vec{r},t) \sim A_1 e^{-\lambda_1 t}\varphi_1(\vec{r})$$

$$= A_1 e^{\left(\frac{k-1}{\ell}\right)t}\varphi_1(\vec{r}) \tag{6-5}$$

where we have identified

$$\ell \equiv \frac{1}{v\Sigma_a(1+L^2B_g^2)} \equiv \text{mean lifetime of neutron in reactor}$$

$$k \equiv \frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_g^2} \equiv \text{multiplication constant}$$

But just how long does it take for the higher spatial modes to decay out? Consider a critical reactor for which

$$D B_1^2 - \nu \Sigma_f + \Sigma_a = 0 \quad \Rightarrow \quad B_1^2 = \frac{\nu \Sigma_f - \Sigma_a}{D} = B_m^2 \tag{6-6}$$

Then the higher modes decay out as

$$e^{-\lambda_n t} = e^{-v D (B_n^2 - B_m^2) t} \tag{6-7}$$

But for thermal neutrons, $D(B_n^2 - B_m^2) \sim n^2$ cm.
Hence, since $v \sim 10^5$ cm/sec,

$$e^{-\lambda_n t} \sim e^{-10^5 n^2 t} \tag{6-8}$$

Hence for $n > 1$, the higher modes decay out very rapidly (indeed, more rapidly than diffusion theory is actually valid for , if we recall our neglect of the $\frac{\partial J}{\partial t}$ term in our earlier derivation of Chapter 5.)

For this reason, one usually uses one-speed diffusion theory to describe the long time behavior of the fundamental mode. Stated in a different way, we assume a flux of the form

$$\Phi(\vec{r}, t) = v n(t) \varphi(\vec{r}) \tag{6-9}$$

where

$$\begin{gathered} \nabla^2 \varphi(\vec{r}) + B_g^2 \varphi(\vec{r}) = 0 \\ \varphi(\tilde{R}_s) = 0 \end{gathered} \tag{6-10}$$

and n(t) satisfies

$$\frac{dn}{dt} = \left(\frac{k-1}{\ell}\right) n(t) \, . \tag{6-11}$$

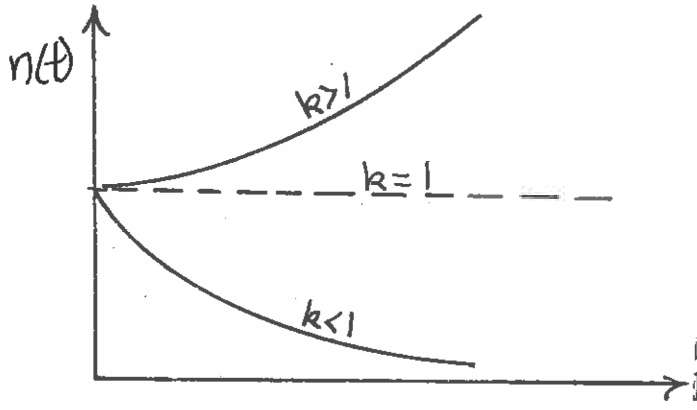
In this sense, n(t) can be interpreted as the total number of neutrons in the reactor at time t [if $\varphi(\vec{r})$ is properly normalized]. Since the normalization of n(t) is arbitrary, we could also scale the dependent variable n(t) to represent the total instantaneous power, say P(t), being generated in the core at any particular time. We will continue to regard n(t) as the neutron population in the core for the present, however.

This equation is known as the "point reactor kinetics equation" in the absence of delayed neutrons, since the space dependence has been separated out by assuming a time independent spatial flux shape, $\varphi(\vec{r})$. In that sense, we have derived a "lumped parameter" model of the reactor, which is characterized by a neutron flux time behavior of the form

$$\Phi(\vec{r},t) = v n_0 e^{\left(\frac{k-1}{\ell}\right)t} \varphi(\vec{r}) \tag{6-12}$$

and a time constant

$$T \equiv \frac{\ell}{k-1} \quad \equiv \text{reactor period} \tag{6-13}$$



This model is of course identical to that developed in our qualitative discussion of chain reaction kinetics in Chapter III--except that one-speed diffusion theory has now given us an explicit expression for the prompt neutron lifetime.

It is of interest to use these expressions to make some simple estimates of how rapidly the neutron flux (or reactor power level) will vary according to this model. In a typical thermal reactor, the prompt neutron lifetime ℓ is roughly 10^{-4} sec. Hence if we make the multiplication factor k greater than unity by a small amount, say by 0.1% such that $k - 1 = .001$, we find that the reactor period is

$$T \sim 10^{-4}/10^{-3} = 0.1 \text{ sec}$$

Hence in one second, the neutron flux in this reactor would increase by $e^{10} = 2.2 \times 10^4$--a very sizeable amount.

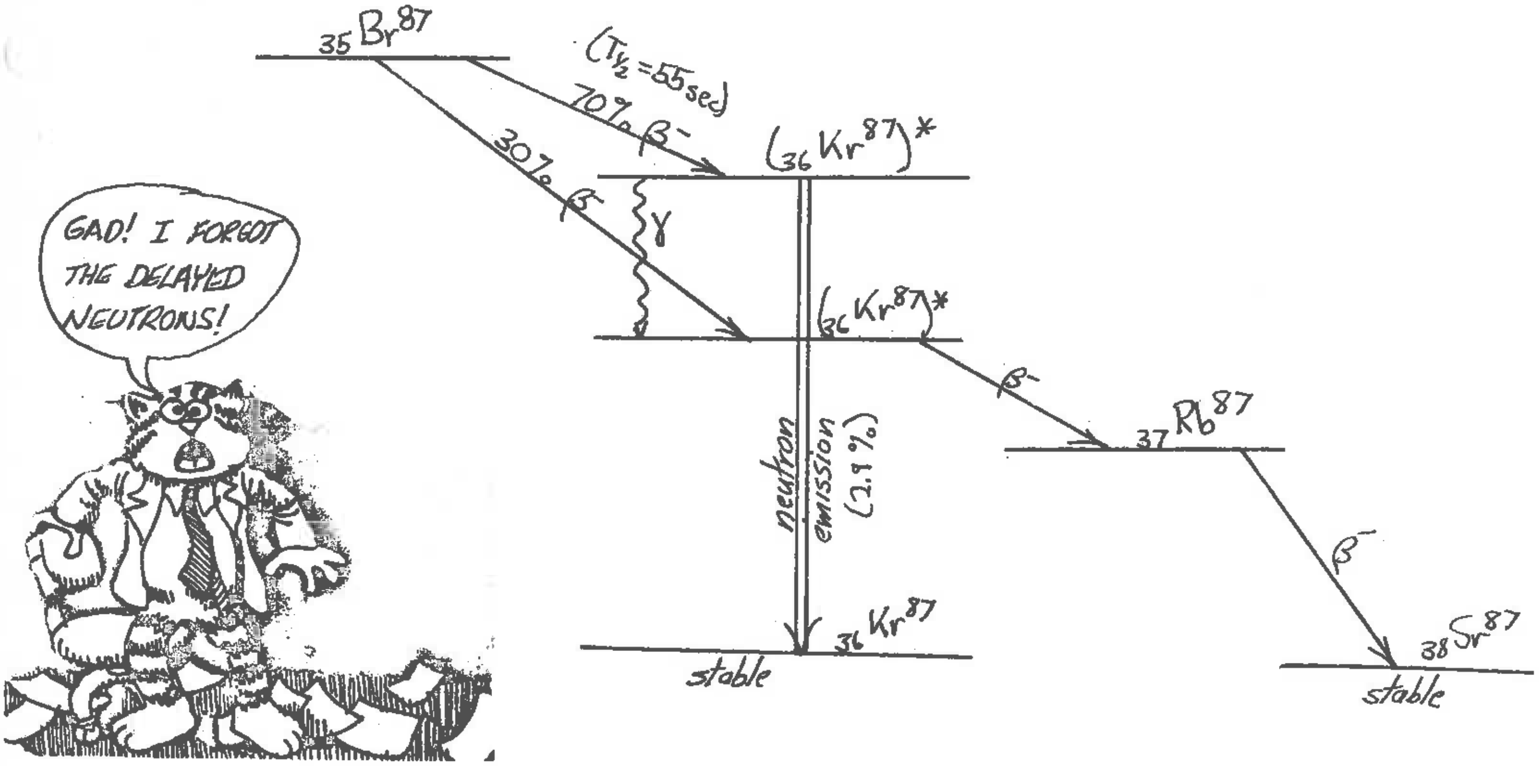
This very rapid response becomes even more severe in fast reactors, in which the prompt neutron lifetime ℓ is more typically 10^{-7}. Then a $k - 1 = .001$ would correspond to a reactor period of only 10^{-4} seconds.

Since there will normally be small fluctuations in the multiplication of even a critical reactor, the analysis above would suggest that the corresponding fluctuation in the reactor power level would be quite excessive, since even a very small change in the multiplication factor k would cause an extremely rapid change in the neutron flux because of the very short neutron lifetime. Such an analysis would suggest that nuclear reactors should be extremely difficult to control.

But in actual fact, we know that reactors are quite easy to control--and that the neutron population usually changes on a time scale of many seconds or even minutes. Hence something is very wrong with the above analysis. The culprit (or saving grace, depending on one's point of view) is our neglect of delayed neutrons. Hence we will now repeat this simple analysis, taking explicit account of the fact that some neutrons appear only after an appreciable time delay after the fission reaction.

II. THE INFLUENCE OF DELAYED NEUTRONS ON REACTOR KINETICS

Thus far we have assumed that all fission neutrons appear promptly at the time of the fission reaction. But recall from our brief discussion of fission physics that a very small fraction ($<$ 0.7%) appear after a time delay due to fission produce decay. For example, consider the decay chain of a typical fission product, ${}_{35}\mathrm{Br}^{87}$



Notice that there is a small possibility for the excited state of ${}_{36}\mathrm{Kr}^{87}$ to decay by emitting a delayed neutron.

Notice in particular that

(i) The effective delay is controlled by the preceding β-decay--in this case, $T_{1/2} = 55$ sec. $_{35}Br^{87}$ is called the "precursor" of the delayed neutron.

(ii) Only (.029) (.7) of the $_{35}Br^{87}$ nuclei yield a delayed neutron.

To be more precise, let's introduce a few definitions:

delayed neutron precursor $\equiv$ that fission fragment whose β-decay yields a daughter nucleus which subsequently decays yielding a delayed neutron

$\lambda_i \equiv$ decay constant (β-decay) of ith kind of precursor

$\beta_i \equiv$ fraction of fission neutrons due to decay of ith kind of precursor

$\beta = \sum_{i=1}^{6} \beta_i \equiv$ total fraction of fission neutrons which are delayed

To date, neutron physicists have found it sufficient to group delayed neutrons into 6 different classes--each characterized by a different decay constant λ_i and fraction β_i. These are tabulated in the tables on p. 219a.

Actually, there are also other processes which can contribute delayed neutrons to the chain reaction. Photoneutron reactions, (γ, n) are particularly important in reactors containing appreciable amounts of deuterium or beryllium (both of which are extremely good moderators). The decay times of these processes are even longer than those characterizing delayed fission neutrons, and hence such photoneutron production may be quite important in certain reactor types (such as D_2O moderated reactors). However, these neutrons can usually be handled by simply including one or more addtional groups of delayed neutrons, hence the

TABLE 6-1

Delayed-Neutron Half-Lives, Decay Constants, and Yields From Fast Fission*

Los Alamos, Ref. 11

Group index, i	Half-life, sec	Decay constant λ_i, sec^{-1}	Relative abundance $a_i \equiv \beta_i/\beta$	Absolute group yield, %
		U^{235} (99.9% 235)		
1	54.51 ± 0.94	0.0127 ± 0.0002	0.038 ± 0.003	0.063 ± 0.005
2	21.84 ± 0.54	0.0317 ± 0.0008	0.213 ± 0.005	0.351 ± 0.011
3	6.00 ± 0.17	0.115 ± 0.003	0.188 ± 0.016	0.310 ± 0.028
4	2.23 ± 0.06	0.311 ± 0.008	0.407 ± 0.007	0.672 ± 0.023
5	0.496 ± 0.029	1.40 ± 0.081	0.128 ± 0.008	0.211 ± 0.015
6	0.179 ± 0.017	3.87 ± 0.369	0.026 ± 0.003	0.043 ± 0.005
		U^{238} (99.98% 238)		
1	52.38 ± 1.29	0.0132 ± 0.0003	0.013 ± 0.001	0.054 ± 0.005
2	21.58 ± 0.39	0.0321 ± 0.0006	0.137 ± 0.002	0.564 ± 0.025
3	5.00 ± 0.19	0.139 ± 0.005	0.162 ± 0.020	0.667 ± 0.087
4	1.93 ± 0.07	0.358 ± 0.014	0.388 ± 0.012	1.599 ± 0.081
5	0.490 ± 0.023	1.41 ± 0.067	0.225 ± 0.013	0.927 ± 0.060
6	0.172 ± 0.009	4.02 ± 0.214	0.075 ± 0.005	0.309 ± 0.024
		U^{233} (100% 233)		
1	55.11 ± 1.86	0.0126 ± 0.0004	0.086 ± 0.003	0.060 ± 0.003
2	20.74 ± 0.86	0.0334 ± 0.0014	0.274 ± 0.005	0.192 ± 0.009
3	5.30 ± 0.19	0.131 ± 0.005	0.227 ± 0.035	0.159 ± 0.025
4	2.29 ± 0.18	0.302 ± 0.024	0.317 ± 0.011	0.222 ± 0.012
5	0.546 ± 0.108	1.27 ± 0.266	0.073 ± 0.014	0.051 ± 0.010
6	0.221 ± 0.042	3.13 ± 0.675	0.023 ± 0.007	0.016 ± 0.005
		Pu^{239} (99.8% 239)		
1	53.75 ± 0.95	0.0129 ± 0.0002	0.038 ± 0.003	0.024 ± 0.002
2	22.29 ± 0.36	0.0311 ± 0.0005	0.280 ± 0.004	0.176 ± 0.009
3	5.19 ± 0.12	0.134 ± 0.003	0.216 ± 0.018	0.136 ± 0.013
4	2.09 ± 0.08	0.331 ± 0.012	0.328 ± 0.010	0.207 ± 0.012
5	0.549 ± 0.049	1.26 ± 0.115	0.103 ± 0.009	0.065 ± 0.007
6	0.216 ± 0.017	3.21 ± 0.255	0.035 ± 0.005	0.022 ± 0.003
		Pu^{240} (81.5% 240)		
1	53.56 ± 1.21	0.0129 ± 0.0004	0.028 ± 0.003	0.022 ± 0.003
2	22.14 ± 0.38	0.0313 ± 0.0005	0.273 ± 0.004	0.238 ± 0.016
3	5.14 ± 0.42	0.135 ± 0.011	0.192 ± 0.053	0.162 ± 0.044
4	2.08 ± 0.19	0.333 ± 0.031	0.350 ± 0.020	0.315 ± 0.027
5	0.511 ± 0.077	1.36 ± 0.205	0.128 ± 0.018	0.119 ± 0.018
6	0.172 ± 0.033	4.04 ± 0.782	0.029 ± 0.006	0.024 ± 0.005
		Th^{232} (100% 232)		
1	56.03 ± 0.95	0.0124 ± 0.0002	0.034 ± 0.002	0.169 ± 0.012
2	20.75 ± 0.66	0.0334 ± 0.0011	0.150 ± 0.005	0.744 ± 0.037
3	5.74 ± 0.24	0.121 ± 0.005	0.155 ± 0.021	0.769 ± 0.108
4	2.16 ± 0.08	0.321 ± 0.011	0.446 ± 0.015	2.212 ± 0.110
5	0.571 ± 0.042	1.21 ± 0.090	0.172 ± 0.013	0.853 ± 0.073
6	0.211 ± 0.019	3.29 ± 0.297	0.043 ± 0.006	0.213 ± 0.031

TABLE 6-2

Delayed-Neutron Half-lives, Decay Constants and Yields from Thermal Fission *

Los Alamos, Ref. 11

Group index, i	Half-life $\tau_{1/2}$, sec	Decay constant λ, sec^{-1}	Relative abundance $a_i \equiv \beta_i/\beta$	Absolute group yield, %
U^{235} (99.9% 235)				
1	55.72 ± 1.28	0.0124 ± 0.0003	0.033 ± 0.003	0.052 ± 0.005
2	22.72 ± 0.71	0.0305 ± 0.0010	0.219 ± 0.009	0.346 ± 0.018
3	6.22 ± 0.23	0.111 ± 0.004	0.196 ± 0.022	0.310 ± 0.036
4	2.30 ± 0.09	0.301 ± 0.011	0.395 ± 0.011	0.624 ± 0.026
5	0.610 ± 0.083	1.14 ± 0.15	0.115 ± 0.009	0.182 ± 0.015
6	0.230 ± 0.025	3.01 ± 0.29	0.042 ± 0.008	0.066 ± 0.008
Pu^{239} (99.8% 239)				
1	54.28 ± 2.34	0.0128 ± 0.0005	0.035 ± 0.009	0.021 ± 0.006
2	23.04 ± 1.67	0.0301 ± 0.0022	0.298 ± 0.035	0.182 ± 0.023
3	5.60 ± 0.40	0.124 ± 0.009	0.211 ± 0.048	0.129 ± 0.030
4	2.13 ± 0.24	0.325 ± 0.036	0.326 ± 0.033	0.199 ± 0.022
5	0.618 ± 0.213	1.12 ± 0.39	0.086 ± 0.029	0.052 ± 0.018
6	0.257 ± 0.045	2.69 ± 0.48	0.044 ± 0.016	0.027 ± 0.010
U^{233} (100% 233)				
1	55.00 ± 0.54	0.0126 ± 0.0003	0.086 ± 0.003	0.057 ± 0.003
2	20.57 ± 0.38	0.0337 ± 0.0006	0.299 ± 0.004	0.197 ± 0.009
3	5.00 ± 0.21	0.139 ± 0.006	0.252 ± 0.040	0.166 ± 0.027
4	2.13 ± 0.20	0.325 ± 0.030	0.278 ± 0.020	0.184 ± 0.016
5	0.615 ± 0.242	1.13 ± 0.40	0.051 ± 0.024	0.034 ± 0.016
6	0.277 ± 0.047	2.50 ± 0.42	0.034 ± 0.014	0.022 ± 0.009

analysis we develop below will apply equally well to delayed photoneutron production.

With these concepts we can now give a very simple minded discussion of the role of delayed neutrons in nuclear reactor kinetics. First recall that the reactor period is given by

$$T = \frac{l}{k-1} \tag{6-14}$$

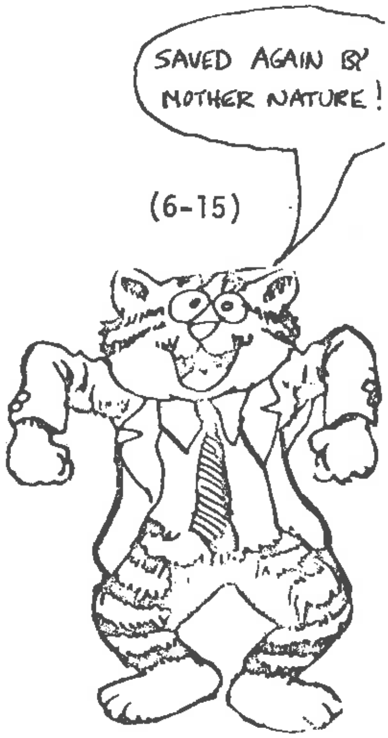
where l is the neutron lifetime. However, in calculating l earlier we assumed all neutrons were prompt. If we now define an average lifetime $\langle l \rangle$ taking into account the delayed neutrons, we find

$$\begin{aligned} \langle l \rangle &= (1-\beta) l + \sum_{i=1}^{6} \beta_i \left[\frac{1}{\lambda_i} + l \right] \\ &\cong (1-\beta) l + \sum_{i=1}^{6} \beta_i / \lambda_i \end{aligned} \tag{6-15}$$

where $l \equiv \left[v \Sigma_a (1 + L^2 B_g^2) \right]^{-1}$ as before. Now

$$l \sim 10^{-4} \text{ sec}$$

$$\sum_{i=1}^{6} \beta_i / \lambda_i \sim 0.1 \text{ sec}$$



Hence we find $\langle l \rangle \sim 0.1$ sec. Thus a (k-1) of 10^{-3} would now yield a period of 100 sec. Hence delayed neutrons substantially increase the time constant of the reactor so that effective control is possible.

This fact suggests a related idea: Suppose we consider a reactor which is very slightly subcritical on prompt neutrons. Suppose further that the fraction β of delayed neutrons provides just enough extra multiplication to achieve criticality. Then this fraction will in fact control the criticality--and hence the time constant. However, if $k-1 > \beta$, the reactor will be critical (or supercritical) on prompt neutrons alone, and the reactor period should become very short, since the delayed neutrons are not needed to sustain the chain reaction.

In actual fact, one cannot proceed so heuristically. We must first set up a set of equations describing the time dependence of the delayed neutrons. To this end, define the precursor atomic number density:

$C_i(\vec{r},t)d^3r \equiv$ expected number of "fictitious" precursors of ith kind in d^3r about $\vec{r}$ which always decay by emitting a delayed neutron (6-16)

Note that $C_i(\vec{r},t)$ is only some fraction of the true isotope concentration, since only a fraction of the ith isotope nuclei eventually decays by delayed neutron emission. For example, in our earlier case

$$C_{Br^{87}}(\vec{r},t) = (.029)(.7)\, Br^{87}(\vec{r},t) \tag{6-17}$$

One can immediately write down a balance relation for these precursor concentrations by noting

$$\begin{pmatrix}\text{\# of precursors} \\ \text{decaying in} \\ d^3r/\text{sec}\end{pmatrix} = \lambda_i C_i(\vec{r},t)\, d^3r \tag{6-18}$$

$$\begin{pmatrix}\text{\# of precursors} \\ \text{being produced} \\ \text{in } d^3r/\text{sec}\end{pmatrix} = \beta_i \nu \Sigma_f \Phi(\vec{r},t)\, d^3r \tag{6-19}$$

[This latter relation assumes the precursors don't migrate or diffuse before decaying.] We can write then that

$$\frac{\partial C_i}{\partial t} = -\lambda_i C_i(\vec{r},t) + \beta_i \nu \Sigma_f \Phi(\vec{r},t) \tag{6-20}$$

Now our old friend, the one-speed diffusion equation, can still be used to describe the flux--provided we treat the delayed neutron contribution to the fission source explicitly:

$$S_f(\vec{r},t) = (1-\beta)\nu\Sigma_f \Phi(\vec{r},t) + \sum_{i=1}^{6} \lambda_i C_i(\vec{r},t) \tag{6-21}$$

Hence our system of equations describing the neutron flux in a reactor <u>including delayed neutrons</u> is

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} - D\nabla^2\Phi + \Sigma_a \Phi(\vec{r},t) = (1-\beta)\nu\Sigma_f \Phi(\vec{r},t) + \sum_{i=1}^{6} \lambda_i C_i(\vec{r},t)$$

$$\frac{\partial C_i}{\partial t} = -\lambda_i C_i(\vec{r},t) + \beta_i \nu \Sigma_f \Phi(\vec{r},t), \qquad i = 1, \ldots, 6 \tag{6-22}$$

We will apply these once again to the asymptotic situation in which

$$\Phi(\vec{r},t) = v n(t) \varphi(\vec{r})$$

$$c_i(\vec{r},t) = c_i(t) \varphi(\vec{r}) \tag{6-23}$$

where

$$\nabla^2\varphi + B_g^2 \varphi(\vec{r}) = 0$$

$$\text{b.c:} \quad \varphi(\tilde{R}_s) = 0 \tag{6-24}$$

If we substitute these forms into Eqs. (6-19), we find

$$\frac{dn}{dt} = -vDB_g^2 n - v\Sigma_a n + (1-\beta)\nu v\Sigma_f n + \sum_{i=1}^{6} \lambda_i C_i \qquad (6\text{-}25)$$

$$\frac{dC_i}{dt} = -\lambda_i C_i(t) + \nu\beta_i\Sigma_f v n(t), \qquad i=1,\ldots,6$$

or re-arranging

$$\frac{dn}{dt} = \left[v\Sigma_a(1+L^2B_g^2)\right]\left[\frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_g^2}(1-\beta) - 1\right]n(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \qquad (6\text{-}26)$$

$$\frac{dC_i}{dt} = -\lambda_i C_i(t) + v\nu\Sigma_f \beta_i n(t), \qquad i=1,\ldots,6$$

But if we recall

$$\frac{1}{v\Sigma_a(1+L^2B_g^2)} \equiv \ell \equiv \text{prompt neutron lifetime} \qquad (6\text{-}27)$$

$$\frac{\nu\Sigma_f/\Sigma_a}{1+L^2B_g^2} \equiv k$$

then we can rewrite these

$$\frac{dn}{dt} = \frac{k(1-\beta)-1}{\ell}n(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \qquad (6\text{-}28)$$

$$\frac{dC_i}{dt} = \beta_i \frac{k}{\ell} n(t) - \lambda_i C_i(t), \qquad i=1,\ldots,6$$

These are known as the point reactor kinetics equations (P.R.K.E.) (including delayed neutrons). One frequently writes these in a somewhat different form by defining:

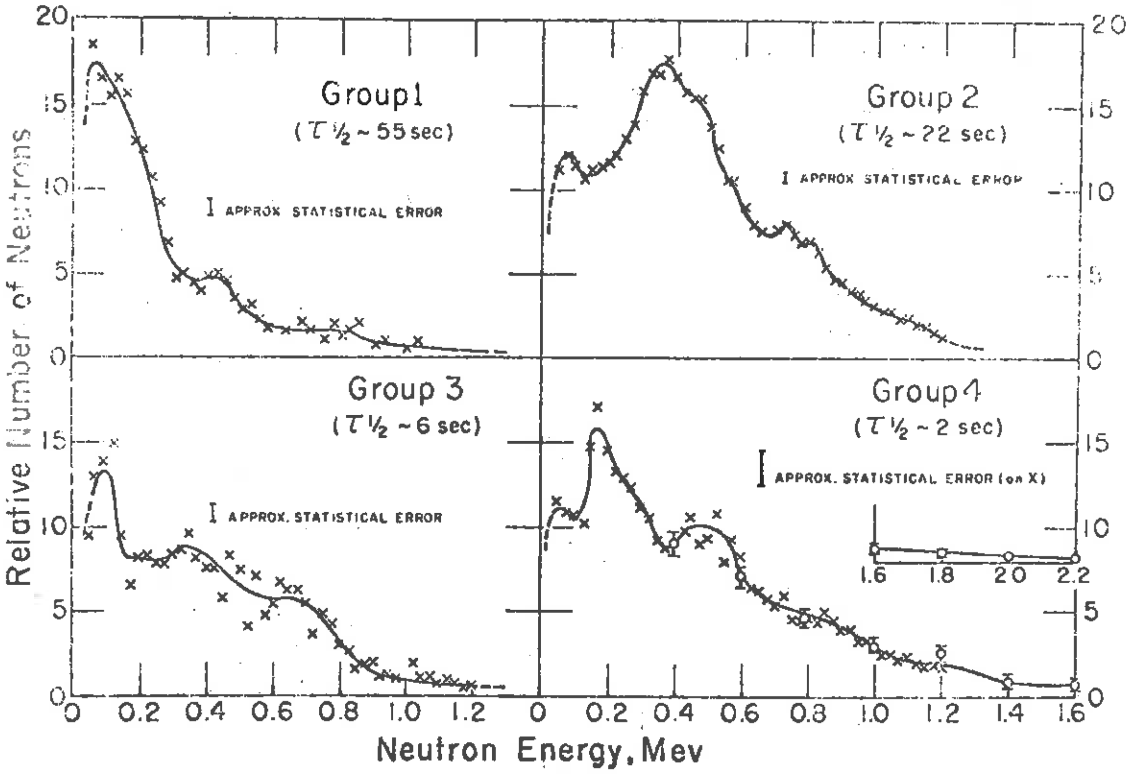


FIGURE 6-1: Measured Delayed Neutron Group Energy Spectra (Keepin)

$\Lambda \equiv \frac{1}{v\nu\Sigma_f} \equiv \frac{\ell}{k}$ mean generation time between birth of neutron and subsequent absorption inducing fission (6-29)

We define also the "reactivity" $\rho(t)$ by

$$\rho(t) = \frac{k(t)-1}{k(t)} \tag{6-30}$$

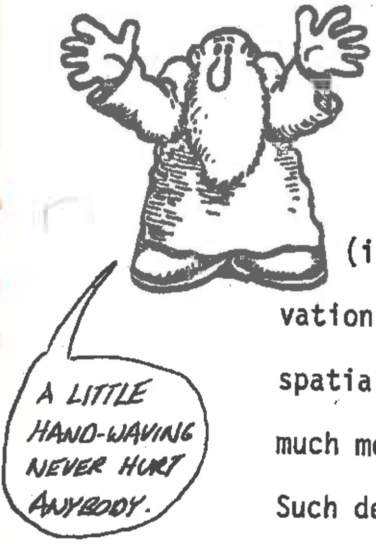
[Notice here we have explicitly indicated that k and hence ρ may be a function of time. We will comment more upon this in a moment.]

Then the PRKE can be written in perhaps their most conventional form

$$\begin{aligned} \frac{dn}{dt} &= \left[\frac{\rho(t)-\beta}{\Lambda}\right] n(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \\ \frac{dC_i}{dt} &= \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t), \qquad i = 1, \ldots, 6 \end{aligned} \tag{6-31}$$

Several comments concerning these equations are necessary at this point:

(i) As they stand, the PRKE are a set of 7 coupled ordinary differential equations in time. However, their solution is not straightforward for several reasons. First, the reactivity, $\rho(t)$, is usually a function of time--and, in fact, frequently depends upon the neutron population n(t). Hence the equations will generally be nonlinear. Furthermore, the time constants characterizing the nuclear processes represented by the equations range all the way from $\Lambda \sim 10^{-4}$ sec to the lifetime of the longest lived precursor, usually about 80 sec. These widely different time scales greatly complicate the numerical solution of these rather simple appearing equations.



(ii) A number of questionable assumptions have entered into the derivation of these equations (e.g., one-speed diffusion theory, a single spatial mode, etc.) However these equations can infact be derived in a much more general fashion in which such assumptions are not necessary. Such derivations usually proceed from the transport equation itself and are also usually very formal. They lead, however, to the set (6-28) in which only the definitions of β, Λ, and ρ are changed. Hence provided one uses more general expressions for these parameters, the point reactor kinetics equations can be regarded as having a much broader domain of validity.

(iii) Even without this more general analysis, one can generalize these equations to account for energy dependent effects. These arise principally because the delayed neutrons appear with a much different energy spectrum than do the prompt fission neutrons (see Figure 6-1). Hence each delayed neutron group will be characterized by a slightly different fast nonleakage probability and resonance escape probability, say P^i_{re} and P^i_{FNL}. To take account of this, we can merely modify the definition of the parameters appearing in the point reactor kinetics equations as

$$k \rightarrow \eta f \epsilon p P_{NTL} P_{NFL} \qquad (6\text{-}32)$$

$$\lambda_i \rightarrow \lambda_i P^i_{re} P^i_{NFL} \qquad (6\text{-}33)$$

$$\beta_i \rightarrow \overline{\beta_i} \equiv \frac{\beta_i P_{re}^i P_{NFL}^i}{(1-\beta) P_{re} P_{NFL} + \sum_i \beta_i P_{re}^i P_{NFL}^i} \equiv \frac{\beta_i P_{re}^i P_{NFL}^i}{\langle P_{re}{}^{\frown}{}_{NFL} \rangle} \qquad (6\text{-}34)$$

$$\beta \rightarrow \bar{\beta} \equiv \sum_{i=1}^{6} \bar{\beta}_i \qquad (6\text{-}35)$$

in which case the point reactor kinetics equations become:

$$\frac{dn}{dt} = \left[\frac{\rho(t) - \bar{\beta}}{\Lambda}\right] n(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \qquad (6\text{-}36)$$

$$\frac{dC_i}{dt} = \frac{\bar{\beta}_i}{\Lambda} n(t) - \lambda_i C_i(t)$$

Let us now re-examine the reactivity, $\rho(t)$, which appears in these equations, by first recalling that

$$\rho = \frac{k-1}{k} \qquad (6\text{-}37)$$

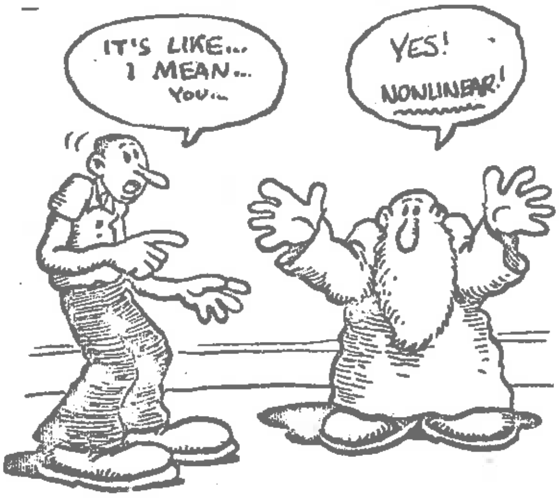
But we know that the multiplication factor k--and hence ρ--depends upon the size and composition of the reactor. In our specific model, in fact, k is explicitly given by

$$k = \frac{(\nu\Sigma_f/\Sigma_a)\langle P_{re} P_{NFL}\rangle}{1+L^2B_g^2} \qquad (6\text{-}38)$$

Hence by changing the size or composition--say by inserting or withdrawing a rod of absorbing material or adjusting a poison concentration--we can change ρ and hence control the reactor. In this sense, ρ will in general be a function of time which is partly under the control of the reactor operator.

But for any reactor operating at power, ρ will also depend upon the flux itself due to several factors. First, the power level will influence the temperature of the components of the reactor core. But the atomic concentrations of materials in the core depend sensitively upon their temperature. As the temperature changes, they may contract or expand or change phase. This in turn will cause a change in the macroscopic cross sections--and hence in the reactivity. Furthermore, the atomic concentration of materials in the core will vary as fission products are produced or fuel nuclei are fissioned and depleted. This will also strongly influence the reactivity.

Such processes whereby the reactor operating conditions will affect the criticality of the core are known as "feedback effects" and play an extremely important role in reactor operation. Stated mathematically, such feedback effects imply that



$$\rho = \rho[n(t), t]$$

Hence the point reactor kinetics equations are actually a coupled set of non-linear ordinary differential equations which are extremely difficult to analyze analytically with the exception of certain very simplified model cases.

Although we will discuss the physics of several of the more prominent feedback mechanisms, we will not initially present a detailed discussion of the study of these equations in which feedback has been explicitly included. Rather we will limit our study to those cases in which $\rho(t)$ is a specified function of time (and hence the point reactor kinetics equations are linear). Such a situation is commonly referred to as the zero-power point reactor model, since it ignores the feedback that would occur due to variations in the reactor power level. Although limited in this sense, this model does reveal quite a bit about the time behavior of the neutron population in a reactor, however.

III. SOLUTION OF THE POINT REACTOR KINETICS EQUATIONS [REACTOR KINETICS]

A. Solution With One Effective Delayed Group

Let us now consider the solution of the point reactor kinetics equations for a constant value of reactivity, $\rho(t) = \rho$. For simplicity, we will only consider one effective group of delayed neutrons characterized by β and λ. [Actually, we can get reasonable numbers from such a model if we choose β and λ properly. For example,

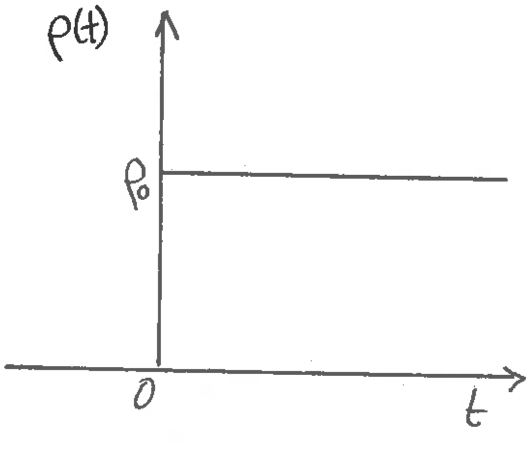
$$\beta = \sum_i \beta_i \cong .0075$$

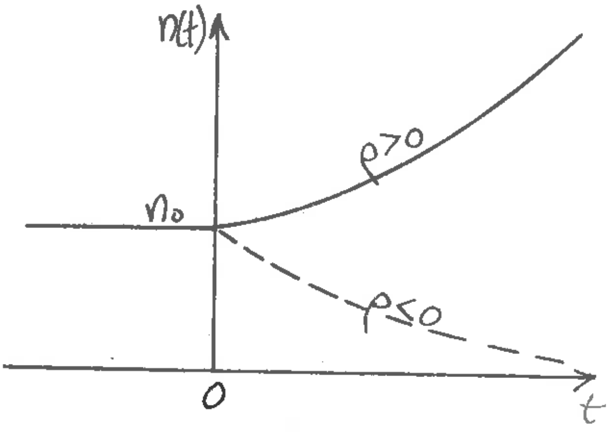
$$\lambda = \langle\lambda\rangle = \left[\frac{1}{\beta}\sum_i \frac{\beta_i}{\lambda_i}\right]^{-1} \cong .08 \text{ sec}^{-1} \Big] \tag{6-40}$$

Then the point reactor kinetics equations become

$$\begin{aligned} \frac{dn}{dt} &= \left(\frac{\rho-\beta}{\Lambda}\right) n(t) + \lambda c(t) \\ \frac{dc}{dt} &= \frac{\beta}{\Lambda} n(t) - \lambda c(t) \end{aligned} \tag{6-41}$$

In particular, we will assume the reactor to be operating at some steady-state level n_0 for $t<0$ $[\text{i.e.}, \rho=0]$, and then introduce a non-zero reactivity ρ for $t \geq 0$.





Note that prior to t = 0,

$$0 = -\frac{\beta}{\Lambda}n_0 + \lambda C_0$$

and $\qquad \Rightarrow \quad C_0 = \frac{\beta}{\lambda\Lambda}n_0$

$$0 = \frac{\beta}{\Lambda}n_0 - \lambda C_0 \tag{6-42}$$

Hence we must solve the coupled ODE's (VI-36) for the initial conditions

$$\begin{aligned} n(0) &= n_0 \\ c(0) &= \frac{\beta}{\lambda\Lambda}n_0 \end{aligned} \tag{6-43}$$

This can be accomplished in a number of ways (the easiest being by Laplace transform, as discussed in Appendix H). Let's use a more pedestrian approach by seeking solutions of the form

$$\begin{aligned} n(t) &= Ne^{\omega t} \\ c(t) &= Ce^{\omega t} \end{aligned} \tag{6-44}$$

Then substituting these into (VI-36) yields

$$\begin{aligned} \omega N &= \left(\frac{\rho-\beta}{\Lambda}\right)N + \lambda C \\ \omega C &= \frac{\beta}{\Lambda}N - \lambda C \end{aligned} \tag{6-45}$$

$$\left(\frac{\rho-\beta}{\Lambda}\right)N + \lambda C = 0$$

$$-\frac{\beta}{\Lambda}N + (\omega+\lambda)C = 0 \qquad (6\text{-}46)$$

This set of homogeneous equations has a solution if and only if

$$\left(\omega - \frac{\rho-\beta}{\Lambda}\right)(\omega+\lambda) - \frac{\lambda\beta}{\Lambda} = 0$$

or

$$\omega^2 + \left[\lambda - \left(\frac{\rho-\beta}{\Lambda}\right)\right]\omega + \left[-\left(\frac{\rho-\beta}{\Lambda}\right)\lambda - \frac{\lambda\beta}{\Lambda}\right] = 0$$

or (6-47)

$$\Lambda\omega^2 + (\lambda\Lambda + \beta - \rho)\omega - \rho\lambda = 0$$

The roots of this polynomial are

$$\omega_{0,1} = \frac{1}{2\Lambda}\left[-(\beta-\rho+\lambda\Lambda) \pm \sqrt{(\beta-\rho+\Lambda)^2 + 4\Lambda\lambda\rho}\right] \qquad (6\text{-}48)$$

Hence we must seek general solutions of the forms

$$n(t) = N_0 e^{\omega_0 t} + N_1 e^{\omega_1 t} \qquad (6\text{-}49)$$

$$c(t) = C_0 e^{\omega_0 t} + C_1 e^{\omega_1 t}$$

To determine the four unknowns, use the initial conditions

$$n(0) = n_o = N_o + N_1$$

$$c(0) = \frac{\beta}{\lambda\Lambda} n_o = C_o + C_1 \tag{6-50}$$

and from the above equations

$$\frac{\beta}{\Lambda} N_o = (\omega_o + \lambda) C_o$$

$$\frac{\beta}{\Lambda} N_1 = (\omega_1 + \lambda) C_1 \tag{6-51}$$

This is still a messy set of equations. To simplify, we will assume $\lambda\Lambda << 1$. Then

$$\omega_o \cong \frac{\lambda\rho}{\beta - \rho} \quad , \quad \omega_1 \cong -\left(\frac{\beta - \rho}{\Lambda}\right) \tag{6-52}$$

Then we find

$$n(t) \sim \frac{\beta}{\beta - \rho} e^{\left(\frac{\lambda\rho}{\beta-\rho}\right)t} - \frac{\rho}{\beta - \rho} e^{-\left(\frac{\beta-\rho}{\Lambda}\right)t} \tag{6-53}$$

for $|\rho| << \beta$.

Notice:

(i) Regardless of the sign of ρ , one of the exponentials is always decaying.

(ii) For $\rho = \beta$, we get garbage--since the approximations fail.

(iii) Consider an example

ρ = .0025

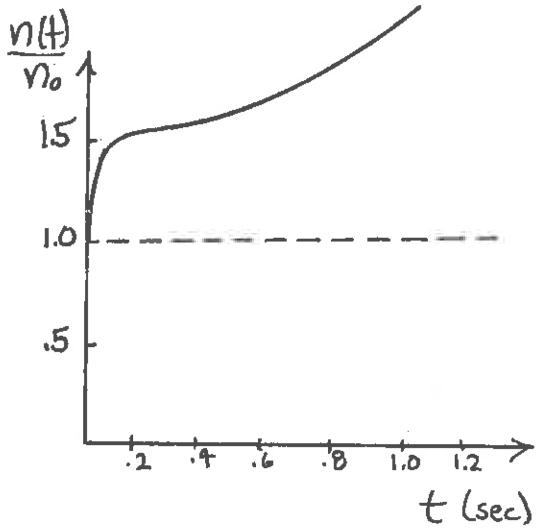
β = .0075

λ = .08 sec^{-1}

Λ = 10^{-3} sec

Then

$$\frac{n(t)}{n_o} = 1.5e^{.04t} - .5e^{-5t}$$



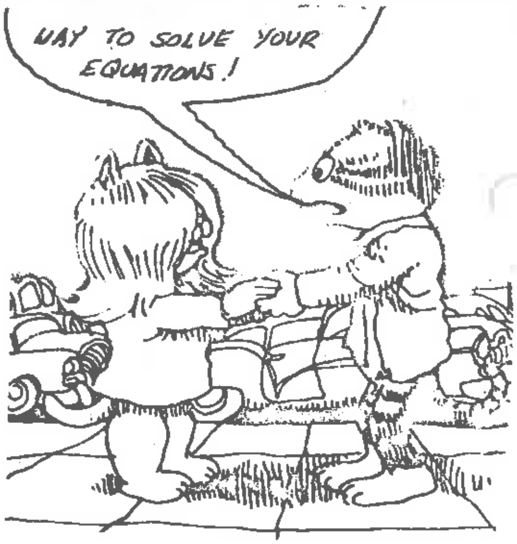
In this example, the role of the delayed neutrons in controlling the period of the reactor for $\rho < \beta$ is evident. The transient term dies out very rapidly so that for times $t > .1$,

$$\frac{n(t)}{n_o} \cong 1.5\, e^{.04t} \tag{6-55}$$

and we say the reactor is on a "stable period" of

$$T = \frac{\beta - \rho}{\rho\lambda} \cong 25 \text{ sec} \tag{6-56}$$

By way of contrast, let us repeat this analysis using Laplace transforms. We will again consider a reactor operating at a steady-state level n_o for $t < 0$ and at $t = 0$, introduce a reactivity ρ



$$\frac{dn}{dt} = \left[\frac{\rho-\beta}{\Lambda}\right] n(t) + \lambda c(t)$$

$$\frac{dc}{dt} = \frac{\beta}{\Lambda} n(t) - \lambda c(t)$$

If we define the Laplace transform (see Appendix H)

$$\tilde{n}(s) \equiv \int_0^\infty dt\, e^{-st} n(t) \equiv \mathcal{L}\{n(t)\} \tag{6-58}$$

and recall

$$\mathcal{L}\left\{\frac{dn}{dt}\right\} = s\tilde{n}(s) - n(0) \tag{6-59}$$

Thus transforming the kinetics equations yields an albegraic system:

$$\begin{aligned} s\tilde{n}(s) - n(0) &= \left(\frac{\rho-\beta}{\Lambda}\right)\tilde{n}(s) + \lambda\tilde{c}(s) \\ s\tilde{c}(s) - c(0) &= \frac{\beta}{\Lambda}\tilde{n}(s) - \lambda\tilde{c}(s) \end{aligned} \tag{6-60}$$

We can solve the second of the these equations for

$$\tilde{c}(s) = \frac{c(0)}{s+\lambda} + \frac{\beta}{\Lambda}\frac{\tilde{n}(s)}{s+\lambda} \tag{6-61}$$

and plug this into Eq. (6-60) to find

$$s\tilde{n}(s) - n(0) = \left(\frac{\rho-\beta}{\Lambda}\right)\tilde{n}(s) + \frac{\lambda\beta}{\Lambda}\frac{\tilde{n}(s)}{s+\lambda} + \frac{\lambda c(0)}{s+\lambda} \tag{6-62}$$

or

$$\tilde{n}(s) = \frac{n(0) + \dfrac{\lambda C(0)}{s+\lambda}}{\left[s - \left(\dfrac{\rho-\beta}{\Lambda}\right) - \dfrac{\beta}{\Lambda}\dfrac{\lambda}{s+\lambda}\right]} \tag{6-63}$$

Further manipulation yields

$$\begin{aligned} \frac{1}{s - \left(\dfrac{\rho-\beta}{\Lambda}\right) - \dfrac{\beta}{\Lambda}\dfrac{\lambda}{s+\lambda}} &= \frac{\Lambda}{s\Lambda - \rho + \beta - \beta\left(\dfrac{\lambda}{s+\lambda}\right)} \\ &= \frac{\Lambda}{s\Lambda - \rho + \dfrac{\beta s}{s+\lambda}} \end{aligned} \tag{6-64}$$

Furthermore, we can utilize our information that the reactor has been operating at constant n_o for $t<0$ to find

$$C(0) = \frac{\beta}{\Lambda} n_o \tag{6-65}$$

Then

$$\begin{aligned} \tilde{n}(s) &= \frac{\Lambda}{s\Lambda - \rho + \dfrac{\beta s}{s+\lambda}}\left[n_o + \frac{\beta n_o/\lambda}{s+\lambda}\right] \\ &= \frac{\Lambda(s+\lambda) + \beta}{\Lambda s^2 + (\lambda\Lambda+\beta-\rho)s - \rho\lambda}\, n_o \end{aligned} \tag{6-66}$$

Now we must invert to find $\mathcal{L}^{-1}\{\tilde{n}(s)\} = n(t)$. Since we have a ratio of two polynomials, we can simply find poles--i.e., zeros of denominator given by

$$s_{0,1} = \frac{1}{2\Lambda}\left[-(\beta-\rho+\lambda\Lambda) \pm \sqrt{(\beta-\rho+\Lambda)^2+4\Lambda\lambda\rho}\right] \tag{6-67}$$

This is still two complicated for our purposes. Consider again the special case: $|\rho| << \beta.$ Then

$$s_0 \cong \frac{\lambda\rho}{\beta-\rho} \quad , \quad s_1 \cong -\left(\frac{\beta-\rho}{\Lambda}\right) \tag{6-68}$$

Hence from

$$\tilde{n}(s) = \frac{\Lambda(s+\lambda)+\beta}{\Lambda(s-s_0)(s-s_1)}\, n_0$$

we can invert to find

$$n(t) = \frac{\Lambda(s+s_0)+\beta}{\Lambda(s_0-s_1)} n_0 e^{s_0 t} + \frac{\Lambda(s+s_1)+\beta}{\Lambda(s_1-s_0)} n_0 e^{s_1 t}$$

$$\sim \frac{\beta}{\beta-\rho} e^{\left[\frac{\lambda\rho}{\beta-\rho}\right]t} - \frac{\rho}{\beta-\rho} e^{-\left[\frac{\beta-\rho}{\Lambda}\right]t} \tag{6-70}$$

$$|\rho| << \beta.$$

just as before.

B. The Inhour Equation

Recall that the time constants ω_0 and ω_1 were given as the roots of

$$\omega\Lambda - \rho + \frac{\beta\omega}{\omega+\lambda} = 0 \tag{6-71}$$

Let's rewrite this in a slightly different form

$$\rho = \frac{k-1}{k} \Rightarrow k = \frac{1}{1-\rho}$$
$$\Rightarrow \Lambda = \frac{l}{k} = l(1-\rho) \tag{6-72}$$

Hence

$$\rho = \omega\Lambda + \frac{\omega\beta}{\omega+\lambda} = \omega l(1-\rho) + \frac{\omega\beta}{\omega+\lambda}$$

or

$$\rho = \frac{\omega l}{\omega l+1} + \frac{1}{\omega l+1}\left(\frac{\omega\beta}{\omega+\lambda}\right) . \tag{6-73}$$

This equation determines the time constants ω for any constant reactivity ρ. In the more general case of 6 delayed groups, this relation becomes

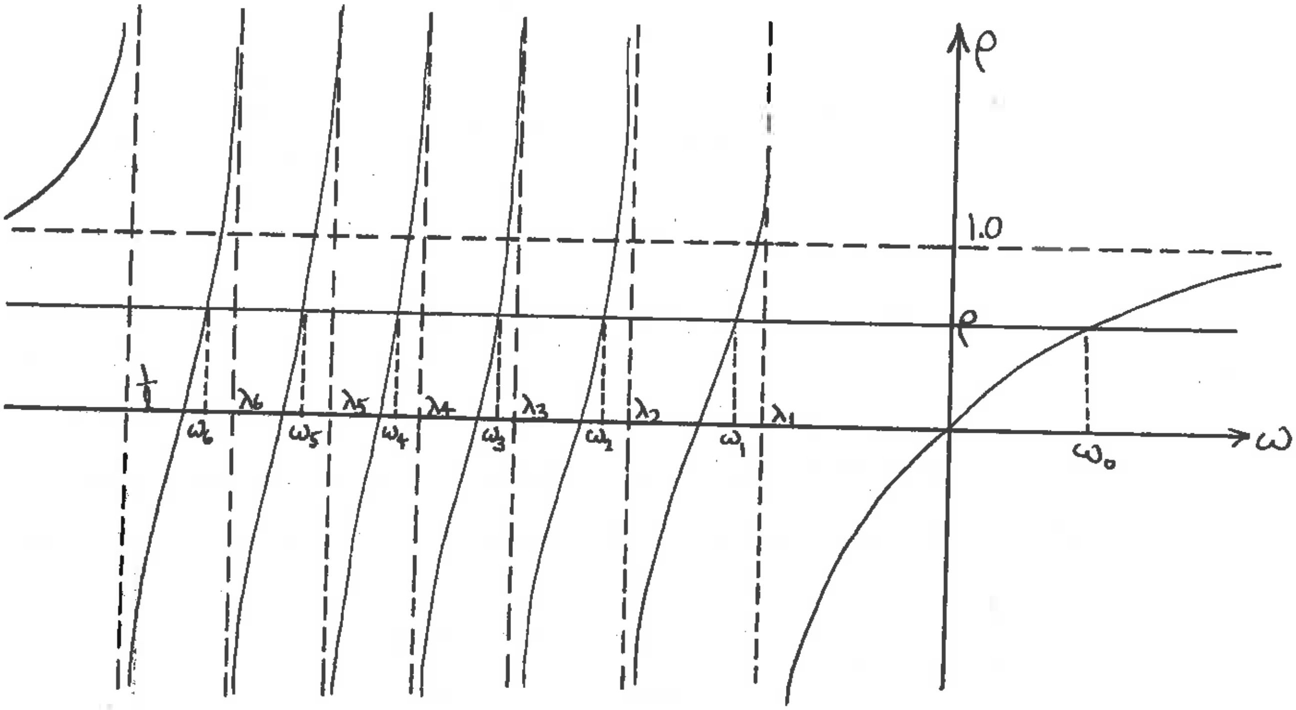
$$\rho = \frac{\omega l}{\omega l+1} + \frac{1}{\omega l+1}\sum_{i=1}^{6}\frac{\omega\beta_i}{\omega+\lambda_i} . \tag{6-74}$$

This is known as the "inhour equation". [Reactivity was first expressed in units of "inverse hour" or

inhour $\equiv$ reactivity which will make the reactor period equal to one hour

Today one measures reactivity in either percentage or another unit called the dollar (see later discussion).]

To determine the roots of the inhour equation, one can plot the right hand side (RHS) of (6-53) vs. ω.



The intersection of these curves with ρ yields the decay constants ω_i characterizing the time behavior

$$n(t) = \sum_{i=0}^{6} n_i e^{\omega_i t} \tag{6-75}$$

In particular, note that the reactor period is defined to be

$$T = 1/\omega_0 \tag{6-76}$$

Several features of these roots should be noted as ρ ranges between

$$-\infty < \rho = \frac{k-1}{k} < 1 \tag{6-77}$$

(i) Notice the limiting cases

$$\begin{aligned} \rho = 0 &\Rightarrow \omega_0 = 0 \qquad \text{critical} \\ \rho \to 1 &\Rightarrow \omega_0 \to \infty \\ \rho \to -\infty &\Rightarrow \omega_0 \to -\lambda_1 \end{aligned} \tag{6-78}$$

This last limit is particularly interesting, for it says that no matter how much negative reactivity we introduce, we cannot shut the reactor down any faster than on a period T = $1/\lambda_1$ (for thermal reactors, $\frac{1}{\lambda_1} \sim 80$ sec).

(ii) Again note that regardless of the sign of ρ, only one root, ω_0, can be positive.

(iii) Some special cases are of interest:

a. ρ small $\Rightarrow$ ω_0 is small

$$|\omega_0| << \lambda_1 < \lambda_2 < \cdots < \frac{1}{\ell} \tag{6-79}$$

Hence in the inhour equation

$$\rho = \frac{\omega_0}{\omega_0 + 1/\ell} + \frac{1/\ell}{\omega_0 + 1/\ell} \sum_{i=1}^{6} \frac{\omega_0 \beta_i}{\omega_0 + \lambda_i}$$

$$\sim \omega_0 \ell + \omega_0 \sum_{i=1}^{6} \beta_i/\lambda_i \tag{6-81}$$

Thus

$$T = \frac{1}{\omega_0} = \frac{1}{\rho}\left[\ell + \sum_{i=1}^{6} \frac{\beta_i}{\lambda_i}\right] = \frac{\langle \ell \rangle}{\rho} \cong \frac{\langle \ell \rangle}{k-1}, \tag{6-82}$$

and this is identical to our earlier heuristic result

b. ρ large $(\rho >> \beta)$

Now

$$\rho \sim \frac{\omega_0}{\omega_0 + 1/\ell} + \frac{1/\ell}{\omega_0 + 1/\ell} \sum_{i=1}^{6} \beta_i$$

or

$$\rho\,(\omega_0 + 1/\ell) = \omega_0 + \beta/\ell \tag{6-83}$$

Hence

$$T = \frac{1}{\omega_0} = \frac{\ell}{k(\rho - \beta)} \cong \frac{\ell}{k-1} \tag{6-84}$$

which is just the result we obtained <u>ignoring</u> delayed neutrons.

c. $\rho \doteq \beta$: This is essentially the "break" point between a reactor controlled by delayed neutrons and that governed by prompt neutrons alone. Recall that

$$\frac{dn}{dt} = \left[\frac{k(1-\beta)-1}{\ell}\right]n(t) + \sum_{i=1}^{6} \lambda_i C_i(t). \tag{6-85}$$

Now for the reactor to be critical on prompt neutrons alone, we require

$$k(1-\beta)-1 = 0$$

or

$$k = \frac{1}{1-\beta}$$

or

$$\rho = \frac{k-1}{k} = \frac{\beta}{1-\beta} \sim \beta \tag{6-86}$$

Hence for

$\rho<\beta$ reactor is subcritical on prompt neutrons alone

$\rho=\beta$ reactor is critical on prompt neutrons alone

$\rho>\beta$ reactor is supercritical on prompt neutrons alone

Some common terminology here is

$0<\rho<\beta$ "delayed critical"

$\rho\geq\beta$ "prompt critical or supercritical"

For this reason, it has become customary to measure reactivity in units of β such that

$$\rho = \beta \cong 1\ \$\ \text{of reactivity} \tag{6-87}$$

This unit of reactivity has led to yet another common form of the point reactor kinetics equations. Suppose we define

$$\$(t) \equiv \rho(t)/\beta \qquad \text{reactivity in dollars} \tag{6-88}$$

$$a_i \equiv \bar{\beta}_i/\beta \qquad \text{relative abundance of delayed neutron group } i \text{ [note } \sum_{i=1}^{6} a_i = 1 \text{]}$$

$$\mathcal{C}_i(t) = c_i(t)\Lambda/\beta$$

Then our equations take the form

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = [\$(t) - 1]P(t) + \sum_{i=1}^{6} \lambda_i \mathcal{C}_i(t) \tag{6-89}$$

$$\frac{d\mathcal{C}_i}{dt} = a_i P(t) - \lambda_i \mathcal{C}_i(t), \qquad i = 1, \ldots, 6$$

For variety, we have also scaled n(t) to represent the reactor power level P(t) in these equations. It is evident from these equations that the conditions $\$ = 1$ leads again to the prompt critical interpretation.

In summary, we have plotted in Figure 6-2 the reactor period $T = 1/\omega_0$ vs. ρ for both positive and negative reactivity insertions (characterizing a typical thermal reactor).

C. The Inverse Method

There are very few problems for which it is possible to obtain an exact solution for n(t) given a specific ρ(t). Actually, it is frequently more convenient to invert the problem by determining that ρ (t) which will yield a desired n(t) behavior, since this is more in line with the philosopy of reactor control.

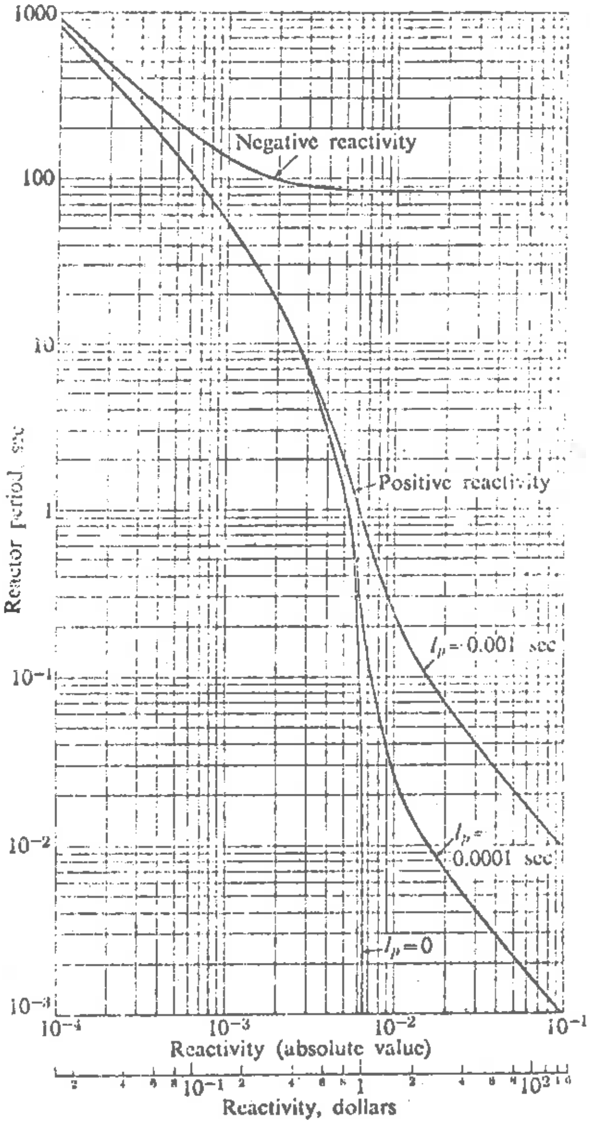


FIGURE 6-2:: Reactor period as a function of positive and negative reactivity for a U^{235} fueled reactor (Lamarsh)

In order to solve for $\rho(t)$ in terms of n(t), let us first derive yet another form of the point reactor kinetics equations. Suppose we begin by formally solving the equations for the precursors in terms of n(t):

$$C_i(t) = C_i(t_0)e^{-\lambda_i(t-t_0)} + \int_{t_0}^{t} dt' a_i n(t') e^{-\lambda_i(t-t')} \tag{6-90}$$

In particular, let $t_0 \to -\infty$, assuming

$$\lim_{t_0\to-\infty} C_i(t_0)\, e^{\lambda_i t_0} = 0 \tag{6-91}$$

to find

$$C_i(t) = \int_{-\infty}^{t} dt' a_i n(t') e^{-\lambda_i(t-t')} = \int_0^\infty d\tau\, a_i e^{-\lambda_i\tau} n(t-\tau) \tag{6-92}$$

where we have let $\tau = t-t'$. Now substitute this into the first of equations (6-89) to find

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = (\$-1)P(t) + \int_0^\infty d\tau \left[\sum_{i=1}^{6} a_i e^{-\lambda_i\tau}\right] n(t-\tau) \tag{6-93}$$

or defining the "delayed neutron kernel"

$$D(\tau) \equiv \sum_{i=1}^{6} \lambda_i a_i e^{-\lambda_i\tau} \tag{6-94}$$

[note $D(\tau)\,d\tau \equiv$ probability that a delayed neutron will be emitted in $d\tau$ about τ following a fission event at $\tau=0$], we find an "integro-differential form" of the point reactor kinetics equations

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = [\$(t)-1]P(t) + \int_0^\infty d\tau\, D(\tau)\, n(t-\tau). \qquad (6\text{-}95)$$

We can now easily solve this to find

$$\$(t) = 1 + \frac{\Lambda}{\beta}\frac{d}{dt}[\ln P(t)] - \int_0^\infty d\tau\, D(\tau)\frac{n(t-\tau)}{n(t)} . \qquad (6\text{-}96)$$

This particular relationship is important for two reasons:

(i) It can in principle be used to determine the time dependence of the applied reactivity required to yield a specific power variation--that is, to program the control rod motion.

(ii) The interpretation of the measured power responses in transient analyses of reactivity changes can be used to provide information about the feedback mechanism in the reactor.

Several specific applications of this relationship are of considerable interest:

1. <u>Periodic Power Variation</u>

Suppose

$$P(t) = P_0 + P_1 \sin\omega t, \qquad (6\text{-}97)$$

Then one finds from Eq. (6-96) that

$$\$(t) = \frac{P_1}{P_0}|Y(i\omega)|\,\frac{\sin(\omega t-\phi)}{1+\frac{P_1}{P_0}\sin\omega t} \qquad (6\text{-}98)$$

$$\phi = \arg\left[\frac{1}{Y(i\omega)}\right]$$

$$Y(i\omega) = i\omega\left(\frac{\Lambda}{\beta} + \sum_{i=1}^{6}\frac{a_i}{i\omega+\lambda_i}\right)$$

Notice in particular that the reactivity insertion which gives rise to a pure sinusoidal power variation is periodic--but <u>not</u> sinusoidal (at least for large power variations).

One can in fact show that \$(t) has a negative bias:

$$\$_{ave} \equiv \frac{1}{T}\int_0^T \$(t)\,dt = -Re\{Y(i\omega)\}\left[\sqrt{1-(P_1/P_0)^2}-1\right] \tag{6-99}$$

It's interesting to note that these features carry through for more general periodic power variations. That is, suppose

$$P(t) = P(t+nT) \qquad n = 0, \pm 1, \cdots \tag{6-100}$$

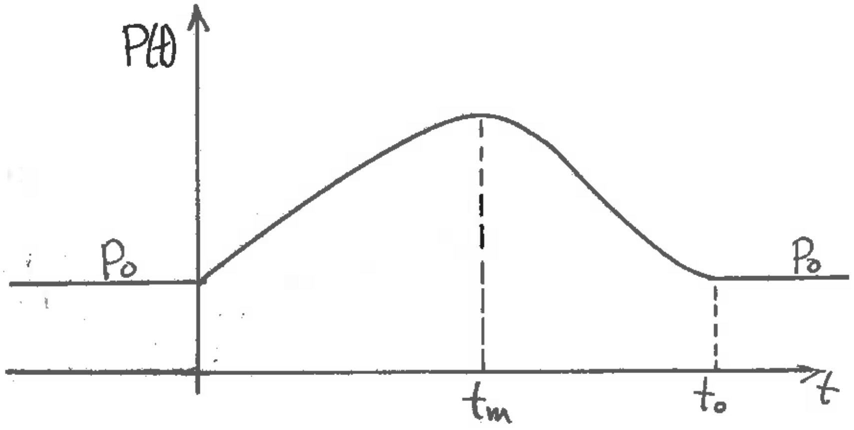
Then

(i) \$(t) must also be periodic with the same period

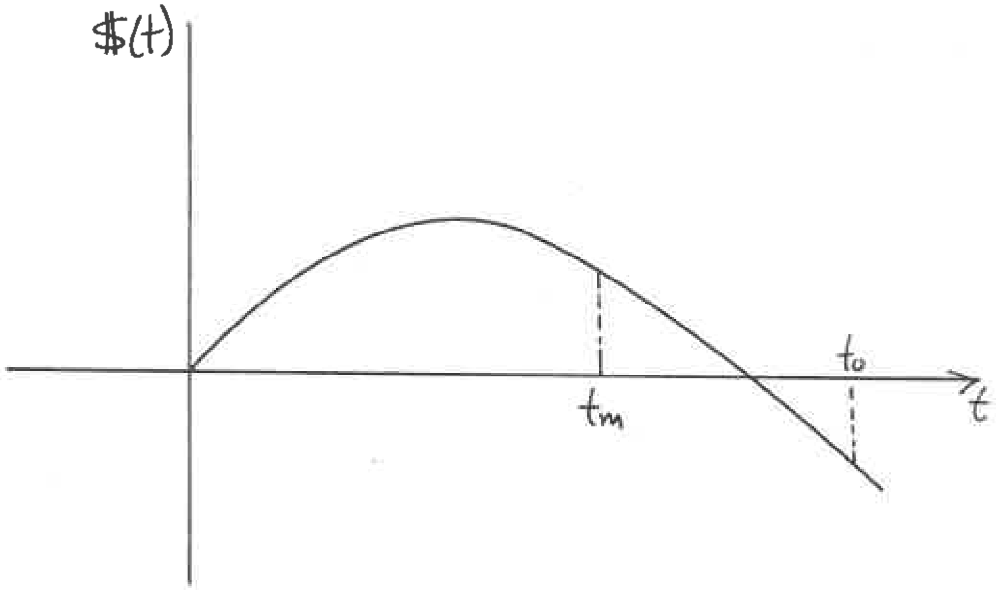
(ii) $\$_{ave} < 0$

2. Reactivity After a Positive Power Excursion

As a second example of the inverse method, consider a positive power excursion of the form



Then in fact we can demonstrate that the reactivity is negative at the time t_0 when the power returns to its initial value P_0



The idea is to use

$$\$(t_0) = \frac{\Lambda}{\beta}\frac{1}{P_0}\frac{dP}{dt}\bigg|_{t_0} - \int_0^{t_0} d\tau\, D(\tau)\left[\frac{P(t_0-\tau)}{P_0} - 1\right] \qquad (6\text{-}101)$$

and note that the integral must be positive $[P(t_0-\tau) > P(t_0)]$ while the slope $dP/dt\big|_{t_0} \leq 0$

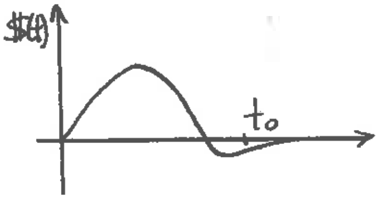
We can, in fact, compute the time dependence of the reactivity if we assume an excursion of very short duration in comparison to delayed neutron rates. For $t > t_0$, assume $P(t) = P_0 = \text{const.}$ Then from (6-107)

$$\$(t) = -\int_0^t d\tau\, D(\tau)\left[\frac{P(t-\tau)-P_0}{P_0}\right] = -\int_0^{t_0} du\, D(t-u)\left[\frac{P(u)-P_0}{P_0}\right]$$

$$\cong -D(t-t_0)\int_0^{t_0} du\left[\frac{P(u)-P_0}{P_0}\right] = -\frac{I}{P_0}\sum_{i=1}^{6} a_i\lambda_i e^{-\lambda_i(t-t_0)}, \quad t \geq t_0 \qquad (6\text{-}102)$$

where

$$I \equiv \int_0^{t_0} du\left[P(u)-P_0\right] \equiv \text{ is excess energy release in excursion} \qquad (6\text{-}103)$$



(i) Note as $t \to \infty$, $\$(t) \to 0$

(ii) $\$(t_0) = -\frac{I}{P_0}\left[\sum_i a_i\lambda_i\right]$ (6-104)

3. Reactivity for $P(t) = P_0 e^{\alpha t^2}$

Assume

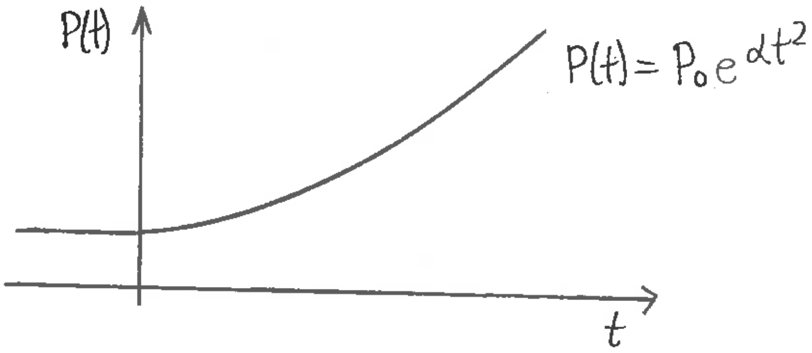
$$\begin{aligned} P(t) &= P_0 & t<0 \\ &= P_0 e^{\alpha t^2} & t\geq 0 \end{aligned} \qquad (6\text{-}105)$$

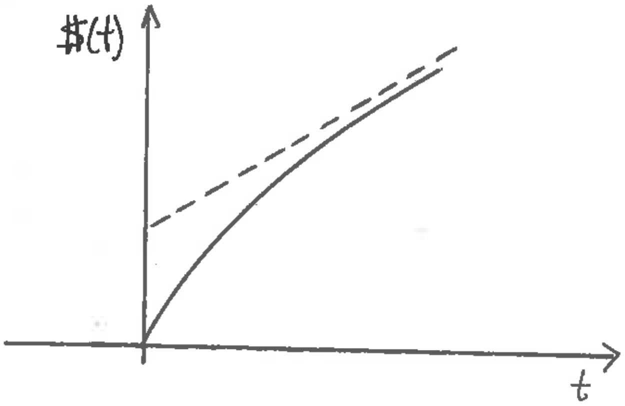
Then

$$\$(t) = 1 + \frac{\Lambda}{\beta}2\alpha t - e^{-\alpha t^2}\sum_{i=1}^{6} a_i e^{-\lambda_i t} - \sum_{i=1}^{6} a_i\lambda_i \int_0^t d\tau\, e^{-\alpha\tau^2 - 2\alpha t\tau - \lambda_i\tau}$$

$$\cong 1 + \frac{\Lambda}{\beta}2\alpha t - \sum_{i=1}^{6}\frac{a_i\lambda_i}{\lambda_i + 2\alpha t} + O(e^{-\alpha t^2}) \qquad (6\text{-}106)$$

Note $(t) approaches a linear function which implies that the response of the reactor power P(t) to a ramp insertion $\$(t) = \gamma t$ should behave as $\exp[\beta\gamma t^2/2\Lambda]$ for large times





D. Approximate Solutions

As we have seen, exact solutions of the PRKE are known only for a few special reactivity insertions. Hence we now turn our attention to approximate schemes for solving these equations in the absence of feedback.

1. Constant Delayed Neutron Production Rate Approximation

In certain problems, such as when the reactor is shut down by rapid insertion of the safety rods, we are interested in the response of the reactor power to a given reactivity insertion in short time intervals following a time t_0. During such short time intervals we can ignore the change in the rate of production of delayed neutrons, replacing $C_i(t)$ by $C_i(0)$. Hence in this approximation, the PRKE becomes

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = [\$(t)-1]P(t) + \frac{\Lambda}{\beta}Q^*(t) \qquad (6\text{-}107)$$

where the "effective source" Q*(t) includes the delayed neutrons

$$Q^*(t) = \frac{\beta}{\Lambda}\sum_{i=1}^{6}\lambda_i C(0) \tag{6-108}$$

Since this is just a first order ODE; it can be integrated to find

$$P(t) = e^{A(t)}\left[P(0) + \int_0^t dt' e^{-A(t')} Q^*(t')\right]$$

where

$$A(t) = \frac{\beta}{\Lambda}\int_0^t dt' \left[\$(t') - 1\right] \tag{6-109}$$

Example: Fast Ramp Reactivity Insertion and Reactor Shut-Down

In the case of an emergency, such as the loss of coolant flow, the reaction is shut down by a rapid insertion of the safety rods. Since the rod insertion takes a finite time, we cannot really treat this as a step reactivity change. A more reasonable model is to assume a negative ramp insertion, i.e., $\$(t) = -\gamma t$. Then, in our earlier notation

$$A(t) = \frac{\beta}{\Lambda}\int_0^t dt' \left[-\gamma t' - 1\right] = -\frac{\beta}{\Lambda}\gamma\frac{t^2}{2} - \frac{\beta}{\Lambda}t \tag{6-110}$$

Using Eq. (6-109), we then find

$$P(t) = e^{-\frac{\beta}{\Lambda}\left[\frac{\gamma t^2}{2} + t\right]} P(0) + \int_0^t dt' e^{-\frac{\beta}{\Lambda}\left[\frac{\gamma(t-t')^2}{2} - (t-t')\right]} \frac{\beta}{\Lambda}\sum_{i=1}^{6}\lambda_i C_i(0) \tag{6-111}$$

Further noting that the initial conditions imply

$$\sum_i \lambda_i C_i(0) = P(0)\sum_i a_i = P(0), \tag{6-112}$$

we can simplify to find

$$\frac{P(t)}{P(0)} = e^{-(T^2-T_0^2)/2}\left[1-\frac{T_0}{\sqrt{2}}F(T_0)\right] + \frac{T_0}{\sqrt{2}}F(T) \qquad \text{(6-113)}$$

where

$$T = (1+\gamma t)T_0, \quad T_0 = \sqrt{\beta/\gamma\Lambda}$$

$$F(T) = \int_0^T dT' e^{(T'^2-T^2)}$$

At the end of the ramp insertion, the reactivity becomes a constant, and we can find P(t) by solving the PRKE for a constant reactivity as we already have done.

3.4.2. The Prompt Jump Approximation

If the relative rate of change of reactor power in a mean prompt generation time is sufficiently small, i.e.,

$$\left|\frac{\Lambda}{\beta}\frac{\dot{P}(t)}{P(t)}\right| << \left|1-\$(t)\right| \qquad \text{(6-114)}$$

then we can neglect the $\frac{\Lambda}{\beta}\frac{dP}{dt}$ in the PRKE and consider

$$0 = [\$(t)-1]P(t) + \sum_{i=1}^{6}\lambda_i C_i(t) \qquad \text{(6-115)}$$

$$\frac{dC_i}{dt} = a_i P(t) - \lambda_i C_i(t), \quad i=1,\ldots,6$$

This is called the "prompt jump approximation" since it predicts a sudden change in the power P(t) following a sudden change in reactivity. Note that in the PJA, a reactivity jump from $\$_1$ to $\$_2$ causes a change from P_1 to P_2 given by

$$\frac{P_2}{P_1} = \frac{\$_1 - 1}{\$_2 - 1} \tag{6-116}$$

Example: This approximation is particularly useful in the case of one delayed group: Then we can estimate C in terms of P to find

$$[1 - \$(t)] \frac{dP}{dt} = [\dot{\$} + \lambda \$] P(t) \tag{6-117}$$

Hence if $\$(t)$ is given, we can solve for P(t):

$$P(t) = e^{A(t)} P(0) \tag{6-118}$$

where

$$A(t) = \int_0^t d\tau \left[\frac{\dot{\$}(\tau) + \lambda \$(\tau)}{1 - \$(\tau)} \right] \tag{6-119}$$

[For example, if $\$(t) = t$, then,

$$P(t) = P(0) e^{-\lambda t} [1 - \gamma t]^{-(1+\lambda/\gamma)} \tag{6-121}$$

Notice from (6-117) that

$$\frac{\dot{P}}{P} = \frac{\dot{\$} + \lambda \$}{1 - \$} \tag{6-122}$$

Hence our condition for the validity of the PJA becomes

$$(1-\$)^2 >> \frac{\Lambda}{\beta}(\dot{\$}+\lambda\$) \sim \frac{\Lambda\$\lambda}{\beta} \qquad (6\text{-}123)$$

Using $\lambda \sim .1\ \mathrm{sec}^{-1}$, $\Lambda = 10^{-5}$ sec, $\beta = 10^{-2}$, this implies that the PJA will be valid until reactivity reaches roughly 80% of prompt criticality. Numerical solutions have demonstrated the PJA to be within 2% to .008% of the true solution after a ρ_0 = .5 \$ step reactivity insertion.

4. Small Amplitude Approximation (Linearization)

Suppose that we assume small reactivity variations will produce only small changes in the reactor power from its equilibrium value P_0. We already know that this assumption is not true for a critical reactor since even a slight positive step in reactivity gives rise to an exponentially increasing power response which eventually grows beyond any bound. However, the assumption will still be true if we consider only short times following the step insertion. Furthermore for certain classes of reactivity changes such as a periodic reactivity insertion with an appropriate negative bias, the resulting power variations remain small for all times. In this case, the PRKE reduce from a set of linear ODE's with variable coefficients to a set of linear ODE's with constant coefficients.

Consider again the integro-differential form of the PRKE

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = [\$(t)-1]P(t) + \int_0^t d\tau\, D(\tau)P(t-\tau) + \sum_{i=1}^{6} \lambda_i C_i(0)e^{-\lambda_i t}. \qquad (6\text{-}124)$$

It is convenient (and conventional) to assume the reactor is operating at a fixed power level P_0 prior to t = 0. Then

$$\sum_{i=1}^{6} \lambda_i C_i(0)e^{-\lambda_i t} = P_0\sum_{i=1}^{6} a_i\lambda_i e^{-\lambda_i t} = -P_0\int_0^t d\tau\, D(\tau) + P_0 \qquad (6\text{-}125)$$

If we now let p(t) denote the power variations about the reference level P_o

$$P(t) = P_o + p(t) \tag{6-126}$$

then (1) becomes

$$\begin{aligned}\frac{\Lambda}{\beta}\frac{dp}{dt} &= \$(t)P_o + \$(t)p(t) \cancel{-P_o} - p(t) + \cancel{\int_0^t d\tau D(\tau) P_o} + \int_0^t d\tau D(\tau)\, p(t-\tau) \\ &\qquad \cancel{-P_o \int_0^t d\tau D(\tau)} + \cancel{P_o} \\ &= \$(t)P_o + \$(t)p(t) + \int_0^t d\tau D(\tau)\, p(t-\tau) - p(t)\end{aligned} \tag{6-127}$$

Our approximation will be to assume that k(t) and p(t) are sufficiently small that we can neglect $\$(t)\, p(t)$ to obtain

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = P_o \$(t) + \int_0^t d\tau D(\tau)\, p(t-\tau) - p(t). \tag{6-128}$$

This approximation is sometimes (incorrectly) referred to as the "linearization approximation". [Note that both (6-127) and (6-128) are linear. Actually, what this approximation does is to linearize the functional relation between $(t) and p(t), which, as we have found earlier, is not linear in general.]

Since (6-128) is now just an integro-differential equation with constant coefficients, we can easily solve it by Laplace transforms to find

$$\tilde{p}(s) = \left[s\left(\frac{\Lambda}{\beta} + \sum_{i=1}^{6} \frac{a_i}{s+\lambda_i}\right)\right]^{-1} P_o\, \tilde{\$}(s) \tag{6-129}$$

or

$$\frac{\tilde{p}(s)}{P_0} = Z(s)\,\tilde{\$}(s) \qquad (6\text{-}130)$$

where we have defined the "zero power transfer function" Z(s)

$$Z(s) \equiv \left[s\left(\frac{\Lambda}{\beta} + \sum_{i=1}^{6} \frac{a_i}{s+\lambda_i}\right)\right]^{-1} \equiv \frac{1}{Y(s)} \qquad (6\text{-}131)$$

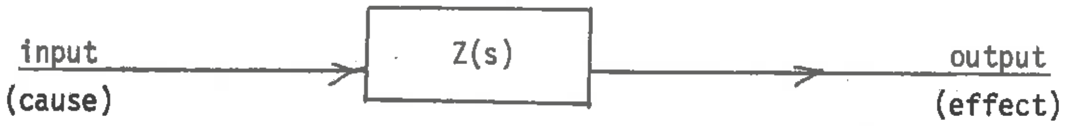
Hence to compute $\tilde{p}(s)$, we need only study the poles of Z(s) and $\tilde{\$}(s)$. However there is a great deal more we can do by employing the very powerful methods of linear systems analysis. In particular, we can study the stability of the reactor when it is operating at power (when we introduce feedback).

a.) Some Elements of Linear System Theory

The response (or output) of any physical system to a signal (or input) applied to it can be expressed in terms of a quantity called the "transfer function" of the system. More precisely, we define

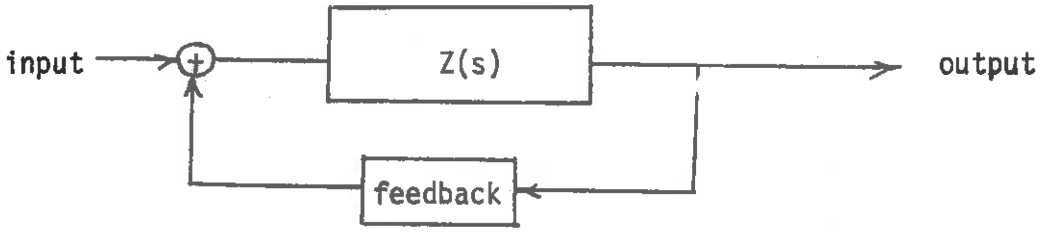
$$\text{Transfer function} = \frac{\text{Laplace transform of response}}{\text{Laplace transform of input}} \equiv Z(s) \qquad (6\text{-}132)$$

This can be conveniently represented by a "block diagram"



In our case, the input is the reactivity \$(t), while the output is the fractional power change $p(t)/P_0$. [Of course other choices are possible, such as the inlet coolant temperature and pressure and so on.]

The transfer function defined for a linear system in this way is sometimes called the "open-loop" transfer function, since we have assumed that the output (power level) does not effect the input (reactivity) in any way. Later we will consider the case in which we allow feedback effects:



[that is, we "close" the feedback loop.]

Comments:

(i) As we have defined it, the transfer function obeys the principle of superposition--that is the sum of the outputs corresponding to two inputs is equal to the output resulting from the sum of the two inputs.

(ii) Notice that $\mathcal{L}\{\delta(t)\} = 1$. Hence the response due to a S-function reactivity input is

$$\frac{\tilde{p}(s)}{P_0} = Z(s) \cdot 1 = Z(s) \qquad (6\text{-}133)$$

or inverting

$$\frac{p(t)}{P_0} = \mathcal{L}^{-1}\{Z(s)\} = \frac{\beta}{\Lambda} + \sum_{j=1}^{6} \frac{e^{\omega_j t}}{\omega_j \left[\frac{\Lambda}{\beta} + \sum_{i=1}^{6} \frac{a_i \lambda_i}{(\omega_j + \lambda_i)^2}\right]} \equiv \mathfrak{z}(t) \qquad (6\text{-}134)$$

Here, $\mathfrak{z}(t)$ is the so-called "unit impulse response"--that is, the power response to a unit impulse reactivity insertion. [$Y(\omega_j) = 0$]

If we return now to the case of more general inputs \$(t), and in particular re-express

$$\frac{\tilde{p}(s)}{P_0} = Z(s)\,\tilde{\$}(s) \tag{6-135}$$

in the "time domain" using the convolution theorem,

$$p(t) = P_0 \int_0^t dt'\, z(t-t')\, \$(t') \tag{6-136}$$

we can see that $z(t)$ is just the Green's function for the linearized point reactor kinetics equation. That is, $z(t-t')$ is the solution to

$$\frac{\Lambda}{\beta}\frac{dz}{dt} = P_0\delta(t-t') + \int_0^t d\tau\, D(\tau)\, z(t-\tau) - z(t) \tag{6-137}$$

Hence it is not surprising that $z(t)$ plays an extremely important role in the study of the linearized PRKE. A couple of interesting points:

a.) $\lim_{t\to\infty} z(t) = \frac{\beta}{\Lambda}$ This implies that the critical reactor has "infinite memory". (6-138)

b.) $$\int_0^\infty |z(t)|\,dt = \infty \tag{6-139}$$

This implies that a critical reactor without feedback is <u>unstable</u> with respect to bounded inputs.

We can derive some more general results. First, let us give a definition of the stability of a system:

<u>Definition</u>: A linear system is said to be <u>stable</u> if its response to any bounded input is also bounded.

Theorem: A necessary and sufficient condition for stability is

$$\int_0^\infty |z(t)|\,dt < \infty \tag{6-140}$$

Proof: To prove sufficiency, note

$$|p(t)| < P_0 \int_0^\infty dt' \, |\$(t-t')|\,|z(t')| < M P_0 \int_0^\infty |z(t)|\,dt \tag{6-141}$$

where M is the bound of the input, i.e., $|\$(t)| < M$.

To prove necessity, we merely construct a bounded input for which the output is unbounded if (6-140) does not hold.

Consider:

$$\$(-t) = z(t)\,/\,|z(t)| \tag{6-142}$$

Then the response at t = 0 is

$$p(0) = P_0 \int_0^\infty dt' \, \$(-t')\,z(t') = P_0 \int_0^\infty dt' \, \frac{z^2(t')}{|z(t')|} = P_0 \int_0^\infty dt\,|z(t)| \tag{6-143}$$

which is unbounded if (6-140) does not hold.

b.) Response to a Small Sinusoidal Input

Consider now a sinusoidal reactivity input

$$\$(t) = \delta k \sin\omega t \tag{6-144}$$

Then

$$\tilde{\$}(s) = \frac{\omega\,\delta k}{s^2+\omega^2} = \frac{\omega\,\delta k}{(s-i\omega)(s+i\omega)} \tag{6-145}$$

We now can solve for

$$p(t)/P_0 = \mathcal{L}^{-1}\left\{\frac{Z(s)\,\omega\delta k}{(s^2+\omega^2)}\right\}$$

$$= \frac{\omega\delta k}{2}\left[\frac{Z(i\omega)e^{i\omega t}}{i\omega} - \frac{Z(-i\omega)e^{-i\omega t}}{i\omega}\right] + \omega\delta k\sum_{j=1}^{6}\frac{e^{\omega_j t}}{(\omega^2+\omega_j^2)\left.\frac{dY}{ds}\right|_{\omega_j}} \qquad (6\text{-}146)$$

where the first two terms arise from the poles of $\$(s)$ on the imaginary axis at $s = i\omega$ and $s = -i\omega$, and the remaining terms are due to the poles of $Z(s)$ which are the roots ω_j of the inhour equation $Y(\omega_j) = 0$. Note that for the critical system we are considering

$$\omega_6 < \omega_5 < \cdots < \omega_0 = 0 \qquad (6\text{-}147)$$

Hence as $t \to \infty$ only the oscillating terms and the $\omega_0 = 0$ term remain, and we find the asymptotic behavior of the power oscillations as

$$\frac{p(t)}{P_0} = \delta k\, G(\omega)\sin(\omega t+\phi) + \frac{\delta k}{\omega}\frac{\beta}{\Lambda} \qquad (6\text{-}148)$$

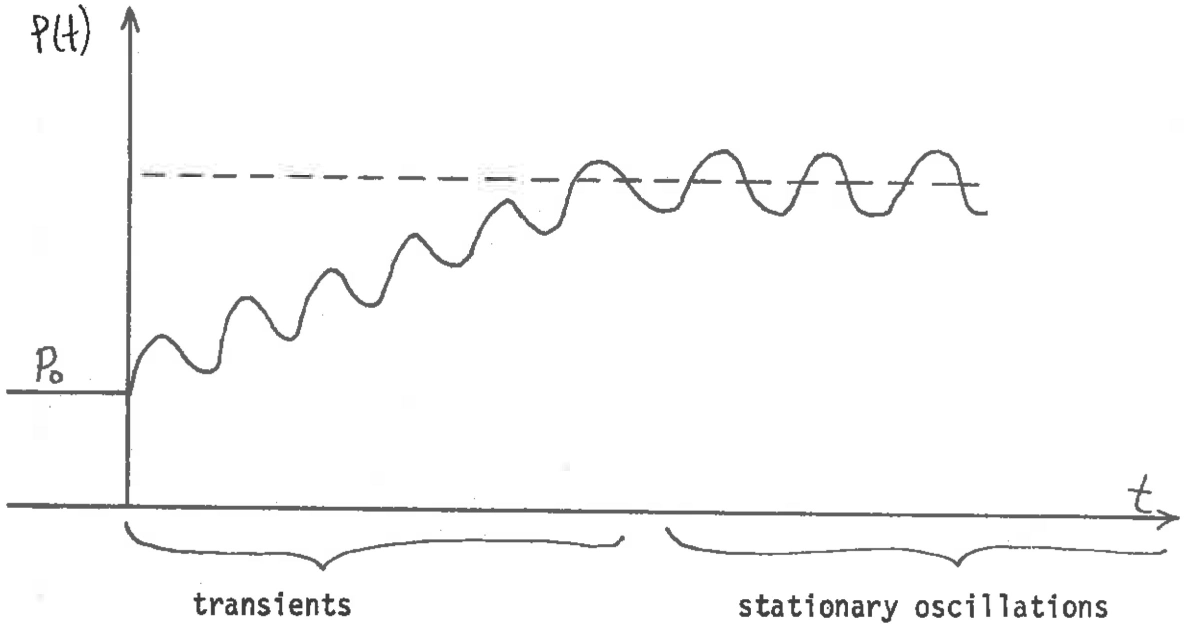
where

$$G(\omega) \equiv |Z(i\omega)| \qquad \text{"gain"}$$

$$\phi(\omega) \equiv \tan^{-1}\left[\mathrm{Im}\{Z(i\omega)\}/\mathrm{Re}\{Z(i\omega)\}\right] \qquad (6\text{-}149) \qquad \text{"phase"}$$

Notice we find a shift in the average power level

$$\delta P_0 = P_0 \lim_{s\to 0}\left[s Z(s)\$(s)\right] = P_0\frac{\delta k}{\omega}\frac{\beta}{\Lambda} \qquad (6\text{-}150)$$



Now it is customary to define

$$\text{gain} \equiv \frac{\text{relative amplitude of power oscillations}}{\text{amplitude of reactivity oscillations}} = \frac{G(\omega)}{1+\frac{\delta k\beta}{\omega\Lambda}}. \qquad (6\text{-}151)$$

To circumvent this difficulty, one can choose an alternative reference power level in this original linearization

$$P(t) = P_r + p(t)$$

where

$$P_r = P_o\left(1 - \frac{\delta k\,\beta}{\omega\Lambda}\right) \qquad (6\text{-}152)$$

Then we find that for long times

$$\frac{p(t)}{P_r} = \delta k \; G(\omega) \sin(\omega t + \phi) \; . \qquad (6\text{-}153)$$

That is, if a reactor operating at a steady-state power level is subjected to a sinusoidal perturbation in reactivity, the power will oscillate with the source frequency, but with a phase shift $\phi \equiv \arg\{Z\}$ (actually a phase lag) and an amplitude proportional to $G(\omega) \equiv |Z(i\omega)|$ Hence we can obtain the values of Z(s) on the imaginary axis in the complex s-plane by measuring experimentally the amplitude and relative phase of power oscillations as a function of frequency, induced by a sinusoidal reactivity insertion with constant amplitude. This is the basis of the zero-power pile-oscillator experiment.

E. Numerical Solutions of the Point Reactor Kinetics Equations

Thus far we have been concerned with methods for obtaining analytical solutions to the PRKE (in the absence of feedback). Such solutions usually involved the introduction of various approximations. The difficulty involved in making headway with analytical solutions should strongly tempt one to simply attempt a brute-force numerical solution, since the PRKE are just a simple system of ordinary differential equations. But as we have mentioned, the principal difficulty here is that these equations contain widely differing time constants. Since the time step size allowed in most standard numerical schemes (e.g., Runge-Kutta or predictor-corrector methods) is by and large controlled by the smallest time constant--in our case, the prompt neutron lifetime--and since the

reactor dynamics occurs on a time scale characterized by the delayed neutrons (in most cases), such direct approaches are quite inefficient.*

Of course, one remedy would be to recognize that those situations for which direct numerical solutions are most inefficient are just those most appropriate for the prompt jump approximation (small ρ and small Λ). It is important, however, to develop numerical schemes which are capable of integrating the PRKE for any values of ρ and Λ. Several such methods have been developed (and are reviewed in Hetrick). We will illustrate the general ideas involved in only one of these methods, that developed by Hanson.

For convenience, consider the PRKE with only one effective delayed neutron group

$$\begin{aligned} \frac{dn}{dt} &= \left(\frac{\rho-\beta}{\Lambda}\right)n(t) + \lambda c(t) \\ \frac{dc}{dt} &= \frac{\beta}{\Lambda}n(t) - \lambda c(t) \end{aligned} \tag{6-154}$$

Now suppose that $\rho(t)$ were essentially constant over a time interval Δt. Then we could integrate these equations to find

$$\begin{aligned} n(t_0+\Delta t) &= n(t_0)\, e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t} + \lambda \int_0^{\Delta t} d\tau\, c(t_0+\tau)\, e^{\left(\frac{\rho-\beta}{\Lambda}\right)(\Delta t-\tau)} \\ c(t_0+\Delta t) &= c(t_0)\, e^{-\lambda\Delta t} + \frac{\beta}{\Lambda}\int_0^{\Delta t} d\tau\, n(t_0+\tau)\, e^{-\lambda(\Delta t-\tau)} \end{aligned} \tag{6-155}$$

Now assume that over this interval of time, Δt,

$$\begin{aligned} n(t_0+\tau) &= n(t_0)\, e^{\omega\tau} \\ c(t_0+\tau) &= c(t_0)\, e^{\omega\tau} \end{aligned} \tag{6-156}$$

---

*It might be remarked that such a wide range of time scales also causes difficulty in analogue similation of the PRKE.

where ω is the largest root of the inhour equation appropriate to ρ. We can then explicitly perform the integrations to find

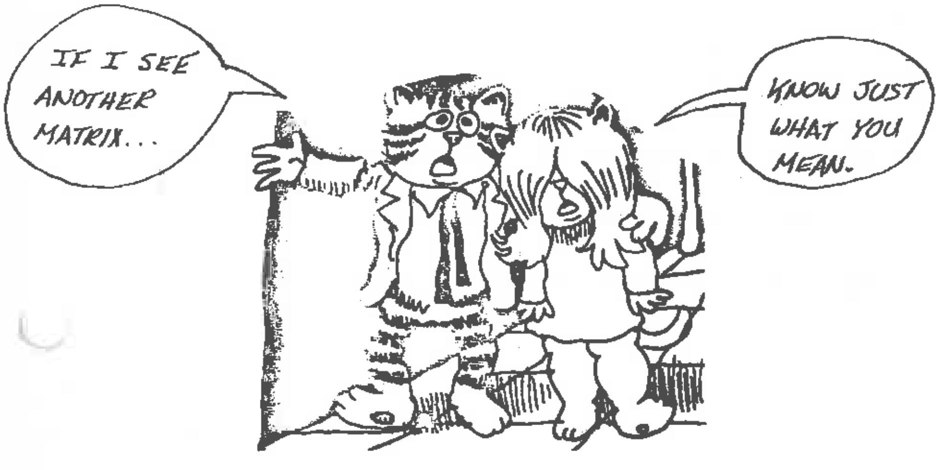
$$n(t_0+\Delta t) = n(t_0)\,e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t} + \frac{\lambda C(t_0)}{\omega-\left(\frac{\rho-\beta}{\Lambda}\right)}\left[e^{\omega\Delta t} - e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t}\right] \quad (6\text{-}157)$$

$$C(t_0+\Delta t) = C(t_0)e^{-\lambda\Delta t} + \frac{(\beta/\Lambda)\,n(t_0)}{\omega+\lambda}\left[e^{\omega\Delta t} - e^{-\lambda\Delta t}\right]$$

Now to account for the fact that $\rho=\rho(t)$, we determine ω from the inhour equation for each time step.

In the more general case of several delayed groups, this yields

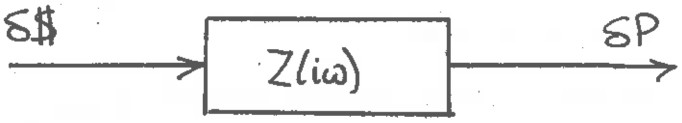
$$\begin{pmatrix} n(t_0+\Delta t) \\ C_1(t_0+\Delta t) \\ \vdots \\ C_m(t_0+\Delta t) \end{pmatrix} = \begin{pmatrix} e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t} & \lambda_1\dfrac{e^{\omega\Delta t}-e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t}}{\omega-\left(\frac{\rho-\beta}{\Lambda}\right)} & \cdots & \lambda_m\dfrac{e^{\omega\Delta t}-e^{\left(\frac{\rho-\beta}{\Lambda}\right)\Delta t}}{\omega-\left(\frac{\rho-\beta}{\Lambda}\right)} \\ \dfrac{\beta_1}{\Lambda}\,\dfrac{e^{\omega\Delta t}-e^{-\lambda_1\Delta t}}{\omega+\lambda_1} & e^{-\lambda\Delta t} & & \vdots \\ \vdots & \vdots & & \vdots \\ \dfrac{\beta_m}{\Lambda}\,\dfrac{e^{\omega\Delta t}-e^{\lambda_m\Delta t}}{\omega+\lambda_m} & 0 & & e^{-\lambda_m\Delta t} \end{pmatrix} \begin{pmatrix} n(t_0) \\ C_1(t_0) \\ \vdots \\ C_m(t_0) \end{pmatrix}$$



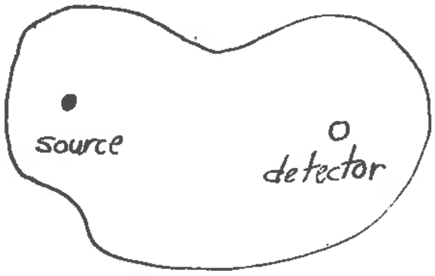
The trick here (and in most of the indirect methods for solving the PRKE) is to assume an exponential time dependence during the time step, which, in turn, allows one to greatly increase the size of such time steps over those that would be required by a standard finite difference scheme (which essentially assumes linear or polynomial time dependences over the time step).

F. Spatial Effects in Reactor Kinetics

Suppose we return for a moment to reconsider the measurement of the transfer function of a reactor (at zero power, for convenience)



Recall that this is accomplished by applying a sinusoidal reactivity variation and measuring the amplitude and phase of the resulting power oscillations for various reactivity frequencies ω. Let us consider these measurements more closely. First, the reactivity perturbation will be localized at a given point (at the location of the oscillating absorber rod). Furthermore, the neutron detector itself is localized at some other point in the reactor. Hence the measurement actually measures a transfer function between two points in the reactor.



Now suppose we were to perform the measurement at various points in the reactor. If the reactor is truly described by the PRKE, then these measurements would give the same results. But in fact, actual measurements will yield different results, depending upon where the oscillator and the detector are placed. An example of this phenomenon is shown in Figure 6-3.

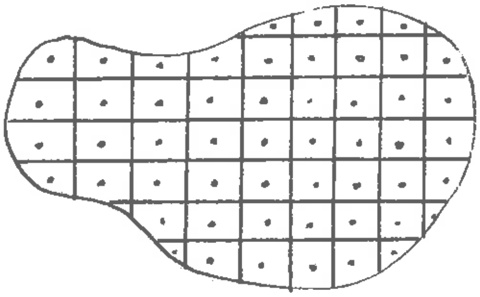
These measurements reveal that the transfer function is actually spatially dependent. They, in fact, also imply a breakdown in the point reactor kinetics model. Recall that in this model, we have assumed that the flux shape in the reactor is time independent:

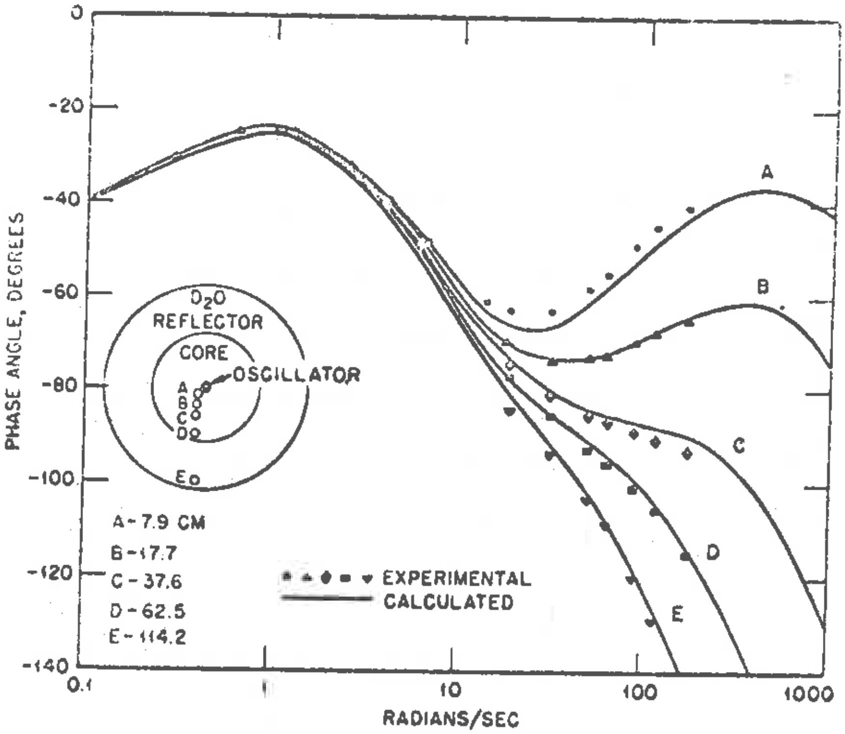
$$\Phi(\vec{r},t) = v\,n(t)\,\phi(\vec{r}) \tag{6-159}$$

But in large cores (particularly those characteristic of today's large power reactors), this assumption is frequently invalid. The core neutronics tend to be quite loosely coupled from point to point in the core. Hence the point reactor kinetics model has a rather limited range of validity (aside from a qualitative study of the reactor kinetics).

For more realistic quantitative estimates of the time behavior of the neutron population in a reactor, one must take explicit account of spatial dependence. Of course, a brute force solution of the neutron diffusion equation (or multigroup diffusion equations) and the delayed neutron precursor equations would be adequate, but such calculations are prohibitively expensive for any realistic reactor configuration. Instead one must turn to other schemes to handle the spatial dependence.

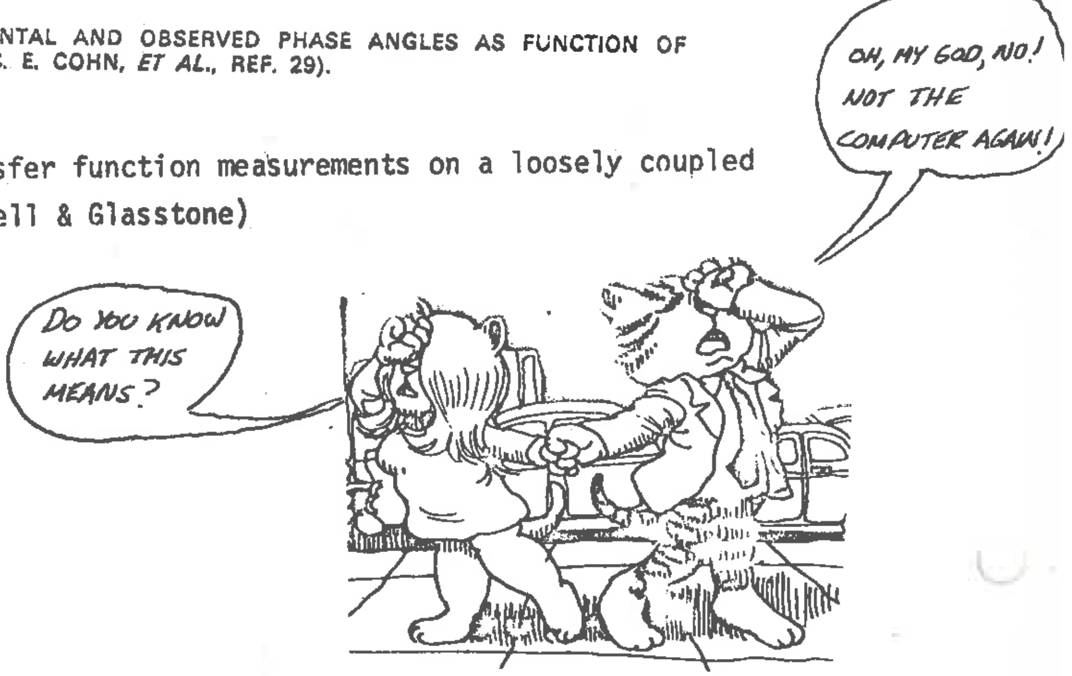
One of the more popular approaches involves dividing the reactor core into a number of regions or nodes. Each node then constitutes a space point in the problem. Of course, the difficulty in this approach is determining the parameters that couple





EXPERIMENTAL AND OBSERVED PHASE ANGLES AS FUNCTION OF POSITION (AFTER C. E. COHN, *ET AL.*, REF. 29).

FIGURE 6-3: Transfer function measurements on a loosely coupled core (Bell & Glasstone)



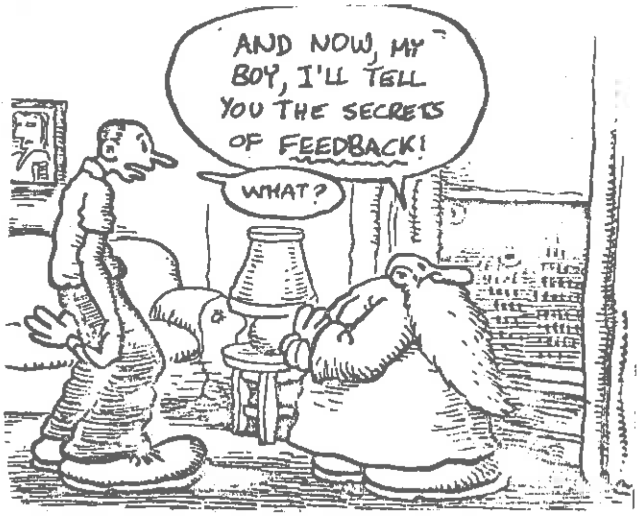
the flux at the various nodal points. There are numerous prescriptions for determining the coupling coefficients (some of which will be discussed later when we consider lattice cell calculations for a nuclear reactor core in Chapter 11).

An alternative approach is to expand the flux in the normal modes (i.e., spatial eigenfunctions) of the system

$$\Phi(\vec{r},t) = \sum_{j} T_j(t)\,\psi_j(\vec{r}) \qquad (6\text{-}160)$$

and then consider the resultant set of equations for the time-dependent coefficients $T_j(t)$. The problem with this approach is that one usually does not know these modes $\psi_j(\vec{r})$ --and, in fact frequently does not know much about them. Various schemes that bypass these difficulties have been suggested (such as "synthesis" methods), but we shall avoid an explicit discussion here and refer the interested reader to existing literature on the subject.

We will return later in Sec. 6-IV to discuss an explicit example of time dependent spatial effects in large power reactors involving oscillations in fission product buildup. For now, however, we turn our attention to consider those mechanisms which cause the reactivity to become dependent upon the power level of the reactor--that is, reactivity feedback.



"Next time, Tonto, I'll go and buy the mask myself."

IV. REACTIVITY FEEDBACK [REACTOR DYNAMICS]

A. Mathematical Description of Feedback

Thus far we have assumed that the reactivity $\rho(t)$ appearing in the point reactor kinetics equations is a given function of time. But we know, in fact, that it depends upon the neutron flux (or power level) itself. This dependence arises because the reactivity depends upon macroscopic cross sections, which themselves involve the atomic number densities of materials in the core:

$$\Sigma(\vec{r},t) = N(\vec{r},t)\,\sigma(\vec{r},t). \tag{6-161}$$

Now it is easily understandable how the atomic density $N(\vec{r},t)$ can depend upon the reactor power level, since

(i) material densities depend upon temperature T, which in turn depends on the power distribution and hence the flux;

(ii) the concentrations of certain nuclei is constantly changing due to neutron interactions (buildup of poison or burnup of fuel).

But it should also be noted that we have explicitly written the microscopic cross sections as explicit functions of $\vec{r}$ and t. This must be done since the cross sections which appear in our one-speed diffusion model are actually averages of the true energy-dependent microscopic cross sections over an energy spectrum characterizing the neutrons in the reactor core. And this neutron energy spectrum will itself depend upon the temperature distribution in the core.

Hence evidently our first task in constructing any model of temperature feedback is to determine the temperature distribution in the core. In a very formal sense, one could write the conventional equation of heat transfer for the core

$$\rho c_p\left[\frac{\partial T}{\partial t}+\vec{u}\cdot\nabla T\right]=\nabla\cdot\kappa\nabla T+H(\vec{r},t) \qquad (6\text{-}162)$$

where c_p is the specific heat of the core material, ρ is its mass density, $\vec{u}(\vec{r},t)$ is its hydrodynamic velocity (usually zero except in the coolant channels), κ is the thermal conductivity, and $H(\vec{r},t)$ is the distributed heat source. This heat source is due, of course, to nuclear processes--predominantly fission, but radiative capture as well. Since the fission fragments travel only short distances before depositing their energy in the form of heat, it is customary to characterize H_f as a localized heat source proportional to the fission rate:

$$H_f(\vec{r},t)=w_f\,\Sigma_f(\vec{r},t)\,\Phi(\vec{r},t) \qquad (6\text{-}163)$$

Of course we are still not through yet, since we must also write down the hydrodynamic equations describing the coolant flow in order to determine the flow velocities.

Needless to say, this collection of neutronic, thermal, and hydraulic equations represents a formidable set of nonlinear partial differential equations. It has become customary to avoid the complexity of a direct solution of the set--at least when only qualitative information about the reactor dynamics is desired--by replacing the spatially dependent description by a "lumped parameter" model similar in philosophy to the point reactor kinetics model, in which the reactor is characterized by a single temperature (or, at most, several temperatures characterizing fuel, moderator, and cooland) and then to postulate a simple dependence of the reactivity upon temperature.

Suppose we go one step further, and assume that the reactivity is given as a simple functional of the reactor power level P(t)

$$\$ = \$[P] \tag{6-164}$$

With this assumption, we can write the PRKE in the presence of feedback as

$$\begin{aligned} \frac{\Lambda}{\beta}\frac{dP}{dt} &= \left\{ \delta\$_{ext}(t) + \delta\$_f[P] - 1 \right\} P(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \\ \frac{dC_i}{dt} &= a_i P(t) - \lambda_i C_i(t) \qquad i=1,\cdots,6 \end{aligned} \tag{6-165}$$

Here we have written the reactivity as the sum of two terms

$$\$ = \delta\$_{ext}(t) + \delta\$_f[P] \tag{6-166}$$

The $\delta\$$ notation signifies that the reactivity is measured with respect to the equilibrium power level P_0. Furthermore, $\delta\$_{ext}(t)$ represents the "external" reactivity insertion such as by adjusting a control rod. $\delta\$_f[P]$ denotes the change in reactivity due to feedback.

When the reactor is operating at a steady-state power level P_0, then there will be a certain feedback reactivity $\$_f(P_0)$. To sustain the criticality of the system, we must supply a counteracting external feedback $\$_0$ such that

$$\$_0 + \$_f[P_0] = 0. \tag{6-167}$$

In this sense we are defining the incremental reactivities

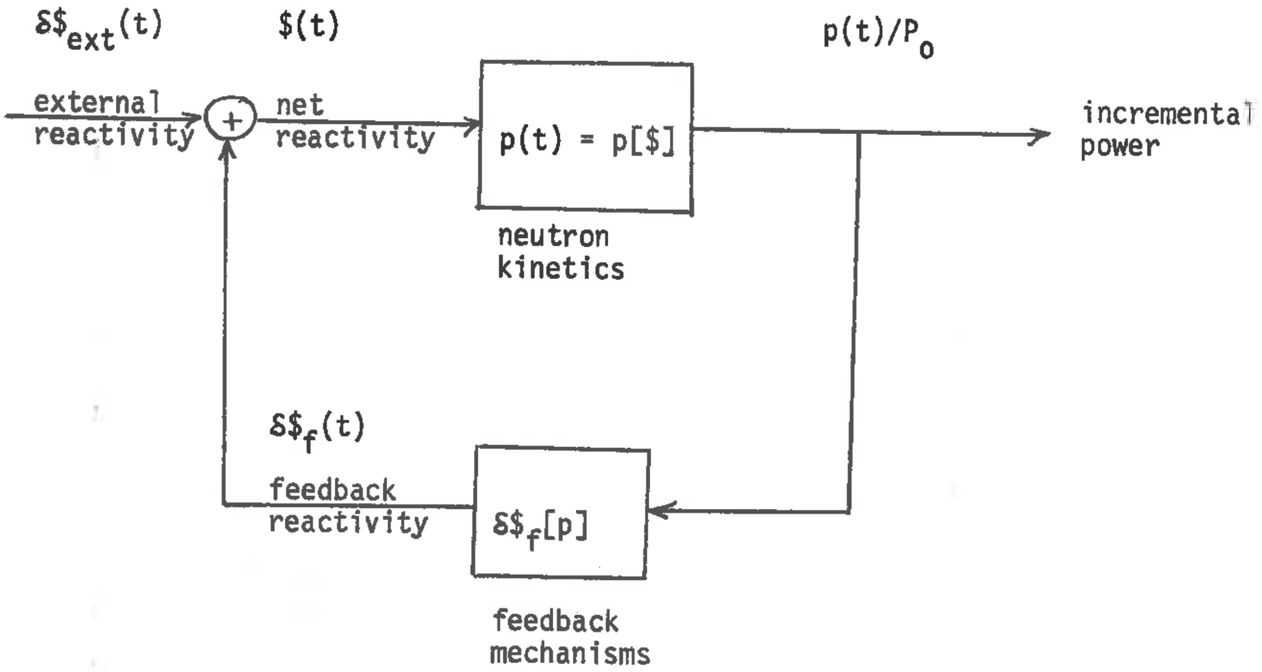
$$\begin{aligned} \delta\$_{ext}(t) &= \$_{ext}(t) - \$_0 \\ \delta\$_f[p] &= \$_f[P] - \$_f[P_0] \end{aligned} \tag{6-168}$$

It is also useful to recall our definition of the incremental power

$$p(t) = P(t) - P_0 \tag{6-169}$$

Note then that $\delta\$_f[p \equiv 0] = \delta\$_f[P_0] = 0$.

We can now sketch the "block" diagram for the reactor with feedback as



We have already analyzed the "black box" describing the neutron kinetics --i.e., the functional p[$] is given by the solution of the PRKE <u>without</u> feedback

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = \$(t)[P_0 + p(t)] + \int_0^\infty d\tau\, D(\tau)\left[p(t-\tau) - p(t)\right] \tag{6-170}$$

Notice that in general we can only determine p[$] <u>approximately</u>, e.g.,

(i) no delayed neutrons

(ii) linearization

$$p[\$] = P_0 \int_0^t d\tau\, z(\tau)\, \$(t-\tau) \tag{6-171}$$

(iii) prompt jump approximation

and so on.

We now turn our attention to a study of the black box describing the feedback functional $\delta\$_f[p]$ by investigating the physical processes involved in temperature feedback.

B. Temperature Coefficient Of Reactivity

Of most concern in a study of short term reactivity feedback is the effect of the core temperature on the multiplication of the core. It has become customary to discuss temperature feedback in terms of a particularly simple model in which the reactivity is assumed to depend linearly upon the temperature--

$$\rho(T) = \rho_0 + \alpha_T T\,, \tag{6-172}$$

where α_T is the temperature coefficient of reactivity defined by

$$\alpha_T \equiv \frac{d\rho}{dT} \tag{6-173}$$

Such a simple model illustrates quite clearly the effect of temperature feedback upon reactor stability. For if a reactor were to possess a positive α_T, then an increase in temperature would produce an increase in ρ, hence the power would increase causing a further increase in temperature, and so on. In this sense, the reactor would be unstable with respect to temperature or power variations.

The more desirable situation is that in which α_T is negative, since then an increase in temperature will cause a decrease in ρ, hence a decrease in reactor power and temperature which tends to stabilize the reactor power level.

The temperature coefficient of reactivity depends upon a great many processes occurring within the core. We will discuss only the more qualitative features which determine α_T.

Suppose we begin by simply using the 6-factor formula for the multiplication factor k

$$k = \eta \epsilon p f P_{NFL} P_{NTL} \tag{6-174}$$

Now if we note

$$\alpha_T = \frac{d\rho}{dT} = \frac{d\rho}{dk}\frac{dk}{dT} \cong \frac{1}{k}\frac{dk}{dT}, \tag{6-175}$$

then we can separate α_T into a sum of contributions from each of the terms in k:

$$\alpha_T = \frac{1}{\eta}\frac{d\eta}{dT} + \frac{1}{\epsilon}\frac{d\epsilon}{dT} + \frac{1}{p}\frac{dp}{dT} + \frac{1}{f}\frac{df}{dT} + \frac{1}{P_{NFL}}\frac{dP_{NFL}}{dT} + \frac{1}{P_{NTL}}\frac{dP_{NTL}}{dT}$$

$$\equiv \sum_i \alpha_T(X_i) \equiv \sum_i \frac{1}{X_i}\frac{dX_i}{dT} \qquad (6\text{-}176)$$

We can now examine each of these terms in turn. Before we begin, however, it should be stressed that there is no single temperature which characterizes the reactor core. Not only will there be a temperature distribution across the core, but in addition the temperature of the fuel will be dramatically different from that of the coolant and moderator. Hence an analysis based upon such "isothermal" reactivity coefficients should be taken with a grain of salt, and used only to illustrate qualitative trends.

$\underline{\alpha_T(\eta)}$: Recall that for a single fissile isotope

$$\eta = \nu \frac{\sigma_f^F}{\sigma_a^F} \qquad (6\text{-}177)$$

Since these are microscopic quantities which do not depend upon atomic concentration, it might be concluded that η does not depend upon temperature. But, in fact, we must remember that ν, σ_f^F, and σ_a^F are actually "averaged" cross sections which appear in our one-speed diffusion model. (This will become more apparent when we develop multigroup models in Chapter 7.) The actual cross sections depend upon energy, and the quantities which appear in η, are in fact these cross sections averaged over some typical neutron energy spectrum--which is, in fact, temperature dependent. In fact, the temperature dependence of η arises from the fact that σ_f^F and σ_a^F do not have the same dependence on neutron energy.

For a mixture of fissile and nonfissile isotopes,

$$\eta = \frac{\sum_i \nu_i \Sigma_f^{(i)}}{\Sigma_a} \tag{6-178}$$

However since the atomic densities of each of these isotopes will have essentially the same temperature dependence, again the temperature dependence of η will be due to the energy dependence of $\sigma_f^{(i)}$ and $\sigma_a^{(i)}$. In all cases, $\alpha_T(\eta)$ is quite small, ranging between $-10^{-4}/°C$ to $+ 4\times10^{-5}/°C$.

$\underline{\alpha_T(f)}$: The thermal utilization is defined for a homogeneous reactor by

$$f \equiv \frac{\Sigma_a^F}{\Sigma_a^F + \Sigma_a^M} \tag{6-179}$$

If we differentiate,

$$\alpha_T(f) = (1-f)\left[\alpha_T(\Sigma_a^F) - \alpha_T(\Sigma_a^M)\right] \tag{6-180}$$

But recalling that $\Sigma = N\sigma$, we find

$$\alpha_T(\Sigma_a) = \alpha_T(N) + \alpha_T(\sigma_a) \tag{6-181}$$

The atomic number density N will vary with temperature as determined by coefficient of volume expansion β

$$\alpha_T(N) = -\beta \quad . \tag{6-182}$$

One can also how that the one-speed absorption cross section depends upon temperature in such a way that

$$\alpha_T(\sigma_a) = a\alpha_T(g_a) - 1/2T \tag{6-183}$$

where g_a measures the departure of the absorption cross section from $1/v$ behavior. One can combine these quantities, noting $N_F \propto N_M$ for a homogeneous reactor, to find

$$\alpha_T(f) = a(1-f)\left[\alpha_T(g_a^F) - \alpha_T(g_a^M)\right] \tag{6-184}$$

This is usually quite small, $\alpha_T(f) \sim 10^{-6}/°C$. The calculation of $\alpha_T(f)$ becomes more complicated for a heterogeneous reactor, since in fact the definition of the thermal utilization must be modified to account for fuel lumping. We will return to consider this in more detail in Chapter 11.

$\underline{\alpha_T(p)}$: The resonance escape probability is a very strong function of temperature because of the so-called "Doppler" effect which broadens absorption resonances as temperature is increased. This is a particularly significant phenomenon in fast reactor calculations. We will return to discuss it in some detail in Chapter 8.

$\underline{\alpha_T(\epsilon)}$: The fast fission factor depends only very weakly on temperature, due to the thermal expansion of the fuel lumps in a heterogeneous reactor core. Its contribution to α_T is usually ignored.

$\underline{\alpha_T(P_{NTL})}$: If we use our one-speed diffusion model, then we can write

$$P_{NTL} = \frac{1}{1+B^2L^2} \tag{6-185}$$

Hence

$$\alpha_T(P_{NTL}) = -\frac{B^2L^2}{1+B^2L^2}\left[\alpha_T(L^2) + \alpha_T(B^2)\right] \tag{6-186}$$

Now

$$L^2 = D/\Sigma_a \tag{6-187}$$

Hence

$$\alpha_T(L^2) = \alpha_T(D) - \alpha_T(\Sigma_a) \tag{6-188}$$

One can usually write

$$\alpha_T(D) = \beta + \frac{m}{T} \quad , \qquad m \sim 0.1 \tag{6-189}$$

We can recall

$$\alpha_T(\Sigma_a) = -\beta - \frac{1}{2T} + f\,\alpha_T(g_a^F) \tag{6-190}$$

Hence

$$\alpha_T(L^2) = 2\beta + \frac{m+\frac{1}{2}}{T} - f\,\alpha_T(g_a^F) \tag{6-191}$$

Now $B^2 \propto$ (characteristic length)$^{-2}$. Hence

$$\alpha_T(B^2) = -\frac{2}{3}\beta \tag{6-192}$$

so that

$$\alpha_T(P_{NTL}) = -\frac{B^2L^2}{1+B^2L^2}\left[\frac{4}{3}\beta + \frac{m+\frac{1}{2}}{T} - f\,\alpha_T(g_a^F)\right] \tag{6-193}$$

<u>$\alpha_T(P_{NFL})$</u>: We have not yet developed an expression for P_{NFL}. We shall do so in Chapter 8, but suffice it to say at this point merely that to a rough approximation,

$$P_{NFL} = e^{-B^2\tau} \tag{6-194}$$

where τ is a parameter characterizing the composition of the system. If one notes that

$$\alpha_T(\tau) = 2\beta \tag{6-195}$$

then

$$\alpha_T(P_{NFL}) = -\frac{4}{3}B^2\tau\beta \tag{6-196}$$

A summary of these contributions is shown below in a table adapted from Lamarsh

Temperature Coefficients of a Heterogeneous Thermal Reactor

Reactor Parameter	Temperature Coefficient
η	+ or -, small (except for Pu^{239})
f	+, small
p	-, large
ϵ	+ or -, small
L^2	+
τ	+
B^2	-, small
P_{NFL}	-
P_{NTL}	-

It is important to keep in mind the rather primitive nature of the isothermal temperature coefficient of reactivity. In a heterogeneous reactor, most of the fission energy release is confined to the fuel elements. This energy must then be transferred by thermal conduction through the fuel element, the clad, and then into the coolant before it can be withdrawn from the core. Hence one has a very non-uniform temperature distribution. Furthermore, the various thermal processes in the core are characterized by widely different time behaviors. The fuel temperature responds relatively rapidly to any power level changes. However it takes an appreciable amount of time to transfer this energy to the coolant, and hence its temperature response is much slower. For this reason, it is convenient to divide up the temperature coefficient of reactivity into prompt and delayed components.

Effects that depend on the instantaneous state of the fuel--e.g., resonance absorption (Doppler effect), thermal distortion of fuel elements --may be regarded as prompt, while effects that depend primarily on the moderator or coolant--e.g., neutron energy spectrum , thermal expansion of moderator material--are delayed. Prompt feedback mechanisms are of particular importance in reactor safety studies, since they play a very important role in limiting any reactor transients which may occur.

Thus far we have only discussed how the reactivity depends upon temperature. The remaining problem of how the temperature depends upon the power level depends sensitively upon the reactor type and involves a thermal-hydraulic analysis of the core. Nevertheless, several simple lumped parameter models have been proposed which are sometimes useful for qualitative studies of reactor dynamics.

One common model assumes a single effective coolant temperature T_c and models the fuel temperature T by Newton's law of cooling

$$\frac{dT}{dt} = KP - \gamma(T-T_c) \tag{6-197}$$

where K and γ are thermal constants characterizing the core. At the opposite extreme would be an adiabatic model in which the heat loss is assumed to be negligible (such as in a very rapid transient)

$$\frac{dT}{dt} = KP \tag{6-198}$$

Still another model assumes constant power removal

$$\frac{dT}{dt} = K(P-P_0) \tag{6-199}$$

All of these models can be considered as special cases of a general linear feedback functional:

$$\rho_f(t) = \int_{-\infty}^{t} d\tau\, h(t-\tau)\,[P(\tau)-P_0] \qquad (6\text{-}200)$$

A little inspection will convince you that the feedback kernel h(t) takes the form:

Newton's Law of cooling: $h(t) = \alpha K e^{-\gamma t}$

Adiabatic model: $h(t) = \alpha K \quad [P_0 = 0]$ (6-201)

Constant power removal: $h(t) = \alpha K$

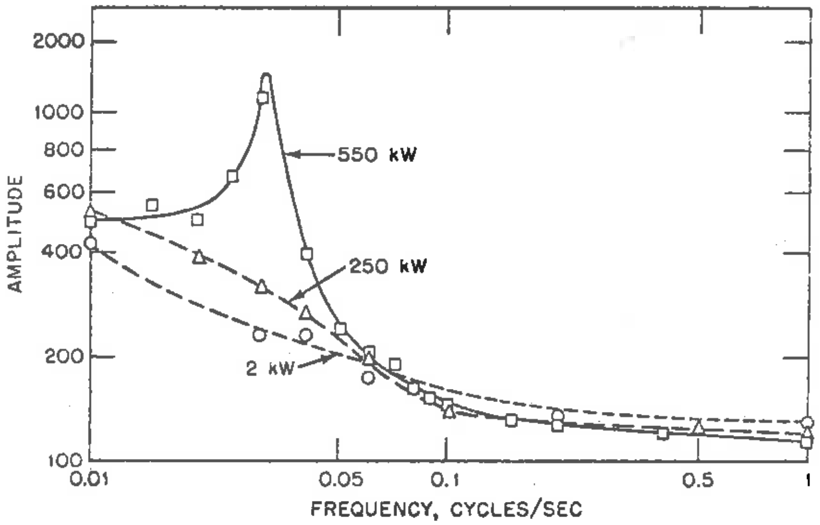
If more reliable design information is required, then one is usually forced to go to a multigroup diffusion calculation coupled with a detailed thermal-hydraulic analysis of the core. One can then calculate the multiplication for several different power levels, and hence determine directly the dependence of reactivity upon power level. We will discuss the coupling between such neutronic and thermal-hydraulic calculations in some detail in Chapter 12.

C. The Transfer Function Of A Reactor With Feedback

1.) Closed Loop Transfer Function

Let us now return to consider the dynamic behavior of a reactor with feedback. In particular, we will consider the effects of feedback on the reactor response to an external reactivity insertion. First we will consider the power oscillations resulting from a periodic reactivity insertion of small amplitude, since this in effect measures the reactivity to power transfer function.

A typical series of reactivity power transfer function gain measurements are shown in Figure 6-4. [These measurements were for EBR-I.]



EXPERIMENTAL TRANSFER FUNCTIONS FOR THE EBR-I (AFTER F. W. THALGOTT, *ET AL.*, REF. 57).

FIGURE 6-4

In particular, notice how different the transfer function at power is from the zero power transfer function. The marked resonance behavior in the vicinity of .03 cps at P_0 = 550 kw is apparent. Such behavior is due to the presence of feedback. As the power level increases, the resonance peak becomes narrower and higher. As we shall see, this implies that for sufficiently large powers, the reactor is unstable.

Let us go back and develop a mathematical expression for the transfer function of the reactor with feedback. Return to the PRKE with $p(t) = P(t) - P_0$

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = \$(t)(p+P_0) + \int_0^\infty d\tau\, D(\tau)\left[p(t-\tau) - p(t)\right] \tag{6-202}$$

where we will use

$$\$(t) = \delta\$_{ext}(t) + \delta\$_f(t) \tag{6-203}$$

We shall now restrict ourselves to small power oscillations about the equilibrium level P_0 so that the feedback functional can be adequately represented as a linear functional

$$\delta\$_f[p] = \int_0^\infty d\tau\, G(\tau)\, p(t-\tau) \tag{6-204}$$

[It should be kept in mind that the feedback kernel $G(\tau)$ actually depends on P_0.] Now (6-202) becomes

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = \left[\delta\$_{ext}(t) + \int_0^\infty d\tau\, G(\tau)p(t-\tau)\right](p+P_0) + \int_0^\infty d\tau\, D(\tau)\left[p(t-\tau) - p(t)\right] \tag{6-205}$$

Of course this equation is still nonlinear. We shall consider only small power variations such that $p(t) \ll P_0$, and we can linearize (6-205) as

$$\frac{\Lambda}{\beta}\frac{dp}{dt} + p(t) = P_0\,\delta\$_{ext}(t) + \int_0^\infty d\tau\left[D(\tau) + P_0 G(\tau)\right]p(t-\tau) \tag{6-206}$$

Now as before, we assume $P(t) = P_0$ for $t < 0$ and Laplace transform to find

$$\frac{\Lambda}{\beta}\left[s\tilde{p} - \underset{\overset{\|}{0}}{p(0)}\right] + \tilde{p}(s) = P_0\,\delta\tilde{\$}_{ext}(s) + \tilde{D}(s)\,\tilde{p}(s) + P_0\,\tilde{G}(s)\,\tilde{p}(s) \tag{6-207}$$

or

$$\frac{\tilde{p}(s)}{P_0} = \left\{\frac{Z(s)}{1 - P_0 H(s) Z(s)}\right\}\delta\tilde{\$}_{ext}(s) \equiv L(s)\,\delta\tilde{\$}_{ext}(s) \tag{6-208}$$

where $Z(s)$ is the usual zero-power transfer function

$$Z(s) = \left[s\left(\frac{\Lambda}{\beta} + \sum_{i=1}^{6}\frac{a_i}{s+\lambda_i}\right)\right]^{-1} \tag{6-209}$$

and $H(s)$ is the "feedback" transfer function

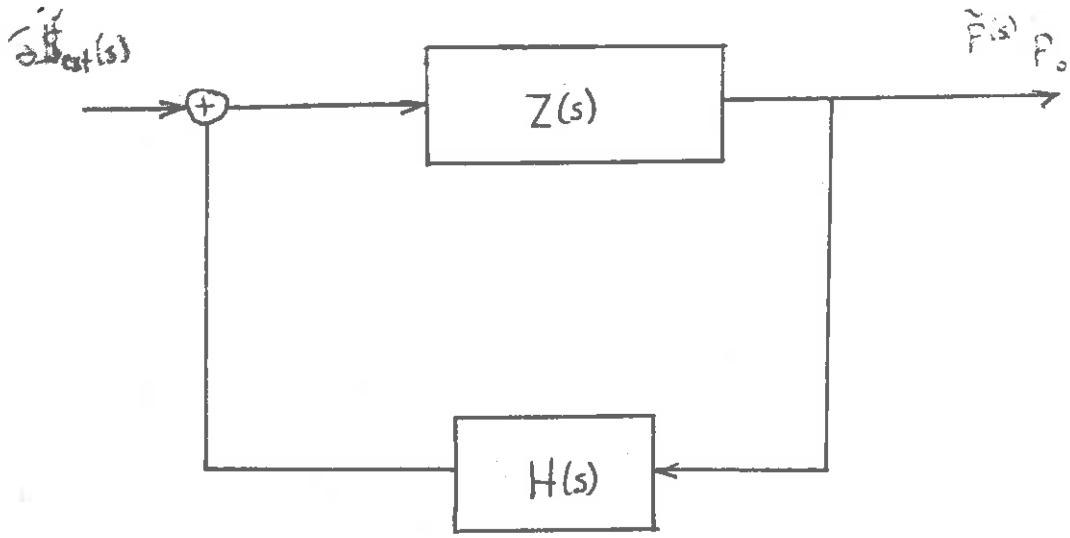
$$H(s) = \tilde{G}(s) \tag{6-210}$$

We have further defined the "reactivity-to-power" or "closed loop" transfer function $L(s)$

$$L(s) \equiv \frac{Z(s)}{1 - P_0 H(s) Z(s)} \tag{6-211}$$

[Note that as $P_0 \to 0$, $L(s) \to Z(s)$, the "zero-power" transfer function.]

This notation is consistent with our earlier block diagram



Note that if we can compute $\ell(t) = \mathcal{L}^{-1}\{L(s)\}$, then we find

$$p(t) = P_0 \int_0^t d\tau \, \ell(t-\tau)\, \delta\$_{ext}(\tau) \tag{6-212}$$

Now let us examine L(s) a bit. First note that unlike Z(s), L(s) is analytical at s = 0 with a value

$$L(0) = \frac{1}{-P_0 H(0)} = \int_0^\infty \ell(t)\, dt \tag{6-213}$$

Hence the long time response to a step reactivity insertion is

$$p(t) = P_0 \delta\$_0 \int_0^t \ell(t')\, dt' \longrightarrow P_0 \delta\$_0 L(0) \tag{6-214}$$

Hence we approach a new equilibrium state

$$P(t\to\infty) = P_0[1 + \delta\$_0 L(0)] \tag{6-215}$$

This in contrast to the zero-power reactor whose power grew exponentially for long time and occurs because the feedback reactivity

$$\delta\$_f(t) = \int_0^t G(t-\tau)p(\tau)d\tau \to p(\infty)H(0) \tag{6-216}$$

such that $\delta\$_f(t) \to -\delta\$_0$

to just compensate the step input.

2.) Response To A Sinusoidal Reactivity Insertion

Now for $\delta\$_{ext}(t) = k_0 \sin\omega t$ we find the long time response

$$\frac{p(t)}{P_0} = |L(i\omega)| \sin(\omega t + \phi) \;, \quad \phi(\omega) = \arg\{L(i\omega)\} \tag{6-217}$$

Now from (6-211), we can see that a resonance in the gain $G(\omega) = [L(i\omega)]$ will occur when

$$1 - P_0 H(i\omega) Z(i\omega) = 1 + P_0 |H(i\omega) Z(i\omega)| e^{i\Phi} \to 0 \tag{6-218}$$

where

$$\Phi(\omega) = \arg\{-Z(i\omega) H(i\omega)\} \tag{6-219}$$

For (6-218) to be satisfied we require

$$\Phi(\omega) = 180^\circ \tag{6-220}$$

and

$$P_o \left| H(i\omega) Z(i\omega) \right| = 1$$

to be simultaneously satisfied. This determines a critical power level P_c and a resonance frequency ω_c. For $P_o < P_c$, there will be a finite resonance peak

$$\left| L(i\omega_c) \right| = \frac{\left| Z(i\omega_c) \right|}{1 - (P_o/P_c)} \tag{6-221}$$

Note that the average power level $P_{ave} = P_o$ when feedback is included. [This is again due to the fact that L(s) is analytic at the origin].

3.) Linear Stability Analysis

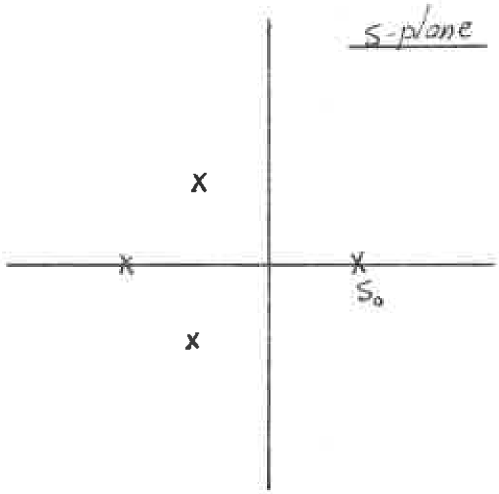
The stability of a reactor with feedback can be investigated by examining the poles of

$$L(s) = \frac{Z(s)}{1 - P_o H(s) Z(s)} \tag{6-222}$$

First note that since Z(s) appears both in the numerator <u>and</u> denominator, its poles ω_j "cancel". Hence the poles of L(s) are merely the zeros of

$$1 - P_o H(s) Z(s) = 0 \tag{6-223}$$

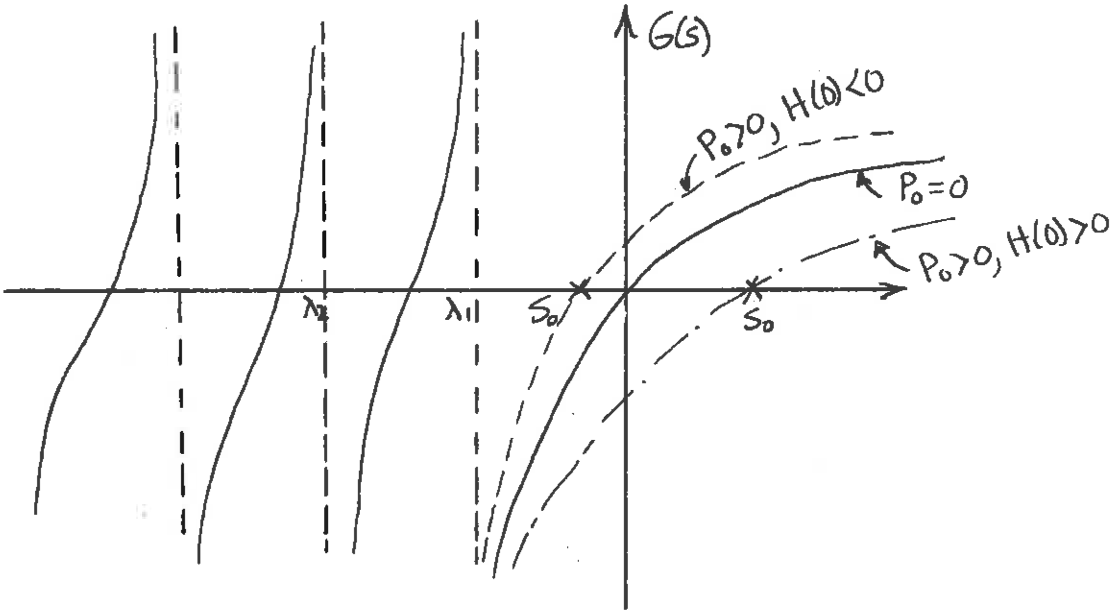
Now suppose (6-223) has a simple root (a pole of L(s)) at $s = s_0$. Then when we invert the Laplace transform, this will contribute a term in p(t) of the form $e^{s_0 t}$. Hence if s_0 is in the RHP, then p(t) will grow exponentially in time, then indicating an unstable response to an applied reactivity perturbation [within the linear approximation, of course.] If the root s_0 lies in the LHP, then $e^{s_0 t}$ will decay in time. Hence to study reactor stability it is obviously important to determine if any of the poles of L(s) [zeros of (6-223) lie in the LHP.



To gain some insight into the outset of unstability, write (6-223) as

$$\mathcal{G}(s) = \frac{1}{Z(s)} - P_0 H(s) = s\left[\frac{\Lambda}{\beta} + \sum_{i=1}^{6} \frac{a_i}{s+\lambda_i}\right] - P_0 H(s) = 0 \qquad \text{(6-224)}$$

Now suppose P_0 is <u>very small</u>. Then the roots of $\mathcal{G}(s)$ are nearly those of $1/Z(s) = Y(s)$--as indicated in the diagram



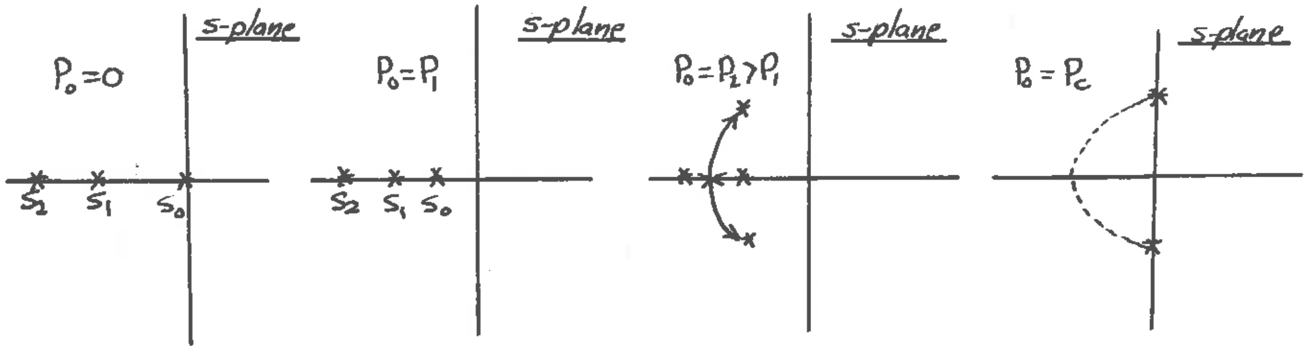
Note now that for a small, nonzero value of P_0, the curve shifts up or down depending upon the sign of the steady-state power coefficient

$$H(0) = \int_0^\infty d\tau\, G(\tau) \qquad (6\text{-}225)$$

In particular, if $H(0) > 0$, s_0 is in the RHP and the system will be unstable

$H(0) < 0$, " " LHP " " stable

For larger powers P_0, the situation is something as shown: For $P_0 = 0$, we can identify the poles of $L(s)$ as just those of $Z(s)$. Then if $H(0) < 0$, as we increase P_0, the root s_0 moves to the left. But other roots will move toward the right



For some sufficiently large P_0, s_0 will encounter s_1, and form a complex conjugate pair. For still larger P_0, this pair moves back to the right, until for some critical power $P_0 = P_c$, the roots move into the RHP and the reactor becomes unstable. When the poles cross the imaginary axis, we observe a "resonance" in the transfer function gain (as we mentioned earlier).

We are interested in the response of a reactor to small power perturbations. The possibility of an unstable response to a small disturbance in the power is characteristic of systems with feedback. We will be concerned with "autonomous" systems in which none of the parameters characterizing the system depend on time. This implies that the external reactivity $\delta\$_{ext}$ and external source S_o are constant. Then the PRKE becomes

$$\frac{\Lambda}{\beta}\frac{dP}{dt} = \left\{\$_{ext} + \$_f[P]\right\}P(t) + \int_0^\infty d\tau\, D(\tau)\left[P(t-\tau) - P(t)\right] + S_o \tag{6-226}$$

For an equilibrium state P_o we require

$$\left\{\$_{ext} + \$_f[P_o]\right\}P_o + S_o = 0 \tag{6-227}$$

For general $\$_f[P_o]$, there might be many equilibrium states. However if $-\$_f[P_o]$ is a non-decreasing function of P_o (as we expect it to be) there will be only one such nontrivial state P_o. [E.g. for a linear functional, we have $\$_f[P_o] = H(0)P_o$, and we have only one equilibrium state.]

Now (6-227) indicates that $P_o = 0$ is always an equilibrium state if $S_o = 0$. But note that in the shutdown state, the net reactivity

$$\$ = \$_{ext} + \$_f[0] = \$_{ext} > 0 \tag{6-228}$$

and hence the power level will increase exponentially if it is perturbed from zero--that is, the shutdown state $P_o = 0$ is unstable.

We will instead direct our attention to the non-zero solution of (6-227) in the absence of sources, i.e.,

$$\$_{ext} + \$_f[P_0] = 0 \tag{6-229}$$

We will again introduce the incremental feedback reactivity and power

$$\begin{aligned} \delta\$_f[p] &= \$_f[P] - \$_f[P_0] \\ p(t) &= P(t) - P_0 \end{aligned} \tag{6-230}$$

in which case (1) becomes

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = \delta\$_f[p]\,(p+P_0) + \int_0^\infty d\tau\, D(\tau)\,[p(t-\tau) - p(t)] \tag{6-231}$$

or linearizing and using a linear feedback functional

$$\frac{\Lambda}{\beta}\frac{dp}{dt} = P_0\int_0^t d\tau\, G(\tau)p(t-\tau) + \int_0^t d\tau\, D(\tau)p(t-\tau) - p(t) \tag{6-232}$$

where we have assumed that the reactor is operated at P_0 prior to $t = 0$. Further, we will introduce an initial perturbation in the power $p(0)$ at $t = 0$. If we now use Laplace transform

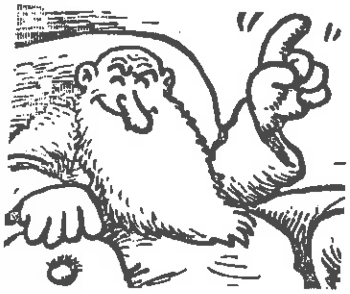
$$\tilde{p}(s) = \frac{p(0)}{\frac{1}{Z(s)} - P_0 H(s)} = L(s)\,p(0) \tag{6-233}$$

The behavior of $p(t)$ is determined by the singularities of $L(s)$ which occur at the zeros of the "characteristic equation"

$$\mathcal{D}(s) = 1 - P_0 H(s) Z(s) \tag{6-234}$$

Hence the problem of the linear stability of our equilibrium state reduces to the problem of determining the sign of the real parts of the roots of the characteristic equation. In particular we have found

CLAIM: A reactor is linearly "strictly stable" when the roots of the characteristic equation all have negative real parts. The response of the power in the critical case, when any of these roots have real parts equal to zero, is not correctly described by linear analysis and depends upon nonlinearities of the PRKE.



There are lots of tricks to determine the signs of the roots of $\mathcal{D}(s)$ without actually solving the characteristic equation. These include methods such as Nyquist diagrams, root-locus plots, Routh-Hurwitz criteria, and so on. But such subjects are more properly the concern of linear system analysis or control theory, so we will simply refer the interested reader to the sources listed at the end of the chapter.

4.) Nonlinear Point Reactor Kinetics

Thus far our study of the PRKE with feedback has been restricted to situations in which the reactivity changes, and corresponding power changes are sufficiently small that these equations can be linearized. In particular, our study of the stability of the reactor has been restricted to the consideration of "<u>stability in the small</u>"--that is, to the study of perturbations and responses sufficiently small for a linear analysis. However, for larger perturbations nonlinear effects must be taken into account. In these cases, the resulting conclusions about stability may be quite different.

For example, we have seen that the linearized PRKE predicts the reactor will be unstable if the power exceeds some critical value P_c. However, even though the reactor is linearly unstable, it may be stable in the nonlinear description. Hence it is of considerable importance to study the significance of linear stability theory within the more general framework of nonlinear stability theory.

It should be remarked, however, that there aremany different approaches to nonlinear point reactor kinetics--none of which is completely satisfactory. Most theories are limited to very simple linear feedback functionals. Further, such theorems as do exist provide only <u>sufficient</u> conditions for stability (as opposed to necessary conditions). Sufficiency conditions are usually much too restrictive for practical applications. Hence, we tend to agree with the conclusion of Bell and Glasstone:

> "From a practical standpoint, nonlinear stability analysis has proved to be much less important than linear analysis. The nonlinear analysis does not lend itself well to experimental verification. Nonlinear studies have usually indicated that the results of linear analysis are not likely to be misleading."

V. FISSION PRODUCT POISONING

A. Introduction

As we have mentioned, the atomic densities of various isotopes in the reactor core are continually changing due to nuclear processes such as fission and radioactive decay. For example, fission reduces the concentration of fissile isotopes such as U^{235} (although subsequent neutron capture may compensate for this fuel depletion to some degree by producing Pu^{239} or U^{233}). In addition, however, one must keep in mind that each fission reaction produces two fission product nuclei. Certain of these nuclei are characterized by extremely large neutron absorption cross sections and may significantly affect the reactivity of the core. For example, Xe^{135} has an enormous thermal neutron cross section of $\sigma_a = 2.7 \times 10^6$ barns. A very small amount of such fission product "poisons" may significantly affect the multiplication of the reactor, since as they accumulate, they will absorb neutrons from the chain reaction.

Although many fission products are characterized by very large thermal absorption cross sections, these cross sections drop off rapidly at higher energies (see Figure 6-5). Hence fission product poisoning is primarily of concern in thermal reactors.

To first order, the effects of such poisons enter through the thermal utilization. If we imagine introducing a poison characterized by a macroscopic cross section Σ_a^P uniformly throughout a homogeneous reactor core, then we can write

$$f = \frac{\Sigma_a^F}{\Sigma_a^F + \Sigma_a^M + \Sigma_a^P} \tag{6-235}$$

Hence we can compute the reactivity change from a critical reactor in which $\Sigma_a^P = 0$ as

$$\Delta\rho \equiv \rho(\Sigma_a^P) - \rho(\Sigma_a^P = 0) \tag{6-236}$$

Now if we recall

$$\rho = \frac{k-1}{k} \quad , \quad k = \eta\epsilon p f P_{NFL} P_{NTL} \tag{6-237}$$

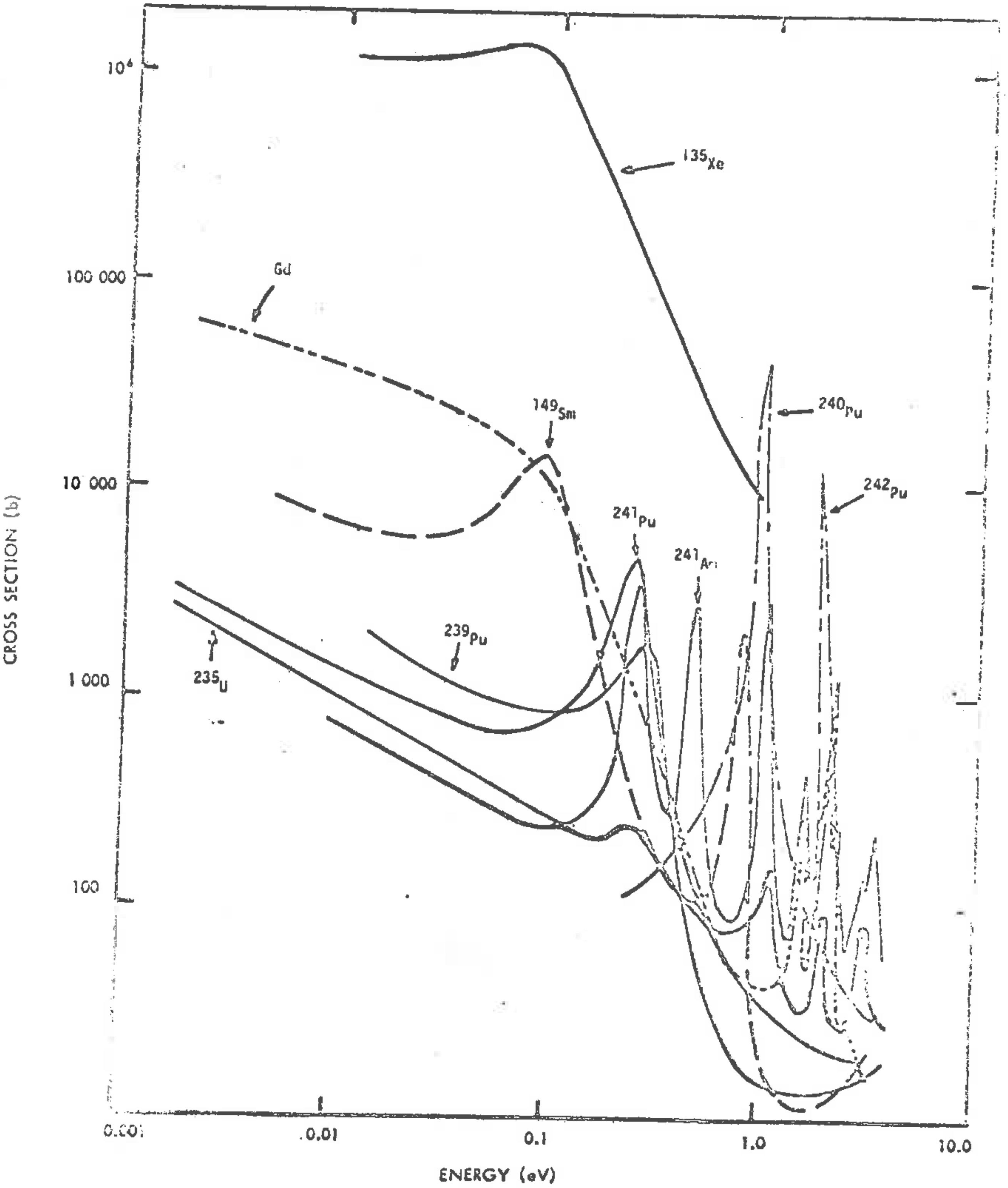


FIGURE 6-5: Thermal cross section behavior

and note that

$$P_{NTL} = \frac{1}{1+L^2B^2} \;, \quad L^2 = \frac{D}{\Sigma_a} = \frac{1}{3\Sigma_{tr}\Sigma_a} \tag{6-238}$$

will also change as Σ_a^P changes, then we can compute

$$\Delta\rho = \frac{f'-f}{f'} + \frac{P'_{NTL} - P_{NTL}}{P'_{NTL}} \tag{6-239}$$

Now

$$\frac{f'-f}{f'} = -\frac{\Sigma_a^P}{\Sigma_a^F + \Sigma_a^M} \tag{6-240}$$

$$\frac{P'_{NTL} - P_{NTL}}{P'_{NTL}} = \frac{L^2B^2}{1+L^2B^2}\left[\frac{\Sigma_a^P}{\Sigma_a} + \frac{\Sigma_{tr}^P}{\Sigma_{tr}}\right] \tag{6-241}$$

Hence we find

$$\begin{aligned}\Delta\rho &= -\frac{\Sigma_a^P}{\Sigma_a}\,\frac{1}{1+L^2B^2}\left[1 - L^2B^2\,\frac{\Sigma_{tr}^P/\Sigma_a}{\Sigma_{tr}/\Sigma_a}\right] \\ &\cong \frac{\Sigma_a^P}{\Sigma_a}\,\frac{1}{1+L^2B^2}\end{aligned} \tag{6-242}$$

Here we have noted that the second term in brackets is usually quite small ($< 10^{-3}$) and can be ignored. If we set $P_{NFL} \sim 1$, then we can use the criticality condition k = 1 for rewrite

$$\Delta\rho = -\frac{\Sigma_a^P/\Sigma_f}{\nu p \epsilon} \tag{6-243}$$

Now we know that the macroscopic cross section for the poison is given by

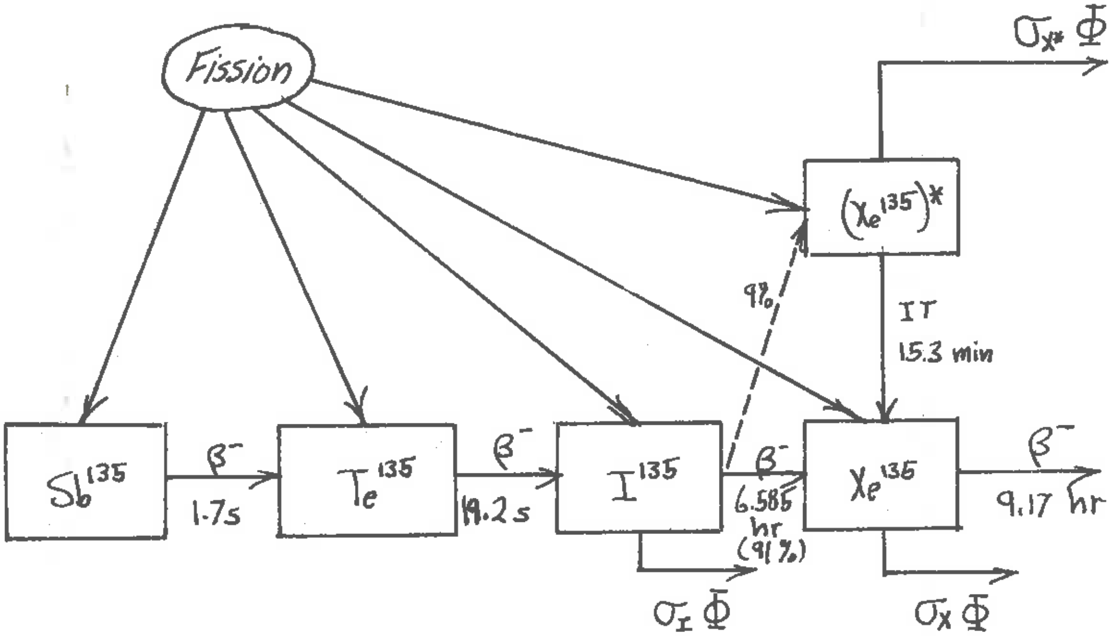
$$\Sigma_a^P = N_P \sigma_a^P \tag{6-244}$$

Hence in order to estimate the reactivity change due to fission product poisoning, we must calculate the number density of the poisoning isotope, N_p, at any time t.

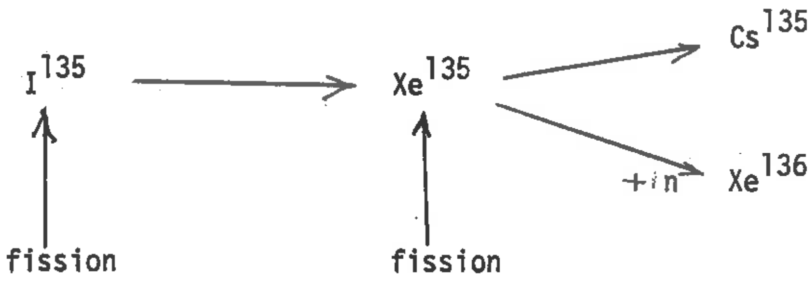
The procedure is simple--at least in concept. To determine $N_p(t)$, we must solve the rate equations describing the various production and decay processes which can affect the poison concentration. We will illustrate this procedure with two simple (but nevertheless important examples):

B. Xenon Buildup

Xe^{135} can be produced either directly as a fission product or following the β-decay of Te^{135}. The full production—decay scheme is



We will assume for convenience that the decay of Te^{135} to I^{135} is instantaneous, while Cs^{135} is stable (at least on the time scale of the I^{135} and Xe^{135} decay). We will also ignore the short-lived isomeric state $(Xe^{135})^*$. Hence the effective decay scheme we will study is



Thus we need to write rate equations, similar to those discussed in Chapter 2, for the atomic densities of I^{135} and Xe^{135}. Call these densities I(t) and X(t). If we define γ_I and γ_X as the effective fraction of the fission products which are I^{135} and Xe^{135}, respectively, then these rate equations are easily seen to be

<u>Iodine</u>

$$\frac{dI}{dt} = \gamma_I \Sigma_f \Phi(\vec{r},t) - \lambda_I I(\vec{r},t) \tag{6-245}$$

<u>Xenon</u>

$$\frac{dX}{dt} = \gamma_X \Sigma_f \Phi(\vec{r},t) + \lambda_I I(\vec{r},t) - \lambda_X X(\vec{r},t) - \sigma_a^X \Phi(\vec{r},t) X(\vec{r},t)$$

Here, λ_I and λ_X are the β-decay constants for I^{135} and Xe^{135}. Notice that we have included a loss term in the xenon balance equation to account for the fact that neutron absorption will deplete the Xe^{135} concentration (as well as the neutrons, of course). Strictly speaking, we should have included a similar term in the iodine equation--but the absorption cross section of I^{135} is sufficiently low that such a term would only be significant for extremely high flux levels. ($\Phi > 10^{16}$ cm^{-2} sec^{-1}).

The values of the yields and decay constants are tabulated in Table 6-3.

Before we can proceed further to solve these equations, we need information about the flux in the reactor, $\Phi(\vec{r},t)$. For the present, we will merely assume that the flux behavior is a known function of space and time. Then we can immediately integrate the iodine equation to find

$$I(\vec{r},t) = \left[I(\vec{r},0) + \gamma_I \int_0^t dt' \, \Sigma_f(\vec{r},t')\Phi(\vec{r},t')e^{\lambda_I t'}\right]e^{-\lambda_I t} \tag{6-246}$$

and then substitute this solution into the xenon equation and integrate it to determine the Xe^{135} concentration as a function of space and time:

$$X(\vec{r},t) = \left[X(\vec{r},0) + \int_0^t \left[\lambda_I I(\vec{r},t') + \gamma_X \Sigma_f(\vec{r},t')\Phi(\vec{r},t')\right] e^{\int_0^{t'} L(t'')dt''}\right] e^{-\int_0^t dt' L(t')} \tag{6-247}$$

where

$$L(t) \equiv \lambda_X + \sigma_X \Phi(\vec{r},t)$$

Of course, for any complicated flux behavior, these solutions will require numerical integrations. For that reason, we will specialize to the situation in which the flux is constant in time.

That is, we will determine the equilibrium levels of I^{135} and Xe^{135} which will exist in a reactor which has been operating at a specified flux level for a very long time. In this sense, we are implying that the concentrations of these fission product poisons will eventually saturate at those equilibrium values for which the production of poisons from fission

TABLE 6-3: Xe^{135} Data

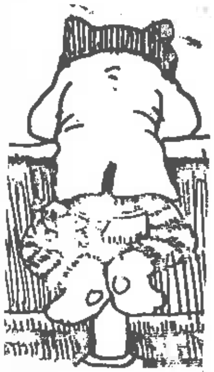
	I-135	Xe-135
σ_a, b	~7	2.64×10^6
$T_{1/2}$, hr.	6.585 ± 0.002	9.172 ± 0.005
λ, sec^{-1}	2.924×10^{-5}	2.099×10^{-5}

	U-233	U-235	Pu-239	Pu-241
$\gamma_I / \gamma_I^{U-235}$	0.7648 ± 0.0112	1.0	0.0552 ± 0.0144	1.2048 ± 0.0304
γ_X / γ_I	0.2790 ± 0.0069	0.0357 ± 0.0019	0.1782 ± 0.0023	0.0332 ± 0.0016
γ_I, %	4.884	6.386	6.100	7.694
γ_X, %	1.363	0.228	1.087	0.255

is just balanced by the decay and neutron capture losses of the poison. To determine these equilibrium levels, we merely set $\Phi(\vec{r},t) = \Phi_o(\vec{r})$ and then examine the case $\frac{dX}{dt} = 0 = \frac{dI}{dt}$ in equation (6-245). These saturation levels are then found to be

$$I_\infty = \frac{\gamma_I \Sigma_f \Phi_o}{\lambda_I}$$

$$X_\infty = \frac{(\gamma_I + \gamma_X)\Sigma_f \Phi_o}{\lambda_X + \sigma_X \Phi_o} \qquad (6\text{-}248)$$



This concentration is plotted for a cylindrical reactor core in Figure (6-6) Using this expression, and recalling

$$\Sigma_a^X = \sigma_a^X X, \qquad (6\text{-}249)$$

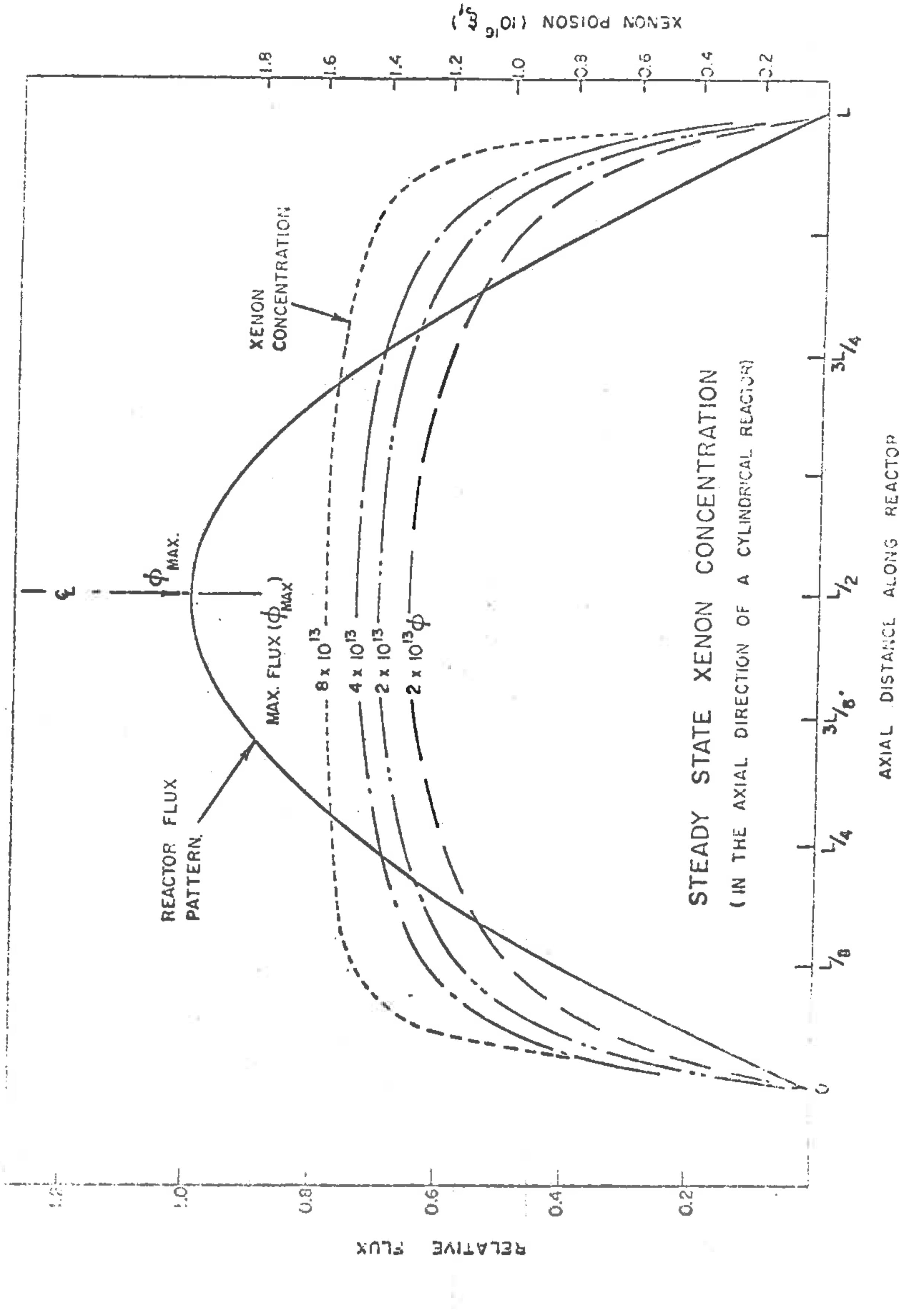
we can calculate the reactivity which must be introduced to compensate for this equilibrium Xe^{135} concentration

$$\Delta\rho = -\frac{(\gamma_I + \gamma_X)\Phi_o}{\nu p \epsilon \left(\frac{\lambda_X}{\sigma_a^X} + \Phi_o\right)} \qquad (6\text{-}250)$$

For example, in a U^{235} fueled thermal reactor, being operated at a large thermal flux--say

$$\Phi_o >> \frac{\lambda_X}{\sigma_a^X} = 0.756 \times 10^{13}\ \text{cm}^{-2}\text{sec}^{-1}, \qquad (6\text{-}251)$$

one finds $\Delta\rho$ assumes a maximum value of



STEADY STATE XENON CONCENTRATION

(IN THE AXIAL DIRECTION OF A CYLINDRICAL REACTOR)

FIGURE 6-6

$$\Delta\rho \cong -\frac{\gamma_I+\gamma_X}{\nu} = -2.62\% \tag{6-252}$$

--a rather sizeable reactivity indeed. This, of course, must be accounted for when determining the initial core loading.

Now suppose that after operating the reactor for a period of time at a constant flux level Φ_o, we suddenly shut the reactor down. Then several things will happen

(i) The removal of Xe^{135} due to neutron capture ceases

(ii) The radioactive decay of I^{135} to Xe^{135} continues

(iii) Since the halflife of I^{135} is shorter than that of Xe^{135}, the Xe^{135} concentration will initially build up before decaying out.

To study this more explicitly, suppose we solve the rate equations (6-245) characterizing the shutdown reactor:

$$\begin{aligned} \frac{dI}{dt} &= -\lambda_I I(\vec{r},t) \\ \frac{dX}{dt} &= \lambda_I I(\vec{r},t) - \lambda_X X(\vec{r},t) \end{aligned} \tag{6-253}$$

subject to the initial conditions that at the time of shutdown (t = 0), the poison concentrations have attained their equilibrium value:

$$\begin{aligned} I(\vec{r},0) &= I_\infty(\vec{r}) = \frac{\gamma_I \Sigma_f \Phi_o(\vec{r})}{\lambda_I} \\ X(\vec{r},0) &= X_\infty(\vec{r}) = \frac{(\gamma_I+\gamma_X)\Sigma_f \Phi_o(\vec{r})}{\lambda_X + \sigma_a^X \Phi_o(\vec{r})} \end{aligned} \tag{6-254}$$

The iodine equation is easy to solve

$$I(\vec{r},t) = I_\infty(\vec{r})e^{-\lambda_I t} \tag{6-255}$$

One can now insert this into the xenon equation and integrate to find

$$X(\vec{r},t) = X_\infty(\vec{r})e^{-\lambda_X t} + \frac{\lambda_I I_\infty(\vec{r})}{\lambda_I - \lambda_X}\left(e^{-\lambda_X t} - e^{-\lambda_I t}\right) \tag{6-256}$$

This concentration has been plotted for various times in Figure 6-7. If we use the explicit forms for X_∞ and I_∞, then we can find the negative reactivity introduced by the Xe^{135} buildup as

$$\rho(t) = -\frac{1}{\nu p \epsilon}\left[\frac{(\gamma_I+\gamma_X)\Phi_0}{\frac{\lambda_X}{\sigma_a^X} + \Phi_0}e^{-\lambda_X t} + \frac{\gamma_I \Phi_0}{\frac{\lambda_I}{\sigma_a^I} - \frac{\lambda_X}{\sigma_a^X}}\left(e^{-\lambda_X t} - e^{-\lambda_I t}\right)\right] \tag{6-257}$$

Some typical values are shown plotted in Figure 6-8 . The maximum value of negative reactivity depends quite sensitively upon the flux level prior to shutdown. In particular, one should note that for a period of about 30 hours after reactor shutdown, a rather sizeable reserve of positive reactivity would be needed to restart the reactor. This, of course, is a major consideration in scheduling shutdown for short periods of time.

C. Samarium Buildup

A very similar analysis can be given for Sm^{149} which is characterized by an absorption cross section σ_a = 58,500 b. The appropriate decay chain is

$$\underset{\substack{\uparrow \\ \text{fission}}}{Nd^{149}} \xrightarrow[2.0\ \text{hr}]{\beta^-} Pm^{149} \xrightarrow[54\ \text{hr}]{\beta^-} Sm^{149}$$

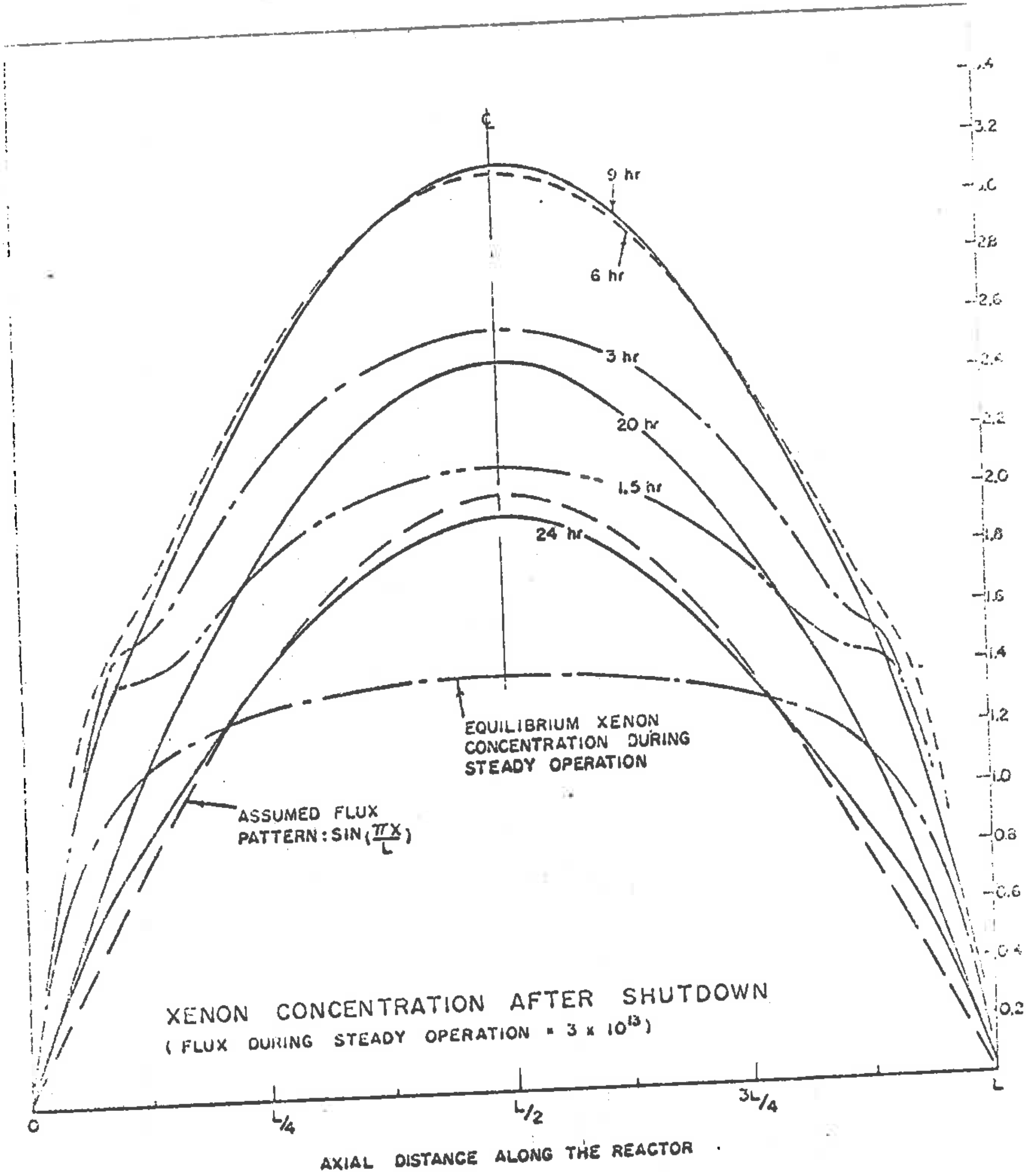
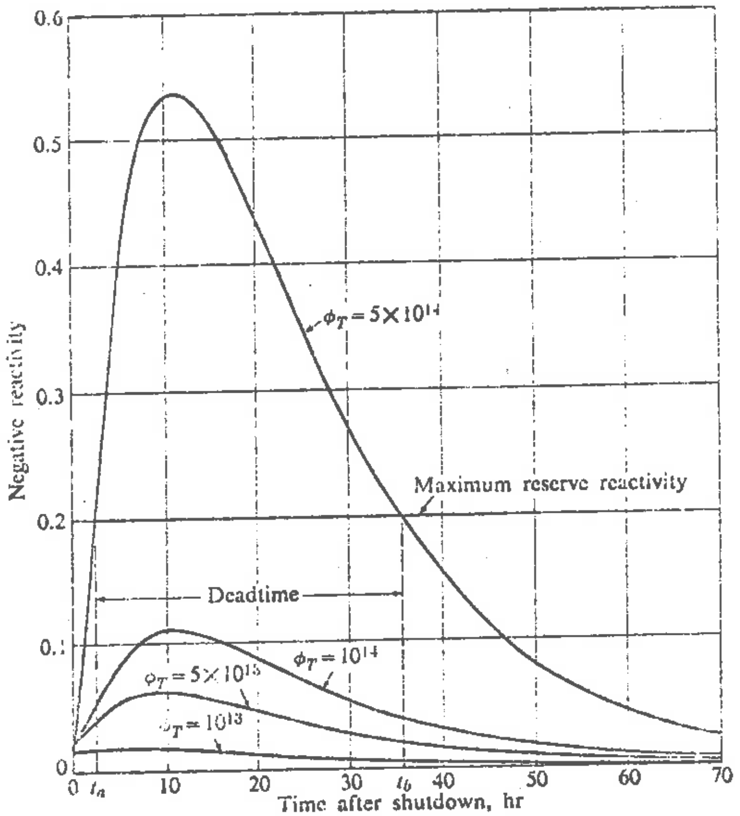

℄
9 hr
6 hr
3 hr
20 hr
1.5 hr
24 hr
EQUILIBRIUM XENON CONCENTRATION DURING STEADY OPERATION
ASSUMED FLUX PATTERN: SIN($\frac{\pi X}{L}$)
XENON CONCENTRATION AFTER SHUTDOWN
(FLUX DURING STEADY OPERATION = 3 x 10^{13})
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
L/4
L/2
3L/4
L
AXIAL DISTANCE ALONG THE REACTOR

FIGURE 6-7



Xenon-135 buildup after shutdown for several values of the operating flux before shutdown.

FIGURE 6-8

Again, it is consistent to neglect the Nd^{149} and assume fission yields Pm^{149} directly with a yield fraction $\gamma_P = .0066$. The corresponding rate equations are then

Promethium:

$$\frac{dP}{dt} = \gamma_P \Sigma_f \Phi - \lambda_P P(t) \tag{6-258}$$

Samarium:

$$\frac{dS}{dt} = \lambda_P P - \sigma_a^S \Phi S$$

where $\lambda_P = .0128\ \text{hr}^{-1}$.

The equilibrium concentrations can again be obtained by setting

$\frac{dP}{dt} = 0 = \frac{dS}{dt}$ to find

$$P_\infty = \frac{\gamma_P \Sigma_f \Phi_0(\bar{r})}{\lambda_P}$$

$$S_\infty = \frac{\gamma_P \Sigma_f}{\sigma_a^S} \tag{6-259}$$

The corresponding negative reactivity is then

$$\Delta\rho = -\frac{\gamma_P}{\nu p \epsilon} \sim 0.463\,\% \tag{6-260}$$

We can again study the shutdown behavior using P_∞ and S_∞ as initial conditions. Notice that since S^{149} is stable (unlike Xe^{135}), it can only be removed by neutron capture. Hence after shutdown it will build up to a steady level

$$S(t) = S_\infty + P_\infty (1 - e^{-\lambda_P t}) \rightarrow S_\infty + P_\infty \qquad (6\text{-}261)$$

The corresponding reacticity is

$$\Delta\rho = \frac{-\gamma_P}{\nu p \epsilon}\left[1 + \frac{\Phi_0 \sigma_a^S}{\lambda_P}(1 - e^{-\lambda_P t})\right] \qquad (6\text{-}262)$$

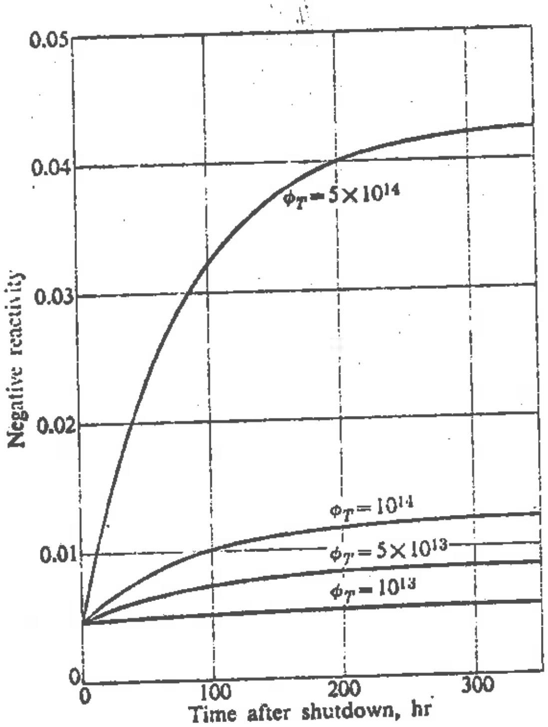
Typical plots of $\Delta\rho(t)$ are given for a U^{235} fueled reactor in Figure 6-9. The much longer time scale of the Sm^{149} should be noticed in particular.

D. Permanent Poisons

There are a great many fission product nuclides other than Xe^{135} and Sm^{149} which have appreciable neutron absorption cross sections. However, the cross sections of these other isotopes are not sufficiently large in most cases, that the poison concentration can be depleted by neutron capture. Hence these fission products to not saturate but rather tend to accumulate in a core indefinitely and must be accounted for in criticality calculations. It has become customary to lump these permanent poisons into several effective groups characterized by an effective cross sections and yields. [For one speed thermal calculations, one frequently assumes that each fission produces a permanent poison nucleus with effective absorption cross section $\sigma_a^P \sim 50$ b.] We will return later in Chapter 11 to discuss how such considerations enter core lifetime and burnup studies.

5.) Xenon-Induced Power Oscillations in Large Power Reactors

Thus far we have ignored the effect of the reactivity introduced by the fission product poisons on the neutronic behavior of the core. Actually, for such long term reactivity changes, the usual form of the neutron



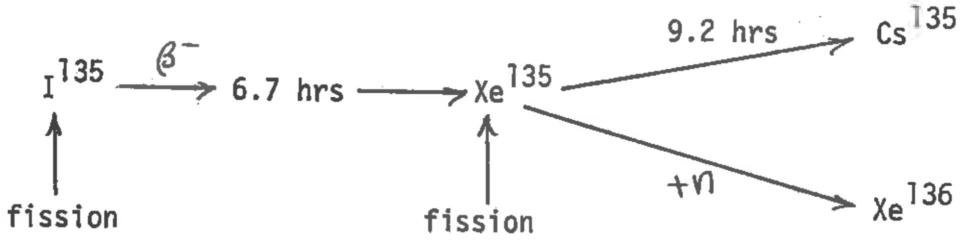
Samarium-149 buildup after shutdown for various values of the operating flux.

FIGURE 6-9

kinetics equations are quite inappropriate, since external control will always be introduced into the core to keep the reactor critical at all times. A very similar situation exists in studying fuel burnup and core lifetime, and we will develop a more general calculational model in Chapter 12 when we consider these topics in some detail.

At this point, however, we wish to illustrate the effects of reactivity feedback on the core flux levels by considering a rather interesting problem of xenon-induced flux oscillations which occur in large thermal power reactors.

We will again consider only a simplified decay chain

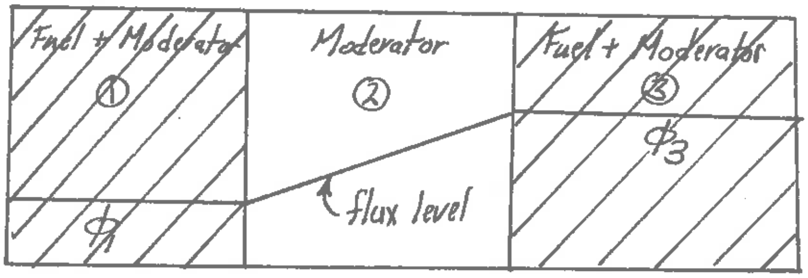


Point Reactor Model: To examine the effect of this decay chain, first consider a point reactor model in which the reactor has been operating at a steady flux level for some time. This will result in a buildup of a steady-state Xe^{135} concentration which results from the balance of Xe^{135} production (via direct fission and I^{135} decay) and loss due to decay to Cs^{135} and transmutation (via neutron absorption) to Xe^{136}. Now suppose a small perturbation increase in the flux occurs. Then Xe^{135} will transmute more rapidly to Xe^{136} (instantaneously), depleting the Xe^{135} concentration, hence decreasing the absorption and increasing the reactivity and the flux. But the increased flux transmutes even more Xe^{135}, and hence the initial flux perturbation grows with time (unstable).

Actually, such an instability can only exist for power levels higher than a certain threshold value. For U^{235} fueled reactors, this threshold is $\Phi \sim 3 \times 10^{11}$ neutrons/cm^2-sec. Below this threshold the stabilizing effect of the direct xenon yield from fission is more important than the destabilizing effect of the xenon decaying from I^{135}.

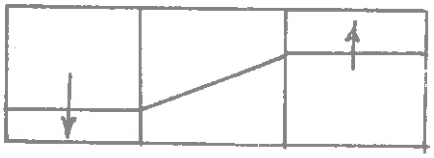
Actually, this type of instability is relatively unimportant in practical reactor operations, since it is easily controlled by normal control rod movement. A much more serious spatial xenon instability can arise, however, which requires a more complex control rod program.

Spatial Xenon Oscillations: An instructive example of a space dependent xenon buildup and decay instability can be given by considering the following very simple model: two coupled xenon unstable point reactors, separated by a moderating material.



Suppose further there is a control system keeping the total power of all three regions a constant (although the flux or power in an individual region is not constant).

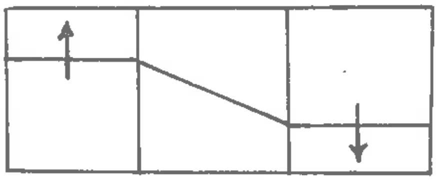
A slight increase in the power level on ons side gives rise to the unstable xenon process described for a point reactor. Since



the control system keeps the total power constant, the flux on the other side decreases. This process continues with a steeper and steeper tilt in the flux resulting. Two effects will limit this tilt:

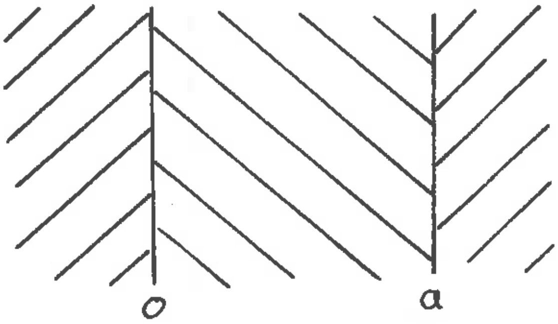
(i) burnup of most of the xenon on the high flux side

(ii) the steep flux tilt creates a flux gradient and hence a current which carries all the excess neutrons being produced to the other side



The flux will remain tilted for several hours. Eventually the high flux side will have created an I^{135} concentration much greater than that originally present. Since the decay constant of I^{135} is 6.7 hours, more xenon will be created after this delay period. Similarly on the low side less xenon will be created. This reverses the flux tilt eventually and produces a side to side oscillation with a period of from 15 to 30 hours. Thus the xenon process tends to be self limiting and produces the effect of a moving "hot spot" to the reactor operator.

The control of such oscillations is of paramount importance, since the flux in the hot spot may be quite large, leading to fuel element damage.



Suppose we consider a more detailed model of this phenomenon using the one-speed diffusion equation. We will treat delayed neutrons as if they appeared promptly, and assume reactivity is represented by $\alpha\Phi(x,t)$ where α is the power coefficient of reactivity. Then the reactor kinetics equations become:

$$\frac{1}{V}\frac{\partial \Phi}{\partial t} = D\frac{\partial^2 \Phi}{\partial x^2} + (k_\infty - 1 + \alpha\Phi)\Sigma_a \Phi - \sigma_x X \Phi \tag{6-263}$$

We will consider the geometry to be that of a well-reflected slab reactor such that the steady-state flux is spatially uniform

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi}{\partial x}\right|_{x=a} \tag{6-264}$$

The equations for iodine and xenon concentration are

$$\frac{\partial I}{\partial t} = \gamma_I \Sigma_f \Phi - \lambda_I I$$

$$\frac{\partial X}{\partial t} = \lambda_I I - \lambda_x X - \sigma_x X \Phi \tag{6-265}$$

Now if the distributions in the steady-state system Φ_o, I_o, and X_o are spatially uniform, we find these equations become

$$(k_\infty - 1 + \alpha\Phi_o)\Sigma_a \Phi_o - \sigma_x X \Phi_o = 0$$

$$I_o = \frac{\gamma_I \Sigma_f \Phi_o}{\lambda_I} \tag{6-266}$$

$$X_o = \frac{\lambda_I I_o}{\lambda_x + \sigma_x \Phi_o} = \frac{\gamma_I \Sigma_f \Phi_o}{\lambda_x + \sigma_x \Phi_o}$$

Here k_∞ is the multiplication factor the reactor would have in the absence of Xe^{135} and power feedback. We can solve for

$$\Phi_0 = \frac{k_\infty - 1}{\dfrac{\sigma_X \gamma_I \Sigma_f}{\Sigma_a(\lambda_X + \sigma_X \Phi_0)} - \alpha} \tag{6-267}$$

which has a solution if $k_\infty > 1$ and $\alpha < 0$.

We shall now linearize our system of equations by assuming the perturbations φ, ι, and χ about these steady-state values are small. Then if we substitute

$$\Phi(x,t) = \Phi_0 + \varphi(x,t)\,;\quad I(x,t) = I_0 + \iota(x,t)\,;\quad X(x,t) = X_0 + \chi(x,t) \tag{6-268}$$

into these equations and neglect second order terms we find

$$\begin{aligned} \frac{1}{v}\frac{\partial \varphi}{\partial t} &= D\frac{\partial \varphi}{\partial x^2} + (k_\infty - 1 + 2\alpha\Phi_0)\Sigma_a\varphi - \sigma_X\left[X_0\varphi + \Phi_0\chi\right] \\ \frac{\partial \iota}{\partial t} &= \gamma_I\Sigma_f\varphi - \lambda_I\iota \\ \frac{\partial \chi}{\partial t} &= \lambda_I\iota - \lambda_X\chi - \sigma_X\left[X_0\varphi + \Phi_0\chi\right] \end{aligned} \tag{6-269}$$

To solve this set of coupled P.D.E's, we will use Laplace transforms in time coupled with a model expansion in space. In this case, the appropriate "modes" are $\cos(n\pi x/a)$, $n = 1, 2, \ldots$ such that we expand

$$\begin{aligned} \varphi(x,t) &= \sum_{n=0}^{\infty} A_n(t)\cos\frac{n\pi x}{a} \\ \iota(x,t) &= \sum_{n=0}^{\infty} I_n(t)\cos\frac{n\pi x}{a} \\ \chi(x,t) &= \sum_{n=0}^{\infty} X_n(t)\cos\frac{n\pi x}{a} \end{aligned} \tag{6-270}$$

In the usual manner, we can substitute these expansions into the linearized set of equations (10-162), multiply by $\cos(n\pi x/a)$, integrate over x, and use orthogonality to find a set of equations for the coefficients A_n, I_n, and X_n. If we also Laplace transform in time, this set becomes

$$\begin{aligned} \frac{s}{V}\tilde{A}_n(s) &= -D\left(\frac{n\pi}{a}\right)^2\tilde{A}_n + (k_\infty - 1 + 2\alpha\Phi_o)\Sigma_a\tilde{A}_n - \sigma_X\left[X_o\tilde{A}_n + \Phi_o\tilde{X}_n\right] \\ s\tilde{I}_n(s) &= \gamma_I\Sigma_f\tilde{A}_n - \lambda_I\tilde{I}_n \qquad\qquad (6\text{-}271) \\ s\tilde{X}_n(s) &= \lambda_I\tilde{I}_n - \lambda_X\tilde{X}_n - \sigma_X\left[X_o\tilde{A}_n + \Phi_o\tilde{X}_n\right] \end{aligned}$$

After a bit of algebra, one can then solve this set for $\tilde{A}_n(s)$. In particular, the poles of $\tilde{A}_n(s)$ are determined by the roots of the characteristic equation

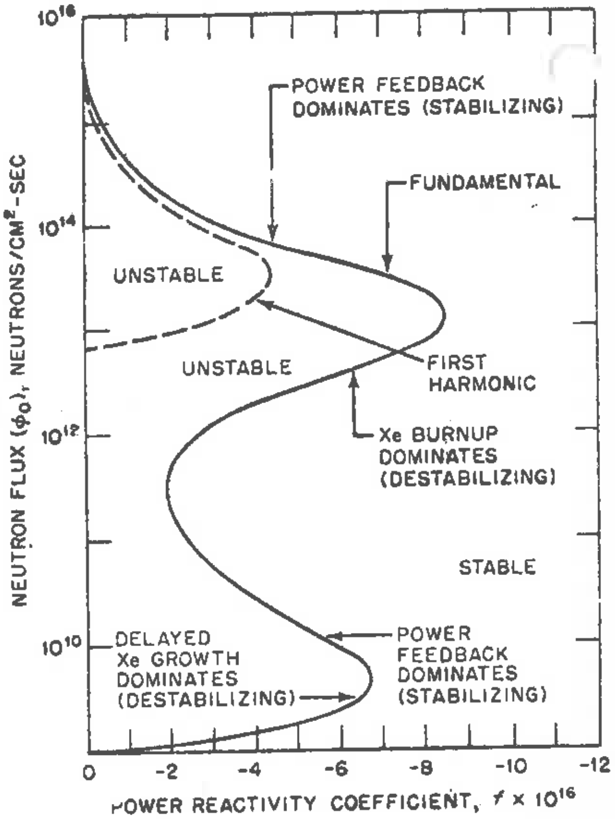
$$\frac{s}{V} = -D\left(\frac{n\pi}{a}\right)^2 + \alpha\Sigma_a\Phi_o - \frac{\sigma_X\gamma_I\lambda_I\Sigma_f\Phi_o}{(s+\lambda_I)(s+\lambda_X+\sigma_X\Phi_o)} + \frac{\sigma_X^2\gamma_I\sigma_f\Phi_o}{(\lambda_X+\sigma_X\Phi_o)(s+\lambda_X+\sigma_X\Phi_o)} \qquad (6\text{-}272)$$

There are three roots to this equation. The threshold of instability occurs when one of the roots becomes imaginary. Suppose we fix D, a, Σ_f, Σ_a, . . . and vary α and Φ_o. Then one can actually sketch an instability parameter region. We have indicated the instability region for the fundamental mode $A_o(t)$. [The dashed region is for the first harmonic $A_1(t)$. Note that it is harder to excite the higher harmonic oscillations.]

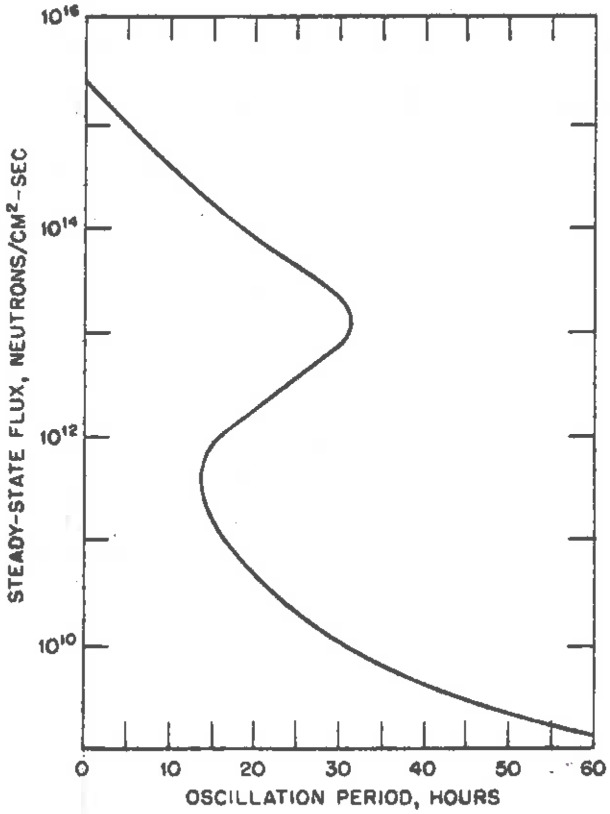
These features hold in general. When the flux Φ_o is less than 10^9 $\text{cm}^{-2}\text{-sec}^{-1}$, the system is stable against Xe^{135} oscillations--regardless of the value of α. [The burnup rate of Xe^{135} is then too small.]

At higher Φ_0, the fundamental mode becomes unstable due to delayed growth of Xe^{135}. For still higher flux, the power feedback will dominate and stabilize--but about 10^{13} the xenon instability takes over again [until Φ_0 exceeds 10^{16}].

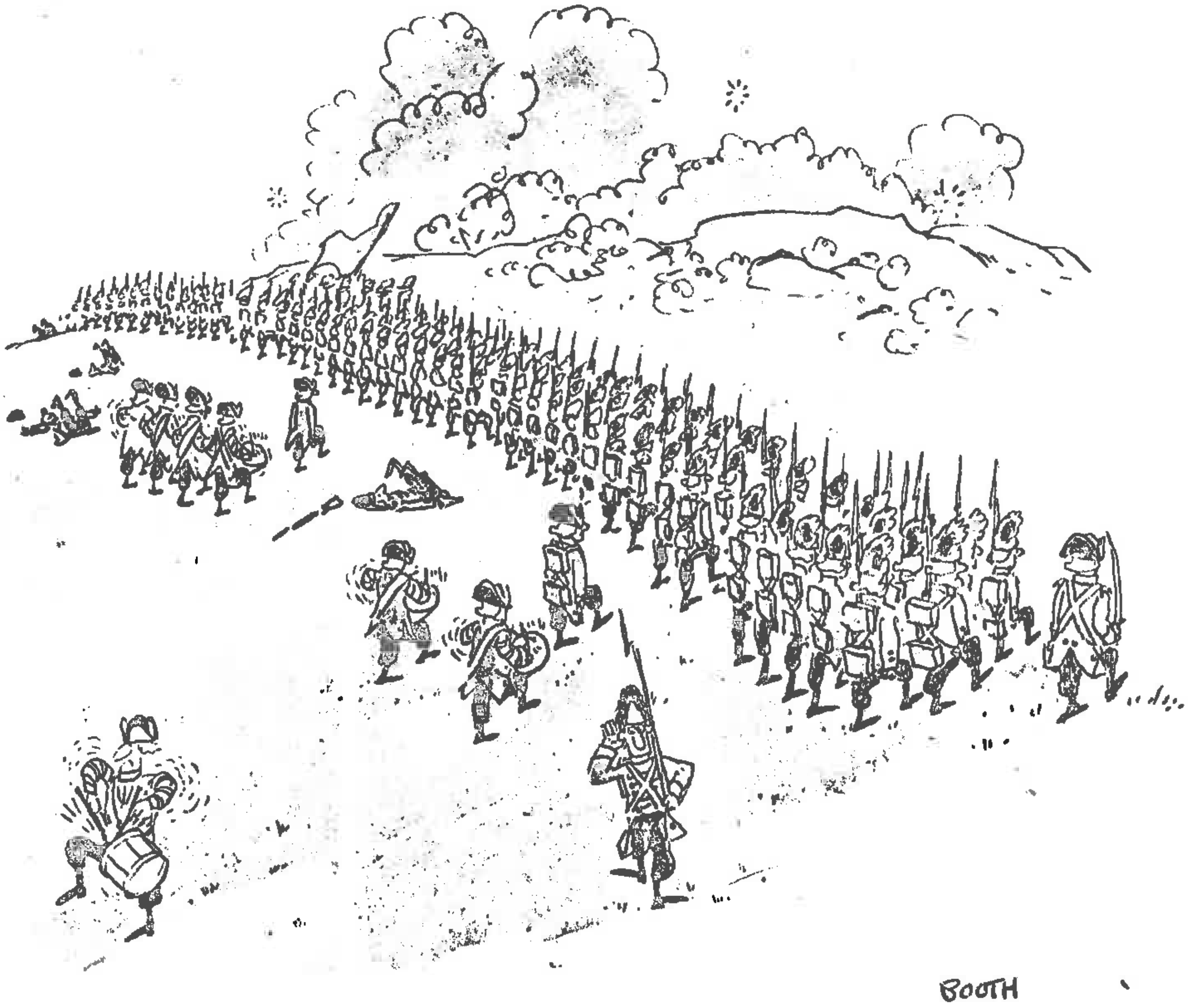
One cannot overlook the higher harmonics however, since sometimes normal control motions tend to aggravate the instability.



One can also plot the period of these oscillations vs. the power level Φ_0.

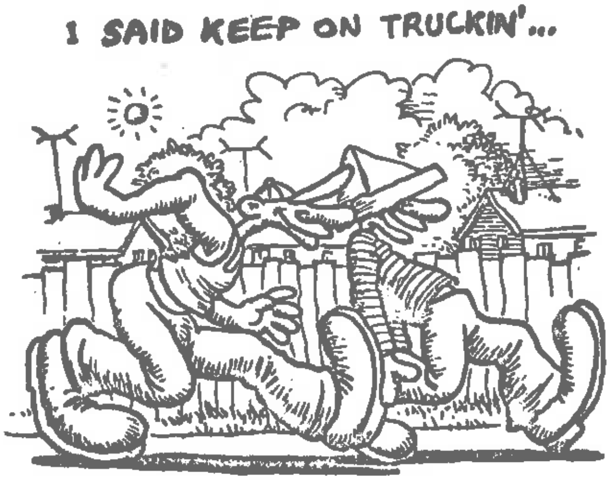


This simple one-speed model, as crude as it is, contains most of the physics of these oscillations, and has proven useful in setting up effective automatic control systems.


BOOTH

PART III

THE MULTIGROUP DIFFUSION METHOD



CHAPTER 7: MULTIGROUP DIFFUSION THEORY

I. INTRODUCTION

Thus far we have based our study of nuclear reactor theory on a particularly simple model of neutron transport: one-speed diffusion theory. This model certainly suffices to introduce most of the important concepts of reactor analysis as well as many of the computational methods used in modern reactor design. It even will provide useful quantitative estimates for certain situations (e.g., preliminary survey studies of thermal reactors). However it is a woefully inadequate model upon which to base any realistic attempt at reactor design.

Recall that two very significant assumptions have been made in the one-speed diffusion model. We first assume that the angular flux is only weakly dependent upon angle so that the diffusion approximation is valid. This assumption is usually reasonably well satisfied in large power reactors (provided we take care to "fudge" up the analysis a bit in the vicinity of strong absorbers).

The principal deficiency of the model is that it assumes that the neutrons can be characterized by only one energy or speed. But, as we have seen, the neutrons in a reactor have energies spanning the range from 10 MeV down to less than 0.01 eV--some 9 orders of magnitude. Furthermore, we have also seen that the cross sections depend rather sensitively upon the incident neutron energy. Hence it is not surprising that any practical reactor calculations will require a more realistic treatment of the neutron energy dependence. (Indeed, it is surprising that one-speed diffusion equation works at all. The fact that it does depends upon a very judicious choice of the one-speed cross sections that appear in the equation.)

We will now allow the neutron flux to depend upon energy. But rather than treat the neutron energy variable E as a continuous variable, we will immediately discretize it into energy intervals or "groups". This is shown schematically below:

Now, in our familiar discrete ordinates fashion, we will only consider the energy dependent neutron flux, $\Phi(\vec{r},E,t)$, at certain discrete points, E_g, inside each of these energy groups:

$$\phi_g(\vec{r},t) \equiv \Phi(\vec{r},E_g,t) \quad , \quad g=1,2,\cdots G \qquad (7\text{-}1)$$

(Actually, this is not quite how we define the discretized fluxes--they are rather defined as integrals of $\Phi(\vec{r},E,t)$ over the energy group. But for pedagogical purposes, we will pretend the standard discrete ordinates method can be applied here.)

Hence our immediate task is to determine equations for the group fluxes $\phi_g(r,t)$. We will first give a heuristic derivation of these "multigroup" equations, and then return in Section III to develop a much more rigorous (and useful) derivation of these equations.

II. HEURISTIC DERIVATION OF THE MULTIGROUP DIFFUSION EQUATIONS

Let us consider any one of the energy groups, say group g. We will now attempt to write down a neutron balance for the group by figuring out all of the ways that neutrons can enter or leave the group. A bit of reflection indicates that such a balance would read as follows:

$$\begin{pmatrix}\text{time rate of}\\ \text{change of}\\ \text{neutrons in}\\ \text{group g}\end{pmatrix} = -\begin{pmatrix}\text{change due}\\ \text{to}\\ \text{leakage}\end{pmatrix} - \begin{pmatrix}\text{absorption}\\ \text{in}\\ \text{group g}\end{pmatrix} + \begin{pmatrix}\text{fission neutrons}\\ \text{born in}\\ \text{group g}\end{pmatrix} - \begin{pmatrix}\text{neutrons}\\ \text{scattering}\\ \text{out of}\\ \text{group g}\end{pmatrix} + \begin{pmatrix}\text{neutrons}\\ \text{scattering}\\ \text{into}\\ \text{group g}\end{pmatrix} \tag{7-2}$$

It should be noted that we have taken explicit account of the fact that a scattering collision can change the neutron energy and hence either remove it from the group g, or if it is initially in another group g', scatter it to an energy in the group g. We will characterize the probability for scattering a neutron from a group g' to the group g by something akin to the differential cross section $\Sigma_s(E_{g'} \rightarrow E_g)$ (a so-called "group transfer" cross section):

$$\Sigma_{sg'g}$$

Note then that the cross section characterizing the probability that a neutron will scatter out of the group g is given by

$$\Sigma_{sg} = \sum_{g'} \Sigma_{sgg'}$$

We will similarly define an absorption cross section characterizing the group g, Σ_{a_g} , and a fission source term S_{fg} which give the rate at which fission neutrons are born in group g. Finally, we will define a diffusion coefficient, D_g, so that the leakage from group g can be written within the diffusion approximation as $\nabla D_g \nabla \phi_g$. If we put all of these terms together, we find a mathematical representation of the balance relation Eq. (7-1).

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} = \nabla D_g \nabla \phi_g - \Sigma_{a_g}\phi_g + S_{fg} - \Sigma_{sg}\phi_g + \sum_{g'=1}^{G} \Sigma_{sg'g}\phi_{g'} \qquad g=1,2,\cdots G \tag{7-3}$$

Actually, we can get a bit more specific with the fission source term by writing it as

$$S_{fg} = \chi_g \sum_{g'=1}^{G} \nu\Sigma_{fg'}\phi_{g'} \tag{7-4}$$

where χ_g is the probability that a fission neutron will be born with an energy in group g, while Σ_{fg} is the fission cross section characterizing a group g'.

Hence we now have a set of G coupled diffusion equations for the G unknown group fluxes $\phi_g(\vec{r},t)$. It shouldn't take much imagination to see that many of the same techniques that we used for the one-speed (or in our present terminology, "one-group") problems will also hold for the G-group system. In fact, we will see later in this chapter that the specific structure of the multigroup equations makes their solution extremely simple in most cases--provided one can handle the diffusion equation within each group.

The more serious problem concerns how one determines the "group constants" which appear in these equations:

$$V_g,\ D_g,\ \Sigma_{ag},\ \Sigma_{sg},\ \Sigma_{sg'g},\ \chi_g,\ \&\ \Sigma_{fg}$$

We have only given a very vague definition of these constants in our heuristic derivation of the multigroup equations. Hence before we can concern ourselves with just how these equations are to be solved, we must go back and give a more careful derivation of these equations in an effort to obtain a more explicit and useful derivation of the group constants.

III. DERIVATION OF THE MULTIGROUP EQUATIONS FROM ENERGY-DEPENDENT DIFFUSION THEORY

Suppose we return to the exact continuity equations we derived long ago in Chapter IV by integrating the transport equation over angle

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} + \nabla\cdot\vec{J}(\vec{r},E,t) + \Sigma_t(E)\Phi(\vec{r},E,t) = \int_0^\infty dE'\,\Sigma_s(E'\to E)\Phi(\vec{r},E',t) + S(\vec{r},E,t) \qquad (7\text{-}6)$$

(Here, $S(\vec{r},E,t)$ includes both external sources and fission sources.) We will assume that we can use a generalization of the diffusion approximation to include energy dependence:

$$\vec{J}(\vec{r},E,t) \cong -D(\vec{r},E)\,\nabla\Phi(\vec{r},E,t) \qquad (7\text{-}7)$$

Actually, this generalization is far from obvious. We will return to consider it in some detail in Chapter 8 when we discuss neutron slowing down. For now, suffice it to say that if the assumption of isotropic scattering is valid, then the energy-dependent diffusion coefficient is given as the expected generalization of our earlier result from Chapter 5:

$$D(E) = \frac{1}{3\Sigma_t(E)} \tag{7-8}$$

In the more general case of anisotropic scattering, a more complicated expression for D(E) must be used

$$D(E) = \frac{1}{3\left[\Sigma_t(E) - \bar{\mu}_0(E)\,\Sigma_s(E)\right]} \tag{7-9}$$

where $\bar{\mu}_0(E)$ represents an average scattering angle: cosine:

$$\bar{\mu}_0(E) = \frac{\int_0^\infty dE' \int d\hat{\Omega}' \,(\hat{\Omega}'\cdot\hat{\Omega})\,\Sigma_s(E\to E', \hat{\Omega}'\cdot\hat{\Omega})}{\int_0^\infty dE \int d\hat{\Omega}\; \Sigma_s(E\to E', \hat{\Omega}'\cdot\hat{\Omega})} \tag{7-10}$$

(These prescriptions for calculating D(E) are extremely important for without them we would be unable to compute the group constants D_g.)

With this understanding, we can now use Eq. (7-7) in Eq. (7-6) to obtain the <u>energy-dependent diffusion equation</u>

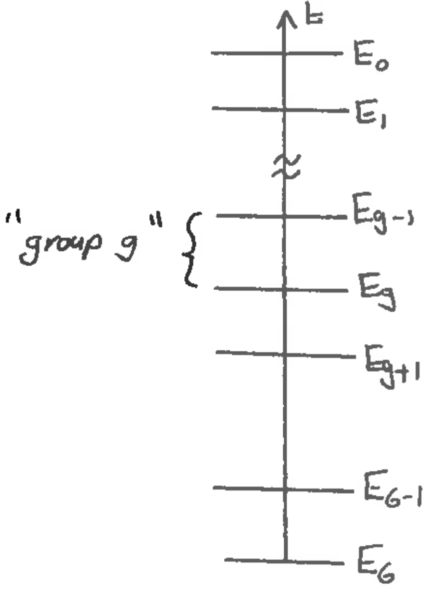
$$\frac{1}{v}\frac{\partial\Phi}{\partial t} - \nabla\cdot D\nabla\Phi + \Sigma_t\Phi = \int_0^\infty dE'\,\Sigma_s(E'\to E)\,\Phi(\vec{r},E',t) + S(\vec{r},E,t) \tag{7-11}$$

This equation will form the basis for our further work. As it stands, the equation is an integrodifferential equation, with an integral term in energy. We will eliminate the energy variable by discretizing this equation in E.

Before we proceed to do this, let us make one additional side comment. We will later find in Chapter 8 that the enormous range of neutron energies present in a reactor makes it convenient to make a variable transformation to a new variable, $u = \ln E_o/E$, where E_o is some suitably chosen reference energy. This logarithmic energy variable is referred to as the neutron "lethargy"--as the neutron slows down, u becomes larger and hence the neutron becomes more "lethargic".

Anyhow, most derivations of the multigroup diffusion equations proceed from a particular approximation to the energy-dependent diffusion equation known as the "age-dffusion" equation (which we will also discuss in Chapter 8) which is written in terms of the lethargy variable. We will utilize this formalism ourselves later when we discuss neutron slowing down. For now, however, it seems most appropriate to remain in the energy variable.

We begin by breaking up the energy range, say from E = 0 to E = 10 MeV, into G intervals, defined as shown below:



We will say that each such interval represents a "group" of energies, e.g., all neutron with energies E between E_g and E_{g-1} are said to be in group g. Notice here that the indexing is a bit backwards--from high energies to low energies. We will later find that this is very convenient, since the fact that the neutron tends to always lose energy in a scattering collision dictates that one solve the multigroup equations starting at high energies and working successively to lower energies.

Next, integrate the energy-dependent diffusion equation (6) over the gth energy group

$$\frac{\partial}{\partial t}\int_{E_g}^{E_{g-1}} dE\,\frac{1}{v}\Phi - \nabla\cdot\int_{E_g}^{E_{g-1}} dE\,D\nabla\Phi + \int_{E_g}^{E_{g-1}} dE\,\Sigma_t\Phi$$
$$= \int_{E_g}^{E_{g-1}} dE\int_0^{\infty} dE'\,\Sigma_s(E'\to E)\,\Phi(\vec{r},E',t) + \int_{E_g}^{E_{g-1}} dE\,S(\vec{r},E,t) \tag{7-12}$$

We will proceed further by making some formal definitions. First define the neutron flux in group g as

$$\phi_g(\vec{r},t) \equiv \int_{E_g}^{E_{g-1}} dE\,\Phi(\vec{r},E,t) \tag{7-13}$$

Next define the total cross section for group g as

$$\Sigma_{tg} \equiv \frac{\displaystyle\int_{E_g}^{E_{g-1}} dE\,\Sigma_t(E)\,\Phi(\vec{r},E,t)}{\displaystyle\int_{E_g}^{E_{g-1}} dE\,\Phi(\vec{r},E,t)} \tag{7-14}$$

the diffusion coefficient for group g as

$$D_g \equiv \frac{\displaystyle\int_{E_g}^{E_{g-1}} dE\,D(E)\,\nabla_j\Phi(\vec{r},E,t)}{\displaystyle\int_{E_g}^{E_{g-1}} dE\,\nabla_j\,\Phi(\vec{r},E,t)} \tag{7-15}$$

the neutron speed characterizing group g as

$$\frac{1}{V_g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \, \frac{1}{v} \Phi(\vec{r},E,t)}{\int_{E_g}^{E_{g-1}} dE \, \Phi(\vec{r},E,t)} \qquad (7\text{-}16)$$

The scattering term requires a bit more work. First break up the integral over E' as

$$\int_0^\infty dE' \, \Sigma_s(E' \to E) \Phi(\vec{r},E',t) = \sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} dE' \, \Sigma_s(E' \to E) \Phi(\vec{r},E',t) \qquad (7\text{-}17)$$

Then if we recognize that the term which appears in equation (1-12) is of the form

$$\int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \Sigma_s(E' \to E) \Phi(\vec{r},E',t) = \sum_{g'=1}^{G} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma_s(E' \to E) \Phi(\vec{r},E',t) \qquad (7\text{-}18)$$

it becomes evident that we want to define the group transfer cross section as

$$\Sigma_{sg'g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g-1}} dE' \, \Sigma_s(E' \to E) \Phi(\vec{r},E',t)}{\int_{E_{g'}}^{E_{g'-1}} dE' \, \Phi(\vec{r},E',t)} \qquad (7\text{-}19)$$

A very similar procedure is followed for the fission term. First write

$$S_f(\vec{r},E,t) = \nu\chi(E)\int_0^\infty dE'\,\Sigma_f(E') \qquad (7\text{-}20)$$

Then if we note that

$$\int_{E_g}^{E_{g-1}} dE\,S_f(\vec{r},E,t) = \int_{E_g}^{E_{g-1}} dE\,\nu\chi(E)\left[\sum_{g'=1}^{G}\int_{E_{g'}}^{E_{g'-1}} dE'\,\Sigma_f(E')\,\Phi(\vec{r},E',t)\right] \qquad (7\text{-}21)$$

it becomes convenient to define the fission cross section for group g' as

$$\Sigma_{f_{g'}} \equiv \frac{\int_{E_{g'}}^{E_{g'-1}} dE'\,\Sigma_f(E')\,\Phi(\vec{r},E',t)}{\int_{E_{g'}}^{E_{g'-1}} dE'\,\Phi(\vec{r},E',t)} \qquad (7\text{-}22)$$

while defining

$$\chi_g \equiv \int_{E_g}^{E_{g-1}} dE\,\chi(E) \qquad (7\text{-}23)$$

If we now use these purely formal definitions to rewrite equation (7-12), we arrive directly at the <u>multigroup diffusion equations</u>:

$$\frac{1}{v_g}\frac{\partial\phi_g}{\partial t} - \nabla\cdot D_g\nabla\phi_g + \Sigma_{t_g}\phi_g(\vec{r},t)$$

$$= \sum_{g'=1}^{G}\Sigma_{s_{g'g}}\phi_{g'} + \nu\chi_g\sum_{g'=1}^{G}\Sigma_{f_{g'}}\phi_{g'} \qquad (7\text{-}24)$$

$$g = 1,2,\cdots G$$

Several comments concerning these equations are necessary. The multigroup diffusion equations (7-24) are still quite exact (within the diffusion approximation, that is)--but they are also quite formal in the sense that the group constants are still undetermined. While it is true that our derivation has yielded explicit expressions for these group constants, it is apparent that in order to calculate them we would need to know the flux $\Phi(\vec{r},E,t)$, and this is just the function we were trying to calculate in the first place by discretizing the energy dependent diffusion equation (7-12). Hence it seems as if we have only gone in a circle.

But maybe you have already guessed the game we will play now. For in fact, we will attempt to guess or approximate the "intragroup" fluxes

$$\Phi(\vec{r},E,t) \cong \Phi_{approx}(\vec{r},E,t) \qquad (7\text{-}25)$$

in our calculation of the group constants, e.g.,

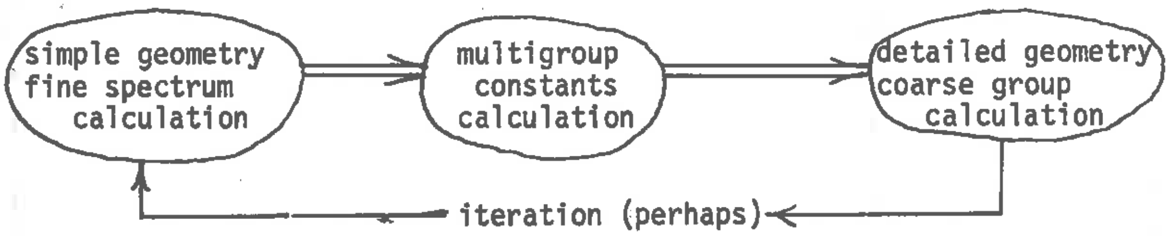
$$\Sigma_{tg} \cong \frac{\displaystyle\int_{E_g}^{E_{g-1}} dE\, \Sigma_t(E)\, \Phi_{approx}}{\displaystyle\int_{E_g}^{E_{g-1}} dE\, \Phi_{approx}} \qquad (7\text{-}26)$$

as averages over these approximate intragroup fluxes.

In the next two chapters we will develop a number of schemes for approximating the flux $\Phi(\vec{r},E,t)$ within a group--usually by first neglecting its spatial and time dependence. The accuracy required of this flux estimate is primarily dictated by the group structure itself. Of course for an extremely fine group structure, the cross sections and hence the flux would tend to be smoothly varying, and hence even a very crude approximation to the flux would be sufficient. For example, in Chapter 8 we will demonstrate that in a thermal reactor, the flux behaves very roughly as $\Phi(E) \sim 1/E$ for energies between 1 eV and 10^5 eV. Hence this functional form could be inserted into our definitions to calculate the group constants characterizing groups in this energy range. However when we remember the very complicated dependence of the cross sections upon energy (in particular, their resonance structure), it becomes apparent that the groups would have to be very finely divided indeed for such a crude approximation to the intragroup fluxes to yield meaningful results.

In actual practice, one usually works with from 4 to 20 groups in reactor calculations. Such few group calculations can only be effective with reasonably accurate estimates of the group constants (and hence the intragroup fluxes). The most common approach is to actually perform two multigroup calculations. In the first of these calculations, the spatial and time dependence is ignored, and a very fine structured multigroup calculation is performed to calculate the intragroup fluxes (usually relying upon various models of neutron slowing down and thermalization). The group constants for this "fine spectrum" calculations are frequently taken to be just the tabulated cross section data in the group of interest.

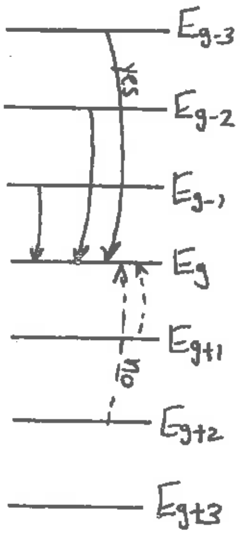
These intragroup fluxes are then used to calculate the group constants for a "coarse" group calculation (including spatial dependence):



This scheme of first calculating a neutron flux spectrum and then "collapsing" the cross section data over this spectrum to generate few group constants is the most common scheme in use today. It should be noted that in a calculation of this type, the spectrum calculation (and hence the few group constants) will depend sensitively upon the particular reactor being analyzed, as well as upon its operating conditions (e.g., fuel loading, isotopic composition, temperature, coolant conditions). Hence spectrum calculations and the generation of few group constants must be performed again and again in reactor design.

How many groups are necessary for a reactor calculation? This will depend upon the problem one is considering. For example, in very crude survey calculations of thermal reactors, 2 groups (one to characterize fast neutrons, one to characterize thermal neutrons) may be sufficient. Most light water reactor calculations are performed using a 4 group diffusion model (3 fast groups, 1 thermal group). For fine detail, one may have to go as high as 20 groups (this is particularly true in fast reactor calculations). And in spectrum calculations, the number of groups can range as high as 1000 (so-called micro-group structure) which is almost as detailed as the tabulated cross section data itself.

It is most convenient to rewrite the multigroup diffusion equations in matrix form. Before doing this, however, let's look a bit closer at the structure of these equations. In particular, consider the scattering term in the equation. Later, in Chapter 8, we will demonstrate that if the neutron



energy is greater than about 1 eV, then it can never gain energy in a scattering collision. That is, fast neutrons only slow down in a collision. Hence in these fast groups, we can set

$$\Sigma_{sg'g} = 0 \quad \text{for} \quad g' < g \tag{7-27}$$

Since most multigroup calculations utilize only one thermal group to describe the neutrons with $E < 1$ eV (assuming that neutrons cannot scatter up out of the thermal group), we can generally simplify the scattering term to write

$$\sum_{g'=1}^{G} \Sigma_{sg'g}\phi_{g'} = \sum_{g'=1}^{g-1} \Sigma_{sg'g}\phi_{g'} + \Sigma_{sgg}\phi_g \tag{7-28}$$

Here we have taken care to separate the "in-group" scattering term

$$\Sigma_{sgg}\phi_g \tag{7-29}$$

It is customary to transfer this term to the left-hand-side of the multigroup equation (7-24) and to define a "removal cross section"

$$\Sigma_{R_g} \equiv \Sigma_{tg} - \Sigma_{sgg} \tag{7-30}$$

which characterizes the probability that a neutron will be removed from the group g by a collision. [Note: Sometimes the removal cross section is defined such that it does not contain absorption, Σ_{a_g}. We will use the above definition in our development however.] We will see later that the neglect of upscattering (that is, the assumption that the neutron can never gain energy or scatter up on energy in a collision) greatly simplified the solution of the multigroup diffusion equations.

Let us now rewrite these equations in matrix form. Since most multigroup calculations are performed for time-independent situations, (e.g., criticality calculations), we will first set

$$\frac{1}{V_g}\frac{\partial\phi_g}{\partial t} = 0 \tag{7-31}$$

so that the multigroup equations can be written as

$$-\nabla D_g \nabla\phi_g + \Sigma_{R_g}\phi_g = \sum_{g'=1}^{g-1}\Sigma_{sg'g}\phi_{g'} + \nu\chi_g\sum_{g'=1}^{G}\Sigma_{f_{g'}}\phi_{g'} \tag{7-32}$$

$$g = 1, 2, \cdots, G$$

In matrix form then

$$\underbrace{\begin{pmatrix} -\nabla D_1\nabla + \Sigma_{R_1} & 0 & 0 & \cdots \\ \Sigma_{s12} & -\nabla D_2\nabla + \Sigma_{R_2} & 0 & \cdots \\ \Sigma_{s13} & \Sigma_{s23} & -\nabla D_3\nabla + \Sigma_{R_3} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}}_{\underline{\underline{M}}} \underbrace{\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \end{pmatrix}}_{\underline{\phi}} = \underbrace{\begin{pmatrix} \nu\chi_1\Sigma_{f_1} & \nu\chi_1\Sigma_{f_2} & \cdots \\ \nu\chi_2\Sigma_{f_1} & \nu\chi_2\Sigma_{f_2} & \cdots \\ \nu\chi_3\Sigma_{f_1} & \nu\chi_3\Sigma_{f_2} & \cdots \\ \vdots & \vdots & \end{pmatrix}}_{\underline{\underline{F}}} \underbrace{\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix}}_{\underline{\phi}}$$

(7-33)

or

$$\underline{\underline{M}}\,\underline{\phi} = \underline{\underline{F}}\,\underline{\phi} \tag{7-34}$$

Notice in particular that the neglect of upscattering has led to a lower triangular form for the "diffusion" matrix $\underline{\underline{M}}$. The fission matrix $\underline{\underline{F}}$ is full, however, since fission neutrons induced by a neutron absorption in a lower group will appear in the higher energy groups.

We will return later to determine a strategy for solving this matrix system of diffusion equations. First, however, it is useful to consider a couple of extremely simple applications of the multigroup equations.

IV. A SIMPLE EXAMPLE: TWO GROUP DIFFUSION THEORY

A. One-Group Diffusion Theory

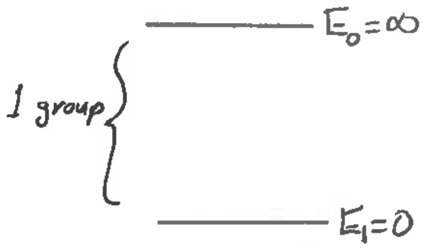
There are very few situations in which analytical solutions to the multigroup diffusion equations are feasible (few groups or few regions). Since these analytical solutions are of little practical value (see Lamarsh, pp. 323-346 for a troll-type example), we will consider only two very simple examples here.

First, suppose we set up the "one-group" diffusion equation by defining $E_0 =$ and $E_1 = 0$. Then if we note that

$$\int_0^\infty dE\,\chi(E) = 1$$

and

$$\int_0^\infty dE\,\Sigma_s(E'\to E) = \Sigma_s(E) \tag{7-35}$$



we find that the multigroup equations yield an old friend

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - D\nabla^2\phi + \Sigma_a \phi(\vec{r},t) = \nu\Sigma_f \phi . \tag{7-36}$$

Of course it should be stressed that this equation is still of only formal significance until we provide some prescription for calculating the group constants (that is, the intragroup flux--which, in this case, is $\Phi(\vec{r},E,t)$). Nevertheless, it is comforting to know that if we chose the group constants properly, even one-speed diffusion theory could give an accurate description of nuclear reactor behavior.

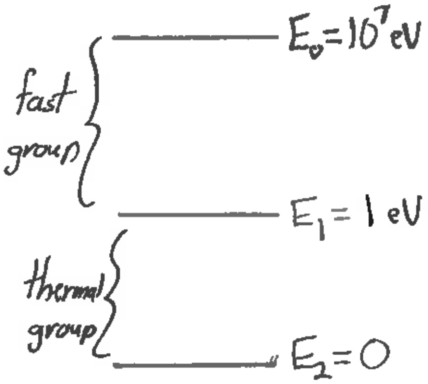
B. Two-Group Diffusion Equations

A more enlighting application involves the study of a bare, homogeneous reactor within two-group diffusion theory. This example, is particularly useful in relating the multigroup description to our earlier work.

First let us choose a group structure. We will break up the neutron energy range into a "thermal group" from $E_2 = 0$ to $E_1 = 1$ eV, and a "fast group" from $E_1 = 1$ eV to $E_0 = 10$ MeV as shown. This allows us to identify

$$\phi_1(\vec{r}) = \int_{E_1}^{E_0} dE\, \Phi(\vec{r},E) \equiv \text{"fast flux"}$$

$$\phi_2(\vec{r}) = \int_{E_2}^{E_1} dE\, \Phi(\vec{r},E) \equiv \text{"thermal flux"}$$

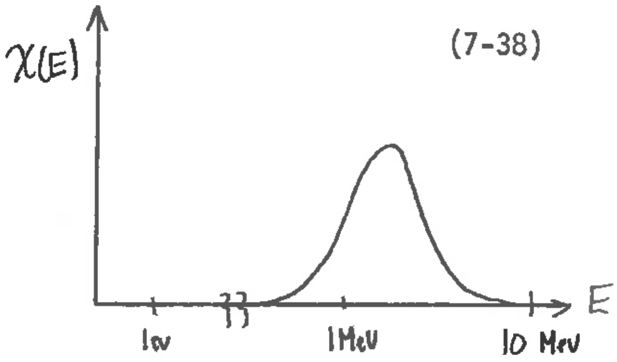


(7-37)

Next, we can simplify the group constants to some degree. First consider the fission spectrum. Since essentially all fission neutrons are born in the fast group, we find

$$\chi_1 = \int_{E_1}^{E_0} dE\, \chi(E) \cong 1$$

$$\chi_2 = \int_{E_2}^{E_1} dE\, \chi(E) \cong 0 \qquad (7\text{-}38)$$



Hence the fission source will only appear in the fast group equation:

$$S_{f_1}(\vec{r}) = \nu_1 \Sigma_{f_1} \phi_1(\vec{r}) + \nu_2 \Sigma_{f_2} \phi_2(\vec{r}) \quad \text{(fast)}$$

$$(7\text{-}39)$$

$$S_{f_2}(\vec{r}) = 0 \quad \text{(thermal)}$$

Continuing on, we can calculate the scattering and removal cross section. First, since there is no slowing down out of the thermal group,

$$\int_{E_2 \sim 0}^{E_1 \sim 1\text{eV}} dE\, \Sigma_s(E' \to E) = \Sigma_s(E') , \qquad E_2 \le E' \le E_1 \qquad (7\text{-}40)$$

Hence

$$\Sigma_{s_{22}} = \frac{\int_{E_2}^{E_1} dE \int_{E_2}^{E_1} dE'\, \Sigma_s(E' \to E)\, \Phi(\vec{r}, E')}{\int_{E_2}^{E_1} dE'\, \Phi(\vec{r}, E')} = \frac{\int_{E_2}^{E_1} dE'\, \Sigma_s(E')\, \Phi(\vec{r}, E')}{\int_{E_2}^{E_1} dE'\, \Phi(\vec{r}, E')} = \Sigma_{s_2} \qquad (7\text{-}41)$$

Thus the removal cross section for the thermal group is just

$$\Sigma_{R_2} = \Sigma_{t_2} - \Sigma_{s_{22}} = \Sigma_{t_2} - \Sigma_{s_2} = \Sigma_{a_2} \tag{7-42}$$

as we might have expected. The remainder of the group constants are defined as before in the previous section. In practice they would be calculated by first performing a fine spectrum calculation for the group of interest, and then collapsing the appropriate cross section data over this spectrum to obtain the group constants. For example, a "fast spectrum" calculation would be performed to calculate the "fast group constants" ν_1, Σ_{f_1}, Σ_{R_1}, and $\Sigma_{s_{12}}$, and D_1 (as described in Chapter 8) while a "thermal spectrum" calculation would be performed to calculate the "thermal group constants" ν_2 and D_2, Σ_{a_2}.

The two group diffusion equations can then be written as

$$\begin{aligned} -D_1\nabla^2\phi_1 + \Sigma_{R_1}\phi_1 &= \frac{1}{k}\left[\nu_1\Sigma_{f_1}\phi_1 + \nu_2\Sigma_{f_2}\phi_2\right] \\ -D_2\nabla^2\phi_2 + \Sigma_{a_2}\phi_2 &= \Sigma_{s_{12}}\phi_1 \end{aligned} \tag{7-43}$$

Notice we have inserted a multiplication factor ($^1/_k$) in front of the fission source term since we are eventually going to be performing a criticality search.

To apply these equations to a bare, homogeneous reactor we will take as boundary conditions

$$\begin{aligned} \phi_1(\tilde{R}_s) &= 0 \\ \phi_2(\tilde{R}_s) &= 0 \end{aligned} \tag{7-44}$$

[Here we are assuming that the extrapolation length is the same for both groups--which is not true in general.] Consistent with our interest in a criticality calculation, we need only use the geometric buckling defined by:

$$\begin{aligned} \nabla^2\phi_1 + B^2\phi_1 &= 0 \\ \nabla^2\phi_2 + B^2\phi_2 &= 0 \end{aligned} \tag{7-45}$$

(Here we have set $B^2 = B_g^2$ = geometric buckling so as not to be confused with the group index g.)

Hence we can rewrite the two-group equations as

$$\begin{aligned} (D_1B^2+\Sigma_{R_1}-\nu_1\Sigma_{f_1})\phi_1 - \nu_2\Sigma_{f_2}\phi_2 &= 0 \\ -\Sigma_{s12}\phi_1 + (D_2B^2+\Sigma_{a_2})\phi_2 &= 0 \end{aligned} \tag{7-46}$$

But this algebraic system has a solution if and only if

$$\left(D_1B^2+\Sigma_{R_1}-\frac{\nu_1\Sigma_{f_1}}{k}\right)(D_2B^2+\Sigma_{a_2}) - \frac{\nu_2\Sigma_{f_2}\Sigma_{s12}}{k} = 0 \tag{7-47}$$

We can now solve for the value of the multiplication factor, k, which will yield a nontrivial solution of the two-group equations:

$$k = \frac{\nu_1\Sigma_{f_1} + \nu_2\Sigma_{f_2}\left(\frac{\Sigma_R}{D_2B^2+\Sigma_{a_2}}\right)}{D_1B^2+\Sigma_{a_1}+\Sigma_R}, \quad \Sigma_R \equiv \Sigma_{R_1}-\Sigma_{a_1} \tag{7-48}$$

C. Relation to 6-Factor Formula

It is of interest for us to see if we can relate this expression to our earlier expressions for k--notably the 6-factor formula. To this end, first set $B^2 = 0$ to obtain an expression for the infinite medium multiplication factor, k_∞:

$$k_\infty = \frac{\nu_1 \Sigma_{f_1} + \nu_2 \Sigma_{f_2}\left(\frac{\Sigma_R}{\Sigma_{a_2}}\right)}{(\Sigma_{a_1} + \Sigma_R)} \tag{7-49}$$

From our earlier definitions of the quantities appearing in the 4-factor formula, it is apparent that we can define

$$\eta f = \nu_2 \frac{\Sigma_{f_2}}{\Sigma_{a_2}} = \left(\nu_2 \frac{\Sigma_{f_2}^F}{\Sigma_{a_2}^F}\right)\left(\frac{\Sigma_{a2}^F}{\Sigma_{a_2}}\right) \tag{7-50}$$

Next, notice that:

number of neutrons leaving group 1/sec = $\Sigma_{R_1}\phi_1$

number of neutrons entering group 2/sec = $\Sigma_{s_{12}}\phi_1$ (7-51)

Hence the probability that a neutron is not absorbed in the fast group must just be the ratio of these quantities. But if we recognize that the principal absorption mechanism in the fast group is due to resonances in the absorption cross section, then we can identify this probability as just the "resonance escape probability"

$$p = \frac{\Sigma_{s_{12}}\phi_1}{\Sigma_{R_1}\phi_1} = \frac{\Sigma_{s_{12}}}{\Sigma_{R_1}} \tag{7-52}$$

We can similarly calculate the fast fission factor by noting

$$\epsilon \equiv \frac{\text{total number of neutrons produced by fission}}{\text{total number of neutrons produced by thermal fission}}$$

$$= \frac{\nu_1 \Sigma_{f_1}\phi_1 + \nu_2 \Sigma_{f_2}\phi_2}{\nu_2 \Sigma_{f_2}\phi_2} \tag{7-53}$$

But in the absence of leakage, Eq. (7-46) implies

$$(\Sigma_{R_1} - \nu_1 \Sigma_{f_1})\phi_1 = \nu_2 \Sigma_{f_2}\phi_2 \qquad (7\text{-}54)$$

Hence we can identify:

$$\epsilon = \frac{\nu_1 \Sigma_f \phi_1 + \Sigma_{R_1}\phi_1 - \nu_1 \Sigma_{f_1}\phi_1}{(\Sigma_{R_1} - \nu_1 \Sigma_{f_1})\phi_1} = \frac{\Sigma_{R_1}}{\Sigma_{R_1} - \nu_1 \Sigma_{f_1}} \qquad (7\text{-}55)$$

To complete our analysis, we must identify the nonleakage probabilities. We might expect these nonleakage probabilities would take the form

$$P_{NFL} = (1 + L_1^2 B^2)^{-1}$$

and (7-56)

$$P_{NTL} = (1 + L_2^2 B^2)^{-1}$$

Hence we must determine the diffusion length for each group.

Recall that the definition of L^2 could be given in terms of the mean square distance to absorption from a point source.

$$L^2 = \frac{1}{6}\langle r^2 \rangle$$

For the fast group, we could attempt to solve

$$-D_1 \nabla^2 \phi_1 + (\Sigma_{R_1} - \nu_1 \Sigma_{f_1})\phi = S_0 \delta(\vec{r}) \qquad (7\text{-}57)$$

for the fast flux, and then calculate $\langle r^2 \rangle$ in order to infer a value for L_1^2. Solving Eq. (7-57) as before in Chapter 5, we find a solution of the form

$$\phi_1(\vec{r}) = A\frac{e^{-\kappa_1 r}}{r}, \quad \kappa_1^2 = \frac{\Sigma_{R_1} - \nu_1 \Sigma_f}{D_1} \qquad (7\text{-}58)$$

Hence

$$L_1^2 = \frac{1}{6} \frac{\int_0^\infty r^2 \phi_1(r)\, 4\pi r^2 dr}{\int_0^\infty \phi_1(r)\, 4\pi r^2 dr} = \frac{1}{\kappa_1^2} \tag{7-59}$$

which implies that we must choose:

$$L_1 = \frac{D_1}{\Sigma_{R_1} - \nu_1 \Sigma_{f_1}} \tag{7-60}$$

If we apply a similar analysis to the thermal group equation

$$-D_2 \nabla^2 \phi_2 + \Sigma_{a_2} \phi_2 = -S_0 \delta(\vec{r}) \tag{7-61}$$

we find we must identify

$$L_2^2 = \frac{D_2}{\Sigma_{a_2}} \tag{7-62}$$

Hence, in summary, we have managed to define the quantities appearing in the 6-factor formula in terms of the group constants characterizing two-group diffusion theory

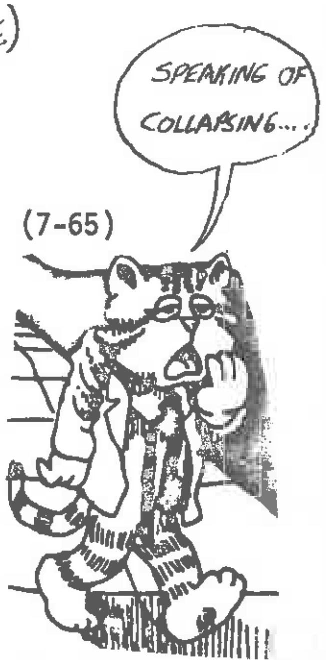
$$\begin{aligned} k &= \left(\frac{\nu_2 \Sigma_{f_2}}{\Sigma_{a_2}^F}\right)\left(\frac{\Sigma_{a_2}^F}{\Sigma_{a_2}}\right)\left(\frac{\Sigma_{S12}}{\Sigma_{R_1}}\right)\left(\frac{\Sigma_{R_1}}{\Sigma_{R_1} - \nu_1 \Sigma_{f_1}}\right)\left(\frac{1}{1+L_1^2B^2}\right)\left(\frac{1}{1+L_2^2B^2}\right) \\ &= \quad \eta \qquad\quad f \qquad\quad p \qquad\qquad \epsilon \qquad\qquad P_{NFL} \qquad\quad P_{NTL} \end{aligned} \tag{7-64}$$

D. Group Collapsing

One can use the definitions of the group constants to obtain expressions for one-group constants in terms of two group constants. For example

$$\Sigma_a = \frac{\int_{E_2}^{E_0} dE\,\Sigma_a(E)\,\Phi(E)}{\int_{E_2}^{E_0} dE\,\Phi(E)} = \frac{\int_{E_1}^{E_0} dE\,\Sigma_a(E)\,\Phi(E) + \int_{E_2}^{E_1} dE\,\Sigma_a(E)\,\Phi(E)}{\int_{E_2}^{E_0} dE\,\Phi(E)}$$

$$= \frac{\Sigma_{R_1}\phi_1 + \Sigma_{a_2}\phi_2 - \Sigma_{S_{12}}\phi_1}{\phi_1 + \phi_2} \qquad (7\text{-}65)$$



or using Eq. (7-46) to eliminate ϕ_2 in terms of ϕ_1:

$$\Sigma_a = \frac{(\Sigma_{R_1} - \Sigma_{S_{12}})(D_2B^2 + \Sigma_{a_2}) + \Sigma_{a_2}\Sigma_{S_{12}}}{D_2B^2 + \Sigma_{a_2} + \Sigma_{S_{12}}} \qquad (7\text{-}66)$$

This is an example of "group collapsing"--that is, generating few group constants from many group constants, which is a common procedure in multigroup methods. The remaining one-group constants can be given as

$$D = \frac{D_1\phi_1 + D_2\phi_2}{\phi_1 + \phi_2} = \frac{(D_2B^2 + \Sigma_{a_2})D_1 + \Sigma_{S_{12}}D_2}{D_2B^2 + \Sigma_{a_2} + \Sigma_{S_{12}}} \qquad (7\text{-}67)$$

$$\nu\Sigma_f = \frac{\nu_1\Sigma_{f_1}\phi_1 + \nu_2\Sigma_{f_2}\phi_2}{\phi_1 + \phi_2} = \frac{(D_2B^2 + \Sigma_{a_2})\nu\Sigma_{f_1} + \nu_2\Sigma_{S_{12}}\Sigma_{f_2}}{D_2B^2 + \Sigma_{a_2} + \Sigma_{S_{12}}} \qquad (7\text{-}68)$$

[These relations can be generalized to the case of collapsing from G groups, but we will leave this development to the problem set at the end of the chapter.]

E. Other Reactor Parameters

1.) Neutron Age

Another parameter of considerable interest is related to the mean square distance $\langle r^2 \rangle$ a fast neutron will travel before it slows down or is absorbed. It is customary to define the "neutron age" τ as one-sixth of this distance

$$\tau \equiv \frac{1}{6}\langle r^2 \rangle \tag{7-69}$$

[We will give an alternative definition in the next chapter.] We can compute this quantity by solving for the fast flux ϕ_1, in

$$-D_1 \nabla^2 \phi_1 + (\Sigma_{a1} + \Sigma_R)\phi_1 = S_0 \delta(\vec{r}) \tag{7-70}$$

We then find

$$\phi_1(r) = A\frac{e^{-\kappa' r}}{r} \quad , \quad \kappa'^2 = \frac{\Sigma_R + \Sigma_{a1}}{D_1} \tag{7-71}$$

and hence we can compute the age (as we computed L_1^2) as

$$\tau = \frac{1}{6}\langle r^2 \rangle = \frac{D_1}{\Sigma_{a1} + \Sigma_R} \tag{7-72}$$

2.) Conversion Ratio

Recall that we defined the conversion ratio CR by

$$\text{CR} \equiv \frac{\text{production rate of fissile nuclei}}{\text{destruction rate of fissile nuclei}} \tag{7-73}$$

For convenience, we will consider a U^{235} fueled reactor. At the beginning of core life, the plutonium concentration, N^{49}, is zero. Then

$$CR = \frac{\Sigma_{c_1}^{28}\phi_1 + \Sigma_{c_2}^{28}\phi_2}{\Sigma_{a_1}^{25}\phi_1 + \Sigma_{a_2}^{25}\phi_2} = \frac{\Sigma_{c_2}^{28} + \Sigma_{c_1}^{28}\left(\frac{\phi_1}{\phi_2}\right)}{\Sigma_{a_2}^{25} + \Sigma_{a_1}^{25}\left(\frac{\phi_1}{\phi_2}\right)} \tag{7-74}$$

But $\frac{\phi_1}{\phi_2} = \Sigma_{a_2}/\Sigma_R$ in an infinite reactor.

Hence

$$CR = \frac{\Sigma_{c_2}^{28} + \Sigma_{c_1}^{28}(\Sigma_{a_2}/\Sigma_R)}{\Sigma_{a_2}^{25} + \Sigma_{a_1}^{25}(\Sigma_{a_2}/\Sigma_R)} \tag{7-75}$$

3.) Critical Poison Concentration

One important method of controlling light water moderated thermal reactors is to dissolve a poison such as boron in the coolant. The two group model can be used to make an estimate of the critical boron concentration, N_p^*, which will make $k_\infty = 1$. Recall

$$k_\infty = \frac{\nu_1\Sigma_{f_1} + \nu_2\Sigma_{f_2}(\Sigma_R/\Sigma_{a_2})}{\Sigma_{a_1} + \Sigma_R} \tag{7-76}$$

Now to a first approximation, the only parameter that changes when the soluble poison is added is Σ_{a_2}(since its absorption cross section is only large for thermal neutrons). Suppose we compute

$$\alpha_p \equiv \frac{\partial k_\infty}{\partial N_p} = \frac{\partial k_\infty}{\partial \Sigma_{a_2}} \frac{\partial \Sigma_{a_2}}{\partial N_p} \tag{7-77}$$

But

$$\frac{\partial k_\infty}{\partial \Sigma_{a_2}} = - \frac{\nu_2 \Sigma_{f_2} \Sigma_R}{\Sigma_{a_2}^2 (\Sigma_{a_1} + \Sigma_R)} = - \frac{k_\infty}{\epsilon \Sigma_{a_2}}$$

$$\frac{\partial \Sigma_{a_2}}{\partial N_p} = \sigma_{a_2}^P \qquad (7\text{-}78)$$

Thus

$$\alpha_p = \frac{\partial k_\infty}{\partial N_p} = - \frac{k_\infty}{\epsilon \Sigma_{a_2}} \sigma_{a_2}^P \qquad (7\text{-}79)$$

Finally, if we start with k_∞ and $N_p = 0$, and want to adjust $N_p = N_p^*$ such that $k_\infty = 1$, we find

$$\delta k_\infty \equiv k_\infty - 1 = \frac{k_\infty}{\epsilon \Sigma_{a_2}} \sigma_{a_2}^P N_p^* \qquad (7\text{-}80)$$

or

$$N_p^* = \left(\frac{k_\infty - 1}{k_\infty}\right) \frac{\epsilon \Sigma_{a_2}}{\sigma_{a_2}^P} \qquad (7\text{-}81)$$

4.) Moderator Coefficient of Reactivity

Frequently we are interested in the change in reactivity associated with a change in moderator density. To this end, we define

$$\alpha_M \equiv \frac{\partial k_\infty}{\partial N_M} \equiv \text{moderator coefficient of reactivity} \qquad (7\text{-}82)$$

where N_M is the moderator atomic density. The three terms in k_∞ that vary as N_M varies are Σ_R, Σ_{a_1}, and Σ_{a_2}. Use

$$k_\infty = \eta f p \epsilon \tag{7-83}$$

Then

$$\frac{1}{k_\infty}\frac{\partial k_\infty}{\partial N_M} = \frac{1}{\eta}\frac{\partial \eta}{\partial N_M} + \frac{1}{f}\frac{\partial f}{\partial N_M} + \frac{1}{p}\frac{\partial p}{\partial N_M} + \frac{1}{\epsilon}\frac{\partial \epsilon}{\partial N_M} \tag{7-84}$$

Here,

$$\eta = \nu_2 \frac{\Sigma_{f_2}}{\Sigma_{a_2}^F} \quad \Rightarrow \quad \frac{\partial \eta}{\partial N_M} = 0 \tag{7-85}$$

Further,

$$f = \frac{\Sigma_{a_2}^F}{\Sigma_{a_2}} \quad \Rightarrow \quad \frac{\partial f}{\partial N_M} = -\frac{\Sigma_{a_2}^F}{\Sigma_{a_2}^2}\sigma_{a_2}^M = -f\frac{\Sigma_{a_2}^M}{\Sigma_{a_2}}\frac{1}{N_M} \tag{7-86}$$

or

$$\frac{1}{f}\frac{\partial f}{\partial N_M} = -\frac{\Sigma_{a_2}^M}{\Sigma_{a_2}}\frac{1}{N_M}$$

Next,

$$p = \frac{\Sigma_R}{\Sigma_R + \Sigma_{a_1}}$$

$$\Rightarrow \frac{\partial p}{\partial \Sigma_R} = \frac{\Sigma_{a_1}}{\Sigma_R^2}p^2$$

$$\frac{\partial p}{\partial \Sigma_{a_1}} = -\frac{1}{\Sigma_R}p^2$$

$$\frac{\partial p}{\partial N_M} = \frac{\Sigma_{a_1}}{\Sigma_R^2}p^2\sigma_R^M - \frac{1}{\Sigma_R}p^2\sigma_{a_1}^M$$

or

$$\frac{1}{p}\frac{\partial p}{\partial N_M} = \frac{p}{\Sigma_R N_M}\left[\frac{\Sigma_{a_1}\Sigma_R^M}{\Sigma_R} - \Sigma_{a_1}^M\right] \tag{7-87}$$

Finally,

$$\epsilon = 1 + \frac{\nu_1 \Sigma_{f_1}\Sigma_{a_2}}{\nu_2 \Sigma_{f_2}\Sigma_R}$$

$$\frac{\partial\epsilon}{\partial\Sigma_{a_2}} = \frac{1}{\Sigma_{a_2}}(\epsilon-1)\,, \quad \frac{\partial\epsilon}{\partial\Sigma_R} = -\frac{1}{\Sigma_R}(\epsilon-1)$$

Hence

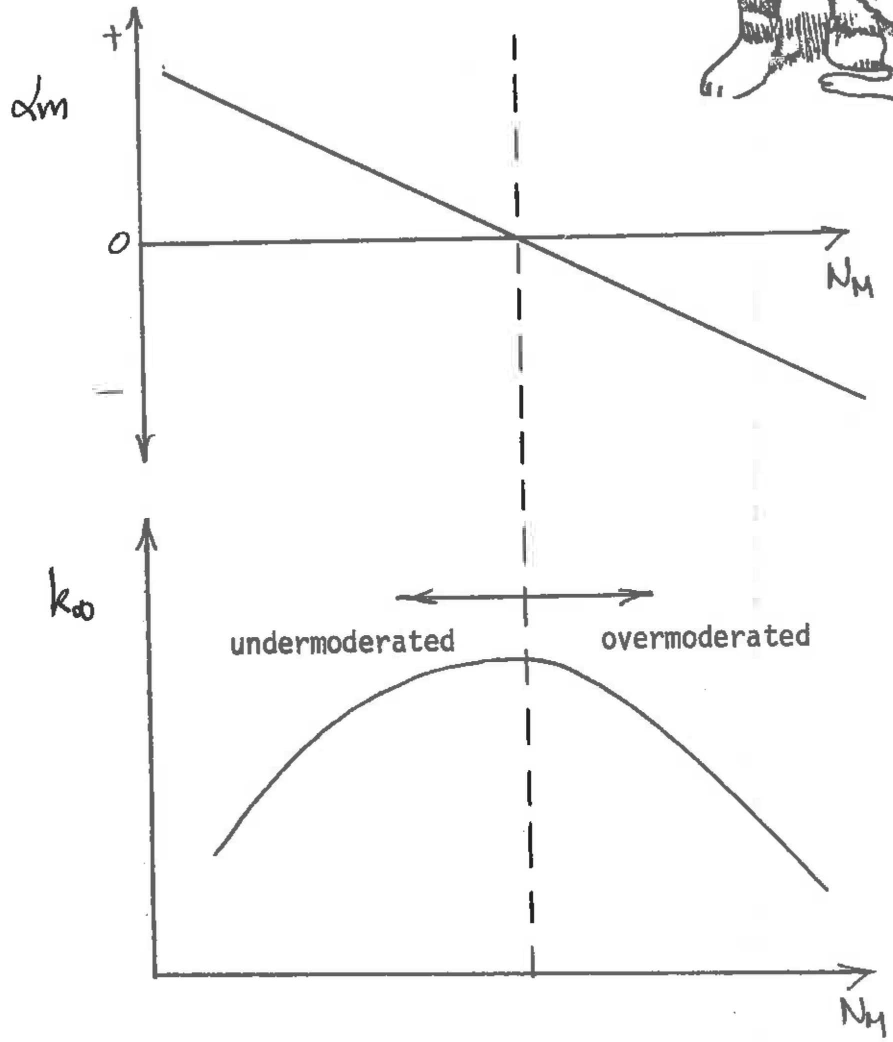
$$\frac{1}{\epsilon}\frac{\partial\epsilon}{\partial N_M} = \left(\frac{\epsilon-1}{\epsilon}\right)\frac{1}{N_M}\left(\frac{\Sigma_{a_2}^M}{\Sigma_{a_2}} - \frac{\Sigma_R^M}{\Sigma_R}\right) \tag{7-88}$$

If we put these together

$$\alpha_M = \frac{k_\infty}{N_M}\left[-\frac{\Sigma_{a_2}^M}{\Sigma_{a_2}} + \frac{p}{\Sigma_R}\left(\frac{\Sigma_{a_1}\Sigma_R^M}{\Sigma_R} - \Sigma_{a_1}^M\right) + \left(1-\frac{1}{\epsilon}\right)\left(\frac{\Sigma_{a_2}^M}{\Sigma_{a_2}} - \frac{\Sigma_R^M}{\Sigma_R}\right)\right] \tag{7-89}$$

$$= \frac{k_\infty}{N_M}\left[\frac{\Sigma_R^M}{\Sigma_R}\left(\frac{1}{\epsilon}-p\right) + p\frac{\Sigma_{a_1}^M}{\Sigma_{a_1}} - \frac{\Sigma_{a_2}^M}{\epsilon\Sigma_{a_2}}\right]$$

The most important term is the one containing the factor $(\frac{1}{\epsilon} - P)$. Recall that as N_M increases, p increases while ϵ stays relatively constant. Hence we can investigate the effect of moderator density on core multiplication



5.) Equilibrium Xenon^{135} and Samarium^{149} Concentrations

We can rewrite our xenon balance equations in the two-group notation as

$$\frac{dI}{dt} = \gamma_I\left[\Sigma_{f_2}\phi_2 + \Sigma_{f_1}\phi_1\right] - \lambda_I I$$

$$\frac{dX}{dt} = \lambda_I I + \gamma_X\left[\Sigma_{f_1}\phi_1 + \Sigma_{f_2}\phi_2\right] - \lambda_X X - \sigma_{a_2}^{X}\phi_2 X \tag{7-90}$$

In equilibrium, we can set $\frac{dI}{dt} = 0 = \frac{dX}{dt}$ and solve for

$$X_\infty = \frac{(\gamma_I + \gamma_X)(\Sigma_{f_1}\phi_1 + \Sigma_{f_2}\phi_2)}{\lambda_X + \sigma_{a_2}^X \phi_2} \tag{7-91}$$

Now to obtain the equilibrium xenon concentration, we need ϕ_1 and ϕ_2 If we use the reactor power

$$P(\text{watts/cm}^3) = w_f\left[\Sigma_{f_1}\phi_1 + \Sigma_{f_2}\phi_2\right] \tag{7-92}$$

where w_f = energy/fission ≅ 200 MeV, as well as the fact that $\phi_1/\phi_2 = \Sigma_{a_2}/\Sigma_R$, then we can obtain absolute values for ϕ_1, and ϕ_2 and use these in Eq. (7-81) to evaluate X_∞.

In a very similar fashion, one can obtain the equilibrium samarium concentration in terms of the two group constants:

$$S_\infty = \frac{\gamma_p\left[\Sigma_{f_1}\phi_1 + \Sigma_{f_2}\phi_2\right]}{\sigma_{a_2}^S \phi_2} \tag{7-93}$$

We have gone through this rather exhaustive study of the two-group model in an effort to demonstrate how multigroup techniques can be used to evaluate many of the quantities of interest in reactor analysis. Of course our examples were extremely simple--they usually ignored spatial dependence (or at best, assumed only a fundamental mode dependence). In any realistic calculation, one must take into account the inhomogeneous nature of the reactor core by actually solving the multigroup diffusion equations in detail. Hence we now turn our attention to the strategy for solving these more general equations.

V. NUMERICAL SOLUTION OF THE MULTIGROUP DIFFUSION EQUATIONS

We now turn our attention to the strategy for solving the multigroup diffusion equations on digital computers. It is helpful to first recall our scheme for solving the one-group diffusion equation with a fission source:

$$-\nabla\cdot D\nabla\phi + \Sigma_a\phi = \nu\Sigma_f\phi = S \tag{7-94}$$

The essential idea was to first guess a fission source and a multiplication factor

$$S(\vec{r}) \cong S^{(0)}(\vec{r}), \qquad k \sim k^{(0)} \tag{7-95}$$

We then solved for the flux resulting from this guessed fission source

$$-\nabla\cdot D\nabla\phi^{(1)} + \Sigma_a\phi^{(1)} = \frac{1}{k^{(0)}} S^{(0)}(\vec{r}), \tag{7-96}$$

Next we calculated a new guess for the fission source

$$S^{(1)}(\vec{r}) = \nu\Sigma_f\phi^{(1)}(\vec{r}) \tag{7-97}$$

and a new value of k as

$$k = \frac{\int d^3r\, S^{(1)}(\vec{r})}{\frac{1}{k^{(0)}}\int d^3r\, S^{(0)}(\vec{r})} \tag{7-98}$$

and continued on in this source iteration until the values of $k^{(n)}$ converged.

This general strategy can also be applied to the multigroup equations. Suppose we begin by writing these equations out in detail

$$\begin{aligned}
-\nabla\cdot D_1\nabla\phi_1 + \Sigma_{R_1}\phi_1 &= \chi_1 S \\
-\nabla\cdot D_2\nabla\phi_2 + \Sigma_{R_2}\phi_2 &= \chi_2 S + \Sigma_{s12}\phi_1 \\
-\nabla\cdot D_3\nabla\phi_3 + \Sigma_{R_3}\phi_3 &= \chi_3 S + \Sigma_{s13}\phi_1 + \Sigma_{s23}\phi_2 \qquad (7\text{-}99) \\
&\ \vdots \qquad\qquad\qquad \vdots \\
-\nabla\cdot D_G\nabla\phi_G + \Sigma_{R_G}\phi_G &= \chi_G S + \Sigma_{s1G}\phi_1 + \cdots \Sigma_{sG-1,G}\phi_{G-1}
\end{aligned}$$

Notice that here we have assumed that there is no upscattering and also defined the fission source as

$$S(\vec{r}) \equiv \nu \sum_{g'=1}^{G} \Sigma_{fg'}\phi_{g'}(\vec{r}) \qquad (7\text{-}100)$$

It is very important to note that the spatial dependence of the fission source is identical in each group diffusion equation.

Now the essential scheme is just as before. We first insert a scale factor 1/k before the fission source in each of the equations (7-99). Then we begin by guessing

$$S(\vec{r}) \sim S^{(0)}(\vec{r}), \qquad k \sim k^{(0)} \qquad (7\text{-}101)$$

Next, we calculate the flux in the first group:

$$-\nabla\cdot D_1\nabla\phi_1^{(1)} + \Sigma_{R_1}\phi_1^{(1)} = \frac{1}{k^{(0)}}\chi_1 S^{(0)}(\vec{r}) \qquad (7\text{-}102)$$

Having obtained this flux, we can then proceed to the diffusion equation characterizing the next lowest energy group

$$-\nabla\cdot D_2\nabla\phi_2^{(1)} + \Sigma_{R_2}\phi_2^{(1)} = \frac{1}{k^{(0)}}\chi_2 S^{(0)}(\vec{r}) + \Sigma_{s12}\phi_1^{(1)} \qquad (7\text{-}103)$$

and solve this for $\phi_2^{(1)}(\vec{r})$ since the right hand side is now known. We can continue on in this fashion to determine all of the group fluxes:

$$\phi_3^{(1)}(\vec{r}),\ \phi_4^{(1)}(\vec{r}),\ \ldots\ \phi_G^{(1)}(\vec{r}) \qquad (7\text{-}104)$$

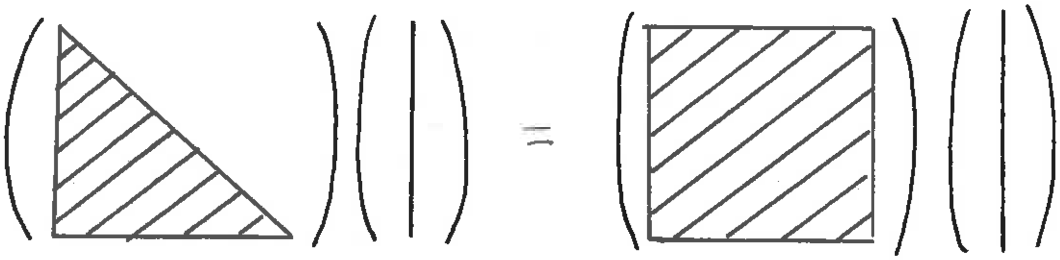
Having done so, we can then calculate a new fission source

$$S(\vec{r}) = \nu\sum_{g'=1}^{G}\Sigma_{fg'}\,\phi_{g'}^{(1)}(\vec{r}) \qquad (7\text{-}105)$$

and a new value of k

$$k^{(1)} = \frac{\int d^3r\, S^{(1)}(\vec{r})}{\frac{1}{k^{(0)}}\int d^3r\, S^{(0)}(\vec{r})} \qquad (7\text{-}106)$$

We can then continue on, performing each source iteration by solving down the multigroup equations towards lower and lower energies. This scheme of solving successively the equations in the direction of lower energies is made possible by the assumption that there is no upscattering. This implies that the flux in the higher energy groups always determines the source term in the lower energy groups. In effect, we are merely inverting a lower triangular matrix (as the matrix formulation in the previous section made apparent):



(If upscattering is present, as it will be if we have more than one thermal group, an iterative solution of the thermal group equations will be necessary.)

A great deal is known about the nature of such multigroup diffusion eigenvalue problems. If we attach the boundary conditions that on the surface of the reactor, the group flux and its normal derivative satisfy a linear relationship of the form

$$\phi_g + b_g \hat{\sigma}\cdot\nabla\phi_g = 0 \tag{7-107}$$

where $\hat{\sigma}$ is an outward normal and b_g is any nonnegative piecewise continuous function defined on the boundary (this includes the usual diffusion theory boundary conditions), furthermore that there is continuity of the flux and current at interfaces, and that the flux has bounded and continuous second derivatives, then one can show that there will always exist a maximum eigenvalue, k_0, which is real and positive. The corresponding eigenfunction is unique and nonnegative everywhere within the reactor. These features are reassuring, because we would anticipate that the largest eigenvalue will characterize the multiplication of the system and the corresponding eigenfunction will describe the flux distribution within the core (which cannot be negative). One can also demonstrate that the above source iteration will converge to this "positive dominant" eigenvalue k_0 and the corresponding eigenfunction. (These features are essentially a consequence of the fact that the multigroup diffusion operators are positive.)

So much for the formal details. In actual practice, one must also discretize the spatial dependence in order to solve the group diffusion equations. That is, one chooses a spatial mesh and a finite difference scheme, just as we did in Chapter 5, and discretizes the diffusion equations for each group. The general structure of the finite--differenced multigroup diffusion equations takes the form

$$\left[\Sigma_{t_i}^g + \sum_j^J \frac{D_{ij}^g}{\Delta_{ij}^2}\right]\phi_i^g - \sum_j^J \frac{D_{ij}^g}{\Delta_{ij}^2}\phi_j^g - \sum_{g'=1}^G \Sigma_{s_i}^{g'\to g}\phi_i^{g'} = \frac{\chi^g}{k}\sum_{g'=1}^G \nu\Sigma_{f_i}^{g'}\phi_i^{g'} \qquad (7\text{-}108)$$

where in Cartesian coordinate geometry

$$\begin{aligned} L_i^g &= \sum_j^J \ell_{ij}^g, \qquad \ell_{ij}^g = \frac{D_{ij}^g}{\Delta_{ij}^2} \\ D_{ij}^g &= (D_i^g + D_j^g)/2 \qquad\qquad (7\text{-}109) \\ \Delta_{ij} &= \underset{i}{\bullet}\longrightarrow\underset{j}{\bullet} \end{aligned}$$

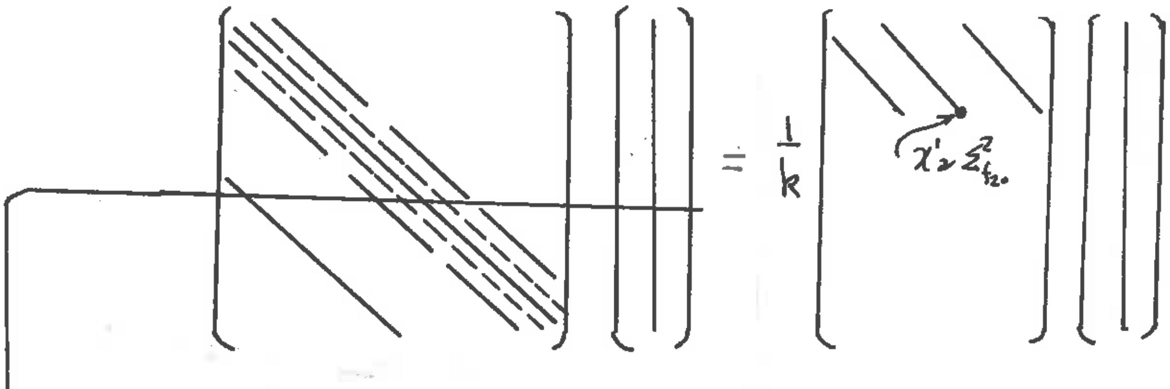
Notice that in addition to the coupling to different energy group fluxes at a given mesh point due to the fission source and scattering, the finite difference equation is coupled to the flux at adjacent spatial mesh points because of the effect of spatial diffusion.

Since each energy-mesh point is defined by such an equation, this problem represents a set of G*N-1 fluxes and the reactor criticality eigenvalue, k. The flux at one energy group-mesh point is arbitrarily normalized so that there are as many unknowns as equations to be solved. In matrix notation, the matrix eigenvalue problem takes the form

$$\underline{\underline{M}}\,\underline{\phi} = \frac{1}{k}\,\underline{\underline{F}}\,\underline{\phi} \tag{7-110}$$

For example, a three energy group, two dimensional 5 x 4 mesh matrix equation takes the following form: Each matrix has (60 by 60) 3600 elements and the flux vector has 60 elements. In a three group problem, $\chi^1 = 1,\ \chi^2 = 0,\ \chi^3 = 0$ and $\Sigma_{sg'g} = 0$ if $g \neq g'+1$

Hence the structure of the matrices are



(7-111)

$$\left(-\Sigma_{s_{1\to2},i}\right)\left(-\frac{D^2_{i,i-5}}{(\Delta_{i,i-5})^2}\right)\left(-\frac{D^2_{i,i-1}}{(\Delta_{i,i-1})^2}\right)\left(\Sigma^2_{ti} + \frac{D^2_{i,i-5}}{(\Delta_{i,i-5})^2} + \frac{D^2_{i,i-1}}{(\Delta_{i,i-1})^2} + \frac{D^2_{i,i+1}}{(\Delta_{i,i+1})^2} + \frac{D^2_{i,i+5}}{(\Delta_{i,i+5})^2}\right)\left(-\frac{D^2_{i,i+1}}{(\Delta_{i,i+1})^2}\right)\left(-\frac{D^2_{i,i+5}}{(\Delta_{i,i+5})^2}\right)\left(\phi^2_i\right)$$

One can now proceed with the standard source iteration:

1.) Make a guess of the flux vector $\underline{\phi}^{(0)}$ and reactor multiplication eigenvalue $k^{(0)}$

2.) Evaluate the fission source

$$\underline{\underline{S}}^{(0)} = \frac{1}{k^{(0)}} \underline{\underline{F}} \ \underline{\phi}^{(0)} \tag{7-112}$$

3.) Solve the inhomogeneous matrix equation

$$\underline{\underline{M}} \ \underline{\phi}^{(n)} = \underline{\underline{S}}^{(n-1)} \tag{7-113}$$

for the unknown flux vector $\underline{\phi}^{(n)}$

4.) Solve for the next iterate eigenvalue, $k^{(n)}$, using the expression

$$k^{(n)} = k^{(n-1)} \frac{(\underline{\underline{F}} \underline{\phi}^{(n)}, \underline{\underline{F}} \underline{\phi}^{(n)})}{(\underline{\underline{F}} \underline{\phi}^{(n-1)}, \underline{\underline{F}} \underline{\phi}^{(n)})} \tag{7-114}$$

(This was determined by multiplying the matrix iterate eigenvalue equation,

$$\underline{\underline{M}} \ \underline{\phi}^{(n)} = \frac{1}{k^{(n-1)}} \underline{\underline{F}} \ \underline{\phi}^{(n-1)} \tag{7-115}$$

by $\underline{\underline{F}} \ \underline{\phi}^{(n)}$, substituting in the assumed equality

$$\underline{\underline{M}} \ \underline{\phi}^{(n)} = \frac{1}{k^{(n)}} \underline{\underline{F}} \ \underline{\phi}^{(n)} \tag{7-116}$$

for $\underline{\underline{M}} \ \underline{\phi}^{(n)}$ and solving for $k^{(n)}$.)

5.) Determine if the change in $k^{(n)}$ or the elements of $\underline{\phi}^{(n)}$ or $\underline{S}^{(n)}$ since the last iteration are small enough to assume convergence to the solution, thus ending the iterative procedure.

6.) Determine the next fission source vector iterate by a

   a.) straight power iteration

$$\underline{S}^{(n)} = \frac{1}{k^{(n)}} \underline{\underline{F}}\, \underline{\phi}^{(n)} \tag{7-117}$$

   b.) or a source extrapolation method such as

$$\underline{S}^{(n)} = \underline{\underline{F}} \left\{ \frac{1}{k^{(n)}} \underline{\phi}^{(n)} + \alpha \left[\frac{1}{k^{(n)}} \underline{\phi}^{(n)} - \underline{S}^{(n-1)} \right] \right\} \tag{7-118}$$

7.) Returning to 3.

This scheme has been diagrammed in Figure (7-2).

As we have mentioned, this fission source iteration algorithm is frequently referred to as the "outer iterations". This terminology arises from the fact that another iterative scheme is necessary to solve the inhomogeneous matrix equation

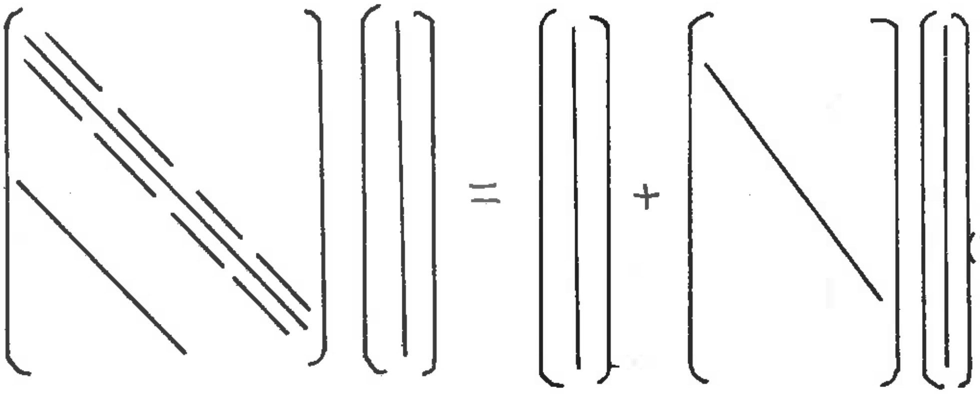
$$\underline{\underline{M}}\, \underline{\phi}^{(n)} = \underline{S}^{(n-1)} \tag{7-119}$$

in two or three dimensional geometries. Such iterations are referred to as "inner iterations" or "flux iterations" and were the subject of Chapter 5. If we have only one thermal group, then upscattering does not arise, and the inhomogeneous matrix equation (7-119) can be solved group-wise in the form of the group inhomogeneous matrix equation

$$\underline{\underline{A}}_g \, \underline{\phi}_g^{(n)} = \underline{S}_g^{(n-1)} + \underline{\underline{R}}_{g-1} \, \underline{\phi}_{g-1} \qquad (7\text{-}120)$$

(where, of course, in the first group: $\underline{\underline{R}} = 0, \ \underline{\phi}_0^{(n)} = 0$)
The slowing down source scattering from the next higher energy group $\underline{\underline{R}}_{g-1} \, \phi_{g-1}^{(n)}$ is based on the present iterate flux just determined in the previous group inhomogeneous matrix equation solution.

For example, the group inhomogeneous matrix equation for our previous 3-group, 2-D (5 x 4 mesh) problem has (20 x 20) 400 element matrices, and the flux and fission source vectors each have 20 elements.

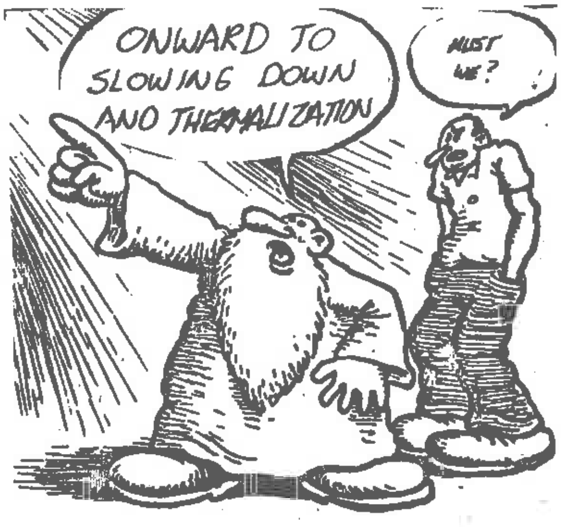


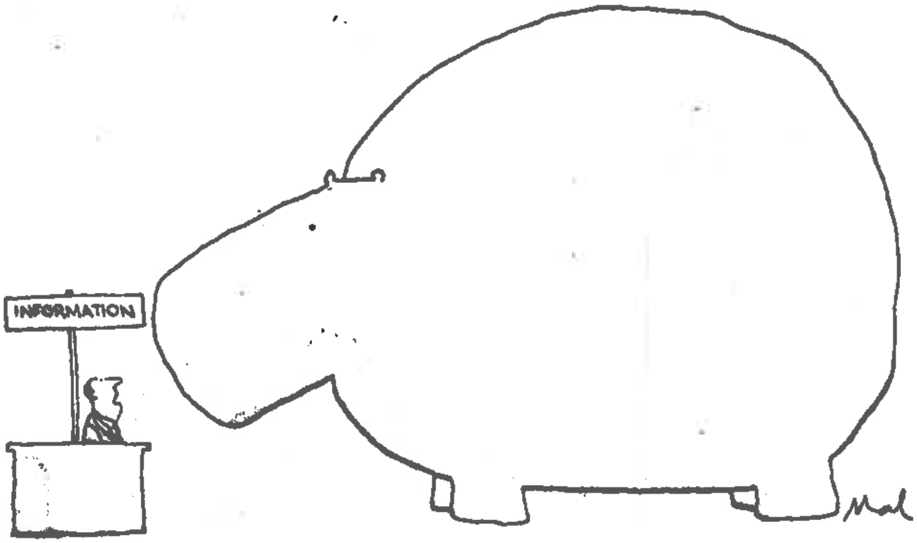
(7-121)

The positive nature of the multigroup diffusion operators imply similar properties for the matrices resulting from finite differencing these equations. Hence many of the formal conclusions concerning convergence to the positive dominant eigenvalue and eigenfunction can also be shown to hold for the finite-differenced multigroup diffusion equations. The theory of such numerical procedures have been placed on firm ground by Varga and Wachspress, and the interested reader is referred to their treatises for more detail.

VI. CONCLUSIONS

We have now developed the multigroup diffusion equations and outlined a strategy for solving them. The big unknown question at this point concerns just how one determines the group constants. These latter calculations rely upon clever guesses or approximations for the intragroup fluxes, and more specifically upon one's ability to determine the neutron energy spectrum characterizing fast and thermal neutrons. This is the subject to which we will next turn our attention as we study the slowing down and thermalization of neutrons.





"You're a hippopotamus."

CHAPTER 8: FAST SPECTRUM CALCULATIONS AND FAST GROUP CONSTANTS

I. NEUTRON SLOWING DOWN IN AN INFINITE MEDIUM

A. Introduction

In the last chapter, we developed the principal tool of nuclear reactor analysis--namely multigroup diffusion theory. The multigroup diffusion equations, viz.

$$-\nabla\cdot D_g\nabla\phi_g + \Sigma_{R_g}\phi_g(\vec{r}) = \sum_{g'=1}^{g}\Sigma_{sgg}\phi_{g'} + \nu\chi_g\sum_{g'=1}^{G}\Sigma_{f_{g'}}\phi_{g'} \qquad (8\text{-}1)$$

$$g=1,\cdots,G$$

contained various group constants which were formally defined in terms of the intragroup fluxes, e.g.,

$$\Sigma_{t_g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE\,\Sigma_t(E)\,\Phi(\vec{r},E)}{\int_{E_g}^{E_{g-1}} dE\,\Phi(\vec{r},E)} \qquad (8\text{-}2)$$

We now turn our attention to suitable approximations to the intragroup fluxes.

If the number of groups is large (>20,), one can frequently get by with rather crude estimates of $\Phi(\vec{r},E)$. For example, for energies above 1 MeV, Φ might be approximated by the fission spectrum, $\chi(E)$; for intermediate energies, .625 eV < E < 1 MeV, we will see that Φ behaves very roughly as $^1/_E$; while for energies below E = 0.625 eV, we might model $\Phi(E)$ by a Maxwell-Boltzmann distribution characterizing neutrons in thermal equilibrium with the reactor core material at a temperature T.

Unfortunately, for most multigroup calculations, one requires a far better treatment of the energy dependence of the flux--that is, of the neutron or reactor "spectrum"--in order to generate satisfactory group constants. Our attention in this and the next chapter will be devoted to studying schemes for calculating such reactor spectra. For reasons which will become apparent as we proceed, it proves very convenient to break these spectrum calculations into two classes: those calculations of the neutron energy spectrum characterizing fast neutrons with energies 0.625 eV $< E <$ 10 MeV, and those characterizing slow or thermal neutrons with energies $0 < E < 0.625$ eV. Then using the results of such fast and thermal spectrum calculations, we will be able to perform the integrals such as indicated in Eq. (8-2) and thereby calculate the fast and thermal group constants. [Actually, since the energy-dependent cross section data is itself frequently tabulated in a microgroup form, the actual scheme will be to collapse this cross section data over the appropriate reactor spectrum.]

Of course we have already derived an exact equation describing $\Phi(\vec{r},E)$, the neutron continuity equation:

$$\nabla\cdot\vec{J}(\vec{r},E) + \Sigma_t(E)\Phi(\vec{r},E) = \int_0^\infty dE'\Sigma_s(E'\to E)\Phi(\vec{r},E') + S(\vec{r},E) \qquad (8\text{-}3)$$

But since $\vec{J}$ is unknown, this equation is only a formality. We will bypass this difficulty, however, by making simple approximations to this term (indeed, even simpler than the diffusion approximation). In fact, we will begin by attempting to calculate the neutron spectrum in an infinite medium in which all spatial dependence disappears--that is, in which $\nabla\cdot\vec{J}\equiv 0$ and $\Phi(\vec{r},E)\to\Phi(E)$. In this case the conservation equation becomes quite simple

$$\Sigma_t(E)\Phi(E) = \int_0^\infty dE'\,\Sigma_s(E'\rightarrow E)\,\Phi(\vec{r},E') + S(E) \tag{8-4}$$

Notice that all of the derivative terms have disappeared, leaving us only with an "integral equation" in the single variable E.

But wait! Before we can solve this equation for the infinite medium neutron energy spectrum, $\Phi(E)$, we need to provide more information about the cross sections. For convenience, we will rewrite $\Sigma_s(E'\rightarrow E)$ as

$$\Sigma_s(E'\rightarrow E) = \Sigma_s(E')\,P(E'\rightarrow E) \tag{8-5}$$

where we define

$P(E'\rightarrow E)dE \equiv$ conditonal probability that if a neutron scatters with an initial energy E', it will emerge with a final energy in dE about E. (8-6)

We will begin by calculating $P(E'\rightarrow E)$ for the simplest (and most important) case:

(i) elastic scattering

(ii) nuclei initially at rest

Of course the nuclei are always in a state of thermal motion. However, if the neutron speed is large compared to the speed of the nucleus, then this assumption will be valid. If we characterize the nuclear speed by their thermal energy kT, then the second assumption amounts to restricting ourselves to neutron energies E>>kT--that is to fast neutrons. In practice, such an assumption will be valid for neutron energies greater than roughly

1 eV [usually the cutoff is chosen as 0.625 eV]. As we will see, the neglect of nuclear motion implies that the neutron will always lose energy or slow down in a collision--hence the phenomenon we first wish to examine is neutron slowing down in an infinite medium.

B. Neutron Energy Loss In Elastic Collisions

We now turn our attention to the calculations of the scattering probability

$P(E_i \rightarrow E_f)$

E_i initial energy
E_f final energy

for elastic scattering collisions from stationary nuclei. We will need a couple of facts from our Appendix on two-body collisions: First we note that the final energy is related to the initial energy by

$$E_f = E_i \left[\frac{A^2 + 2A\cos\theta + 1}{(A+1)^2} \right] \tag{8-7}$$

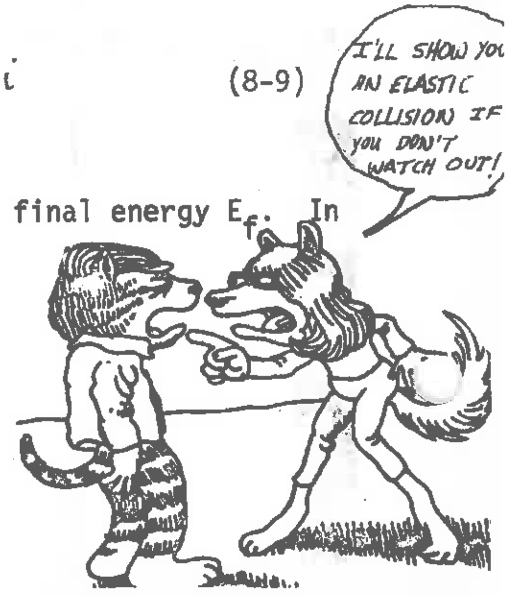
where θ is the scattering angle in the CM system. If we define

$$\alpha \equiv \left(\frac{A-1}{A+1} \right)^2 \tag{8-8}$$

then we can rearrange this into a more convenient form

$$E_f = \frac{1}{2} \left[(1+\alpha) + (1-\alpha)\cos\theta \right] E_i \tag{8-9}$$

Notice that to each θ, there corresponds a definite final energy E_f. In particular



$$\theta = 0 \Rightarrow E_f = E_i \qquad \text{("misses")}$$

$$\theta = 180° \Rightarrow E_f = \alpha E_i \qquad \text{("backscatter")}$$

Obviously the maximum energy is lost in a backscatter collision. For example

Nucleus	A	α	Maximum ΔE
H	1	0	100%
D	2	0.111	88.9%
C	12	0.716	28.4%
U	238	0.983	1.7%

Hence it is apparent that the neutron will lose the most energy in an elastic collision with a light nucleus such as $_1H^1$. As a corollary, we notice that if we desire to prevent the neutrons from slowing down (as we would in a fast reactor, for example), then we want to make sure the core contains only high mass number material.

From these considerations it is apparent that:

(i) the neutron cannot gain energy in such a scattering collision, i.e., $E_f < E_i$;

(ii) the neutron cannot emerge with energies $E_f < \alpha E_i$.

Hence we must require that our scattering probability $P(E_i \rightarrow E_f)$ vanish unless $\alpha E_i < E_f < E_i$. We need only calculate $P(E_i \rightarrow E_f)$ in this interval.

To calculate the distribution of final energies for a given initial energy E_i, we can use the fact that the final energy is related to the scattering angle θ, and the probability of scattering through a given angle θ is given by the differential scattering cross section

$$P(E_i \rightarrow E_f)\,dE_f = -\frac{\sigma_s(\theta)}{\sigma_s}\,d\hat{\Omega}$$

$$= -\frac{2\pi\sigma_s(\theta)}{\sigma_s}\sin\theta\,d\theta \qquad (8\text{-}10)$$

[The negative dign appears because the final energy E_f decreases as θ increases.]

If we use equation (8-9), we find

$$dE_f = -\frac{E_i}{2}(1-\alpha)\cos\theta\,d\theta \qquad (8\text{-}11)$$

Hence using this in (8-10), we find

$$P(E_i \rightarrow E_f) = \begin{cases} \dfrac{4\pi\sigma_s(\theta)}{\sigma_s(1-\alpha)E_i}, & \alpha E_i < E_f < E_i \\ 0, & \text{otherwise} \end{cases} \qquad (8\text{-}12)$$

We still need to know the differential scattering cross section in the CM system, however.

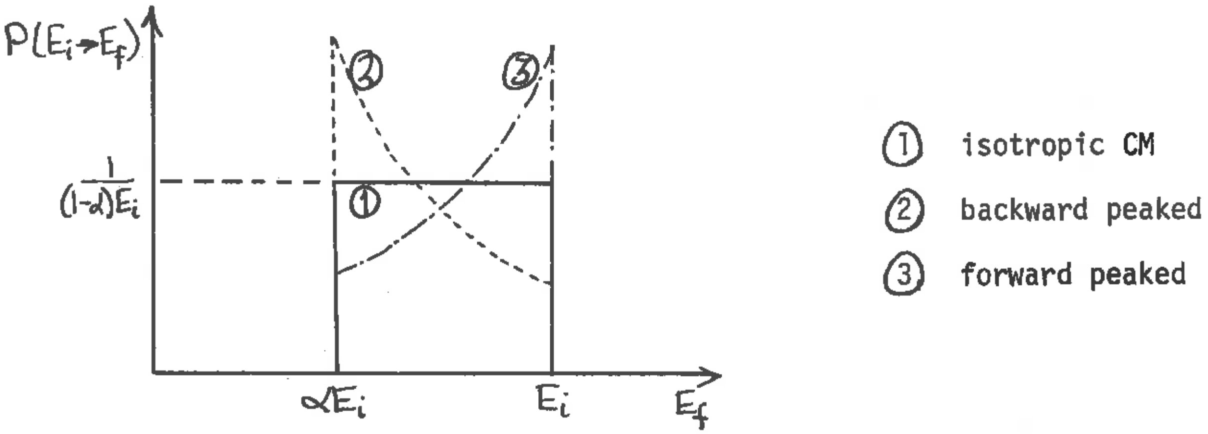
For low energies (say E < 100 keV), we recall from Chapter 2 that the potential scattering cross section $\sigma_s(\theta)$ is isotropic in the CM system--that is, we have "s-wave" scattering:

$$\sigma_s(\theta) = \frac{\sigma_s}{4\pi} \qquad (8\text{-}13)$$

In this case (which we will be mostly concerned with) therefore

$$P(E_i \rightarrow E_f) = \begin{cases} \dfrac{1}{(1-\alpha)E_i}, & \alpha E_i < E_f < E_i \\ 0, & \text{otherwise} \end{cases} \qquad (8\text{-}14)$$

We can represent this scattering probability schematically by plotting $P(E_i \rightarrow E_f)$ vs the final energy E_f



We have also sketched for comparison how this behavior changes when anisotropic scattering must be considered.

Now that we have the scattering probability for s-wave elastic scattering, we can calculate several quantities of interest.

normalization:

$$\int_0^\infty dE_f \, P(E_i \rightarrow E_f) = \int_{\alpha E_i}^{E_i} \frac{dE_f}{(1-\alpha)E_i} = 1 \tag{8-15}$$

[This guarantees that $\int_0^\infty dE' \, \Sigma_s(E \rightarrow E') = \Sigma_s(E)$.] (8-16)

average final energy:

$$\langle E_f \rangle = \int_{\alpha E_i}^{E_i} dE_f \, E_f \, P(E_i \rightarrow E_f) = \left(\frac{1+\alpha}{2}\right) E_i \tag{8-17}$$

average energy loss:

$$\langle \Delta E \rangle = E_i - \langle E_f \rangle = \left(\frac{1-\alpha}{2}\right) E_i \tag{8-18}$$

average fractional energy loss:

$$\frac{\langle \Delta E \rangle}{E_i} = \frac{1-\alpha}{2} \tag{8-19}$$

We can now use this information to write the scattering kernel for s-wave elastic scattering from stationary nuclei as

$$\Sigma_s(E' \to E) = \begin{cases} \dfrac{\Sigma_s(E')}{(1-\alpha)E'} , & \alpha E' < E < E' \\ 0 , & \text{otherwise} \end{cases} \tag{8-20}$$

Hence our "infinite medium slowing down equation" becomes

$$[\Sigma_s(E) + \Sigma_a(E)]\,\Phi(E) = \int_E^{E/\alpha} dE' \frac{\Sigma_s(E')\,\Phi(E')}{(1-\alpha)E'} + S(E) \tag{8-21}$$

This, then, is the equation we must examine to determine suitable approximations for the intragroup fluxes. As it stands, Eq. (8-21) is a very complicated equation (although it looks deceptively simple). We will first study its solution for the special case of slowing down in hydrogen (which we can solve exactly), and then turn to the more difficult case of treating slowing down in media of arbitrary mass number A.

C. Neutron Moderation in Hydrogen

1.) Slowing Down in the Absence of Absorption

For slowing down in hydrogen, we set A = 1. Hence

$$\alpha_H = \left(\frac{A-1}{A+1}\right)^2 \Bigg|_{A=1} = 0 \tag{8-22}$$

and our infinite medium slowing down equation becomes

$$\Sigma_s(E)\Phi(E) = \int_E^{\infty} dE' \frac{\Sigma_s(E')\Phi(E')}{E'} + S(E) . \qquad \text{(8-23)}$$

We will first consider the situation in which we have a monoenergetic source S_0 at an energy E_0. Now the slowing down equation will only be applied to describe those energies $E < E_0$. Hence we don't count the source neutrons until they suffer a scattering collision and slow down to an energy E below the source energy E_0. Hence the effective source term representing neutrons slowing down to an energy E after suffering a scattering collision at the source energy E_0 is just

$$S(E) = S_0 P(E_0 \to E) = \frac{S_0}{E_0} , \quad E < E_0 . \qquad \text{(8-24)}$$

Thus the equation we must solve is

$$\Sigma_s(E)\Phi(E) = \int_E^{\infty} dE' \frac{\Sigma_s(E')\Phi(E')}{E'} + \frac{S}{E_0} , \quad E < E_0 \qquad \text{(8-25)}$$

Notice that we have still not specified the form of the macroscopic scattering cross section $\Sigma_s(E)$. It turns out that one doesn't need to specify it in order to solve the equation, so we will leave it arbitrary for now.

To solve this equation, it is convenient to first make a change of dependent variables by defining the collision rate density

$$R(E) = \Sigma_s(E)\Phi(E) \qquad \text{(8-26)}$$

Then we can rewrite Eq. (8-25) as

$$R(E) = \int_E^{E_0} dE' \, \frac{R(E')}{E'} + \frac{S}{E_0} \, , \quad E < E_0 . \tag{8-27}$$

[We have chopped off the upper limit of integration at E_0, since there are no source neutrons and hence no scattering neutrons above this energy.] We can solve this integral equation by differentiating it to convert it into a simple ordinary differential equation

$$\frac{dR}{dE} = \frac{d}{dE}\left[\int_E^{E_0} dE' \, \frac{R(E')}{E'} \right] + \frac{d}{dE}\underbrace{\left(\frac{S_0}{E_0}\right)}_{\overset{\shortparallel}{0}} \tag{8-28}$$

or

$$\frac{dR}{dE} = -\frac{1}{E} R(E) \tag{8-29}$$

[Here we have used the formula for differentiating an integral of the form

$$I(x) = \int_{a(x)}^{b(x)} dy \, f(x,y) \tag{8-30}$$

$$\frac{dI}{dx} = \int_{a(x)}^{b(x)} dy \, \frac{\partial f}{\partial x}(x,y) + \frac{db}{dx} f[x, b(x)] - \frac{da}{dx} f[x, a(x)] \tag{8-31}$$

]

The general solution to this ODE is just

$$R(E) = \frac{C}{E} \tag{8-32}$$

To determine the constant C, note that we can infer an initial condition at $E = E_0$ from Eq. (8-27)

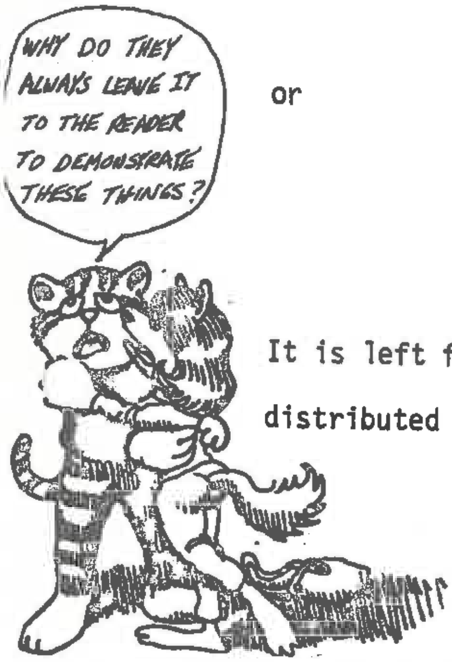
$$R(E_0) = \frac{S_0}{E_0} \tag{8-33}$$

Hence we must choose $C = S_0$ to find

$$R(E) = \frac{S_0}{E} \tag{8-34}$$

or

$$\Phi(E) = \frac{S_0}{\Sigma_s(E)E} \tag{8-35}$$



It is left for a problem set to demonstrate that for a more general distributed source, S(E), the solution to (8-23) is just

$$\Phi(E) = \frac{1}{\Sigma_s(E)E} \int_E^{\infty} dE' S(E') \tag{8-36}$$

It should be noted that in both of these solutions, if the scattering cross section is weakly dependent upon energy (which it usually is), the flux assumes a 1/E form. This functional form could in fact be used as a crude estimate of the flux in generating group constants characterizing neutron slowing down, but we will continue to develop more sophisticated models.

It is useful to introduce several new definitions at this point in order to faciliate our later analysis. We first want to define the neutron "slowing down density", q(E), which describes the rate at which neutrons slow down past a given energy E. To be more general, we define

$q(\vec{r},E)d^3r$ = number of neutrons slowing down past energy E per second in d^3r about $\vec{r}$ (8-37)

If we recall that the differential scattering cross section describes the probability that a neutron will scatter from an initial energy E' to a final energy E" in dE", then we can write

$$\text{rate at which neutrons which suffer collision at energy } E' \text{ in } dE' \text{ slow down past } E = \left[\int_0^E \Sigma_s(E'\to E'')\,\Phi(\vec{r},E)\,dE''\right]dE' \qquad (8\text{-}38)$$

Hence the total slowing down density resulting from all initial energies E' > E is given by

$$q(\vec{r},E) = \int_E^\infty dE' \int_0^E dE''\,\Sigma_s(E'\to E'')\,\Phi(\vec{r},E'') \qquad (8\text{-}39)$$

We can apply this definition to slowing down in hydrogen (if we take care to include in addition the source term)

$$q(E) = \int_0^E dE'' \left[\int_E^{E_0} dE' \frac{\Sigma_s(E')\Phi(E')}{E'} + \frac{S_0}{E_0}\right] \qquad (8\text{-}40)$$

$$= E\left[\int_E^{E_0} dE' \frac{R(E')}{E'} + \frac{S_0}{E_0}\right] = ER(E) = S_0 \qquad (8\text{-}41)$$

Hence for this simple problem, the slowing down density is constant and equal to the source.

An alternative derivation of this result is informative. Note that

$$\text{fraction of collisions in hydrogen which scatter neutrons from } E' \text{ past } E = \int_0^E P(E'\to E'')dE'' = \int_0^E \frac{dE''}{E'} = \frac{E}{E'} \qquad (8\text{-}42)$$

Hence the number slowed down past E after scattering at E' is just

$$\int_E^{E_0} dE'\, R(E')\left(\frac{E}{E'}\right) \tag{8-43}$$

The number from the first collisions of source neutrons is

$$S_0\left(\frac{E}{E_0}\right) \tag{8-44}$$

Hence the total number slowing down past E is

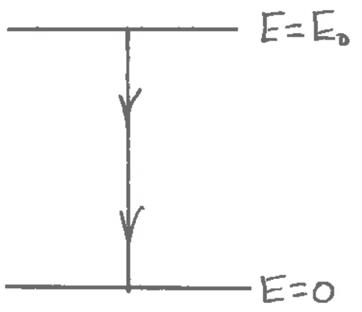
$$q(E) = E\left[\int_E^{E_0} dE'\,\frac{R(E')}{E'} + \frac{S_0}{E_0}\right] = ER(E) = S_0 \tag{8-45}$$

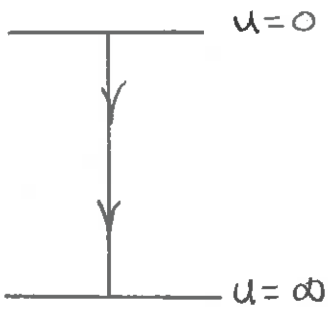
The energy range spanned by neutron slowing down is extremely broad--from 10^6 to 1 eV. If we note that in hydrogen, the collision density R(E) is proportional to 1/E, then there are 10^6 times as many collisions occurring per second at 1 MeV as at 1 eV. Furthermore, we have found that in elastic scattering the neutron tends to lose a fraction of its initial energy, rather than a fixed amount of energy. These considerations suggest that it would be more convenient to use as an independent variable, the logarithm of the neutron energy E. To this end, we define the "neutron lethargy"

$$u \equiv \ln\frac{E_0}{E} \equiv \quad \text{lethargy} \tag{8-46}$$

Here, the energy E_0 is chosen to be the maximum energy which neutrons can achieve in the problem. It is either set at the source energy for a monoenergetic source problem, or chosen as 10 MeV for a reactor calculation.

Notice that as a neutron's energy E decreases, its lethargy u increases (that is, the neutron becomes more "lethargic")





We now must convert all of our earlier equations over to this new variable. To accomplish this, we first compute the relationship between differentials:

$$du = \left(\frac{E}{E_0}\right)\left(-\frac{E_0}{E^2}\right)dE = -\frac{dE}{E} \qquad (8\text{-}47)$$

For example, we can calculate the collision density in terms of lethargy by writing

$$R(u)\,du = -R(E)\,dE \qquad (8\text{-}48)$$

[The minus sign appears because lethargy increases as energy decreases.] Hence using Eq. (8-47), we find that

$$R(u) = E\,R(E) = S_0 \qquad (8\text{-}49)$$

Thus the collision density in the lethargy variable is a constant for hydrogen.

As a second example, we can compute the scattering probability function P(E'→E) in lethargy by noting

$$P(u'\rightarrow u)\,du = -P(E'\rightarrow E)\,dE \qquad (8\text{-}50)$$

Thus

$$P(u'\to u) = -\frac{dE}{du}P(E'\to E) = E\,P(E'\to E)$$

$$= \frac{1}{(1-\alpha)}\left(\frac{E}{E'}\right) = \frac{e^{u'-u}}{(1-\alpha)} \tag{8-51}$$

Also

$$\alpha E' < E < E' \quad \Longrightarrow \quad u' + \ln(1/\alpha) > u > u' \tag{8-52}$$

Hence we find

$$P(u'\to u) = \begin{cases} \dfrac{e^{u'-u}}{(1-\alpha)}, & u' < u < u' + \ln(1/\alpha) \\ 0, & \text{otherwise} \end{cases} \tag{8-53}$$

We can now rewrite our slowing down equation in terms of the lethargy variable as

$$\Sigma_s(u)\,\Phi(u) = \int_0^u du'\,e^{u'-u}\,\Sigma_s(u')\,\Phi(u') + S(u) \tag{8-54}$$

Now notice something rather interesting: From Eq. (8-39) and (8-53), it is apparent the slowing down density in the lethargy variable is given by

$$q(u) = \int_0^u du'\,\Sigma_s(u')\,\Phi(u')\,e^{u'-u} \tag{8-55}$$

Now suppose we differentiate this expression with respect to u

$$\frac{dq}{du} = -\int_0^u du' \Sigma_s(u') \Phi(u') e^{u'-u} + \Sigma_s(u) \Phi(u) \qquad (8\text{-}56)$$

Hence we can re-identify q(u) from Eq. (8-55) to write

$$\frac{dq}{du} + q(u) = \Sigma_s(u) \Phi(u) \qquad (8\text{-}57)$$

These equations relating the slowing down density to the flux are peculiar to slowing down in hydrogen, but we will later find that they hold also when absorption and spatial dependence is included. They will prove to be of considerable use in numerical studies of neutron slowing down.

As a final exercise involving the lethargy variable, let us compute the average lethargy gain (corresponding to the average energy loss) of a neutron in a collision with a nucleus of arbitrary mass number:

$$\begin{aligned} \langle \Delta u \rangle \equiv \xi &= \int_{\alpha E_i}^{E_i} \left[\ln\left(\frac{E_0}{E_f}\right) - \ln\left(\frac{E_0}{E_i}\right) \right] \frac{1}{(1-\alpha)E_i} dE_f \\ &= \frac{1}{(1-\alpha)E_i} \int_{\alpha E_i}^{E_i} \ln\left(\frac{E_i}{E_f}\right) dE_f = \frac{1}{(1-\alpha)} \int_1^{\alpha} \ln x \, dx \end{aligned} \qquad (8\text{-}58)$$

or

$$\xi = 1 + \frac{\alpha}{1-\alpha} \ln \alpha = 1 - \frac{(A-1)^2}{2A} \ln \frac{A+1}{A-1} \qquad (8\text{-}59)$$

By way of example,

A	1	2	12	238
ξ	1	.725	.158	.00838

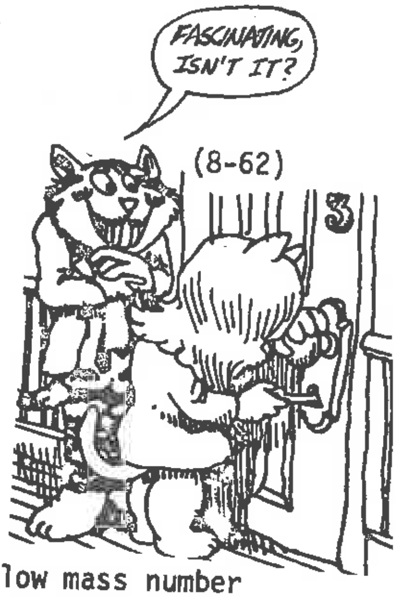
(8-60)

In particular for large mass number A, one can express ξ asymptotically as

$$\xi \sim \frac{2}{A+2/3} \quad , \quad A >> 1 \tag{8-61}$$

An interesting application of this quantity is to compute the average number of collisions necessary to thermalize a fission neutron, i.e., to slow it down from 2 MeV to 0.025 eV. This is given by

$$\langle \# \rangle = \frac{\ln \frac{2\times 10^6}{.025}}{\xi} = \frac{18.2}{\xi} \tag{8-62}$$



Again several examples are of interest:

A	1	2	12	238
$\langle \# \rangle$	18	25	114	2172

We can see rather dramatically how much more effective low mass number nuclei are at moderating fast neutrons.

2. Slowing Down with Absorption

We will now include an absorption term in our infinite medium slowing down equation. Actually, the absorption cross section of hydrogen is negligible. The physical situation we want to describe is that of a strongly absorbing isotope mixed in hydrogen (such as U^{238}). However this isotope can also scatter, and since its mass number is not unity, it would invalidate our analysis. For simplicity, therefore, we will assume the absorber to be "infinitely massive" so that it does not slow down neutrons--it only absorbs them. Then the appropriate slowing down equation (again with a monoenergetic source at energy E_0) is just

$$[\Sigma_a(E)+\Sigma_s(E)]\Phi(E) = \int_E^{E_0} dE' \frac{\Sigma_s(E')\Phi(E')}{E'} + \frac{S}{E_0}, \quad E<E_0 \tag{8-63}$$

As in our earlier analysis, we define the collision density

$$R(E) = \Sigma_t(E)\Phi(E) \tag{8-64}$$

such that the slowing down equation becomes

$$F(E) = \int_E^{E_0} dE' \frac{\Sigma_s(E')F(E')}{E'\Sigma_t(E')} + \frac{S}{E_0}, \quad E<E_0 \tag{8-65}$$

We again solve this equation by first differentiating to find

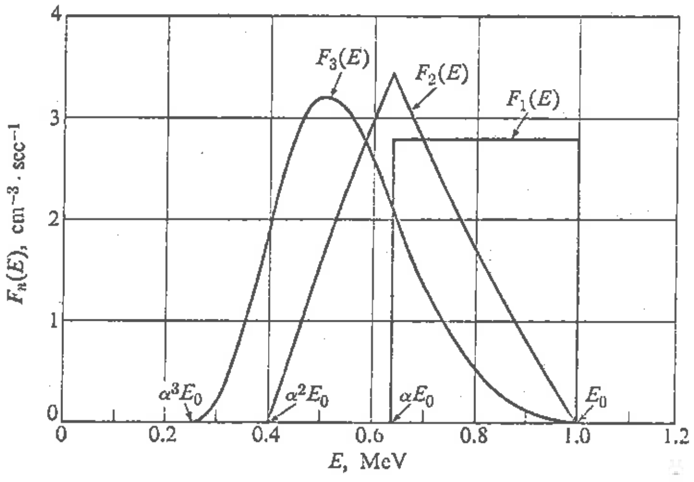
$$\frac{dR}{dE} = \left[\frac{\Sigma_s(E)}{E\Sigma_t(E)}\right] R(E) \tag{8-66}$$

We can easily integrate this ODE to find

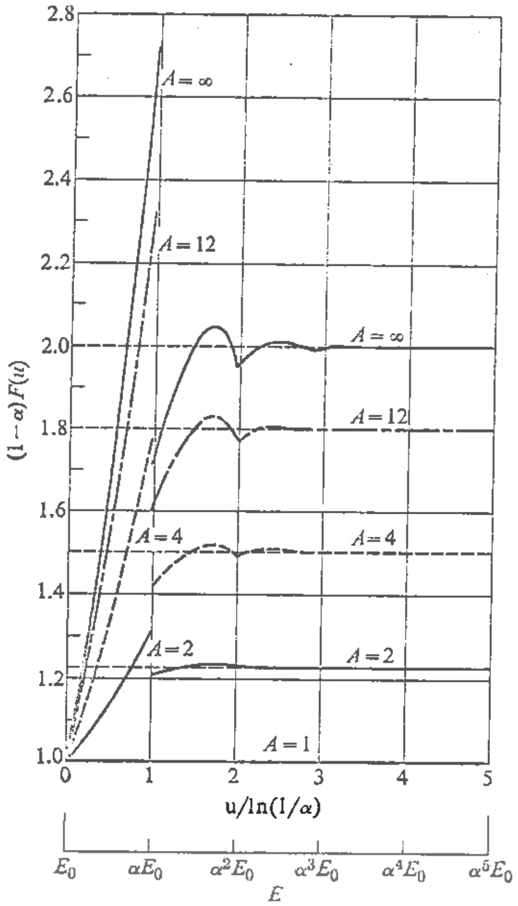
$$R(E) = \frac{C}{E} \exp\left[-\int_E^{E_0} \frac{\Sigma_a(E')dE'}{\Sigma_t(E')E'}\right] \tag{8-67}$$

To determine the constant C, we again use an an initial condition

$$R(E_0) = S_0/E_0 \tag{8-68}$$



The first, second, and third collision densities for unit source of 1-MeV neutrons in beryllium.



The collision density per unit lethargy for various moderators. (After A. M. Weinberg and E. P. Wigner, *The Physical Theory of Neutron Chain Reactors*. Chicago: University of Chicago Press, 1958.)

FIGURE 8-1

We can integrate this to write

$$R_n(u) = R_n(n\ln 1/\alpha)\, e^{\left(\frac{\alpha}{1-\alpha}\right)(u - n\ln 1/\alpha)} - \frac{1}{1-\alpha}\int_{n\ln 1/\alpha}^{u} du'\, R_{n-1}(u' - \ln 1/\alpha)\, e^{\left(\frac{\alpha}{1-\alpha}\right)(u-u')} \tag{8-86}$$

Since we know $R_0(u)$, we can use this expression to generate higher order $R_n(u)$. For example

$$R_1(u) = \left(\frac{1-\alpha^{\frac{1}{1-\alpha}}}{1-\alpha}\right) e^{\left(\frac{\alpha}{1-\alpha}\right)u} - \frac{\alpha^{\frac{\alpha}{1-\alpha}}}{(1-\alpha)^2}(u - \ln 1/\alpha)\, e^{\left(\frac{\alpha}{1-\alpha}\right)u} \tag{8-87}$$

There is a discontinuity between $R_0(u)$ and $R_1(u)$ at $u = \ln 1/\alpha$:

$$R_0(\ln 1/\alpha) - R_1(\ln 1/\alpha) = \frac{\alpha}{1-\alpha} \tag{8-88}$$

These functions (so-called "Placzek functions") are illustrated in Figure (8- 1). Notice in particular how these functions appear to be smoothing out as the neutrons suffer more and more collisions. In fact, for $u >> \ln 1/\alpha$, we can use an asymptotic solution to equation (8-79) in which the source term is neglected

$$R(u) = \int_{u-\ln 1/\alpha}^{u} du' \,\frac{R(u')}{(1-\alpha)}\, e^{u'-u} \tag{8-89}$$

It is evident that R(u) = constant = C is a solution to this equation. However it is not evident just what relationship this solution appears to $R_n(u)$ for large u. Furthermore, there is no apparent prescription for determining C.

Perhaps the most direct way to generate the asymptotic solution is to use Laplace transforms in lethargy. To this end, consider Eq. (8-79) with the source term retained

$$R(u) = \int_{u-\ln 1/\alpha}^{u} du' \, R(u') \left(\frac{e^{u'-u}}{1-\alpha} \right) + S_o \, S(u) \tag{8-90}$$

If we define the Laplace transform

$$\tilde{R}(s) \equiv \int_0^{\infty} du \, e^{-su} R(u) \tag{8-91}$$

we find

$$\tilde{R}(s) = \tilde{R}(s) \tilde{K}(s) + S_o \tag{8-92}$$

where

$$\tilde{K}(s) = \frac{1-\alpha^{s+1}}{(1+\alpha)(s+1)} \tag{8-93}$$

Hence we can solve for

$$\tilde{R}(s) = S_o + \frac{S_o (1-\alpha^{s+1})}{(1-\alpha)(s+1) - (1-\alpha^{s+1})} \tag{8-94}$$

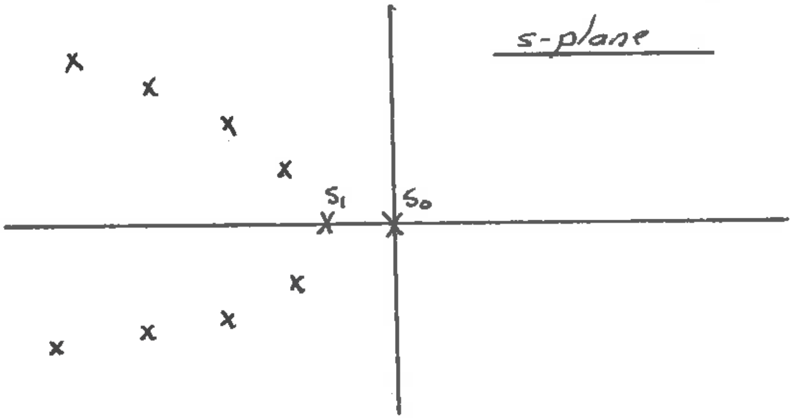
If we define the roots of the denominator as s_j

$$(1-\alpha)(s_j+1) - (1-\alpha^{s_j+1}) = 0 \tag{8-95}$$

then we can invert the Laplace transform to find

$$R(u) = S_0\delta(u) + S_0\sum_{j=0}^{\infty}\frac{[1-\alpha^{s_i+1}]e^{s_i u}}{(1-\alpha)+\alpha^{s_i+1}\ln\alpha} \tag{8-96}$$

The location of these roots s_j in the complex plane are shown below



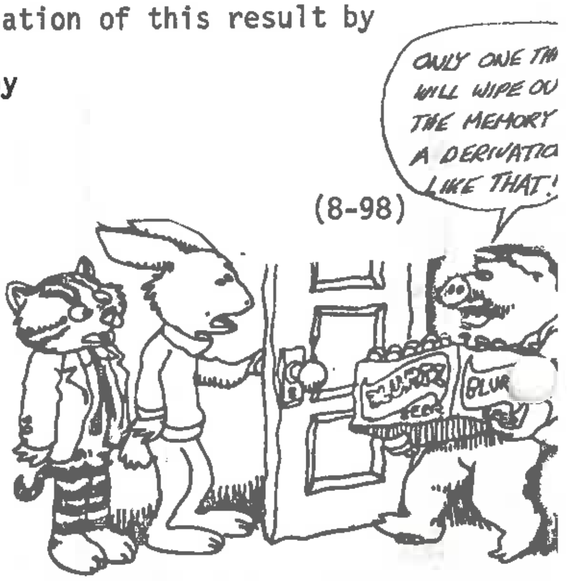
It is apparent that the least damped root is $s_0 = 0$. This root will dominate the solution for large u such that

$$R(u) \sim \frac{S_0(1-\alpha)}{1-\alpha+\alpha\ln\alpha} = \frac{S_0}{1+\frac{\alpha}{1-\alpha}\ln\alpha} = \frac{S_0}{\xi} \tag{8-97}$$

[Note for hydrogen, $\alpha = 1$ and only the root $s_0 = 0$ appears.] The contributions from the higher order roots correspond to the transient solutions such as those we obtained in our collision interval analysis.

It is possible to give a less formal derivation of this result by noting that the slowing down density is given by

$$q(u) = \int_{u-\ln 1/\alpha}^{u} du' R(u') \int_{u}^{u'+\ln 1/\alpha} du'' \frac{e^{u'-u''}}{(1-\alpha)} \tag{8-98}$$



Now if we substitute in our asymptotic form, $R(u) = C$, we find

$$q(u) = C\xi \tag{8-99}$$

But in a non-absorbing media we know that $q(u)$ must be constant and equal to the source rate S_o. Hence we find

$$C = \frac{S_o}{\xi} \tag{8-100}$$

which, together with $R(u) = C$, again yields

$$R(u) = \frac{S_o}{\xi} \tag{8-101}$$

or

$$\Phi(u) = \frac{S_o}{\xi \Sigma_s(u)} \tag{8-102}$$

or, in the energy variable

$$\Phi(E) = \frac{S_o}{\xi E \Sigma_s(E)} \tag{8-103}$$

Hence, asymptotically at least, the flux characterizing neutron slowing down in a nonabsorbing medium of mass number A is very similar to that found in hydrogen, with the exception of an additional factor, the mean lethargy loss per collision, ξ .

More frequently, one is concerned with neutron slowing down in a mixture of nuclides. To this end, define the partial collision density for a given ith species as

$$R^{(i)}(u) = \Sigma_s^{(i)}(u)\,\Phi(u) = \frac{\Sigma_s^{(i)}}{\Sigma_s}\,R(u) \tag{8-104}$$

The asymptotic form of the slowing down equation is then

$$R(u) = \sum_i \int_{u-\ln 1/\alpha_i}^{u} du'\, R^{(i)}(u)\, \frac{e^{u'-u}}{(1-\alpha)} \tag{8-105}$$

Again one finds an asymptotic solution

$$R^{(i)}(u) = C_i \tag{8-106}$$

We can compute the slowing down density as

$$\begin{aligned} q(u) &= \sum_i \int_{u-\ln 1/\alpha_i}^{u} du'\, R^{(i)}(u') \int_{u}^{u'+\ln 1/\alpha_i} du'\, \frac{e^{u'-u''}}{1-\alpha} \\ &= \sum_i C_i \left[1 + \frac{\alpha_i}{1-\alpha_i} \ln \alpha_i\right] = \sum_i C_i \xi_i = \sum_i R^{(i)}(u)\, \xi_i \end{aligned} \tag{8-107}$$

If we again equate $q(u) = S_0$ and define

$$\overline{\xi}(u) \equiv \frac{1}{\Sigma_s(u)} \sum_i \xi_i\, \Sigma_s^{(i)}(u) \tag{8-108}$$

we find

$$R(u) = \frac{S_0}{\overline{\xi}(u)} \tag{8-109}$$

Now if we substitute in our asymptotic form, $R(u) = C$, we find

$$q(u) = C\xi \tag{8-99}$$

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The asymptotic form of the slowing down equation is then

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Again one finds an asymptotic solution

$$R^{(i)}(u) = C_i \tag{8-106}$$

We can compute the slowing down density as

$$\begin{aligned} q(u) &= \sum_i \int_{u-\ln 1/\alpha_i}^{u} du'\, R^{(i)}(u') \int_{u}^{u'+\ln 1/\alpha_i} du'\, \frac{e^{u'-u''}}{1-\alpha} \\ &= \sum_i C_i \left[1 + \frac{\alpha_i}{1-\alpha_i} \ln \alpha_i\right] = \sum_i C_i \xi_i = \sum_i R^{i}(u)\, \xi_i \end{aligned} \tag{8-107}$$

If we again equate q(u) = S_0 and define

$$\bar{\xi}(u) \equiv \frac{1}{\Sigma_s(u)} \sum_i \xi_i\, \Sigma_s^{(i)}(u) \tag{8-108}$$

we find

$$R(u) = \frac{S_0}{\bar{\xi}(u)} \tag{8-109}$$

or

$$\Phi(u) = \frac{S_o}{\overline{\xi(u)}\ \Sigma_s(u)} \qquad (8\text{-}110)$$

or

$$\Phi(E) = \frac{S_o}{\overline{\xi(E)}\ E\ \Sigma_s(E)} \qquad (8\text{-}111)$$

Hence provided we interpret the mean lethargy loss per collision as an averaged quantity over the scattering cross sections characterizing the isotopes of interest, we can use our earlier results. It should be noted that this average quantity, $\overline{\xi(E)}$, is in fact energy-dependent because of the energy dependence of the scattering cross sections.

2.) Slowing Down With Absorption

We could now include absorption (again assuming an infinitely massive absorber) into our earlier Eq. (8-74)

$$[\Sigma_a(E) + \Sigma_s(E)]\,\Phi(E) = \int_E^{E/\alpha} dE' \frac{\Sigma_s(E')\Phi(E')}{(1-\alpha)\,E'} + S(E) \qquad (8\text{-}112)$$

or in terms of the collision density

$$F(E) = \int_E^{E/\alpha} dE' \left[\frac{\Sigma_s(E')}{\Sigma_t(E')}\right] \frac{F(E')}{(1-\alpha)E'} + S(E) \qquad (8\text{-}113)$$

Now the presence of the factor $\left[\Sigma_s(E)/\Sigma_t(E)\right]$ makes it very difficult to make much progress towards an analytical solution to this equation, with the exception of very special cross section behaviors and elaborate approximation techniques. Rather than discuss such techniques here, we will recognize that one is usually most interested in the effects of resonance absorption, and so we will proceed directly to a discussion of the various methods used to calculate the resonance escape probability.

E. Inelastic Scattering

Thus far we have concerned ourselves with neutron moderation via elastic collisions in which a neutron merely bounces off of a nucleus in a billiard ball fashion, losing some energy in the process. However for higher energy neutrons (> 10 keV), inelastic scattering processes are possible in which an appreciable fraction of the incident neutron energy goes into exciting the nucleus into a higher nuclear quantum state. Such scattering is extremely important in heavy mass nuclei in which slowing down by elastic scattering is negligible. For example, if we consider a 10 MeV neutron incident upon a U^{238} nucleus, then the average energy lost in an elastic scattering collision would be

$$\overline{\Delta E}(\text{elastic}) = \left(\frac{1-\alpha}{2}\right)10 = .085 \text{ MeV}$$

By way of comparison, the average energy lost via inelastic scattering is

$$\overline{\Delta E}(\text{inelastic}) \simeq 8.68 \text{ MeV}$$

Since inelastic scattering is much more significant for fast neutrons in high mass number materials, it might be expected to be of considerable consequence in fast reactors. Indeed, inelastic scattering in materials such as sodium is the dominant slowing down mechanism in fast reactors, and as such, is extremely important to study.

Unfortunately, the details of the inelastic scattering cross sections are quite complicated, and analytical investigations such as those we have applied to elastic scattering are restricted to very simple nuclear models (e.g., the Weisskopf evaporation model or few level models). Instead one must usually proceed in practice with a brute force fine-structure multigroup calculation. That is, one writes the infinite medium slowing down equation in multigroup form as:

$$\Sigma_{Rg}\phi_g = \sum_{g'=1}^{g} \Sigma_{sg'g}^{in}\phi_g + S_g \qquad (8\text{-}114)$$

This can then be solved directly for many groups in order to obtain the intragroup fluxes for calculating the few group constants. Such fine spectrum calculations may require as many as a thousand or more microgroups to adequately treat the details of inelastic scattering. We will return to discuss this topic in more detail when we specifically consider several of the problems which arise in fast reactor analysis.

II. RESONANCE ABSORPTION

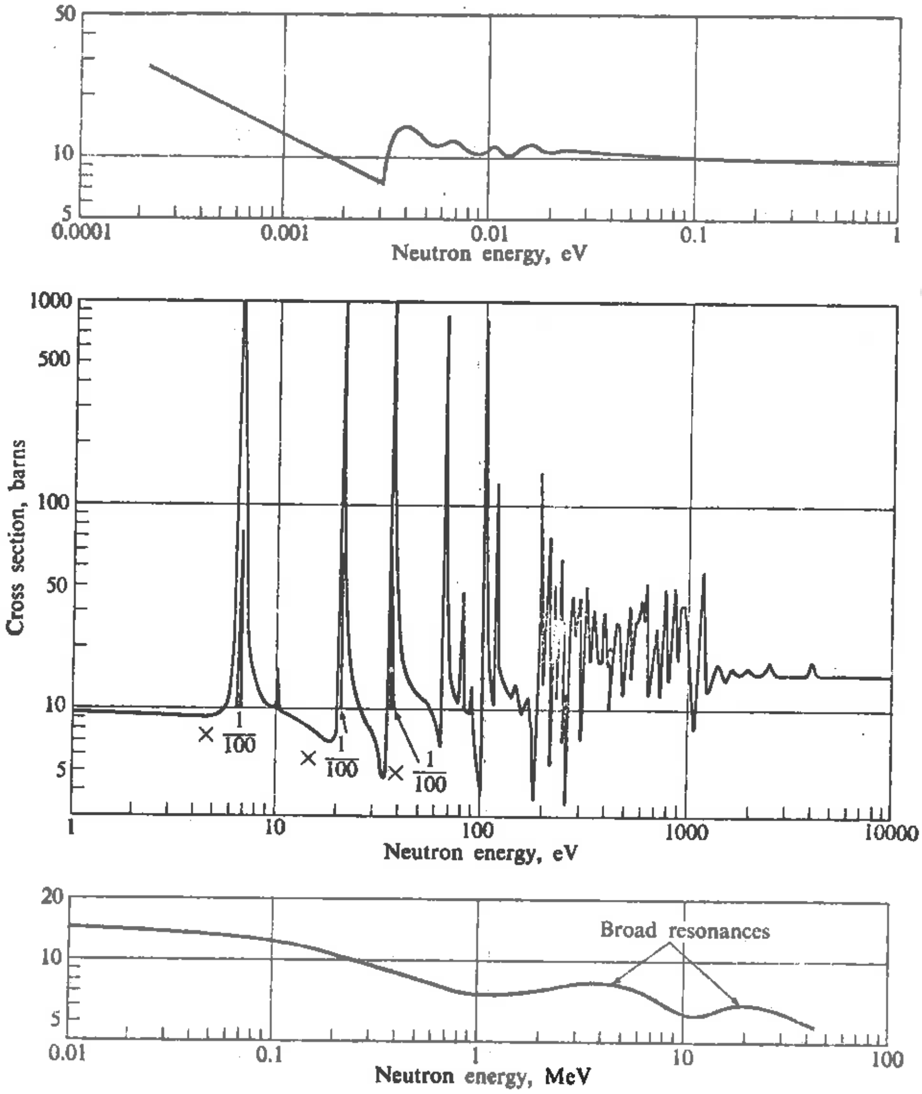
Thus far our study of neutron slowing down has been concerned with the energy range from roughly 1 eV to 100 keV. In this energy range, most neutron absorption occurs in heavy nuclei at sharp capture resonances. This phenomenon of resonance absorption is extremely important in both thermal and fast reactors. An accurate treatment of resonance absorption is essential to reactor criticality calculations. In general there will be depression in the neutron flux at those energies in the vicinity of a strong resonance, and such flux depressions are of considerable importance in determining multigroup constants. Furthermore, the resonance absorption is quite sensitive to the temperature of the fuel due to Doppler broadening of the resonances. This is of particular importance in determining the fast temperature coefficient of reactivity, as we have seen in Chapter 6.

In this section we will attempt to introduce some of the more elementary concepts and approximations useful in the study of resonance absorption. We will begin by reviewing the behavior of the neutron cross section in the vicinity of an isolated resonance, and generalize this analysis to include the effects of temperature upon the resonance behavior. We will then turn to a study of resonance absorption in an infinite medium (consistent with our earlier study of neutron slowing down) and develop the principal approximations useful in the calculation of the resonance escape probability and fast group constants. Later in Chapter 10 we will return to re-examine this subject once again in an effort to include the effects of spatial neutron transport.

A. Resonance Cross Section Behavior

The cross sections characterizing heavy nuclei exhibit many sharp resonances in the range of neutron slowing down. By way of example, we have shown the cross section for U^{238} (perhaps the most significant resonance absorber in today's generation of power reactors) in Figure (8-2). Below roughly 1 KeV, these resonances are well separated, with an average spacing of $\sim$ 18 eV and a resonance width ranging between 0.03 and 0.1 eV. The lowest such resonance occurs at 6.7 eV. Above a kilovolt, the resonances merge together because experimental methods cannot resolve the resonance structure. This region of unresolved resonances is of particular importance in fast reactor analysis and requires rather specialized treatment.

In this study, however, we will confine ourselves to well separated resonances for which the cross section can be described by the Breit-Wigner

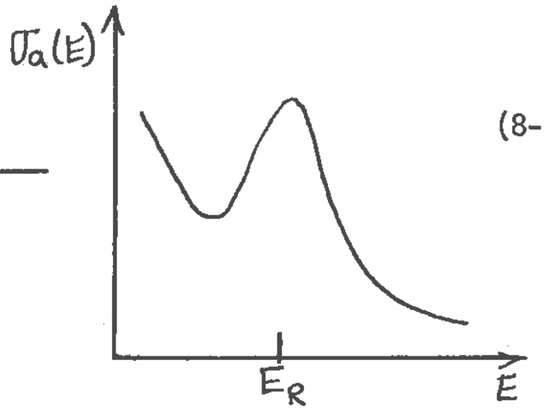


The total cross section of U^{238}. [From BNL-325, Second Edition (1958).]

FIGURE 8-2

formula. For example, the absorption cross section is given by

$$\sigma_a(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_R}{E}}\;\frac{1}{4\frac{(E-E_R)^2}{\Gamma^2}+1} \qquad (8\text{-}115)$$



where σ_0 is the cross section at resonance energy E_R

$$\sigma_0 = g\, 4\pi \lambda\!\!\!^{-2} \frac{\Gamma_n}{\Gamma} \qquad (8\text{-}116)$$

g is a statistical factor

$$g = \frac{2J+1}{2(2I+1)} \qquad (8\text{-}117)$$

J = target spin + neutron spin
I = target spin

while Γ_n is the neutron line width which varies in energy as

$$\Gamma_n = \Gamma_n^0 \sqrt{\frac{E}{E_R}} \qquad (8\text{-}118)$$

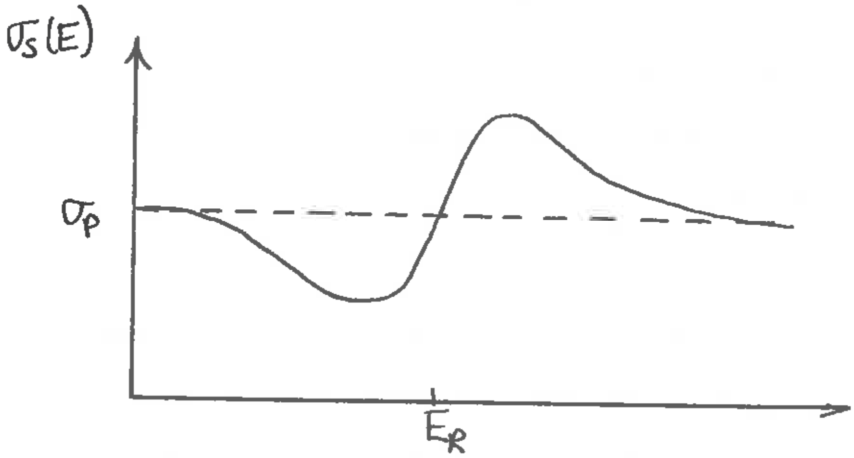
Γ_γ is the gamma emission line width and Γ is the total line width. $\lambda\!\!\!^{-}$ is the reduced neutron wavelength in the CM system

$$\lambda\!\!\!^{-} = \frac{\hbar}{\mu v} \quad , \quad \mu \equiv \frac{Am}{A+1}$$

There will also be a resonance in the scattering cross section

$$\sigma_s(E) = \underbrace{\sigma_0 \frac{\Gamma_n^0}{\Gamma} \frac{1}{4\frac{(E-E_R)^2}{\Gamma^2}+1}}_{\text{resonance scattering}} + \underbrace{\sqrt{\sigma_0 \sigma_p g \frac{\Gamma_n^0}{\Gamma}}\, \frac{2(E-E_R)/\Gamma}{4\frac{(E-E_R)^2}{\Gamma^2}+1}}_{\text{interference scattering}} + \underbrace{\sigma_p}_{\text{potential scattering}}$$

Notice in particular here that resonance and potential scattering combine to yield in addition an interference term, as we see below



It will be very useful to define yet another parameter characterizing resonances. We define the "practical width" Γ_p of the resonance as that range of energies for which the sum of the absorption cross section and the resonance scattering cross section are larger than the potential scattering cross section, i.e.,

$$\Gamma_p \ : \quad \text{all } E \text{ for which} \quad \sigma_a(E) + \sigma_{sR}(E) > \sigma_p \tag{8-120}$$

As a general trend, one finds that the practical width is much larger than the total resonance width--in fact, if we compare

$$\sigma_0 \frac{1}{4\frac{(E-E_R)^2}{\Gamma^2}+1} = \sigma_p \qquad (8\text{-}121)$$

then we find

$$\Gamma_p \sim \Gamma\sqrt{\frac{\sigma_0}{\sigma_p}} \qquad (8\text{-}122)$$

Typically for low lying resonances in U^{238}, $\sigma_0 \sim 10^4$ barns while 10 barns. Hence $\Gamma_p \sim 30\,\Gamma \sim 30$ eV. The practical width is a useful quantity since it is essentially a measure of the extent of the influence of a sharp resonance.

B. The Doppler Effect

The cross section depends upon the relative speed between the neutron and the target nucleus. We must remember that the nuclei themselves are in thermal motion, hence the relative speed V_r may be greater than or less than the neutron speed

This difference in relative speeds gives rise to a "Doppler shift" effect in the absorption cross section.

To take account of this effect, we must average the Breit-Wigner resonance formulas for the cross sections over the thermal distribution of the velocities of the target nuclei. To be more specific, define

$$\eta(\vec{V})\, d^3V \equiv \text{number of target atoms/cm}^3 \text{ with } \vec{V} \text{ in } d^3V \tag{8-123}$$

We will define the average of the cross section $\sigma(v_r)$ over this distribution by writing down an expression for the interaction rate induced by a neutron beam of intensity I

$$\text{interaction rate} = I N_A \bar{\sigma}(E) = \int d^3V \eta(\vec{V}) N\, v_r \sigma(v_r), \tag{8-124}$$

where N_A is the atomic number density and N is the neutron density. If we now recall that I = Nv, then we can find

$$\bar{\sigma}(E) = \frac{1}{N_A v} \int d^3V\; v_r \sigma(v_r)\, \eta(\vec{V}) \tag{8-125}$$

In this sense, we have defined $\bar{\sigma}(E)$ by averaging the reaction rate, $v\sigma(v)$, rather than the cross section itself.

We will assume that the nuclei obey a Maxwell-Boltzmann distribution characteristic of a temperature T

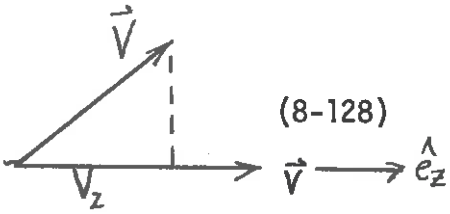
$$\eta(\vec{V}) = N_A \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-MV^2/2kT} \tag{8-126}$$

Strictly speaking, such a distribution would only characterize a perfect gas. However at those temperatures characteristic of a reactor core, a Maxwell distribution is found to yield adequate results.

To perform this average, we first note that the energy available in the CM system is

$$E_c = \frac{1}{2}\mu v_r^2 = \frac{1}{2}|\vec{v} - \vec{V}|^2 \qquad (8\text{-}127)$$

where $\vec{v}$ is the neutron velocity, $\vec{V}$ is the nuclear velocity, and μ is the reduced mass $\mu = mM/(m + M)$. Hence,



$$\begin{aligned} E_c &= \frac{1}{2}\mu v^2 + \frac{1}{2}\mu V^2 - \mu \vec{v}\cdot\vec{V} \qquad (8\text{-}128) \\ &= \frac{M}{m+M}E + \frac{m}{m+M}E_A - \mu\sqrt{\frac{2E}{m}}\,V_z \end{aligned}$$

where we have chosen the z-axis of $\vec{V}$ along $\vec{v}$,

If we note $M \gg m$ for most resonance absorbers ($A \gg 1$), then

$$E_c \cong E - \mu\sqrt{\frac{2E}{m}}\,V_z \qquad (8\text{-}129)$$

Now since σ depends only upon E_c and hence upon V_z, we can perform the integrations over V_x and V_y to find

$$\bar{\sigma}(E) = \frac{1}{v}\int_{-\infty}^{\infty} dV_z\, v_r \sigma(E_c)\left(\frac{M}{2\pi kT}\right)^{1/2} e^{-MV_z^2/2kT} \qquad (8\text{-}130)$$

If we note that for $M \gg m$, $\mu \sim m$ and hence

$$\frac{v_r}{v} = \frac{\sqrt{2E_c/\mu}}{\sqrt{2E/m}} \sim \sqrt{\frac{E_c}{E}} \qquad (8\text{-}131)$$

and also recall the Breit-Wigner form

$$\sigma_a(E_c) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_R}{E_c}} \; \frac{1}{4\left(\frac{E_c-E_R}{\Gamma}\right)^2+1} \tag{8-132}$$

then this integral becomes

$$\overline{\sigma_a}(E) = \left(\sigma_0 \frac{\Gamma_\gamma}{\Gamma}\right)\sqrt{\frac{E_R}{E}}\left(\frac{M}{2\pi kT}\right)^{1/2}\int_{-\infty}^{\infty} dV_z \; \frac{e^{-MV_z^2/2kT}}{4\left(\frac{E_c-E_R}{\Gamma}\right)^2+1} \tag{8-133}$$

Unfortunately, this integral cannot be evaluated analytically. It is customary to introduce a variable transformation to

$$\begin{aligned} x &= \frac{2}{\Gamma}(E-E_R) \\ y &= \frac{2}{\Gamma}(E_c-E_R) \end{aligned} \tag{8-134}$$

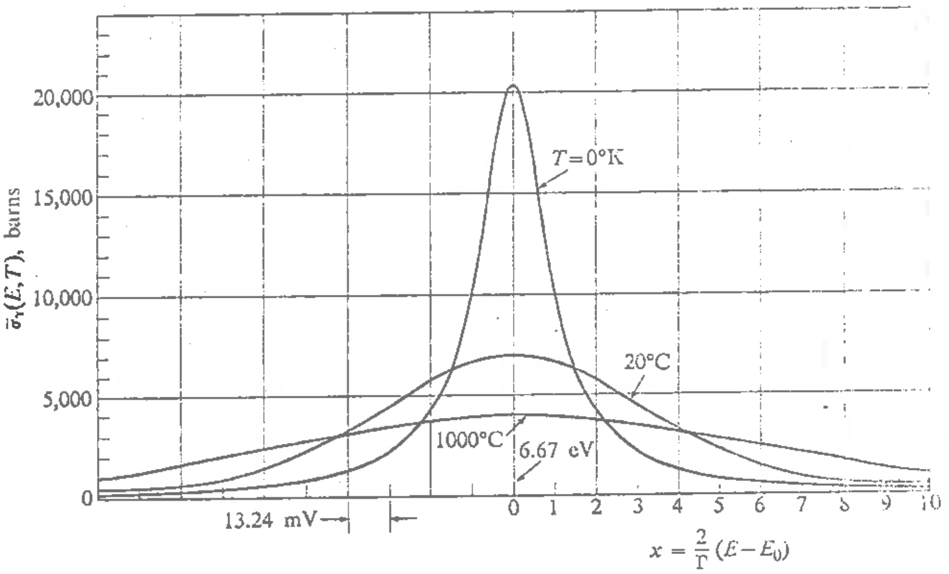
and define $\xi = \frac{\Gamma}{\Gamma_D}$ where $\Gamma_D \equiv \sqrt{\frac{4E_RkT}{A}}$ is the so-called "Doppler width" of the resonance. Then we can write

$$\overline{\sigma_a}(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_R}{E}}\,\psi(\xi,x) \sim \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\,\psi(\xi,x) \tag{8-135}$$

(since $E \sim E_R$ in the vicinity of the resonance). Here $\psi(\xi,x)$ is a tabulated function defined by

$$\psi(\xi,x) \equiv \frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty} \frac{e^{-\frac{1}{4}(x-y)^2\xi^2}}{1+y^2}\,dy \tag{8-136}$$

Several features of this averaged cross section are extremely important. Suppose we plot $\overline{\sigma_a}(E)$ for various values of temperature T



Doppler broadening of the capture cross section of U^{238} at the 6.67 eV resonance.

Notice that as the temperature increases, the resonance is broadened. For low temperatures, $T \to 0 \implies \xi \to \infty$ which yields

$$\psi(\xi,x) \sim \frac{\xi}{2\sqrt{\pi}} \frac{1}{1+x^2} \int_{-\infty}^{\infty} e^{-\frac{1}{4}\xi^2(x-y)^2} dy = \frac{1}{1+x^2} \qquad (8\text{-}137)$$

and hence we arrive at just the Breit-Wigner form

$$\overline{\sigma_a}(E)\Big|_{T=0} = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_R}{E}} \frac{1}{4\left(\frac{E_c-E_R}{\Gamma}\right)^2+1} \qquad (8\text{-}138)$$

At the other extreme, as $T \to \infty$ one finds

$$\bar{\sigma}_a(E) \longrightarrow \sigma_0 \frac{\Gamma}{\Gamma_D} \frac{\sqrt{\pi}}{2} e^{-(E-E_R)^2/\Gamma_D^2} \tag{8-139}$$

which is a Gaussian shape characterized by the Doppler width Γ_D rather than the natural line width Γ.

Regardless of the temperature, it is important to note that the area under the resonance remains constant

$$\int_{\text{resonance}} dE\, \bar{\sigma}_a(E) \cong \frac{\Gamma_\gamma}{\Gamma} \sigma_0 \int_{-\infty}^{\infty} dx\, \psi(\xi,x) = \frac{\pi}{2} \sigma_0 \Gamma_\gamma \tag{8-140}$$

This is extremely important, for it will imply that increasing the temperature, thereby broadening the resonance without changing its area, will lead to much higher absorption in the resonance.

In a similar manner, one can calculate the Doppler broadened scattering cross section to find

$$\bar{\sigma}_s(E) = \sigma_0 \frac{\Gamma_n^0}{\Gamma} \psi(\xi,x) + \left(\sigma_0 \sigma_p g \frac{\Gamma_n^0}{\Gamma}\right)^{1/2} \chi(\xi,x) + \sigma_p \tag{8-141}$$

Here we have had to define a new tabulated function to characterize the interference term

$$\chi(\xi,x) = \frac{\xi}{\sqrt{4\pi}} \int_{-\infty}^{\infty} y \, \frac{e^{-\frac{1}{4}\xi^2(x-y)^2}}{1+y^2} \, dy \tag{8-142}$$

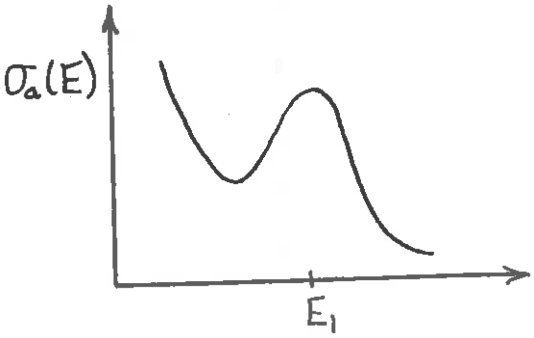
We will now proceed to use these cross sections to study resonance absorption in an infinite medium. Although we have denoted the Doppler broadened cross section with a bar, e.g., $\overline{\sigma_a}(E)$, henceforth we will omit this notation and regard all resonance cross sections as having been Doppler broadened.

C. Resonance Absorption In Hydrogen

We will begin by studying resonance absorption due to an infinitely massive absorber distrubuted through an infinite medium of hydrogen. This case is of particular interest, since we can obtain an exact expression for the resonance escape probability

$$p(E) = \exp\left[-\int_E^{E_o} dE' \frac{\Sigma_a(E')}{\Sigma_t(E')E'}\right] \tag{8-143}$$

We will apply this to calculate the resonance escape probability for a single resonance at an energy E_1. For convenience, we will ignore the scattering from the absorber (infinitely massive) and the absorption in the hydrogen-e.g.,



$$\sigma_s^H >> \sigma_s^A \quad , \quad \sigma_\gamma^H << \sigma_\gamma^A \tag{8-144}$$

If we denote the resonance escape probability for this particular resonance as p_1, then we find

$$P_1 = \exp\left[- \int_{E_1} \frac{N_A \sigma_\gamma^A(E')}{N_H \sigma_s^H(E') + N_A \sigma_\gamma^A(E')} \frac{dE'}{E'} \right] \qquad (8\text{-}145)$$

Suppose we first ignore Doppler broadening (T = 0) such that

$$\sigma_\gamma^A(E') = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \frac{1}{4\left(\frac{E'-E_1}{\Gamma}\right)^2 + 1} \qquad (8\text{-}146)$$

It is customary to assume that the absorber concentration N_A is sufficiently low that

$$N_A \sigma_\gamma^A << N_H \sigma_s^H \qquad (8\text{-}147)$$

[This is known as the "infinite dilution" approximation.] One then finds

$$P_1 \rightarrow \exp\left[- \frac{N_A}{N_H \sigma_s^H} \int_{E_1} \sigma_\gamma^A(E') \frac{dE'}{E'} \right] \equiv P_1^\infty \qquad (8\text{-}148)$$

Now

$$\int_{E_1} \sigma_\gamma^A(E') \frac{dE'}{E'} \cong \frac{1}{E_1} \int_{E_1} \sigma_\gamma^A(E') dE' \cong \frac{\sigma_0 \Gamma_\gamma}{2E_1} \int_{-\infty}^{\infty} \frac{dx}{1+x^2} \qquad (8\text{-}149)$$

Hence

$$P_1^\infty = \exp\left[- \frac{\pi N_A \sigma_0 \Gamma_\gamma}{2 N_H \sigma_s^H E_1} \right] \qquad (8\text{-}150)$$

The case of finite dilution is actually not much more difficult in this case

$$P_1 = \exp\left[-\frac{N_A\sigma_0\Gamma_\gamma}{2N_H\sigma_s^H E_1}\int_{-\infty}^{\infty}\frac{dx}{a^2+x^2}\right], \quad a^2 = 1 + \frac{N_A\sigma_0\Gamma_\gamma}{N_H\sigma_s^H\Gamma} \tag{8-151}$$

$$= \exp\left[-\frac{\pi N_A\sigma_0\Gamma_\gamma}{2N_H\sigma_s^H E_1 a}\right]$$

[As a check, note when $N_A\sigma_0 \ll N_H\sigma_s^H$, $a \rightarrow 1$ and we find $P_1 \rightarrow P_1^\infty$.]

Now to include Doppler broadening we use

$$\sigma_\gamma^A(E) = \sigma_0\frac{\Gamma_\gamma}{\Gamma}\psi(\xi,x), \quad \xi = \Gamma\sqrt{\frac{A}{4E_1kT}} \tag{8-152}$$

Again we first calculate the infinite dilution limit

$$P_1^\infty = \exp\left[-\frac{N_A\sigma_0\Gamma_\gamma}{2N_H\sigma_s^H E_1}\int_{-\infty}^{\infty}\psi(\xi,x)\,dx\right] \tag{8-153}$$

Notice that in particular the infinite dilution resonance escape probability does not depend upon temperature.

However in the case of finite dilution, we find

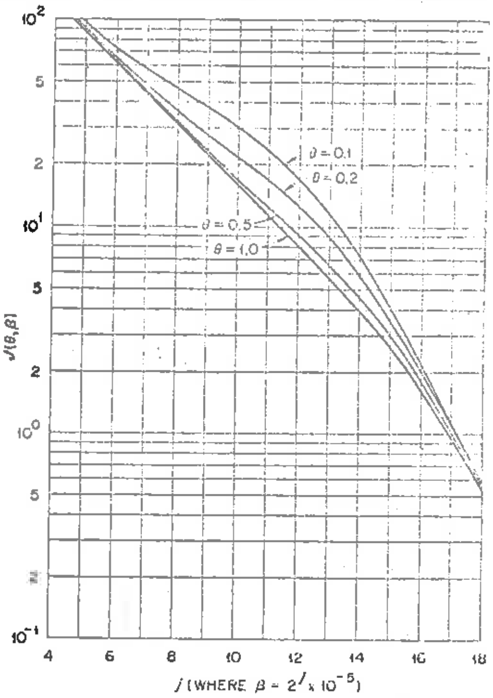
$$P_1 = \exp\left[-\frac{\Gamma}{E_1}J(\xi,\beta)\right] \tag{8-154}$$

where

$$J(\xi,\beta) \equiv \int_0^\infty \frac{\psi(\xi,x)}{\beta+\psi(\xi,x)}\,dx \tag{8-155}$$

$$\beta \equiv \frac{N_H\sigma_s^{\#}\Gamma}{N_A\sigma_0\Gamma_\gamma} \tag{8-156}$$

Here, $J(\xi,\beta)$ is another tabulated function. It is apparent that p_1 is indeed temperature dependent. If we examine the sketch of $J(\xi,\beta)$ vs. β then it is apparent that



The Doppler broadening function $J(\theta, \beta)$ vs. β for various θ.

$$T\uparrow \;\Rightarrow\; \xi\downarrow \;\Rightarrow\; J(\xi,\beta)\uparrow \;\Rightarrow\; p_1\downarrow \tag{8-157}$$

This implies that the resonance escape probability decreases as the temperature increases. This is the very important "Doppler effect" referred to earlier in our discussion of temperature coefficients of reactivity. We will see later that this arises because the broadened resonance leads to a decrease in the flux depression in the vicinity of the resonance energy.

But since the area under the resonance is constant, there will be an increase in the product of the flux and the cross section--hence in the absorption probability.

D. Resonance Integrals

Suppose we consider neutron slowing down in an infinite medium from a source S_0 at energy E_0. Then if we recognize that the rate at which neutrons are absorbed while slowing down from E_0 to E is just

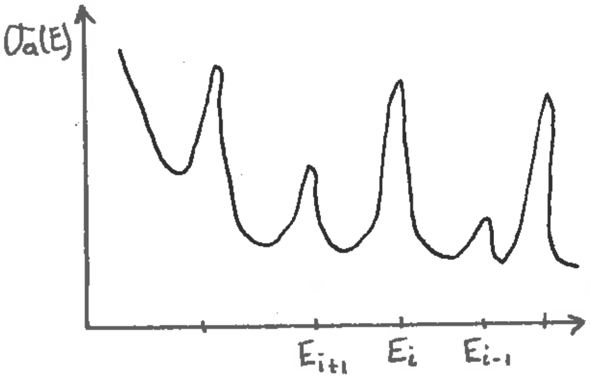
$$\int_E^{E_0} dE'\Sigma_a(E')\Phi(E') \tag{8-158}$$

it is apparent that the resonance escape probability can be formally defined as

$$p(E) = \frac{S - \text{neutron. absorption rate}}{S} = 1 - \frac{1}{S}\int_E^{E_0} dE'\Sigma_a(E')\Phi(E') \tag{8-159}$$

In particular, we can break this up for each resonance by defining

$$P_i = 1 - \frac{1}{S}\int_{E_i} dE'\Sigma_a(E')\Phi(E') \tag{8-160}$$



as the resonance escape probability characterizing each resonance. But, of course, we don't know the flux $\Phi(E)$ within the resonances, so these expressions are only formal.

Now between the resonances, we know the flux eventually approaches its asymptotic form

$$\Phi(E) \sim \Phi_{as}(E) = \frac{C}{\xi\Sigma_s(E)E} \tag{8-161}$$

If we now assume that all of the resonances are widely spaced, we find that the flux at energies below all of the resonances should be of the form

$$\begin{aligned}\Phi(E) &= \frac{S_0}{\xi\Sigma_s(E)E}\prod_i P_i \\ &= \frac{S_0}{\xi\Sigma_s(E)E}\prod_i\left[1 - \frac{1}{S_0}\int_{E_i} dE'\,\Sigma_a(E')\Phi(E')\right]\end{aligned} \tag{8-162}$$

Now suppose we define the "effective resonance integral"

$$I_i \equiv \xi\Sigma_s \int_{E_i} dE'\,\sigma_\gamma^i(E')\,\Phi(E') \tag{8-163}$$

where $\Phi(E')$ is defined to be the flux within the resonance resulting from a flux $\Phi(E) \sim \frac{1}{E}$ above the resonance. Then noting that $1 - P_i \ll 1$, we find

$$\Phi(E) \cong \frac{S_0}{\xi\Sigma_s(E)E}\exp\left[-\frac{N_A}{\xi\Sigma_s}\sum_i I_i\right] \tag{8-164}$$

The effective resonance integral is a very useful concept since it is largely independent of the properties of the moderator. It is also the quantity which appears directly in the calculation of the multigroup constants.

For recall our definition of the multigroup absorption cross section for a group g

$$\Sigma_{a_g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE\, \Sigma_a(E)\, \Phi(E)}{\int_{E_g}^{E_{g-1}} dE\, \Phi(E)} \tag{8-165}$$

Now since the resonances are quite narrow, then over most of the group energy range the flux behaves asymptotically such that

$$\int_{E_g}^{E_{g-1}} dE\, \Phi(E) = \frac{1}{\xi \Sigma_s} \ln\left(\frac{E_{g-1}}{E_g}\right) \tag{8-166}$$

Furthermore, essentially all neutron absorption will occur in those resonances contained in the group g. Hence using our earlier definition of the effective resonance integral, we find

$$\Sigma_{a_g} = \frac{N_A \sum\limits_{i \in g} I_i}{\ln\left(\frac{E_{g-1}}{E_g}\right)} \tag{8-167}$$

where $i \in g$ is written to indicate that only those resonances contained in the group g contribute to Σ_{a_g}. Hence we can generate multigroup constants characterizing absorption directly by using resonance integrals.

Now "all" we need to do is figure out a way to calculate or measure the resonance integrals themselves. We will now turn our attention towards several approximate schemes for doing this.

E. Approximate Calculations Of Resonance Integrals

1.) The Narrow Resonance (NR) Approximation

We now will consider in more detail neutron slowing down and resonance in infinite homogeneous mixture of moderator (denoted by M) and absorber (denoted by A). The basic assumption behind the first approximation we will study is that the average energy loss in a scattering collision with <u>either</u> the absorber or moderator nucleus is large compared to the practical width of the resonance. Since the average energy loss is smallest in collisions with the absorber, we can write the criterion for validity of the "narrow resonance" approximation as

$$\overline{\Delta E}\Big|_A = \left(\frac{1-\alpha_A}{2}\right) E_1 >> \Gamma_p \tag{8-168}$$

To utilize this assumption, we first write down the infinite medium slowing down equation in material containing both an absorbing and a moderating isotope

$$\Sigma_t(E)\Phi(E) = \int_E^{E/\alpha_M} dE' \frac{\Sigma_s^M \Phi(E')}{(1-\alpha_M)E'} + \int_E^{E/\alpha_A} dE' \frac{\Sigma_s^A \Phi(E')}{(1-\alpha_A)E'} \tag{8-169}$$

Now the NR assumption implies that neutrons can only arrive in the resonance by scattering from above it. Hence we can replace the $\Phi(E)$ which occurs inside the scattering integrals by their asymptotic forms to find

$$\int_E^{E/\alpha_M} dE' \frac{\Sigma_s^M \Phi(E')}{(1-\alpha_M)E'} \cong \frac{\Sigma_s^M}{(1-\alpha_M)} \int_E^{E/\alpha_M} dE' \left(\frac{1}{E'}\right) \frac{1}{\bar{\xi}\Sigma_s E'} = \frac{\Sigma_s^M}{\bar{\xi}\Sigma_s E} \tag{8-170}$$

where $\bar{\xi} = \dfrac{\xi_M \Sigma_s^M + \xi_A \Sigma_p^A}{\Sigma_s^M + \Sigma_p^A}$

$$\int_{E}^{E/\alpha_A} dE' \frac{\Sigma_s^A \Phi(E')}{(1-\alpha_A)E'} \cong \frac{\Sigma_p^A}{(1-\alpha_M)} \int_{E}^{E/\alpha_A} dE' \left(\frac{1}{E'}\right) \frac{1}{\bar{\xi}\Sigma_s E'} = \frac{\Sigma_p^A}{\bar{\xi}\Sigma_s E} \tag{8-171}$$

In the second integral we have noted that the absorber scattering cross section is characterized by potential scattering in this asymptotic energy region for above the resonance.

Using these results in Eq. (8-169) we find

$$\Sigma_t(E)\Phi(E) = \frac{\Sigma_s^M + \Sigma_p^A}{\bar{\xi}\Sigma_s E} \tag{8-172}$$

Hence the narrow resonance approximation to the flux is

$$\Phi_{NR}(E) = \frac{\Sigma_s^M + \Sigma_p^A}{\Sigma_t(E)\,(\bar{\xi}\Sigma_s E)} \tag{8-173}$$

The corresponding expression for the resonance integral becomes

$$I_{NR} = \bar{\xi}\Sigma_s \int_{E_i} dE' \, \sigma_\gamma^i(E')\Phi(E') = \int_{E_i} dE' \, \frac{\sigma_\gamma^i(E')(\Sigma_s^M + \Sigma_p^A)}{\Sigma_t(E)E} \tag{8-174}$$

This integral can now be computed using our Doppler broadened resonance shapes, just as it was for hydrogen. Such an approximate expression for the resonance integral is good for higher energy resonances. For lower energy resonances, the energy loss in collisions with absorber nuclei will no longer be larger than the practical width of the resonance, Γ_p. Then we will need to use an alternative approximation.

2.) The Narrow Resonance - Infinite Mass Absorber (NRIM) Approximation

We will now assume

$$\overline{\Delta E}\Big|_A = \left(\frac{1-\alpha_A}{2}\right)E_1 << \Gamma_p \tag{8-175}$$

although we will still continue to treat the resonance width as large compare to the energy loss in scattering from the moderator nuclei

$$\overline{\Delta E}\Big|_M = \left(\frac{1-\alpha_M}{2}\right)E_1 >> \Gamma_p \tag{8-176}$$

We again start from the slowing down equation

$$\Sigma_t(E)\Phi(E) = \int_E^{E/\alpha_M} dE'\,\frac{\Sigma_s^M(E')\Phi(E')}{(1-\alpha_M)E'} + \int_E^{E/\alpha_A} dE'\,\frac{\Sigma_s^A(E')\Phi(E')}{(1-\alpha_A)E'} \tag{8-177}$$

We again will assume that the flux in the moderator scattering integral is given by its asymptotic form such that

$$\int_E^{E/\alpha_M} dE'\,\frac{\Sigma_s^M(E')\Phi(E')}{(1-\alpha_M)E'} \sim \frac{\Sigma_s^M}{\bar{\xi}\Sigma_s E} = \frac{\Sigma_s^M}{(\xi_M \Sigma_s^M + \xi_A \Sigma_p^A)E} \tag{8-178}$$

To handle the absorber scattering term, we will implement the criterion (8-175) by evaluating this term in the limit as $\alpha_A \to 1$ [i.e., letting the absorber mass number $A \to \infty$ such that $\alpha = \left(\frac{A-1}{A+1}\right)^2 \to 1$]. Then

$$\lim_{\alpha_A \to 1} \int_E^{E/\alpha_A} dE'\,\frac{\Sigma_s^A(E')\Phi(E')}{(1-\alpha_A)E'} \to \frac{\Sigma_s^A(E)\Phi(E)}{E}\int_E^{E/\alpha_A} \frac{dE'}{(1-\alpha_A)} \to \Sigma_s^A(E)\,\Phi(E) \tag{8-179}$$

If we now substitute these into Eq. (8-177)

$$\Sigma_t(E)\,\Phi(E) = \frac{\Sigma_s^M}{\xi\Sigma_s E} + \Sigma_s^A(E)\,\Phi(E) \tag{8-180}$$

we can solve for

$$\Phi_{NRIM}(E) = \frac{\Sigma_s^M}{\left[\Sigma_t(E) - \Sigma_s^A(E)\right]\xi\Sigma_s E} \tag{8-181}$$

The corresponding resonance integral is

$$I_{NRIM} = \int_{E_i} dE'\,\frac{\sigma_\gamma^i(E')\;\Sigma_s^M}{\left[\Sigma_t(E) - \Sigma_s^A(E)\right]E} \tag{8-182}$$

Notice that the NR and NRIM approximations differ only in the way in which scattering form absorber nuclei is treated. The key parameter here is the average energy loss suffered in a collision with an absorber nucleus:

$$\overline{\Delta E}\Big|_A = \left(\frac{1-\alpha_A}{2}\right)E_1 \tag{8-183}$$

As we might expect, the NR should be good for larger energies ($\overline{\Delta E} >> \Gamma_p$) while the NRIM should be more appropriate for lower energies ($\overline{\Delta E} << \Gamma_p$).

One can go even further and introduce the Doppler broadened Breit-Wigner line shapes to calculate these resonance integrals in terms of resonance parameters. To this end it is convenient to neglect interference scattering such that

$$\sigma_s^A(E) \cong \sigma_0 \frac{\Gamma_n}{\Gamma}\psi(\xi,x) + \sigma_p$$

$$\sigma_\gamma^A(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\psi(\xi,x) \tag{8-184}$$

Then for the ith resonance

$$I_{NR}^{(i)} = \frac{\sigma_p \Gamma_\gamma^{(i)}}{E_i} J(\xi,\beta) \; , \quad \beta = \frac{\sigma_p}{\sigma_0}\frac{N_M}{N_A} \tag{8-185}$$

and

$$I_{NRIM}^{(i)} = \frac{\Gamma^{(i)}\sigma_s^M}{E_i} J(\xi,\beta') \; , \quad \beta' = \frac{\sigma_s^M \Gamma^{(i)}}{\sigma_s^A \Gamma_\gamma^{(i)}}\frac{N_M}{N_A} \tag{8-186}$$

In Table (8-1) we have given examples of such calculations for several resonances in U^{238}. These are compared with direct numerical calculations of the resonance integral. Although neither approximation seems to yield satisfactory results for the resonances at intermediate energy, when large numbers of resonances are accounted for, the errors tend to average out.

We will return later in Chapter 10 to discuss the modifications which must be made in these results in order to account for heterogeneities (i.e., fuel lumping). Now, however, we will continue with our study of neutron slowing down in an effort to take account of spatial effects (i.e., finite media).

TABLE 8-1

E_o	ev	6.68	103.00	81.00	475.00
Γ_γ	ev	0.024	0.024	0.024	0.024
Γ_n	ev	0.00148	0.072	0.0021	0.005
Γ/Γ_D		0.474	0.455	0.139	0.0639
Γ_p	ev	1.26	3.98	0.76	0.26
$\alpha_0 E_0$	ev	0.11	1.73	1.36	8.0
	N.R.		0.613	0.259	0.0432
		(5.40)	(0.601)	(0.258)	(0.0432)
	I.M.		0.555	0.226	———
		(4.75)	(0.554)	(0.226)	———
	INT	4.94	0.518	0.259	0.0434
		(4.84)	(0.424)	(0.251)	(0.0431)

Resonance Integrals for Uranium Rods of 0.422 cm radius at 300°K

III. NEUTRON SLOWING DOWN IN FINITE MEDIA

A. Derivation of the Energy Dependent P_1 Equations

Before we proceed to develop more sophisticated models of neutron slowing down, we first have to backtrack a bit and develop a generalization of the P_1 equations we derived in Chapter 5 to include energy dependence. This will also touch upon the subject of energy dependent diffusion theory which we so cavalierly accepted in deriving the multigroup diffusion equations of Chapter 7.

The general approach is exactly the same as in the one-speed case. We first integrate the transport equation (ignoring time dependence) over angle to obtain the neutron continuity equation

$$\nabla\cdot\vec{J}(\vec{r},u) + \Sigma_t(u)\Phi(\vec{r},u) = \int_0^\infty du'\,\Sigma_{s_0}(u'\to u)\,\Phi(\vec{r},u') + S_0(\vec{r},u) \quad (8\text{-}187)$$

Here we have chosen to work with the lethargy variable, and furthermore have denoted

$$\Sigma_{s_0}(u'\to u) \equiv \int d\hat{\Omega}\,\Sigma_s(u'\to u, \hat{\Omega}'\cdot\hat{\Omega}) \quad (8\text{-}188)$$

$$S_0(\vec{r},u) \equiv \int d\hat{\Omega}\,S(\vec{r},\hat{\Omega},u) \quad (8\text{-}189)$$

Next, we multiply the transport equation by $\hat{\Omega}$ and again integrate to find

$$\nabla\cdot\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\phi(\vec{r},\hat{\Omega},u) + \Sigma_t(u)\vec{J}(\vec{r},u) \quad (8\text{-}190)$$
$$= \int_0^\infty du'\,\Sigma_{s_1}(u'\to u)\,\vec{J}(\vec{r},u') + S_1(\vec{r},u)$$

where now we have noted

$$\int d\hat{\Omega}\,\hat{\Omega}'\,\Sigma_s(u'\to u,\hat{\Omega}'\cdot\hat{\Omega}) = \hat{\Omega}\,\Sigma_{s_1}(u'\to u) \tag{8-191}$$

if we define

$$\Sigma_{s_1}(u'\to u) \equiv \int d\hat{\Omega}\,(\hat{\Omega}'\cdot\hat{\Omega})\,\Sigma_s(u'\to u,\hat{\Omega}'\cdot\hat{\Omega}) \tag{8-192}$$

while

$$\vec{S}_1(\vec{r},u) \equiv \int d\hat{\Omega}\,\hat{\Omega}\,S(\vec{r},\hat{\Omega},u) \tag{8-193}$$

Notice here that $\Sigma_{s_1}(u'\to u)$ represents the linearly anisotropic part of the double-differential scattering cross section. If one assumes that scattering is isotropic in the laboratory system, then of course $\Sigma_{s_1}(u'\to u)=0$.

Finally, we insert the usual approximation to the angular flux

$$\phi(\vec{r},\hat{\Omega},u) \cong \frac{1}{4\pi}\Phi(\vec{r},u) + \frac{3}{4\pi}\vec{J}(\vec{r},u)\cdot\hat{\Omega} \tag{8-194}$$

and note then that

$$\nabla\cdot\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\phi(\vec{r},\hat{\Omega},u) \cong \frac{1}{3}\nabla\Phi(\vec{r},u) \tag{8-195}$$

to find the coupled P_1 equations

$$\nabla\cdot\vec{J}(\vec{r},u) + \Sigma_t(u)\Phi(\vec{r},u) = \int_0^\infty du'\,\Sigma_{s_0}(u'\to u)\Phi(\vec{r},u') + S_0(\vec{r},u)$$

$$\frac{1}{3}\nabla\Phi(\vec{r},u) + \Sigma_t(u)\vec{J}(\vec{r},u) = \int_0^\infty du'\,\Sigma_{s_1}(u'\to u)\vec{J}(\vec{r},u') + S_1(\vec{r},u) \quad (8\text{-}196)$$

This is an appropriate point at which to stop and reconsider how one would now derive the diffusion approximation from these equations. The first step would be to assume an isotropic source such that $S_1 \equiv 0$. If, in addition, we assumed isotropic scattering, then $\Sigma_{s_1}(u'\to u) \equiv 0$ and we could obtain Fick's law directly from the second equation:

$$\vec{J}(\vec{r},u) = -\frac{1}{3\Sigma_t(u)}\nabla\Phi(\vec{r},u) \quad (8\text{-}197)$$

But the assumption of isotropic scattering is far too gross for most reactor calculations. We, in fact, must retain the scattering term $\Sigma_{s_1}(u'\to u)$ in the second equation.

But now our quandary becomes apparent. For since this term involves an integration over lethargy, we are not allowed to separate out $\vec{J}(\vec{r},u)$ --and hence, strictly speaking, it is not possible to derive a Fick's law type of relation from Eq. (8-196b). We could proceed <u>formally</u>, however, and define an energy dependent diffusion coefficient

$$D(\vec{r},u) = \frac{1}{3}\left[\Sigma_t(\vec{r},u) - \frac{\int_0^\infty du'\,\Sigma_{s_1}(u'\to u)J_i(\vec{r},u')}{J_i(\vec{r},u)}\right]^{-1} \quad (8\text{-}198)$$

which would automatically yield

$$\vec{J}(\vec{r},u) = -D(\vec{r},u)\nabla\Phi(\vec{r},u) \tag{8-199}$$

Of course this is highly artificial because $D(\vec{r},u)$ still depends upon $\vec{J}(\vec{r},u)$.

A very heuristic way to avoid this difficulty is to assume that in some sense

$$\int du'\,\Sigma_{s_1}(u'\to u)J_i(\vec{r},u') \cong \int du'\,\Sigma_{s_1}(u\to u')J_i(\vec{r},u) \tag{8-200}$$

Then, in fact, we find

$$D(\vec{r},u) = \frac{1}{3}\left[\Sigma_t(\vec{r},u) - \bar{\mu}_0(u)\Sigma_s(\vec{r},u)\right]^{-1} \tag{8-201}$$

where we have defined the average scattering angle cosine $\bar{\mu}_0(u)$ as

$$\bar{\mu}_0(u) \equiv \frac{\int_0^\infty du'\,\Sigma_{s_1}(u\to u')}{\int_0^\infty du'\,\Sigma_{s_0}(u\to u')} \tag{8-202}$$

We will return momentarily to give a more satisfactory derivation of this result (the so-called age diffusion approximation). For the present, however, we will avoid introducing the diffusion approximation and continue working with the lethargy dependent P_1 equations. For convenience, we will rewrite them in one-dimensional form as

$$\frac{\partial J}{\partial x} + \Sigma_t(u)\Phi(x,u) = \int_0^u du' \Sigma_{s_0}(u' \to u)\Phi(x,u') + S_0(x,u)$$

$$\frac{1}{3}\frac{\partial \Phi}{\partial x} + \Sigma_t(u) J(x,u) = \int_0^u du' \Sigma_{s_1}(u' \to u) J(x,u) + S_1(x,u) \tag{8-203}$$

In practice, such a one-dimensional treatment is sufficient for calculating fast spectra. Notice that we have also restricted these equations to the description of neutron slowing down by cutting off the upper limit of integration at u' = u (that is, ignoring upscattering).

One further bit of notation is frequently used. Recall that we defined the slowing down density $q(\vec{r},E)$ by

$$q(\vec{r},E) = \int_0^E dE' \int_E^\infty dE'' \Sigma_s(E'' \to E')\Phi(\vec{r},E'') \tag{8-204}$$

One can verify by direct differentiation that

$$\frac{\partial q}{\partial E} = \int_E^\infty dE' \Sigma_s(E' \to E)\Phi(\vec{r},E') - \underbrace{\int_0^E dE' \Sigma_s(E' \to E)\Phi(\vec{r},E)}_{\Sigma_s(E)\Phi(\vec{r},E)} \tag{8-205}$$

If we take this over into the lethargy variable, we find

$$\frac{\partial q_0}{\partial u} = -\int_0^u du' \Sigma_{s_0}(u' \to u)\Phi(\vec{r},u') + \Sigma_s(u)\Phi(\vec{r},u) \tag{8-206}$$

where we have denoted the usual definition of the slowing down density as $q_0(\vec{r},u)$. We will also define an analogous quantity for $\Sigma_{s_1}(u' \to u)$ and $\vec{J}$ by first noting

$$\vec{q}_1(\vec{r},E) = \int_0^E dE' \int_E^\infty dE'' \Sigma_{s_1}(E'' \to E')\vec{J}(\vec{r},E'')$$

so that we can write

$$\frac{\partial \vec{q}_1}{\partial u} = -\int_0^u du' \, \Sigma_{s_1}(u' \to u) \vec{J}(\vec{r},u') + \bar{\mu}_0(u) \Sigma_s(u) \vec{J}(\vec{r},u) \tag{8-207}$$

Hence we can formally rewrite our P_1 equations characterizing neutron slowing down as

$$\begin{aligned} \frac{\partial J}{\partial x} + \Sigma_s(u)\Phi(x,u) &= -\frac{\partial q_0}{\partial u} + S_0(x,u) \\ \frac{1}{3}\frac{\partial \Phi}{\partial x} + \underbrace{[\Sigma_t(u) - \bar{\mu}_0(u)\Sigma_s(u)]}_{\Sigma_{tr}(u)} J(x,u) &= -\frac{\partial q_1}{\partial u} + S_1(x,u) \end{aligned} \tag{8-208}$$

B. Approximate Treatments of Neutron Slowing Down

1.) Age-Diffusion Theory

We will temporarily confine ourselves to the study of neutron slowing down via elastic scattering. We then know that

$$\Sigma_{s_0}(u' \to u) = \begin{cases} \dfrac{\Sigma_s(u)\, e^{u'-u}}{(1-\alpha)} , & u - \ln 1/\alpha < u' < u \\ 0 , & \text{otherwise} \end{cases} \tag{8-209}$$

One can similarly show that

$$\Sigma_{s_1}(u' \to u) = \tag{8-210}$$

Now suppose that $\Sigma_s(u')\,\Phi(x,u')$ were a slowly varying function over a collision interval $u - \ln 1/\alpha < u' < u$. [For zero absorption in a infinite medium we know $\Sigma_s(u)\,\Phi(u)$ is damn slowly varying--it is just a constant

$$\Sigma_s(u)\Phi(u) = R(u) = \frac{S}{\xi} \tag{8-211}$$

Hence for systems which are not too strongly absorbing, and for which the collision interval is not too large--i.e., A is large--this assumption should be reasonable.] Then we can expand $\Sigma_s(u')\Phi(u')$ about u and retain only low order terms as

$$\Sigma_s(u')\Phi(u') \cong \Sigma_s(u)\Phi(u) + (u'-u)\frac{\partial}{\partial u}\left[\Sigma_s(u)\Phi(u)\right] \tag{8-212}$$

Now let's plug this into our scattering integral to find

$$\int_{u-\ln 1/\alpha}^{u} du' \frac{\Sigma_s(u')\Phi(u')e^{u'-u}}{(1-\alpha)} \cong \Sigma_s(u)\Phi(u)\underbrace{\int_{u-\ln 1/\alpha}^{u} du'\frac{e^{u'-u}}{(1-\alpha)}}_{1} + \frac{\partial}{\partial u}\left[\Sigma_s(u)\Phi(u)\right]\underbrace{\int_{u-\ln 1/\alpha}^{u} du'\frac{e^{u'-u}}{(1-\alpha)}(u'-u)}_{-\xi}$$

$$= \Sigma_s(u)\Phi(u) - \frac{\partial}{\partial u}\left[\xi\Sigma_s(u)\Phi(x,u)\right] \tag{8-213}$$

If we compare this with Eq. (8-208), we note that this approximation is equivalent to writing

$$q_0(x,u) \cong \xi\Sigma_s(u)\Phi(x,u) \tag{8-214}$$

[More generally, for several isotope species one writes $q_0(x,u) = \sum_i \xi_i \Sigma_s^i \Phi$ $= \bar{\xi}(u)\Sigma_s(u)\Phi(x,u)$]. This is known as the "age approximation" or as "continuous slowing down theory". The former name will only become apparent in Sec. IV-C. The latter name arises because the neglect of higher order terms in the expansion of the collision density $\Sigma_s(u')\Phi(x,u')$ effectively implies that neutrons lose only an infinitesimal amount of energy in each collision.

To proceed further, we will now make two additional approximations:

(i) Assume only isotropic sources--i.e., $S_1 \equiv 0$

(ii) Assume $q_1(x,u) \equiv 0$

Under these assumptions, we can now write the second of equations (8-208) as

$$J(x,u) = -\frac{1}{3}\left[\Sigma_t(u) - \bar{\mu}_0 \Sigma_s(u)\right]^{-1} \nabla\Phi = -D(u)\nabla\Phi(x,u) \tag{8-215}$$

and then substitute this into the first equation (8-208) to find

$$-\frac{\partial}{\partial x} D(x,u)\frac{\partial \Phi}{\partial x} + \Sigma_a(u)\Phi(x,u) = -\frac{\partial}{\partial u}\left[\xi(u)\Sigma_s(u)\Phi\right] + S(x,u) \tag{8-216}$$

This is known as the "age-diffusion equation". It is sometimes also referred to as the "inconsistent P_1 equation", since we have not treated the slowing down density $q_1(x,u)$ in the same fashion as we treated $q_0(x,u)$.

This equation is primarily of historical importance in reactor analysis since it is restricted to slowing down in heavy mass moderators (certainly not hydrogeneous moderators). It is of interest primarily because it can be solved exactly in certain special cases (as we will see in Section IV-C). At this point, however, we will continue on to develop more accurate descriptions of neutron slowing down.

2.) Consistent P_1 Equations

Of course one simple adjustment we could make would be to treat both q_1 and q_0 on the same footing. That is, we could expand

$$\Sigma_s(u')J(x,u') \cong \Sigma_s(u)J(x,u) + (u'-u)\frac{\partial}{\partial u}\left[\Sigma_s(u)J(x,u)\right] \qquad (8\text{-}217)$$

in

$$\int_0^u du'\,\Sigma_s(u')P_1(u'\to u)J(x,u') \cong \bar{\mu}_0\,\Sigma_s(u)J(x,u) - \frac{\partial}{\partial u}\left[\xi(u)\Sigma_s(u)J(x,u)\right] \qquad (8\text{-}218)$$

where

$$\xi(u) \equiv \frac{1}{\Sigma_s(u)}\int_0^u du'\,(u'-u)\mu_0(u)\,\Sigma_s(u'\to u) \qquad (8\text{-}219)$$

Then we can identify

$$q_1(x,u) = \xi(u)\Sigma_s(u)J(x,u) \qquad (8\text{-}220)$$

and hence arrive at the coupled set of equations

$$\frac{\partial J}{\partial x} + \Sigma_a(u)\Phi(x,u) = -\frac{\partial}{\partial u}\left[\bar{\xi}(u)\Sigma_s(u)\Phi(x,u)\right] + S_0(x,u)$$

$$\frac{1}{3}\frac{\partial \Phi}{\partial x} + \Sigma_{tr}(u)J(x,u) = -\frac{\partial}{\partial u}\left[\bar{\xi}(u)\Sigma_s(u)J(x,u)\right] + S_1(x,u) \qquad (8\text{-}221)$$

which are known as the "consistent P_1 equations." Unfortunately, once again these equations are limited to the description of slowing down in heavy mass moderators. Hence we will turn our attention now towards methods more suitable for the treatment of low mass number moderators.

3.) The Selengut-Goertzel Method

The Selengut-Goertzel method is designed to describe neutron slowing down in a mixture of hydrogen plus heavy mass number nuclei. The essential idea is to use an exact treatment of slowing down in hydrogen, while treating the heavy mass species using age theory (inconsistent P_1).

We begin by first writing out the P_1 equations, but taking care to separate out hydrogen from the nonhydrogeneous elements (denoted by the superscript NH)

$$\frac{\partial J}{\partial x} + \Sigma_a(u)\Phi(x,u) = -\frac{\partial q_0^H}{\partial u} - \sum_i \frac{\partial q_{0i}^{NH}}{\partial u} + S_0(x,u) \qquad (8\text{-}222)$$

$$\frac{1}{3}\frac{\partial \Phi}{\partial x} + \Sigma_{tr}(u)J(x,u) = -\frac{\partial q_1^H}{\partial u} - \sum_i \frac{\partial q_{1i}^{NH}}{\partial u} + S_1(x,u)$$

Now our sequence of approximations will be

(i) Heavy elements (NH): age theory

$$q_{0i}^{NH}(x,u) = \xi_i^{NH}\Sigma_{s_i}^{NH}(u)\Phi(x,u)$$
$$q_{1i}^{NH}(x,u) = 0 \qquad (8\text{-}223)$$

(ii) Hydrogen: Here we will use an exact treatment. Recall that the scattering terms for hydrogen take the form

$$\int_{u-\ln 1/\alpha_H}^{u} du'\,\Sigma_{s_0}^H(u'\to u)\Phi(x,u') = \int_0^u du'\,\Sigma_s^H(u')e^{u'-u}\Phi(x,u')$$
$$\int_{u-\ln 1/\alpha_H}^{u} du'\,\Sigma_{s_1}^H(u'\to u)J(x,u') = \int_0^u du'\,\Sigma_s^H(u')e^{-\frac{3}{2}(u'-u)}J(x,u') \qquad (8\text{-}224)$$

But we can recall from Section 8-I-C that

$$q_0^H(x,u) = \int_0^u du' \, \Sigma_s^H(u') e^{u'-u} \, \Phi(x,u') \tag{8-225}$$

Similarly

$$q_1^H(x,u) = \int_0^u du' \, \Sigma_s^H(u') e^{-3/2(u'-u)} \, J(x,u') \tag{8-226}$$

If we now differentiate each of these equations, we find

$$\begin{aligned} \frac{\partial q_0^H}{\partial u} + q_0^H(x,u) &= \Sigma_s^H(u)\,\Phi(x,u) \\ \frac{\partial q_1^H}{\partial u} + \frac{3}{2} q_1^H(x,u) &= \frac{2}{3}\Sigma_s^H(u)\,J(x,u) \end{aligned} \tag{8-227}$$

In summary, then, the equations which comprise the Selengut-Goertzel model are

$$\begin{aligned} \frac{\partial J}{\partial x} + \Sigma_a(u)\,\Phi(x,u) &= -\frac{\partial q_0^H}{\partial u} - \sum_i^{NH} \xi_i \Sigma_s^{(i)} \Phi(x,u) + S_0(x,u) \\ \frac{1}{3}\frac{\partial \Phi}{\partial x} + \Sigma_{tr}(u)\,J(x,u) &= -\frac{\partial q_1^H}{\partial u} + S_1(x,u) \\ \frac{\partial q_0^H}{\partial u} + q_0^H(x,u) &= \Sigma_s^H(u)\,\Phi(x,u) \\ \frac{\partial q_1^H}{\partial u} + \frac{3}{2} q_1^H(x,u) &= \frac{2}{3}\Sigma_s^H(u)\,J(x,u) \end{aligned} \tag{8-228}$$

We will return momentarily to discuss how one solves such equations.

4.) The Greuling-Goertzel Approximation

Thus far we have provided prescriptions for handling neutron slowing down in either very heavy isotopes (age theory) or in hydrogen (exact solution). However neither of these schemes are adequate for light, nonhydrogeneous materials--with deuterium, D^2 being a prime villian. Hence we are motivated to construct an alternative to the age approximation for nonhydrogeneous media.

Suppose we try to seek equations very similar to those describing slowing down in hydrogen

$$\lambda_0 \frac{\partial q_0}{\partial u} + q_0(x,u) = \beta_0 \Phi(x,u) \tag{8-229}$$

$$\lambda_1 \frac{\partial q_1}{\partial u} + q_1(x,u) = \beta_1 J(x,u)$$

Now suppose we proceed formally as we did in the age approximation by expanding the collision density in the scattering integral to find

$$q_0(x,u) = -\sum_{n=0}^{\infty} \frac{d^n}{dx^n}\left[G_0^{(n+1)}\Phi\right] \tag{8-230}$$

where $$G_0^{(n)}(u) = -\int_0^{\ln 1/\alpha} (u'-u)^n \Sigma_{s_0}(u'\to u)\,du'$$

Then

$$\frac{\partial q_0}{\partial u} = -\sum_{n=0}^{\infty} \frac{d^{n+1}}{du^{n+1}}\left[G_0^{(n+1)}\Phi\right] = -\sum_{n=1}^{\infty} \frac{d^n}{du^n}\left[G_0^{(n)}\Phi\right] \tag{8-231}$$

Now compute

$$q_0 - \frac{G_0^{(2)}}{G_0^{(1)}}\frac{\partial q_0}{\partial u} = -G_0^{(1)}\Phi - \frac{\partial}{\partial u}\left(G_0^{(2)}\Phi\right) + \frac{G_0^{(2)}}{G_0^{(1)}}\frac{\partial}{\partial u}\left(G_0^{(1)}\Phi\right)$$

$$+\underbrace{\sum_{n=2}^{\infty}\left\{G_0^{(2)}\frac{d^n}{du^n}\left[G_0^{(n)}\Phi\right] - G_0^{(1)}\frac{d^n}{du^n}\left[G_0^{(n+1)}\Phi\right]\right\}}_{\text{neglect}} \tag{8-232}$$

$$\cong \left[\frac{G_0^{(2)}}{G_0^{(1)}}\frac{\partial G_0^{(1)}}{\partial u} - \frac{\partial G_0^{(2)}}{\partial u} - G_0^{(1)}\right]\Phi$$

Hence we now have arranged things in the form of (8-229) if we identify

$$\lambda_0 = -\frac{G_0^{(2)}}{G_0^{(1)}}$$

$$\beta_0 = -\frac{G_0^{(2)}}{G_0^{(1)}}\frac{\partial G_0^{(1)}}{\partial u} - \frac{\partial G_0^{(2)}}{\partial u} - G_0^{(1)} \qquad (8\text{-}233)$$

For the specific case of s-wave scattering, these reduce to

$$\lambda_0^{(i)} = \frac{1-\alpha_i\left[1+\ln 1/\alpha_i + \frac{1}{2}\ln^2\frac{1}{\alpha_i}\right]}{1-\alpha_i\left[1+\ln 1/\alpha_i\right]} \qquad (8\text{-}234)$$

$$\beta_0^{(i)} = \xi_i \Sigma_s^{(i)}$$

We can go through a very similar analysis for $\beta_1^{(i)}$ and $\lambda_1^{(i)}$ to find

$$\lambda_1^{(i)} = \qquad (8\text{-}235)$$

$$\beta_1^{(i)} = \xi_i \Sigma_s^{(i)}$$

Augmenting the set of P_1 equations (8-208) with Eq. (8-229) yields what is known as the Greuling-Goertzel approximation. Notice in particular that this approximation will result in an exact treatment of hydrogen.

5.) Summary of the P_1 Slowing Down Equations

We can summarize all of these various approximations by writing the P_1 equations as

$$\frac{\partial J}{\partial x} + \Sigma_a(u)\Phi(x,u) = -\frac{\partial q_0^H}{\partial u} - \sum_i \frac{\partial q_{0i}^{NH}}{\partial u} + S_0(x,u) \qquad (8\text{-}236)$$

$$\frac{1}{3}\frac{\partial \Phi}{\partial x} + \Sigma_{tr}(u)J(x,u) = -\frac{\partial q_1^H}{\partial u} - \sum_i \frac{\partial q_{1i}^{NH}}{\partial u} + S_1(x,u)$$

$$\left.\begin{aligned}\frac{\partial q_0^H}{\partial u} + q_0^H(x,u) &= \Sigma_s^H \Phi(x,u)\\ \frac{2}{3}\frac{\partial q_1^H}{\partial u} + q_1^H(x,u) &= \frac{4}{9}\Sigma_s^H J(x,u)\end{aligned}\right\}\ \text{exact treatment of H} \qquad (8\text{-}237)$$

$$\left.\begin{aligned}\lambda_{0i}\frac{\partial q_{0i}^{NH}}{\partial u} + q_{0i}^{NH}(x,u) &= \beta_{0i}\Phi(x,u)\\ \lambda_{1i}\frac{\partial q_{1i}^{NH}}{\partial u} + q_{1i}^{NH}(x,u) &= \beta_{1i} J(x,u)\end{aligned}\right\}\ \text{approximate treatment of NA} \qquad (8\text{-}238)$$

where

(i) age approximation--Selengut-Goertzel

$$\lambda_{0i} = \lambda_{1i} = \beta_{1i} = 0$$
$$\beta_{0i} = \xi_i \Sigma_s^{(i)} \qquad (8\text{-}239)$$

(ii) consistent age approximation

$$\lambda_{0i} = \lambda_{1i} = 0$$
$$\beta_{0i} = \xi_i \Sigma_s^{(i)}, \quad \beta_{1i} = \xi_i \Sigma_s^{(i)} \qquad (8\text{-}240)$$

(iii) Grueling-Goertzel approximation (s-wave scattering)

$$\lambda_0^{(i)} = \frac{1-\alpha_i\left[1+\ln 1/\alpha_i + \tfrac{1}{2}\ln^2 1/\alpha_i\right]}{1-\alpha_i\left[1+\ln 1/\alpha_i\right]}$$
$$\lambda_1^{(i)} = \qquad (8\text{-}241)$$
$$\beta_{0i} = \xi_i \Sigma_s^{(i)}, \quad \beta_{1i} = \xi_i \Sigma_s^{(i)}$$

6.) Treatment of the Spatial Dependence in the P_1 Slowing Down Equations

Recall that we are going to use the solution of the P_1 slowing down equations to generate fast group constants. Hence we only need a crude method to account for leakage. In particular, we will assume that the lethargy and spatial dependence of the flux is separable

$$\Phi(x,u) = \phi(u)\,\varphi(x) \tag{8-242}$$

and furthermore characterize the spatial dependence by a simple buckling mode--i.e.,

$$\begin{aligned}&\Phi(x,u)=\phi(u)e^{iBx}, \quad q_0(x,u)=q_0(u)e^{iBx}, \quad S_0(x,u)=S_0(u)e^{iBx}\\ &J(x,u)=J(u)e^{iBx}, \quad q_1(x,u)=q_1(u)e^{iBx}, \quad S_1(x,u)=S_1(u)e^{iBx}\end{aligned} \tag{8-243}$$

[That is, we approximate the spatial dependence by a single Fourier mode.] Here, B will characterize the leakage in each region of the core in which the neutron spectrum $\phi(u)$ is to be calculated, and must be chosen from other considerations. For example, if we were considering a bare, homogeneous reactor we know that B would be determined by

$$\nabla^2\varphi(\vec{r}) + B^2\varphi(\vec{r}) = 0 \tag{8-244}$$

--that is, as the geometric buckling characterizing the core.

If we substitute these forms into the P_1 equations, we arrive at

$$\begin{aligned}&iBJ(u)+\Sigma_a(u)\phi(u) = -\frac{dq_0^H}{du} - \sum_i \frac{dq_{0i}^{NH}}{du} + S_0(u)\\ &\frac{iB}{3}\Phi(u)+\Sigma_{tr}(u)J(u) = -\frac{dq_1^H}{du} - \sum_i \frac{dq_{1i}^{NH}}{du} + S_1(u)\end{aligned} \tag{8-245}$$

augmented by the set

$$q_{0}^{H} + \frac{dq_{0}^{H}}{du} = \Sigma_s^{H} \Phi$$
$$q_{1}^{H} + \frac{2}{3}\frac{dq_{1}^{H}}{du} = \frac{4}{9} \Sigma_s^{H} J \tag{8-246}$$

and

$$q_{0i}^{NH} + \lambda_{0i} \frac{dq_{0i}^{NH}}{du} = \beta_{0i} \Phi$$
$$q_{1i}^{NH} + \lambda_{1i} \frac{dq_{1i}^{NH}}{du} = \beta_{1i} J \tag{8-247}$$

Hence we now have arrived at a set of simple, first order differential equations which we can integrate numerically. Before discussing how one solves such equations, there are two modifications we must make to include both fission and inelastic scattering.

7.) Fission Sources

We shall regard our source term as consisting of two parts due to fission and inelastic scattering, respectively:

$$S_0(x,u) = S_{\text{fission}}(x,u) + S_{\text{in}}(x,u) \tag{8-248}$$

Since we are only using these equations to generate few group constants, we can treat the fission source as a steady state external source with the fission spectrum as its energy dependence. This source is also considered to be isotropic. Hence

$$S_{0\,\text{fission}}(x,u) = \chi(u)\; e^{iBx}$$
$$S_{1\,\text{fission}}(x,u) \equiv 0 \tag{8-249}$$

8.) Inelastic Scattering

Thus far we have only considered slowing down via elastic scattering. Inelastic scattering is also a very important process. Unfortunately, however, its treatment is not amenable to the various approximations we have used to describe elastic scattering. Hence we must deal directly with the differential cross section for inelastic scattering (as obtained from some suitable nuclear data set). We will, however, assume that such scattering is isotropic in the LAB system such that

$$S_{0_{in}}(x,u) = e^{iBx}\sum_{i}\int_0^u du'\,\Sigma_{in}^{(i)}(u'\to u)\,\Phi(u') \qquad (8\text{-}250)$$

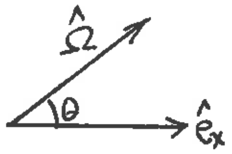
$$S_{1in}(x,u) \equiv 0$$

9.) An Alternative Treatment of Spatial Dependence--The B_1 Method

Thus far we have considered approximating the spatial dependence of the solutions to the P_1 slowing down equations by a single mode of the form exp(iBx). There is an alternative scheme which bypasses the P_1 equations entirely, and for completeness we will sketch its derivation here. To do so, we must return to the steady-state transport equation, written in its one-dimensional form as

$$\mu\frac{\partial\phi}{\partial x} + \Sigma_t(u)\,\phi(x,\mu,x) = \int_{-1}^{+1}d\mu'\int_0^{\infty}du'\,\Sigma_s(u'\to u,\mu'\to\mu)\,\phi(x,\mu',u') + S(x,\mu,u) \qquad (8\text{-}251)$$

Here, $\mu = \hat{\Omega}\cdot\hat{e}_x = \cos\theta$ has been chosen as a more convenient angular variable. Note $\theta \in [0,\pi] \Rightarrow \mu \in [-1,+1]$.



Now assume an angular flux and source spatial dependence of the form

$$\phi(x,\mu,u) = \varphi(\mu,u)\,e^{iBx} \qquad (8\text{-}252)$$

$$S(x,\mu,u) = \frac{S(u)}{2}\,e^{iBx}$$

[Note we have assumed an isotropic source, consistent with our earlier assumptions concerning fission and inelastic scattering.] Then we find

$$\left(\Sigma_t(u) - iB\mu\right)\varphi = \int_{-1}^{+1} d\mu' \int_0^{\infty} du'\,\Sigma_s(u'\to u, \mu'\to\mu)\,\varphi(\mu',u) + \frac{S(u)}{2} \qquad (8\text{-}253)$$

At this point, if we multiplied by 1 or μ and integrated over μ and then expanded $\varphi = \frac{1}{2}\Phi(u) + \frac{3}{2}\mu J(u)$, we would rederive the P_1 equations. Instead, suppose we first divide by $(\Sigma_t - iB\mu)$, and <u>then</u> perform this sequence of steps. That is, write

$$\varphi(\mu,u) = \frac{1}{\Sigma_t - iB\mu} \int_{-1}^{+1} d\mu' \int_0^{\infty} du'\,\Sigma_s(u'\to u, \mu'\to\mu)\left[\tfrac{1}{2}\Phi(u) + \tfrac{3}{2}J(u)\mu\right] \qquad (8\text{-}254)$$

$$+ \frac{S(u)}{2(\Sigma_t - iB\mu)}$$

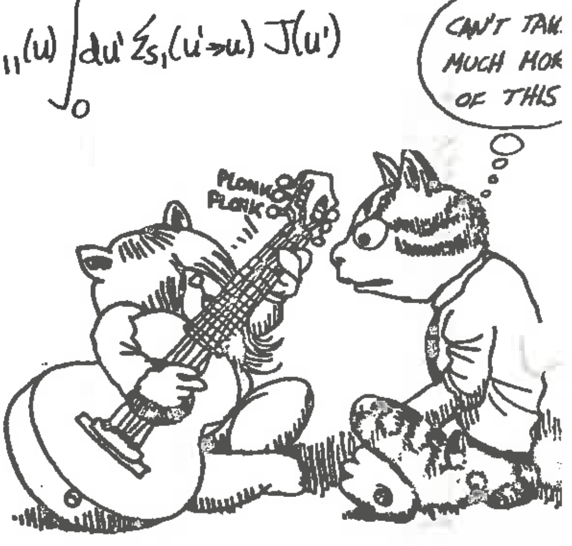
Now integrating over μ yields

$$\Sigma_t(u)\Phi(u) = A_{00}(u)\int_0^u du'\,\Sigma_{s0}(u'\to u)\,\Phi(u') + A_{01}(u)\int_0^u du'\,\Sigma_{s1}(u'\to u)\,J(u') + A_{00}(u)\,S($$

$$(8\text{-}255)$$

$$\Sigma_t(u)J(u) = A_{10}(u)\int_0^u du'\,\Sigma_{s0}(u'\to u)\,\Phi(u') + A_{11}(u)\int_0^u du'\,\Sigma_{s1}(u'\to u)\,J(u')$$

where



$$A_{ij}(u) \equiv \frac{1}{2}\int_{-1}^{+1} d\mu \, \frac{P_i(u)\,P_j(u)}{1 - \frac{iB\mu}{\Sigma_t(u)}}$$

$$P_0(u) = 1$$
$$P_1(u) = \mu \qquad (8\text{-}256)$$

$$A_{00}(u) = \frac{\tanh^{-1}\left(\frac{iB}{\Sigma_t}\right)}{\left(\frac{iB}{\Sigma_t}\right)}$$

After some rearranging, one can rewrite these equations as

$$\Sigma_a(u)\,\Phi + iBJ = \int_0^u du' \,\Sigma_{s0}(u' \to u)\,\Phi(u') + \frac{S_0(u)}{2} \qquad (8\text{-}257)$$

$$\gamma(u)\,\Sigma_{tr}(u)\,J + \frac{1}{3}iB\Phi = \int_0^u du' \,\Sigma_{s1}(u' \to u)\,J(u')$$

where

$$\gamma(u) = \frac{\left(\frac{B}{\Sigma_t}\right)^2 \tan^{-1}\left(\frac{B}{\Sigma_t}\right)}{3\left[\frac{B}{\Sigma_t} - \tan^{-1}\left(\frac{B}{\Sigma_t}\right)\right]} \cong 1 + \frac{4}{15}\left(\frac{B}{\Sigma_t}\right)$$

Upon rewriting the scattering integrals in terms of slowing down densities, one can recognize that the B_1 equations above are very similar to the P_1 equations (8-245), except for the appearance of the factor γ. For bare slab geometries, the B_1 equations are found to yield more accurate spectra. However, for more complicated geometries, both methods yield very similar results, and one customarily relies upon the P_1 equations in practice.

IV. FAST SPECTRUM CALCULATIONS AND FAST GROUP CONSTANTS

We now turn our attention towards the application of the P_1 and B_1 equations to the calculation of fast neutron spectra suitable for the generation of fast group constants to be used in few-group diffusion codes. We will actually examine three different schemes. The first such scheme will be the numerical solution of the P_1 (or B_1) equations characterizing neutron slowing down in hydrogeneous systems. This scheme is commonly known as the MUFT technique, and for many years has been the mainstay of light water reactor calculations. We will next consider the calculation of fast reactor spectra in which inelastic scattering is of primary importance and for which a direct solution of the P_1 equations is required. Then finally for completeness (and historical sentiment), we will briefly develop the analytical age-diffusion model (although such a model has very little relevance to modern day reactor calculations).

A. The MUFT Technique

We will consider the P_1 equations applied to describe neutron slowing down in a mixture of hydrogen plus a single heavy isotope, A. To be specific, we will utilize the age approximation to describe slowing down from this heavy isotope (and an exact treatment of hydrogen), although the procedure we develop applies equally well to the other approximate schemes we have discussed (e.g., Goertzel-Grueling method).

Hence the P_1 equations we will consider can be written as

$$\underset{①}{iBJ} + \left[\underset{②}{\Sigma_a^S} + \underset{③}{\Sigma_a^R} + \underset{④}{\Sigma_{in}}\right]\Phi = \underset{⑤}{\chi(u)} + \underset{⑥}{\int_0^u du' \, \Sigma_{in}^A(u' \to u)\,\Phi(u')} \underset{⑦}{- \frac{dq_{b0}^H}{du}} \underset{⑧}{- \frac{dq_{b0}^A}{du}}$$

$$\underset{⑨}{\frac{iB}{3}\Phi} + \underset{⑩}{\Sigma_{tr} J(u)} = \underset{⑪}{-\frac{dq_{b1}^H}{du}}$$

$$\underset{⑫}{q_{b0}^H} + \underset{⑬}{\frac{dq_{b0}^H}{du}} = \underset{⑭}{\Sigma_s^H \Phi} \tag{8-258}$$

$$\underset{⑮}{q_{b1}^H} + \underset{⑯}{\frac{2}{3}\frac{dq_{b1}^H}{du}} = \underset{⑰}{\frac{4}{9}\Sigma_s^H J}$$

$$\underset{⑱}{q_{b0}^A} = \underset{⑲}{\xi_A \Sigma_s^A} \Phi$$

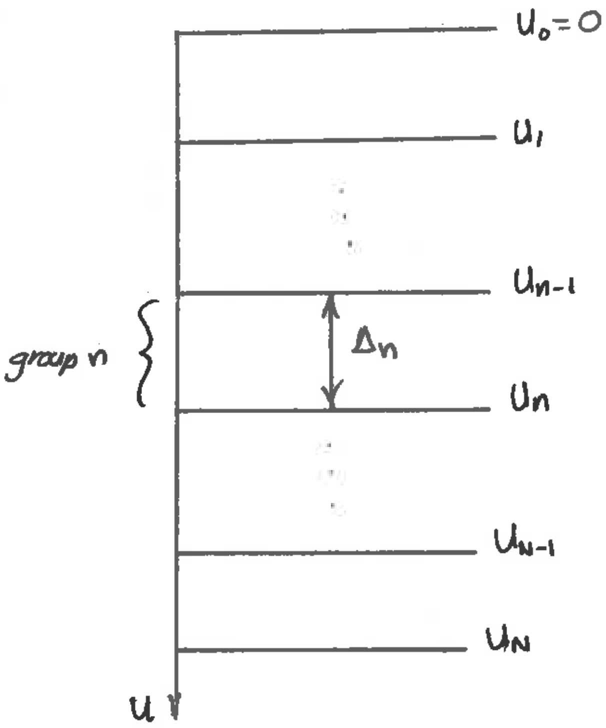
Here we have found it convenient to separate the removal cross section into three parts

Σ_a^S = "smooth" absorption cross section

Σ_a^R = "resonance" absorption cross section (8-259)

$\Sigma_{in} = \int_0^\infty du' \, \Sigma_{in}^A(u \to u') \equiv$ inelastic scattering cross section

To solve these equations, we will now discretize them into multigroup form by performing simple averages over lethargy intervals. [In MUFT type codes, one usually utilizes 54 lethargy groups.] First define the group structure as shown



Now integrate the P_1 equations over a typical group n. Considering each of the terms in these equations:

① [also ⑨]

$$\int_{U_{n-1}}^{U_n} iBJ(u)du = iB\int_{U_{n-1}}^{U_n} J(u)du = iBJ^n\Delta_n \tag{8-260}$$

where $$J^n \equiv \frac{1}{\Delta_n}\int_{U_{n-1}}^{U_n} J(u)du$$

② [also ④, ⑩, ⑭, ⑰, ⑲]

$$\int_{u_{n-1}}^{u_n} \Sigma_a^s(u)\,\Phi(u)\,du = \Sigma_a^{sn}\,\Phi^n\,\Delta_n$$

$$\text{where} \quad \Sigma_a^{sn} \equiv \frac{\int_{u_{n-1}}^{u_n} \Sigma_a^s(u)\,\Phi(u)\,du}{\int_{u_{n-1}}^{u_n} \Phi(u)\,du} \cong \frac{1}{\Delta_n}\int_{u_{n-1}}^{u_n} \Sigma_a^s(u)\,du \tag{8-261}$$

Note that to compute these "fine group constants", we are merely performing an average of the cross section over the lethargy group

⑤

$$\int_{u_{n-1}}^{u_n} \chi(u)\,du = \chi^n\,\Delta_n \quad \text{where} \quad \chi^n \equiv \frac{1}{\Delta_n}\int_{u_{n-1}}^{u_n} \chi(u)\,du \tag{8-262}$$

⑫ [also ⑮, ⑱]

$$\int_{u_{n-1}}^{u_n} q_0^H(u)\,du \cong \left[\frac{q_0^{H^n} + q_0^{H^{n-1}}}{2}\right]\Delta_n \tag{8-263}$$

$$\text{where} \quad q^{H^n} = q_0^H(u_n) \,, \quad q_0^{H^{n-1}} = q_0^H(u_{n-1})$$

⑦ [also ⑧, ⑪, ⑬, ⑯]

$$\int_{u_{n-1}}^{u_n} \frac{dq_0^H}{du}\,du = q_0^H(u_n) - q_0^H(u_{n-1}) = q_0^{H^n} - q_0^{H^{n-1}} \tag{8-264}$$

③

$$\int_{u_{n-1}}^{u_n} \Sigma_a^R(u)\,\Phi(u)\,du$$

= Resonance absorption rate for group n

$$= (1-P_n)\left[q_{bo}^{H^{n-1}} + q_{bo}^{A^{n-1}}\right] \qquad (8\text{-}265)$$

where P_n = resonance escape probability for group n

⑥

$$\int_{u_{n-1}}^{u_n} du \int_0^{u} du'\, \Sigma_{in}^A(u'\to u)\,\Phi(u') = \sum_{j=1}^{N} \underbrace{\int_{u_{n-1}}^{u_n} du \int_{u_{j-1}}^{u_j} du'\, \Sigma_{in}^A(u'\to u)\,\Phi(u')}_{\Sigma_{jn}^A\,\Phi^j\,\Delta_j\Delta_n} \qquad (8\text{-}266)$$

where

$$\Sigma_{jn}^A \equiv \frac{\displaystyle\int_{u_{n-1}}^{u_n} du \int_{u_{j-1}}^{u_j} du'\, \Sigma_{in}^A(u'\to u)\,\Phi(u)}{\displaystyle\int_{u_{n-1}}^{u_n} du \int_{u_{j-1}}^{u_j} du'\, \Phi(u')} \cong \frac{\displaystyle\int_{u_{n-1}}^{u_n} du \int_{u_{j-1}}^{u_j} du'\, \Sigma_{in}^A(u'\to u)}{\Delta_n\Delta_j} \qquad (8\text{-}267)$$

Notice that since there is no upscattering, i.e.,

$$\Sigma_{in}^A(u'\to u) = 0 \quad \text{if} \quad u' > u \qquad (8\text{-}268)$$

we have

$$\Sigma_{jn}^A = 0 \quad \text{if} \quad n \leq j$$

--that is, the inelastic scattering matrix is lower triangular

$$\underline{\underline{\Sigma}}^A = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ \Sigma_{12}^A & 0 & 0 & \cdots \\ \Sigma_{13}^A & \Sigma_{23}^A & 0 & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{8-269}$$

Thus

$$\int_{u_{n-1}}^{u_n} du \int_0^u du'\, \Sigma_{in}^A(u' \to u)\, \Phi(u') = \Delta_n \sum_{j=1}^{n-1} \Sigma_{jn}^A\, \Phi^j \Delta_j \tag{8-270}$$

If we now substitute all of these terms back into the P_1 equations, we find

$$iBJ^n \Delta_n + \Sigma_a^{s^n} \Phi^n \Delta_n + \Sigma_{in}^n \Phi^n + (1-P_n)\left[q_0^{H^{n-1}} + q_0^{A^{n-1}}\right]$$
$$= \chi^n \Delta_n + \Delta_n \sum_{j=1}^{n-1} \Sigma_{jn}^A \Phi^j \Delta_j - \left(q_0^{H^n} - q_0^{H^{n-1}}\right) - \left(q_0^{A^n} - q_0^{A^{n-1}}\right)$$

$$\frac{iB}{3} \Phi^n \Delta_n + \Sigma_{tr}^n J^n \Delta_n = -\left(q_1^{H^n} - q_1^{H^{n-1}}\right)$$

$$\left[\frac{q_0^{H^n} + q_0^{H^{n-1}}}{2}\right]\Delta_n + \left(q_0^{H^n} - q_0^{H^{n-1}}\right) = \Sigma_s^{H^n} \Phi^n \Delta_n$$

(8-271)

$$\left[\frac{q_1^{H^n} + q_1^{H^{n-1}}}{2}\right]\Delta_n + \frac{2}{3}\left(q_1^{H^n} - q_1^{H^{n-1}}\right) = \frac{4}{9} \Sigma_s^{H^n} J^n \Delta_n$$

$$\left[\frac{q_0^{A^n} + q_0^{A^{n-1}}}{2}\right]\Delta_n = \left(\xi_{SA} \Sigma_s^A\right)^n \Phi^n \Delta_n$$

These are now a set of 5N algebraic equations for $J^n, \Phi^n, q_{b0}^{H^n}, q_{b1}^{H^n}, q_{b0}^{A^n}$. Since $q_{b0}^{H^0} = q_{b1}^{H^0} = q_{b0}^{A^0} = 0$, we can easily solve for J^0 and Φ^0 and then continue on to obtain $J^1, \Phi^1, q_{b0}^{H^1}, q_{b1}^{H^1}, q_{b0}^{A^1}$, and so on, solving succesively for the variables characterizing higher and higher lethargy groups.

Once we have obtained Φ^n, we can then use it to generate few group constants. For example, if we utilized a 54 group MUFT calculation to generate one-fast-group constants, we would find

$$\Sigma_{a_1} = \frac{\int_0^{u_{thermal}} \Sigma_a(u)\Phi(u)du}{\int_0^{u_{thermal}} \Phi(u)du} = \frac{\sum_{n=1}^{54} \Sigma_a^n \Phi^n \Delta_n}{\sum_{n=1}^{54} \Phi^n \Delta_n}$$

or (8-272)

$$D_1 = \frac{\sum_{n=1}^{54} \frac{1}{3\Sigma_{tr}^n} \Phi^n \Delta_n}{\sum_{n=1}^{54} \Phi^n \Delta_n}$$

Sometimes an alternative scheme is used to calculate the group diffusion coefficients. This procedure comes from requiring that D_g be defined such that for a group of lethargy width Δu

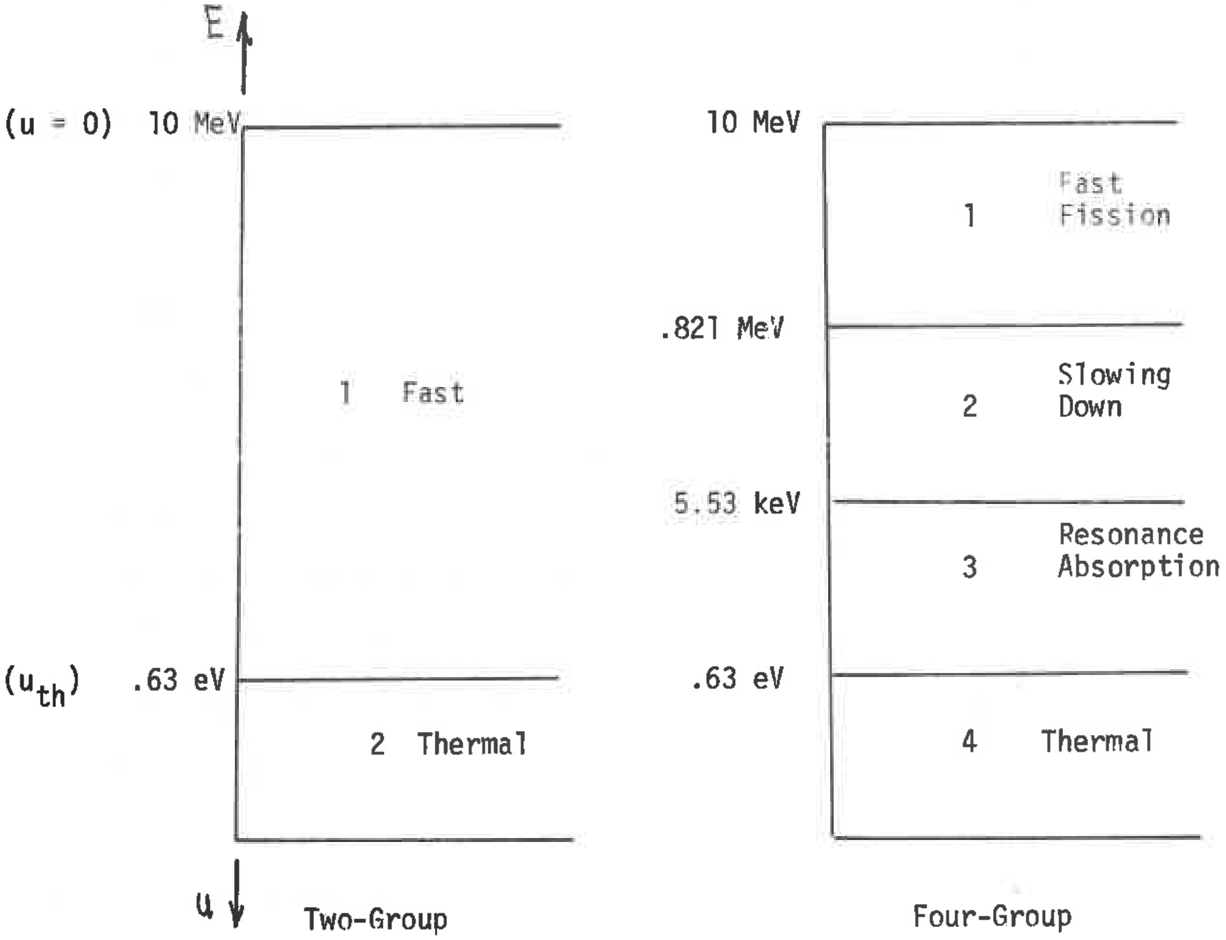
$$\int_{\Delta u_g} du\, J(x,u) = -D_g \frac{d}{dx} \int_{\Delta u_g} du\, \Phi(x,u) \qquad (8\text{-}273)$$

If we use our single buckling mode forms for J(x,u) and $\Phi(x,u)$, we find that D_g is then defined by

$$D_g = \frac{1}{iB} \frac{\int_{\Delta u_g} du\, J(u)}{\int_{\Delta u_g} du\, \Phi(u)} \tag{8-274}$$

In summary then, MUFT is a scheme which will generate a fast neutron spectrum and calculate few group constants by using the P_1 (or B_1) slowing down equations, approximating the spatial dependence by a single spatial mode characterized by an "equivalent bare core buckling" B^2, treating elastic scattering by a continuous slowing down model (an exact treatment for hydrogen and either the age approximation or the Goertzel-Greuling model for materials with mass number $A > 1$), and handling inelastic scattering using a multigroup transfer matrix. We have not dwelt in detail on the treatment of resonance absorption, because a typical MUFT type of calculation will correct the infinite medium resonance escape probabilities we considered earlier for fuel lumping (heterogeneous) effects. We will return to discuss this in some detail in Chapter 11.

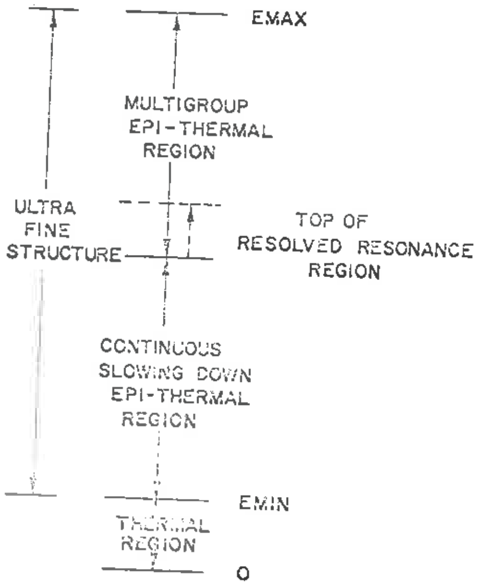
Most typically the MUFT scheme is used to generate either 1-group or 3-group constants for light water reactor calculations with the group structure as shown (we have also indicated the thermal group which must be handled by methods to be discussed in the next chapter).



B. The Generation Of Fast Group Constants For Fast Reactor Calculations

The generation of few group constants for fast reactor applications involves much more in the way of brute force techniques than comparable thermal reactor calculations. To a large degree this is because of the relatively limited experience in fast reactor design and hence the desire for as accurate a calculation as possible. It also arises, however, because of the increased complexity of the array of nuclear process which influence a fast reactor spectrum--particularly resonance absorption and inelastic scattering. In a thermal reactor, the strong elastic scattering present in the system and the fact that most fissions are induced by thermal neutrons will tend to wash out many of these details. However in a fast reactor, essentially all fissions are induced by neutrons with energies in just those ranges in which inelastic scattering and resonance absorption are most important.

At the present time, the most general code for generating few group constants for fast reactor calculations is the MC^2 code and its variants. This code begins with evaluated cross section data (ENDF/B), and proceeds to perform a sequence of group averages, from ultra fine groups with $\Delta u \sim 1/120$, to fine groups with $\Delta u \sim 1/4$, and finally to broad groups with $\Delta u \sim 1/2$ to 1. In the more advanced versions of this code, a direct multigroup spectrum calculation is performed at higher energies, whereas a continuous slowing down calculation is used to handle elastic scattering at lower energies. This is shown schematically below:



Schematic Diagram of the MC^2-2 Energy Structure.

Notice that the form of this equation is very similar to that of the time-dependent diffusion equation. For this reason, τ is known as

$$\tau(u) \equiv \text{“Fermi age”} \tag{8-282}$$

even though its units are [cm^2] rather than [sec].

By noting the similarity between the age equation (8-151) and the time-dependent diffusion equation, we can adapt all our earlier analysis to solve this equation. We won't do this here, however, because age theory is primarily of historical interest and is only of limited utility in present day reactor design.

2.) Nonzero Absorption, $\Sigma_a \neq 0$

Now the age equation becomes

$$\frac{D(u)}{\xi\Sigma_s(u)}\nabla^2 q_a - \frac{\Sigma_a(u)}{\xi\Sigma_s(u)} q_a(\vec{r},u) = \frac{\partial q_a}{\partial u} \tag{8-283}$$

where the subscript "a" has been affixed to denote that absorption is included in this calculation of q. Now to solve this, let

$$\begin{aligned} q_a(\vec{r},u) &= q(\vec{r},u)\exp\left[-\int_0^u \frac{\Sigma_a(u')}{\xi\Sigma_s(u')}du'\right] \\ &= q(\vec{r},u)\ p(u) \end{aligned} \tag{8-284}$$

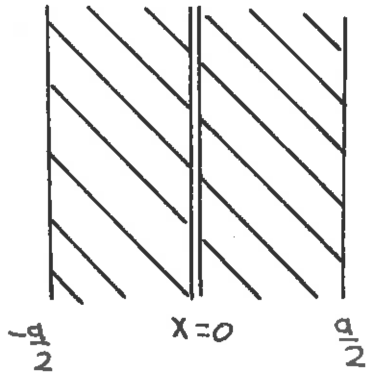
We then find that q(r,u) satisfies

$$\frac{D(u)}{\xi\Sigma_s(u)}\nabla^2 q = \frac{\partial q}{\partial u} \tag{8-285}$$

--which is identical to our equation without absorption. Hence, to handle the case in which absorption is present, we need only multiply the solution $q(\underline{r},u)$ for zero absorption by the resonance escape probability to lethargy u, p(u),

$$p(u) = \exp\left[-\int_0^u du' \frac{\Sigma_a(u')}{\xi\Sigma_s(u')}\right] \tag{8-286}$$

3.) An Example



Consider an infinite planar source emitting neutrons of energy E_0 at the center of a non-absorbing slab of width a (as we have seen, absorption can be easily included). We will define the lethargy variable with respect to the source energy E_0, such that u = 0 corresponds to the source energy. If we also note

$$\tau(u) = \int_0^u \frac{D(u)}{\xi\Sigma_s(u)} du = \int_E^{E_0} \frac{D(E)\,dE}{\xi\Sigma_s(E)E} \tag{8-287}$$

then we can write the appropriate form of the age equation as

$$\frac{\partial^2 q}{\partial x^2} = \frac{\partial q}{\partial \tau} \tag{8-288}$$

subject to: initial condition: $q(x,0) = S\delta(x)$

boundary conditions: $q(-\frac{a}{2},\tau) = 0 = q(\frac{a}{2},\tau)$

To solve this, we will try an eigenfunction expansion

$$q(x,\tau) = \sum_n f_n(\tau)\cos B_n x, \quad B_n = \frac{n\pi}{a} \tag{8-289}$$

If we substitute this into the age equation

$$-\sum_n B_n^2 f_n(\tau)\cos B_n x = \sum_n \frac{df_n}{d\tau}\cos B_n x \tag{8-290}$$

Now using orthogonality, we find

$$\frac{df_n}{d\tau} = -B_n^2 f_n(\tau) \tag{8-291}$$

or

$$f_n(\tau) = A_n e^{-B_n^2\tau} \tag{8-292}$$

Hence the general solution is

$$q(x,\tau) = \sum_n A_n e^{-B_n^2\tau}\cos B_n x \tag{8-293}$$

Now using the initial condition at $\tau = 0$

$$q(x,0) = \sum_n A_n \cos B_n x = S\delta(x) \tag{8-294}$$

Multiplying by cos $B_m x$ and integrating

$$S\underbrace{\int_{-\tilde{a}/2}^{\tilde{a}/2} dx \cos B_m x\, \delta(x)}_{1} = \sum_n A_n \underbrace{\int_{-\tilde{a}/2}^{\tilde{a}/2} dx \cos B_m x \cos B_n x}_{\frac{\tilde{a}}{2}\delta_{mn}}$$

Hence

$$A_n = \frac{2S}{\tilde{a}} \tag{8-295}$$

and our solution is

$$q(x,\tau) = \frac{2S}{\tilde{a}} \sum_n e^{-B_n^2 \tau} \cos B_n x \tag{8-296}$$

Now far below the source energy--i.e., large τ, we find only the fundamental mode is significant

$$q(x,\tau) \sim \frac{2S}{\tilde{a}} e^{-B_g^2 \tau} \cos B_g x, \qquad B_g = B_1 \tag{8-297}$$

Now notice something interesting: The total number of neutrons/sec slowing down to age τ is

$$\int_{-\tilde{a}/2}^{\tilde{a}/2} dx\, q(x,\tau) = \frac{2S}{\tilde{a}} e^{-B_g^2 \tau} \int_{-\tilde{a}/2}^{\tilde{a}/2} dx \cos B_g x = S e^{-B_g^2 \tau} \tag{8-298}$$

Hence the probability of slowing down to age τ (or the corresponding energy E) withoug leaking out of the slab is just

$$\frac{Se^{-B_g^2\tau}}{S} = e^{-B_g^2\tau} \tag{8-299}$$

This leads us to identify the fast non-leakage probability introduced earlier (Chapter III) in the "6-factor formula" for k as

$$P_{NFL} = e^{-B_g^2\tau_{th}} \tag{8-300}$$

where τ_{th} is the age corresponding to thermal energies (usually taken as .025 eV):

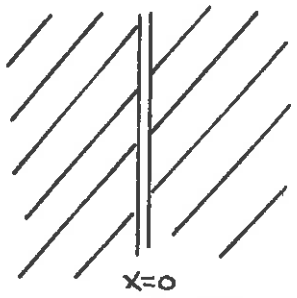
$$\tau_{th} = \int_{E_{th}}^{E_0} \frac{D(E)\,dE}{\xi\Sigma_s(E)E} \tag{8-301}$$

Of course this expression for P_{FNL} is valid only in the age approximation.

A couple of other simple examples are enlightening:

Example: Plane source in an infinite medium

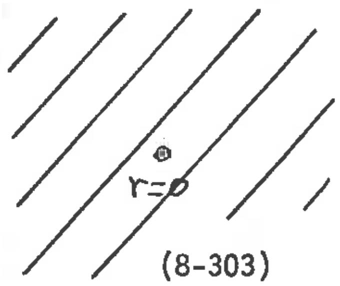
$$q_{pl}(x,\tau) = S\frac{e^{-x^2/4\tau}}{\sqrt{4\pi\tau}}$$



(8-302)

Example: Point source in an infinite medium

$$q_{pt}(r,\tau) = S\frac{e^{-r^2/4\tau}}{(4\pi\tau)^{3/2}}$$



(8-303)

The continuous slowing down calculation uses an improved Goertzel-Grueling approximation, similar to that we discussed in the previous section. Spatial dependence is handled in either the P_1 or B_1 approximation with again a single spatial mode characterizing leakage with an effective buckling B^2. A number of rather sophisticated techniques are used to handle resonance absorption--particularly for the overlapping or unresolved resonance regions (the isolated resonances are most typically handled by the narrow resonance (NR) approximation).

As we have mentioned, codes such as MC^2 are much too elaborate for day to day use in reactor design, and are intended more for the evaluation of calculational techniques and comparison with critical experiments. As more experience is acquired in the design of cores for commercial fast reactors, less elaborate (although sufficiently accurate) techniques will evolve in a manner similar to the MUFT scheme used in light water reactor design.

C. Age-Diffusion Theory

For historical completeness, let us return to consider the age-diffusion equation

$$-D(u)\nabla^2\Phi(\vec{r},u)+\Sigma_a(u)\Phi(\vec{r},u)=-\frac{\partial q}{\partial u}+S(\vec{r},u) \qquad (8\text{-}275)$$

where

$$q(\vec{r},u)\cong\xi\Sigma_s(u)\Phi(\vec{r},u) \qquad (8\text{-}276)$$

Now we know that this equation is only valid for neutron slowing down in moderators with reasonably large mass numbers (such as graphite, for example). Nevertheless, age-diffusion theory has been thoroughly studied in the past because one can frequently obtain an explicit solution of this equation in certain cases:

1.) Zero Absorption, $\Sigma_a \equiv 0$

If we assume that the source term is zero, the age-diffusion equation becomes

$$-D(u)\nabla^2\Phi = -\frac{\partial q}{\partial u} \tag{8-277}$$

But using Eq. (8-276), we find

$$\frac{D(u)}{\xi\Sigma_s(u)}\nabla^2 q(\vec{r},u) = \frac{\partial q}{\partial u} \tag{8-278}$$

To solve this equation, we first make a change of independent variable by defining

$$\tau(u) \equiv \int_0^u du' \frac{D(u')}{\xi\Sigma_s(u')} \tag{8-279}$$

and note

$$\frac{\partial}{\partial u} = \frac{\partial\tau}{\partial u}\frac{\partial}{\partial\tau} = \frac{D(u)}{\xi\Sigma_s(u)}\frac{\partial}{\partial\tau} \tag{8-280}$$

Hence we can rewrite Eq. (8-148) as

$$\nabla^2 q(\vec{r},\tau) = \frac{\partial q}{\partial\tau} \tag{8-281}$$

One can use this last result to demonstrate that

$\tau = \frac{1}{6}\langle r^2 \rangle$ = 1/6 the average (crow-flight distance)^2 from the point where a neutron enters a system with E_0 to the point at which it slows down to an age

(8-304)

One usually calculates or measures the age-to-thermal energies, τ_{th} or more commonly, the age to the indium resonance at 1.45 eV, τ_{IN} (since this is the most common measurement)

Moderator	H_2O	D_2O	Be	BeO	Graphite
τ_{IN}	26	111	85	80	311 cm^2

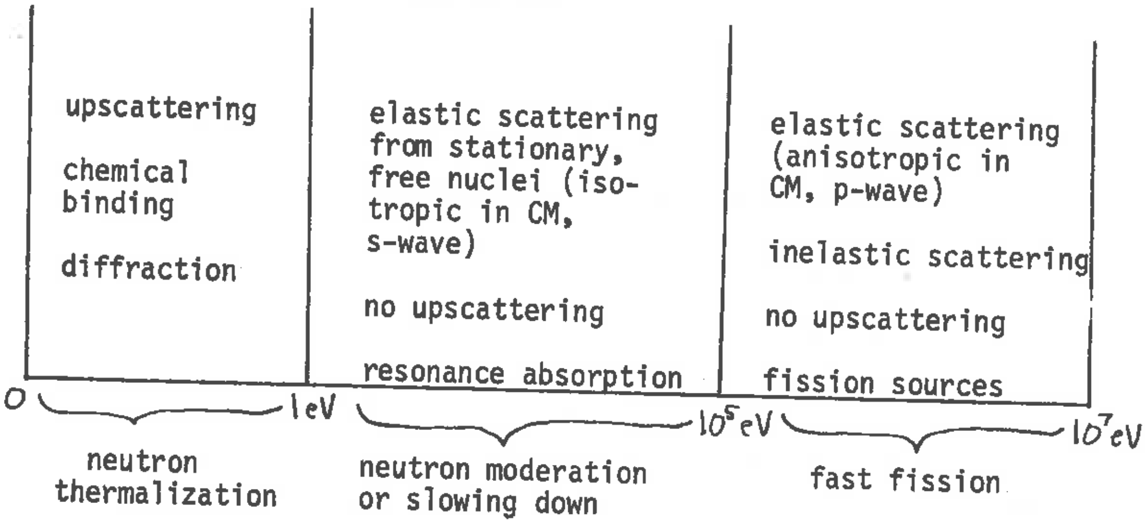
"We're getting busted every day and I can't shake the nagging suspicion that we've been infiltrated."

CHAPTER 9: THERMAL SPECTRA AND THERMAL GROUP CONSTANTS

I. INTRODUCTION

A. Neutron Thermalization

It is customary to divide the range of neutron energies into three different regions, each characterized by different types of neutron interactions as shown below:



We shall direct our attention towards the lowest of these energy ranges, that corresponding to neutron thermalization which characterizes neutron energies between 0 and 1 eV. The terminology of "neutron thermalization" actually refers to two separate problems:

(i) the calculation of the cross sections for thermal neutrons;

(ii) the use of these cross sections to determine the energy spectrum characterizing such low energy neutrons (e.g., for use in determining thermal group constants for few-group diffusion calculations).

These subjects are actually quite interrelated since those features characteristic of thermal neutron cross sections actually have a rather significant influence on thermal spectra.

There are essentially three features which are characteristic of cross sections for thermal neutrons. First, since the energy of thermal neutrons is comparable to the thermal energy of the scattering nuclei ($kT \sim 0.05$ eV), we can no longer neglect thermal motions of the nuclei by assuming them to be stationary (as one does in neutron slowing down theory). In fact, it will now be possible for neutrons to gain energy (i.e., upscatter) in a collision with these moving nuclei. Of similar importance is the fact that the energy of thermal neutrons is comparable to the chemical binding energy of the scattering nuclei (e.g., in a molecule or a crystal lattice). Hence the nucleus will no longer recoil freely, and thus binding will become significant in determining the energy and angle change of a neutron in a collision. The final characteristic of thermal neutron scattering involves coherent interference effects. For low energies, the neutron wavelength,

$$\lambda = 2.86 \times 10^{-9} \quad E^{-\frac{1}{2}} \quad \text{cm} \tag{9-1}$$

is comparable to the interatomic spacing of the scattering material. Hence the neutron wave function experiences diffraction effects (just as light is diffracted). Such interference effects can be quite important in determining the neutron scattering cross section for the material.

Needless to say, such considerations greatly complicate the calculation of thermal neutron spectra. The subject of thermal neutron cross sections is an extraordinarily complex one, being essentially a subfield of statistical mechanics and solid state physics. Since the measurement and calculation of such cross sections can infer information about the microscopic structure and dynamics of materials, thermal neutron scattering has received a voluminous treatment in the scientific literature, and we will not attempt to duplicate that treatment in this text.

Fortunately, most of the complicated details of thermal neutron cross section behavior are of little concern in nuclear reactor analysis. This is particularly true in light water reactor calculations in which the moderator can frequently be modeled as a simple gas of protons (totally ignoring binding and diffraction effects). For other types of thermal reactors, such as the high temperature gas cooled reactor in which graphite is the moderator, somewhat more sophisticated models are used. However in all cases, the models of thermal neutron cross sections utilized in practical reactor design are very crude indeed compared to the sophisticated theories and measurements which exist for the interpretation of thermal neutron scattering data.

Hence our concern in this chapter will be to first illustrate some of the simple ideas involved in neutron thermalization, and then to develop those tools which form the bases for thermal spectra calculations and which are used to generate thermal group constants.

B. Equilibrium Neutron Spectra

We will begin by pointing out some interesting consequences of thermal neutron cross section behavior. Suppose we consider once again the infinite medium "slowing down equation", although we will now extend the range of integration down to $E = 0$ in order to include the thermal range.

$$\left[\Sigma_a(E)+\Sigma_s(E)\right]\Phi(E) = \int_0^\infty dE'\,\Sigma_s(E'\to E)\,\Phi(E') + S(E) \tag{9-2}$$

Now the differential scattering cross section can be shown to possess a very interesting and general property:

$$v'\Sigma_s(E'\to E)\,M(E') = v\,\Sigma_s(E'\to E)\,M(E) \tag{9-3}$$

where M(E) is the Maxwell-Boltzmann distribution

$$M(E) = \frac{2\pi n}{(\pi kT)^{3/2}}\,E^{1/2}\,e^{-E/kT} \tag{9-4}$$

This is known as the <u>principle of detailed balance</u>, and it must be obeyed by any neutron cross section characterizing neutron scattering from a system of nuclei in thermal equilibrium at a temperature T (regardless of their structure or detailed dynamics). This property is essentially a consequence of the laws of statistical mechanics characterizing the scattering material. It implies an extremely important consequence for the neutron energy spectrum in a reactor.

Let's consider the special case in which we set the absorption and source terms equal to zero. Then Eq. (9-2) becomes

$$\Sigma_s(E)\,\Phi(E) = \int_0^\infty dE'\,\Sigma_s(E'\to E)\,\Phi(E') \tag{9-5}$$

We now claim that the solution to this equation, regardless of the detailed form of the scattering cross section, is just a Maxwellian flux:

$$\Phi(E) = v\,M(E) \equiv \Phi_M(E) \tag{9-6}$$

This result is a consequence of the principal of detailed balance, for if we substitute in Eq. (9-6) into Eq. (9-5), we find

$$\begin{aligned}\Sigma_s(E)\,\Phi_M(E) &= \int_0^\infty dE'\,\Sigma_s(E'\to E)\,v'\,M(E') \\ &= \int_0^\infty dE'\,\Sigma_s(E\to E')\,v\,M(E) = \Sigma_s(E)\,\Phi_M(E)\end{aligned} \tag{9-7}$$

Hence the principle of detailed balance insures that the equilibrium spectrum of the neutrons (in the absence of absorption, sources, leakage, etc.) will be a "Maxwellian" characterized by the moderator temperature T

$$\Phi_M(E) = \frac{2\pi n}{(\pi kT)^{3/2}}\sqrt{\frac{2}{m}}\,E\,e^{-E/kT} \tag{9-8}$$

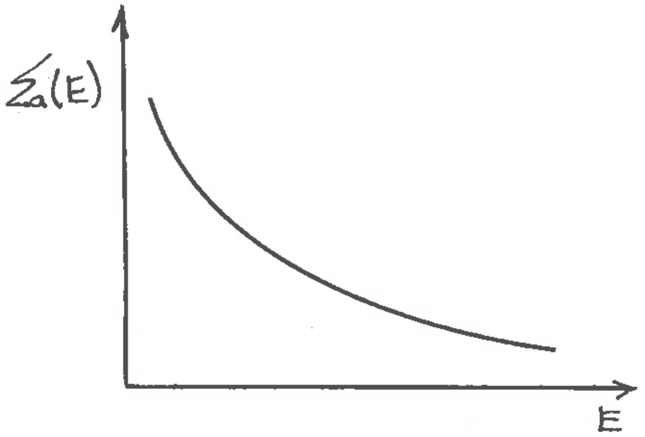
--that is, that the neutrons will eventually come into thermal equilibrium with the moderator nuclei. In particular, we can find that the most probable neutron energy and speed for such a distribution are

$$\begin{aligned}&\text{most probable energy} = E_T = kT = 8.6\times10^{-5}\,T \quad (\text{eV}) \\ &\text{most probable speed} = v_T = \sqrt{\frac{2kT}{m}} = 1.28\times10^{4}\sqrt{T} \quad (\text{cm/sec})\end{aligned} \tag{9-9}$$

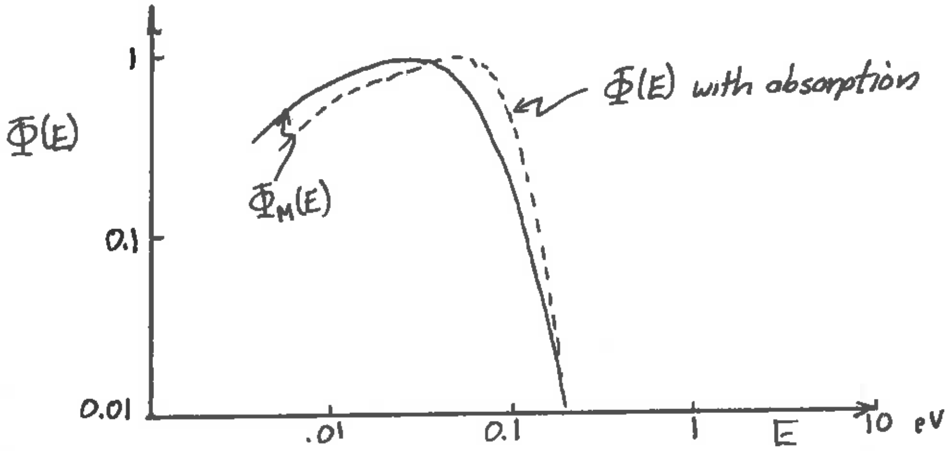
C. Nonequilibrium Thermal Spectra

Now detailed balance only guarantees that in the absence of any nonequilibrium perturbation, the neutrons will tend to come into thermal equilibrium with the moderator. Any perturbation such as absorption or sources or leakage will tend to distort this spectrum away from its equilibrium shape.

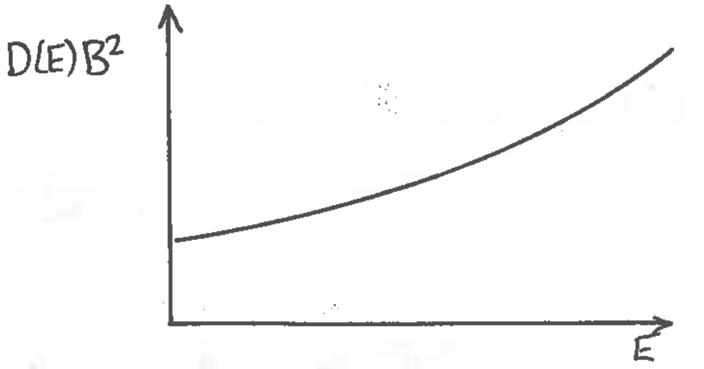
Consider, for example, the addition of an absorption term to Eq. (9-5). If we recall that absorption cross sections are characterized by a 1/v behavior at low energies, then we can see that the addition of absorption



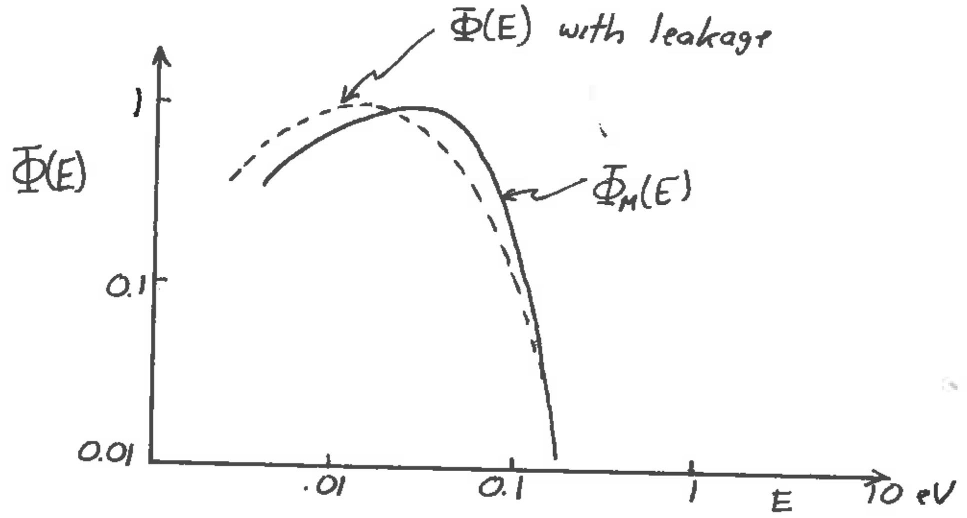
will preferentially tend to deplete neutrons with lower energies. The net effect is to shift the spectrum towards higher energies



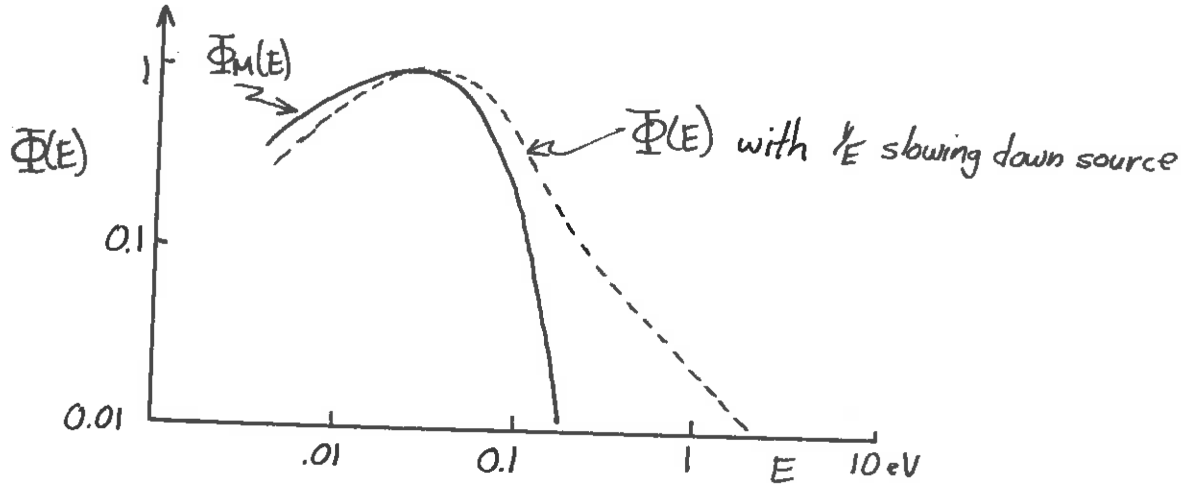
By way of contrast, one can model the addition of leakage by adding a term of the form D(E) B^2 to the infinite medium equation. This term acts as an effective absorption, except that it tends to be largest



at higher energies. The net effect is to deplete higher energy neutrons from the system, tending to shift the spectrum to lower energies



Finally, the addition of a slowing down source will cause the higher energy portion of the spectrum to behave in a characteristic 1/E fashion



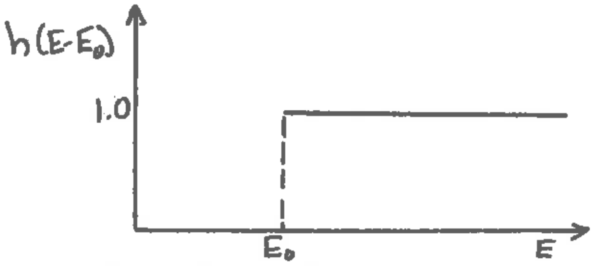
These perturbations can crudely be interpreted as shifting the neutron temperature, T_n, from the moderator temperature T_m. In that sense, one refers to "absorption heating" or "diffusion cooling" of the thermal spectrum. One could use such an interpretation for the calculation of thermal group constants. For example, if the thermal groups were very fine, one might be able to get away with a simple Maxwellian for the intragroup flux

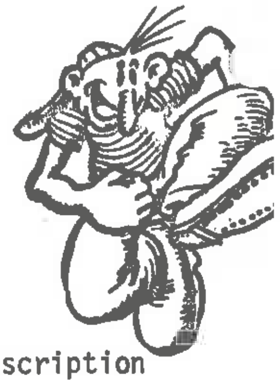
$$\Phi(\vec{r},E) \cong \Phi_M(E) = \frac{2\pi n}{(\pi kT)^{3/2}}\sqrt{\frac{2}{m}}\,E\,e^{-E/kT} \tag{9-10}$$

A slightly more sophisticated form would arise from characterizing the neutrons by an effective temperature, T_n, and adding on a "1/E" tail component

$$\Phi(\vec{r},E) \cong \frac{2\pi n}{(\pi kT_n)^{3/2}}\sqrt{\frac{2}{m}}\,E\,e^{-E/kT_n} + \lambda\frac{h(E-E_0)}{E} \tag{9-11}$$

Here, T_n would be fudged to account for the spectrum shift due to absorption or leakage, while h(E) is a "step" function





which "cuts in" a 1/E slowing down spectrum above 4 kT. This prescription was originally proposed by Westcott and represents perhaps the simplest way to take account of nonequilibrium spectrum effects.

Unfortunately, neither of these prescriptions is of much use in generating thermal group constants when the group size is large (and in most calculations, only one such thermal group is used). Hence we now turn our attention to more accurate schemes for generating the thermal neutron spectrum.

II. NEUTRON THERMALIZATION IN A PROTON GAS

Perhaps the simplest model of neutron thermalization which yields results of sufficient accuracy for use in reactor design is that which pictures the reactor core as a proton gas (mass number A = 1) in thermal equilibrium at a temperature T. Such a model obviously ignores both chemical binding and diffraction. However it does describe upscattering and has proven to be remarkable successful for generating thermal spectra useful in light water reactor design.

To be more specific, we will consider the solution of the infinite medium spectrum problem

$$[\Sigma_a(E)+\Sigma_s(E)]\,\Phi(E) = \int_0^\infty dE'\,\Sigma_s(E'\to E)\,\Phi(E') \qquad (9\text{-}12)$$

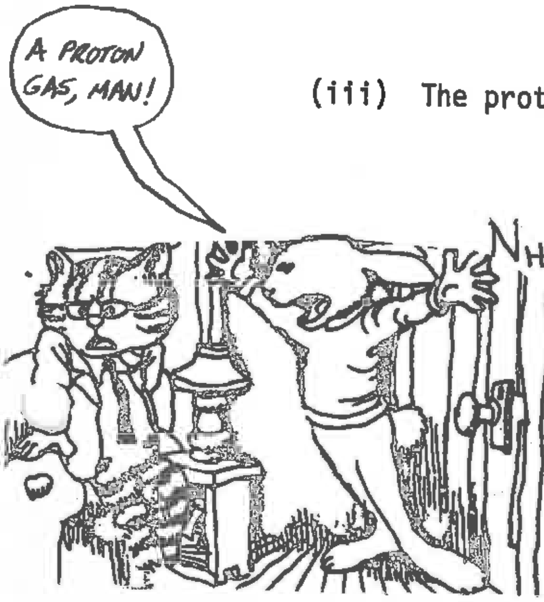
assuming

(i) The microscopic scattering cross section, σ_s, is independent of the relative velocity V_r between neutron and proton.

(ii) The absorption cross section behaves as

$$\sigma_a(V_r) = \gamma/V_r \qquad (9\text{-}13)$$

(iii) The proton gas is in thermal equilibrium such that



$$N_H(\vec{V}) = N_H\left(\frac{M}{2\pi kT}\right)^{3/2} e^{-MV^2/2kT} \qquad (9\text{-}14)$$

In this case, the differential scattering cross section can be written as

$$\Sigma_s(E'\to E) = \frac{\Sigma_{sf}}{E}\begin{cases} \operatorname{erf}\sqrt{E'/kT}\,, & E'<E \\ \exp[(E-E')/kT]\operatorname{erf}\sqrt{E/kT}\,, & E'>E \end{cases} \tag{9-15}$$

where $\Sigma_{sf} = N_H\,\sigma_s^H$ = "free atom cross section of hydrogen"

Using this cross section, we find

$$\Sigma_s(E) = \frac{1}{v}\int v_r\sigma_s^H N_H(\vec{V})\,d\vec{V} = \int_0^\infty dE'\,\Sigma_s(E\to E') = \frac{\sigma_s^H}{v}\mathcal{V}(E) \tag{9-16}$$

where

$$\mathcal{V}(E) \equiv N_H\sqrt{\frac{2kT}{M}}\left[\frac{e^{-x^2}}{\sqrt{\pi}} + \left(x+\frac{1}{2x}\right)\operatorname{erf}(x)\right] \tag{9-17}$$

and $x^2 = E/kT$

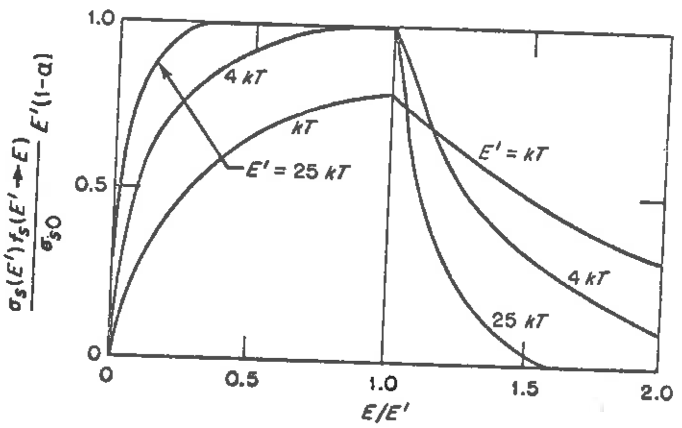
It is also useful to note

$$\Sigma_a(E) \equiv \frac{1}{v}\int v_r\,\frac{\gamma}{v_r}\,N_A(\vec{V})\,d^3V = N_A\frac{\gamma}{v} \tag{9-18}$$

Before continuing, it is useful to look at the differential scattering probability $P(E'\to E)$

$$P(E'\to E) = \frac{\Sigma_s(E'\to E)}{\Sigma_s(E')} = f(E)\begin{cases} \operatorname{erf}\sqrt{E'/kT}\,, & E'<E \\ e^{E-E'/kT}\operatorname{erf}\sqrt{E/kT}\,, & E'>E \end{cases} \tag{9-19}$$

We have plotted P(E'   E) vs. final energy below



In particular, note that for large incident energies E' >> kT, the scattering probability approaches the form we found in slowing down studies in which the nuclear motion was neglected

$$P(E'\to E) \to \frac{1}{E}, \qquad E' >> kT \tag{9-20}$$

As the incident energy E' approaches kT, there is more and more probability of the neutron experiencing an increase in energy--that is, upscattering.

Before proceeding to solve for the neutron energy spectrum characterizing such a scattering cross section, we will first manipulate Eq. (9-12) into a slightly more convenient form. Recall (and verify explicitly) that $\Sigma_s(E'\to E)$ must satisfy detailed balance

$$v'\Sigma_s(E'\to E)M(E') = v\Sigma_s(E\to E')M(E) \tag{9-21}$$

or

$$\Sigma_s(E')\,P(E'\to E) = \Sigma_s(E)\,P(E\to E')\,\frac{vM(E)}{v'M(E')} \qquad (9\text{-}22)$$

Then we can rewrite Eq. (9-12) as

$$\Sigma_a(E)\Phi(E) = \Sigma_s(E)\int_0^\infty dE'\,P(E\to E')\left[\frac{vM(E)}{v'M(E')}\Phi(E') - \Phi(E)\right] \qquad (9\text{-}23)$$

or

$$\Sigma_a(E)\psi(E) = \Sigma_s(E)\int_0^\infty dE'\,P(E\to E')\left[\psi(E') - \psi(E)\right] \qquad (9\text{-}24)$$

where

$$\psi(E) \equiv \frac{\Phi(E)}{vM(E)} \qquad (9\text{-}25)$$

If we next substitute in for the cross sections, we find

$$\frac{N_A\gamma}{v}\psi = \frac{\sigma_s^H}{v}V(E)\int_0^\infty dE'\,P(E'\to E)\left[\psi(E') - \psi(E)\right] \qquad (9\text{-}26)$$

or noting $\int_0^\infty dE'\,P(E\to E') = 1$,

$$\left[\frac{N_A\gamma}{\sigma_s^H} + V(E)\right]\psi(E) = V(E)\int_0^\infty dE'\,P(E\to E')\,\psi(E') \qquad (9\text{-}27)$$

Notice now that P(E' → E) has a discontinuous first derivative at E' = E. Its structure is very similar to that of a Green's function for a second order differential equation. Using this fact and several straightforward manipulations, one can recast Eq. (9-24) into the following form

$$-\frac{d}{dx}\left\{\frac{1}{P(x)}\frac{d}{dx}\left[V(x)+\Gamma\right]\psi(x)\right\}+\left[W(x)\left[V(x)+\Gamma\right]-\frac{4}{\sqrt{\pi}}\right]\psi(x)=0$$

where

$$W(x)=\frac{x^2}{P(x)}-\frac{e^{-x^2}}{P^2(x)}\ ,\quad x=\sqrt{E/kT} \tag{9-28}$$

$$P(x)=e^{-x^2}+\sqrt{\pi}\,x\,\mathrm{erf}(x)$$

$$\Gamma=\frac{\gamma}{V_0\sigma_s^H}\ ,\qquad V_0=\sqrt{\frac{2kT}{m}}$$

This equation is sometimes referred to as the Wigner-Wilkins equation after the investigators which first studied the proton gas problem. One final step can then be taken: By introducing a transformation of dependent variable, one can recast Eq. (9-28) into a nonlinear <u>first</u> order differential equation (a Ricatti equation) more suitable for numerical solution:

$$\frac{dJ}{dE}=\frac{S(E)}{2kT}+\left[\frac{1-2P(E)}{2E}\right]J(E)-\frac{P(E)}{2E}J^2(E) \tag{9-29}$$

where

$$\Phi(E)=\frac{E}{Q(E)}\exp\left\{\frac{1}{2}\int_0^E\frac{dE'}{E'}\left[P(E')\left[J(E')+1\right]-\left[1+E'/kT\right]\right]\right\} \tag{9-30}$$

while

$$S(E) = \frac{1}{x^2}\left[1-P(x)\right] + \frac{x^2}{P(x)} - \frac{e^{-x^2}}{P^2(x)} - \frac{4}{Q} \qquad (9\text{-}31)$$

$$Q(E) = P + \frac{1}{x}\,\frac{\sqrt{\pi}}{2}\,\mathrm{erf}\,x + \sqrt{\frac{\pi}{kT}}\left(\frac{\Sigma_a(E)+DB^2}{\Sigma_s^H}\right) \qquad (9\text{-}32)$$

Here we have modified this derivation to include a non-$^1/_v$ absorption and modeled leakage with a $D(E)B^2$ term where

$$D(E) = \frac{1}{3\Sigma_{tr}} = \frac{1}{3\left[\Sigma_a + \Sigma_s^H(1-\bar{\mu})\right]} \quad \leftarrow \tfrac{2}{3}\text{ for, } H! \qquad (9\text{-}33)$$

Although the equation for J(E) looks rather complicated, it is in fact quite simple to solve numerically. Thermal spectrum codes based upon solutions of the Wigner-Wilkins equation are occasionally referred to as SOFOCATE-type methods (after one of the early thermal spectrum codes used for light water reactor calculations).

In most of these codes, Eq. (9-29) is first solved for J(E) numerically using Milne's predictor-corrector method. To get this method started, an asymptotic solution for $E \ll kT$ is used. Once J(E) is known, $\Phi(E)$ is then determined from Eq. (9-30) using a numerical integration (e.g., trapezoidal rule). Typically on the order of 50-60 mesh points are found to yield sufficient accuracy over the interval

In Figure (9-2) we have illustrated the shape of the Wigner-Wilkins spectrum for several values of $^1/_v$ absorption (characterized by the parameter $\Gamma = \frac{\gamma}{V_0\sigma_s^H}$) and a slowing down source. We have also compared

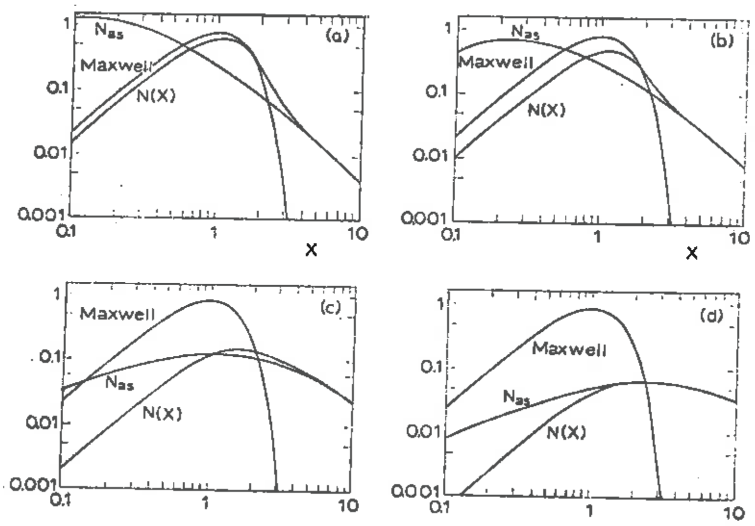
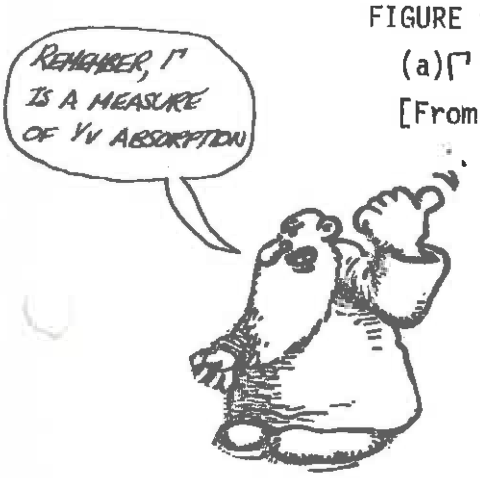


FIGURE 9-2: Neutron density in a proton gas for (a)Γ = .226, (b) Γ = .451, (c) Γ = 2.257, and (d) Γ = 5.0 [From: ANL 6498]



these results with an asymptotic solution valid for large speeds

$$N_{as}(v) = \frac{C_0 v}{\left[1+\frac{1}{\Gamma}\left(\frac{v}{v_0}\right)\right]^2} \tag{9-34}$$

Notice in particular that as we increase absorption (Γ), the spectrum "hardens" by shifting to higher energies, hence verifying our earlier comments concerning absorption "heating".

One can now use these computed spectra to generate thermal group constants. For example, if we wished to utilize a single thermal group, we would define

$$\Sigma_{s_{th}} = \frac{\int_0^{.63}\left[\sum_i N_i \sigma_s^i\right]\Phi(E)\,dE}{\int_0^{.63}\Phi(E)\,dE} \tag{9-35}$$

and similarly for $\Sigma_{a_{th}}$ and $\Sigma_{f_{th}}$ [Note we have included a summation over the various isotopes which may be present.] Finally,

$$D_{th} = \frac{\int_0^{.63}\frac{1}{3}\left[\sum_i N_i\sigma_a^i + \sum_i N_i(1-\mu_i)\sigma_s^i\right]^{-1}\Phi(E)\,dE}{\int_0^{.63}\Phi(E)\,dE} \tag{9-36}$$

It is very important to take into account the spatial heterogeneities present in a reactor core when generating thermal groups constants because the thermal neutron mfp is frequently rather small compared to the distances characterizing the core lattice structure. Fortunately, there are procedures available which can make simple modifications to simple infinite medium spectrum calculations to account for this, thereby avoiding a detailed multigroup diffusion calculation. We will return to discuss these methods in some detail in Chapter 11.

It should be noted that the proton gas model effectively converts an integral equation (9-12) into a ordinary differential equation. Such a result is of some significance when contemplating numerical solutions, since these differential equations are considerably easier to solve than the full matrix equations which arise from discretizing the integral equation directly. We will see momentarily that there are other approximate methods used for converting such integral equations into ordinary differential equations suitable for machine calculations.

III. THE HEAVY GAS MODEL

Obviously the proton gas model is of limited utility in analyzing neutron thermalization in nonhydrogeneous moderators. Alternative models are needed for heavier mass moderators such as graphite which is used in gas-cooled reactors. One of the simplest thermalization models is based upon expanding the cross section for a free gas of arbitrary mass M in $\frac{1}{M}$, hence arriving at an approximation which should be valid for large mass numbers.

The differential scattering cross section for a free gas can be derived in a straightforward, if somewhat cumbersome, consideration of two body kinematics (similar to Appendix A). This cross section can be written as

$$\Sigma_s(E'\rightarrow E) = \begin{cases} \dfrac{\Sigma_s\theta^2}{2E'} e^{-(\epsilon-\epsilon')} \Bigl\{ \operatorname{erf}(\theta\sqrt{\epsilon'}-\xi\sqrt{\epsilon}) + \operatorname{erf}(\theta\sqrt{\epsilon'}+\xi\sqrt{\epsilon}) \\ \qquad + \operatorname{erf}(\theta\sqrt{\epsilon}-\xi\sqrt{\epsilon'}) - \operatorname{erf}(\theta\sqrt{\epsilon}+\xi\sqrt{\epsilon'}) \Bigr\} & \epsilon' < \epsilon \\ \dfrac{\Sigma_s\theta^2}{2E'} e^{-(\epsilon'-\epsilon)} \Bigl\{ \operatorname{erf}(\theta\sqrt{\epsilon'}-\xi\sqrt{\epsilon}) - \operatorname{erf}(\theta\sqrt{\epsilon'}+\xi\sqrt{\epsilon}) \\ \qquad + \operatorname{erf}(\theta\sqrt{\epsilon}-\xi\sqrt{\epsilon'}) + \operatorname{erf}(\theta\sqrt{\epsilon}+\xi\sqrt{\epsilon'}) \Bigr\} & \epsilon' > \epsilon \end{cases} \qquad (9\text{-}37)$$

where

$$\theta = \frac{(A+1)}{2\sqrt{A}}\ ,\quad \xi = \frac{(A-1)}{2\sqrt{A}}\ ,\quad \epsilon = \frac{E}{kT}\ ,\quad \mu = \frac{1}{A} = \frac{m}{M}$$

If we now expand in inverse mass number, A^{-1}, we find

$$\Sigma_s(E'\rightarrow E) = \Sigma_s \left\{ \delta(E'-E) + \frac{(E+E')}{A}\sqrt{\frac{E}{E'}}\left[-\delta'(E'-E) + kT\delta''(E'-E)\right] \right. \qquad (9\text{-}38)$$

Here, δ' and δ" are the first and second derivatives of the Dirac δ-function, defined in Appendix D . The corresponding total scattering cross section for this model is

$$\Sigma_s(E) = \Sigma_s\left(1 + \frac{kT}{2AE}\right) \qquad (9\text{-}39)$$

If we now substitute this rather singular scattering kernel back into our integral equation and note that from the definition of δ' and δ"

$$\int_0^\infty dE'\Sigma_s(E'\rightarrow E)\,\Phi(E') = \frac{2\Sigma_s}{A}\left[kTE\frac{d^2\Phi}{dE^2} + E\frac{d\Phi}{dE} + \Phi\right] + \Sigma_s\left(1+\frac{kT}{2AE}\right)\Phi, \qquad (9\text{-}40)$$

then we find that Eq. (9-12) becomes

$$\Sigma_a(E)\,\Phi(E) = \frac{2\Sigma_s}{A}\left[EkT\frac{d^2\Phi}{dE^2} + E\frac{d\Phi}{dE} + \Phi(E)\right] \qquad (9\text{-}41)$$

This simple second order differential equation is known as the heavy gas equation. In many ways the heavy gas approximation is similar to the age approximation we developed to describe neutron slowing down in heavy mass moderators--and, indeed, in the large energy limit the heavy gas model just reduces to age theory.

Using the usual techniques from the the theory of second order ODE's, one can laborously generate asymptotic solutions to this equation for different absorption cross section energy dependences--e.g., $\Sigma_a(E)$ = constant = Σ_a , or $\Sigma_a(E) = \gamma/_v$. It can also be integrated directly to generate thermal neutron spectra for moderators such as graphite.

For example, if we assume $^1/_v$ absorption:

$$\Sigma_a(E) = \frac{\gamma}{v} \tag{9-42}$$

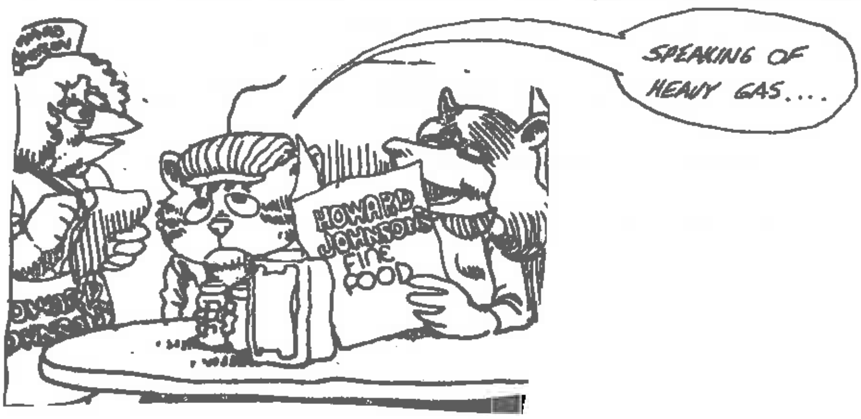
then we can rewrite the heavy gas equation as

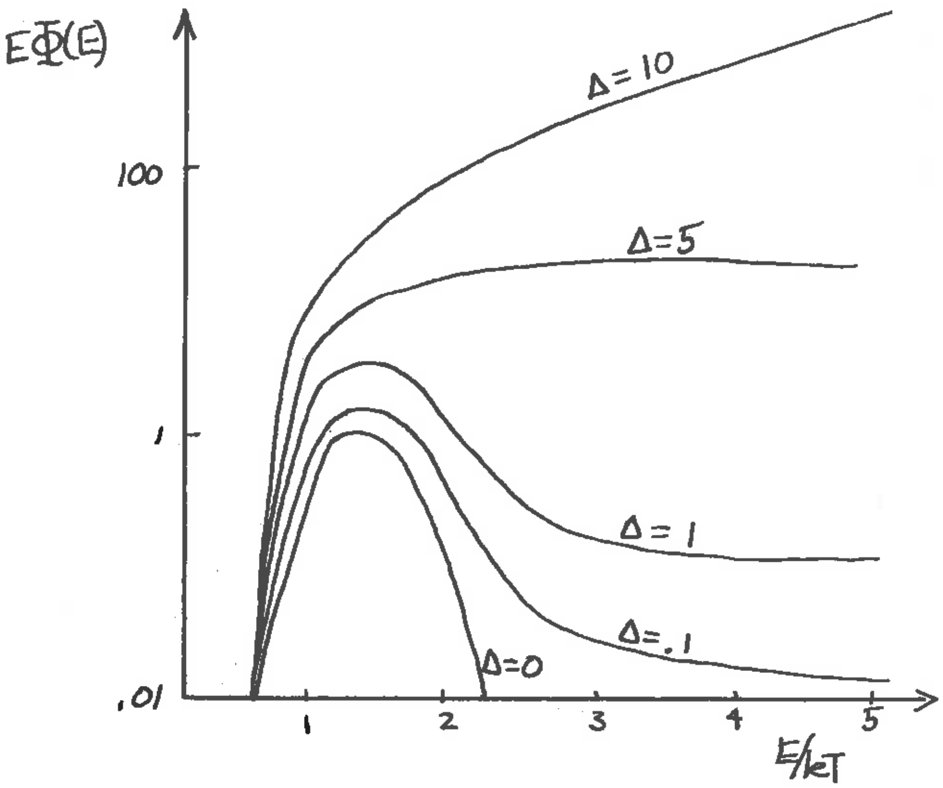
$$x\frac{d^2\psi}{dx^2} + (3-2x^2)\frac{d\psi}{dx} - \Delta\psi = 0 \tag{9-43}$$

where

$$x = \sqrt{\frac{E}{kT}} \quad , \qquad \Delta = \frac{2\Sigma_a(kT/m)}{\Sigma_s} \tag{9-44}$$

This equation can be solved numerically to yield the spectrum shown below





Note as we make the moderator mass heavier and heavier, the moderator is less and less capable of slowing down neutrons and hence the spectrum hardens. In this approximation, a heavier gas is equivalent to the addition of absorption.

Unfortunately, the heavy gas (or even free gas) model is far less effective at predicting thermal spectra in graphite moderated reactors than is the proton gas model for light water reactors. This has led to a rather limited use of this model in practice. More frequently one must use more realistic scattering kernels characterizing material such as graphite (e.g., the Parks kernel) and solve the integral equation describing thermalization directly.

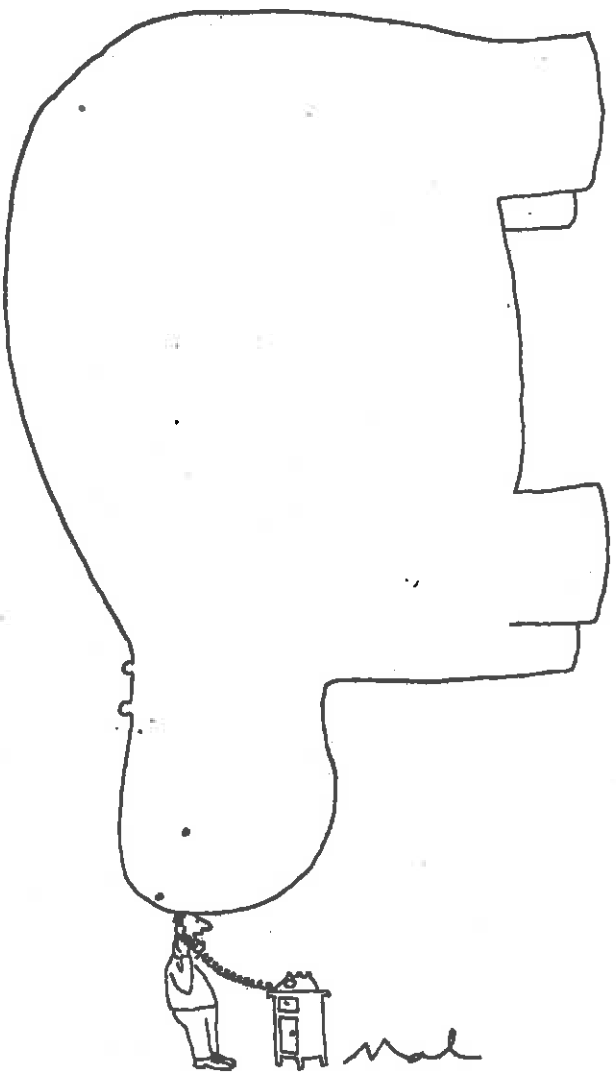
IV. GENERAL THERMAL SPECTRUM CALCULATIONS

Outline:

- Cross section generation: GASKET-FLANGE
  - (i) incoherent approximation
  - (ii) phonon frequency distribution
- Spectrum generator: GATHER [B_1 or P_1, 101 groups]
- Lattice effects: THERMOS, SPECTROX
- Synthetic kernels

PART IV

AN INTRODUCTION TO THE DESIGN
OF
NUCLEAR POWER REACTORS



“Now you tell me the Sullivan show is canceled!”

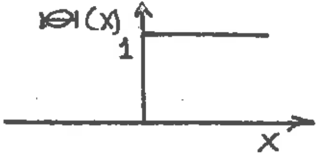
APPENDIX C

"STEP FUNCTIONS, DELTA FUNCTIONS, AND OTHER EXOTIC BEASTS"*

I. INTRODUCTION

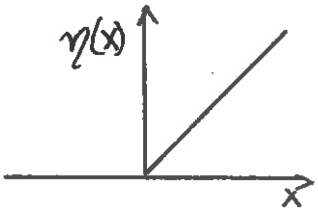
Consider the discontinuous function $\Theta(x)$ defined by the properties

$$\Theta(x) = \begin{cases} 0 & x<0 \\ 1 & x\geqslant 0 \end{cases} \qquad \text{(C-1)}$$



$\Theta(x)$ is the unit "step function" introduced by Heaviside in his development of operational calculus (now known as Laplace transform analysis). One can perform numerous operations on $\Theta(x)$. In particular, it can be integrated to yield the ramp function

$$\eta(x) = \int_{-\infty}^{x} dx'\,\Theta(x') = \begin{cases} 0 & x<0 \\ x & x\geqslant 0 \end{cases} \qquad \text{(C-2)}$$



Let's try something a bit more unusual by taking the derivative of $\Theta(x)$. Clearly this is ridiculous, because this derivative, call it $\delta(x)$, is undefined at x = 0 because $\Theta(x)$ is discontinuous at this point:

$$\delta(x) = \begin{cases} 0 & x\neq 0 \\ \infty & x=0 \end{cases} \qquad \text{(C-3)}$$

Nevertheless, Dirac, Heaviside, and others have made very good use of this strange "function". [Actually it is not a function, but rather must be regarded as a "generalized function".] To be more specific, the Dirac δ-function, $\delta(x)$, has the properties

$$\delta(x-x_0) = \begin{cases} 0, & x\neq x_0 \\ \infty, & x=x_0 \end{cases}, \qquad \int_{-\infty}^{\infty} dx\,\delta(x-x_0) = 1 \qquad \text{(C-4)}$$

---

*A. Messiah, "Quantum Mechanics", Vol. I (John Wiley, 1965) pp. 468-470
M. J. Lighthill, "Fourier Analysis and Generalized Functions" (Cambridge,1959)

[In this sense, it resembles a generalization of the Kronecker δ-function

$$\delta_{mn} = \begin{cases} 0 , & m \neq n \\ 1 , & m = n \end{cases}$$
]

The most useful property of the Dirac δ-function occurs when it is integrated along with a well-behaved function, say f(x):

$$\int dx\, f(x)\, \delta(x-x_0) = f(x_0) . \tag{C-5}$$

This property not only is very interesting, but it is extremely useful in mathematical physics. Unfortunately, the proof of this property--and, indeed, all of the <u>theory</u> of such generalized functions--requires a rather potent dose of mathematics. [Such generalized functions are really not functions at all, but rather a class of linear functionals called "distributions" which are defined on some set of suitable test functions (which are "indefinitely differentiable with compact support").]

Fortunately, one does not need all of this high-powered mathematics in order to <u>use</u> δ-functions. Only a knowledge of their properties is necessary.

II. PROPERTIES OF THE DIRAC δ-FUNCTION

A. Alternative Representations

$$\delta(x-x_0) = \frac{1}{\pi} \lim_{\lambda \to \infty} \frac{\sin \lambda (x-x_0)}{(x-x_0)} \tag{C-6}$$

$$\delta(x-x_0) = \frac{1}{\pi} \lim_{\kappa \to \infty} \frac{1-\cos \kappa (x-x_0)}{\kappa (x-x_0)^2} \tag{C-7}$$

$$\delta(x-x_0) = \frac{1}{\pi} \lim_{\epsilon \to 0^+} \frac{\epsilon}{(x-x_0)^2 + \epsilon^2} \tag{C-8}$$

$$\delta(x-x_0) = \lim_{\eta \to 0} \frac{\Theta(x-x_0+\eta) - \Theta(x-x_0)}{\eta} = \frac{d}{dx} \Theta(x-x_0) \tag{C-9}$$

B. Properties

$$\delta(x) = \delta(-x) \tag{C-10}$$

$$\delta(ax) = \frac{1}{|a|}\,\delta(x)\,, \quad a \neq 0 \tag{C-11}$$

$$\delta[g(x)] = \sum_n \frac{1}{|g'(x_n)|}\,\delta(x - x_n) \tag{C-12}$$

where x_n are the zeros of $g(x)$, $g(x_n) = 0$, such $g'(x_n) \neq 0$.

$$x\,\delta(x) = 0 \tag{C-13}$$

$$f(x)\,\delta(x-a) = f(a)\,\delta(x-a) \tag{C-14}$$

$$\int \delta(x-y)\,\delta(y-a)\,dy = \delta(x-a) \tag{C-15}$$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx} \tag{C-16}$$

Actually, these properties only make sense when inserted in an integral. For example, property (C-10) really should be interpreted as

$$\int dx\, f(x)\,\delta(x) = \int dx\, f(x)\,\delta(-x) = f(0) \tag{C-17}$$

C. Derivatives

One can differentiate a δ -function as many times as one wishes. The mth derivative is given by

$$\int_{-\infty}^{\infty} \delta^{[m]}(x)\, f(x)\, dx = (-1)^m \left.\frac{d^m f}{dx^m}\right|_{x=0} \tag{C-18}$$

One can show

$$\delta^{[m]}(x) = (-1)^m \delta^{[m]}(-x) \tag{C-19}$$

$$\int \delta^{[m]}(x-y)\delta^{[n]}(y-a)\,dy = \delta^{[m+n]}(x-a) \tag{C-20}$$

$$x^{m+1}\delta^{[m]}(x) = 0 \tag{C-21}$$

Perhaps of more direct use is the application of these properties to the first derivative

$$\int_{-\infty}^{\infty} \delta'(x) f(x)\,dx = -f'(0) \tag{C-22}$$

$$\delta'(x) = -\delta'(-x) \tag{C-23}$$

$$\int \delta'(x-y)\,\delta(y-a)\,dy = \delta'(x-a) \tag{C-24}$$

$$x\delta'(x) = -\delta(x) \tag{C-25}$$

$$x^2\delta'(x) = 0 \tag{C-26}$$

$$\delta'(x) = \frac{i}{2\pi}\int_{-\infty}^{\infty} k e^{ikx}\,dk \tag{C-27}$$

APPENDIX D

"THE ZOOLOGY OF SPECIAL FUNCTIONS"

I. INTRODUCTION

It is almost impossible to proceed very far in the study of science or engineering without running into one or more of the special functions which prowl the jungles of applied mathematics. It is rather essential that the engineer learn at least enough about these functions so that he will not quake with fear when he encounters face-to-face an error function or a Hankel function or, God-forbid, a hypergeometric function. These exotic sounding beasts are just functions, in everyway analogous to more common species such as sin(x) or e^x--except that they don't arise nearly as frequently. For this reason, it really isn't essential that you become an expert on, say, Hankel functions--just knowing where to look up their properties is usually enough.

This appendix will be a very brief tour through the zoo of special functions. We'll try to define each of the beasts you are likely to encounter as nuclear engineers, describe several of their anatomical features, and give examples of their habitats. For more detailed information, I will refer you to the standard references:

H. Margenau and G. Murphy, "The Mathematics of Physics and Chemistry", (D. Van Nostrand, 1956) Chapter 3

M. Abramowitz and I. Stegun, ed., "Handbook of Mathematical Functions", A.M.S. 55 (Dover, 1964)

E. T. Copson, "Introduction to the Theory of Functions of a Complex Variable", (Oxford University Press, 1935)

II. FUNCTIONS ARISING AS SOLUTIONS TO SECOND ORDER DIFFERENTIAL EQUATIONS

A. Exponential and Trigometric Functions

Defining Equation:

$$a\frac{d^2f}{dz^2} + b\frac{df}{dz} + cf(z) = 0$$

$$f(z): \ e^{\alpha z}, e^{-\alpha z}, \sin\beta z, \cos\beta z$$

$$\alpha = -\frac{b \pm \sqrt{b^2-4ac}}{2a}, \quad \beta = i\alpha$$

Habitat: everywhere

Properties: well known

B. Legendre Functions

Defining Equation: $(1-z^2)\frac{d^2f}{dz^2} - 2z\frac{df}{dz} + \ell(\ell+1)f(z) = 0$ (Legendre's Equation)

$f(z)$: $P_\ell(z)$ Legendre polynomial of the first kind

$Q_\ell(z)$ Legendre polynomial of the second kind

Representations:

$$P_\ell(z) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dz^\ell}(z^2-1)^\ell : P_0(z)=1;\ P_1(z)=z;\ P_2(z)=\tfrac{1}{2}(3z^2-1)$$

$$Q_\ell(z) = \frac{1}{2}P_\ell(z)\ln\left(\frac{1+z}{1-z}\right) - \sum_{m=1}^{\ell}\frac{1}{m}P_{m-1}(z)P_{\ell-m}(z) :$$

$$Q_0(z) = \frac{1}{2}\ln\left(\frac{1+z}{1-z}\right);\ Q_1(z) = \frac{z}{2}\ln\left(\frac{1+z}{1-z}\right) - 1;\ Q_2(z) = \frac{(3z^2-1)}{4}\ln\left(\frac{1+z}{1-z}\right) - \frac{3z}{2}$$

(Note $Q_\ell(z)$ is singular at $z = \pm 1$. For this reason it is not used very frequently.)

Habitat:

(i) Differential equations solved in spherical coordinates--
e.g., diffusion equation for a spherical reactor,
Schrodinger equation for spherically symmetric potential

(ii) Expanding functions $f(\mu)$, $-1 \le \mu \le 1$
e.g., P_N expansion of angular flux $\varphi(x,\mu) = \sum_{\ell=1}^{\infty}\varphi_\ell(x)P_\ell(\mu)$

Properties: $\{P_\ell(x)\}$ is a complete, orthogonal set on range $-1 \le x \le 1$

$$\int_{-1}^{+1} dx\, P_\ell(x)P_{\ell'}(x) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

Useful recursion relations:

$$\frac{dP_{\ell+1}}{dx} - x\frac{dP_\ell}{dx} = (\ell+1)P_\ell, \quad (\ell+1)P_{\ell+1} = (2\ell+1)xP_\ell - \ell P_{\ell-1}$$

$$\frac{dP_{\ell+1}}{dx} - \frac{dP_{\ell-1}}{dx} = (2\ell+1)P_\ell,$$

$$(x^2+1)\frac{dP_\ell}{dx} = \ell x P_\ell(x) - \ell P_{\ell-1}(x),$$

Generating function:

$$\frac{1}{\sqrt{1-2xy+y^2}} = \sum_{\ell=0}^{\infty}P_\ell(x)y^\ell$$

Associated Legendre Functions

Defining Equation:

$$(1-z^2)\frac{d^2f}{dz^2} - 2z\frac{df}{dz} + \left[\ell(\ell+1) - \frac{m^2}{1-z}\right]f(z) = 0$$

$$f(z):\quad P_\ell^m(z),\ Q_\ell^M(z)$$

Representation:

$$P_\ell^m(z) = (1-z^2)^{m/2}\,\frac{d^m}{dz^m}P_\ell(z)$$

Generating function:

$$\frac{(2m)!\,(1-x^2)^{m/2}\,y^m}{2^m m!\,(1-2xy+y^2)^{m+1/2}} = \sum_{\ell=m}^{\infty} P_\ell^m(x)\,y^\ell$$

Habitat: Occur most frequently as solutions to the angular part part of equations involving ∇^2 in spherical coordinates--e.g.,

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} + \lambda Y = 0$$

has as solutions

$$Y_{\ell m}(\theta,\phi) = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi}$$

Here $Y_{\ell m}(\hat{\Omega}) = Y_{\ell m}(\theta,\phi)$ are referred to as the "spherical harmonic" functions.

Properties: $\{Y_{\ell m}\}$ are complete and orthonormal

$$\int_0^\pi d\theta\int_0^{2\pi}d\phi\, Y_{\ell m}^*(\theta,\phi)Y_{\ell' m'}(\theta,\phi)\sin\theta \equiv \int d\hat{\Omega}\,Y_{\ell m}^*(\hat{\Omega})\,Y_{\ell' m'}(\hat{\Omega}) = \delta_{\ell\ell'}\delta_{mm'}$$

where $\hat{\Omega} \equiv (\theta,\phi)$, $d\hat{\Omega} \equiv \sin\theta\, d\theta\, d\phi$

by definition

$$Y_{0,0}(\hat{\Omega}) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0}(\hat{\Omega}) = \sqrt{\frac{3}{4\pi}}\cos\theta,\quad Y_{1,\pm1}(\hat{\Omega}) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$Y_{2,0}(\hat{\Omega}) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1),\quad Y_{2,\pm1}(\hat{\Omega}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi},\quad Y_{2,\pm2}(\hat{\Omega}) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm}$$

Of particular usefulness is the addition theorem for Legendre polynomials:

$$P_\ell(\hat{\Omega}\cdot\hat{\Omega}') = \left(\frac{4\pi}{2\ell+1}\right)\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\Omega})Y_{\ell m}(\hat{\Omega}')$$

C. Hermite Functions

Defining Equation: (Hermite's Equation)

$$z\frac{d^2f}{dz^2} - 2z\frac{df}{dz} + 2nf(z) = 0$$

$$f(z):\ H_n(z)$$

Representation:

$$H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}e^{-z^2}$$

$$H_0(z) = 1,\quad H_1(z) = 2z,\quad H_2(z) = 4z^2-2,\ \ldots$$

Habitat: Schrodinger equation for a simple harmonic oscillator

Properties: $\{H_n\}$ is complete and orthogonal with weight function e^{-x^2}

$$\int_{-\infty}^{\infty} dx\, e^{-x^2}H_n(x)H_m(x) = 2^n n!\sqrt{\pi}\,\delta_{nm}$$

$$\frac{dH_n}{dx} = 2nH_{n-1}(x),\quad \frac{d^2H_n}{dx^2} = 4n(n-1)H_{n-2},\ \ldots$$

Generating function:

$$e^{x^2-(z-x)^2} = \sum_{n=0}^{\infty}\frac{1}{n!}H_n(x)z^n$$

D. Laguerre Functions

Defining Equation: (Laguerre's Equation)

$$z\frac{d^2f}{dz^2} + (1-z)\frac{df}{dz} + nf(z) = 0$$

$$f(z):\ L_n(z)$$

Representations: $L_n(z) = e^z\frac{d^n}{dz^n}(z^ne^{-z})$

$$L_0(z) = 1,\quad L_1(z) = 1-z,\quad L_2(z) = 2-4z-z^2$$

Habitat: One more frequently encounters the associated Laguerre defined below.

Properties:

$$\frac{dL_n}{dz} - n\frac{dL_{n-1}}{dz} = -nL_{n-1}$$

$$L_{n+1} = (2n+1-z)L_n(z) - n^2 L_{n-1}$$

Generating function:

$$\frac{1}{1-z}e^{-\frac{xz}{1-z}} = \sum_{n=0}^{\infty}\frac{1}{n!}L_n(x)$$

Associated Laguerre Function:

Defining Equation:

$$z\frac{d^2f}{dz^2} + (k+1-z)\frac{df}{dz} + (n-k)f(z) = 0$$

$f(z)$: $L_n^{(k)}(z)$

Representation: $L_n^{(k)}(z) = (-1)^k \frac{d^k}{dz^k}L_{n+k}(z)$

$L_n^{(0)}(z) = L_n(z)$, $L_0^{(1)}(z) = z$, $L_1^{(1)}(z) = 18-6z$, $L_2^{(1)}(z) = 18-18z+3z^2$,

Habitat: Schrodinger equation for hydrogen atom

$$\left[e^{-r/2}r^{\ell}L_{n+1}^{2\ell+1}(r)\right]$$

Properties: $\{L_n^{(k)}(x)\}$ complete and orthogonal with weight function x^k

$$\int_0^{\infty} dx\, x^k e^{-x} L_m^{(k)}(x)L_n^{(k)}(x) = \delta_{mn}\frac{[\Gamma(k+n+1)]^3}{\Gamma(n+1)}$$

Generating function:

$$\frac{(-1)^k}{1-z}\left(\frac{z}{1-z}\right)^k e^{-\frac{xz}{1-z}} = \sum_{n=k}^{\infty}\frac{1}{n!}L_n^{(k)}(x)$$

E. Bessel Functions

Defining Equation:

$$z^2\frac{d^2f}{dz^2} + z\frac{df}{dz} + (z^2-\nu^2)f(z) = 0$$

(Bessel's Equation)

$f(z)$:
$J_{\pm\nu}(z)$ Bessel function of the first kind
$Y_\nu(z)$ Bessel function of the second kind
$H_\nu^{(1)}(z)$, $H_\nu^{(2)}(z)$ Hankel functions

Representations:

$$J_\nu(z) = \left(\frac{z}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{\left(-\frac{1}{4}z^2\right)^k}{k!\,\Gamma(\nu+k+1)}$$

$$Y_\nu(z) = \frac{J_\nu(z)\cos(\nu\pi) - J_{-\nu}(z)}{\sin\nu\pi}$$

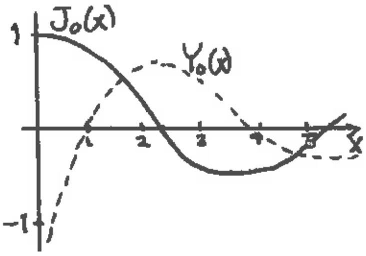
$$H_\nu^{(1)}(z) = J_\nu(z) + i\,Y_\nu(z)$$

$$H_\nu^{(2)}(z) = J_\nu(z) - i\,Y_\nu(z)$$

Habitat: Differential equations in cylindrical or polar coordinates (e.g., cylindrical reactors).

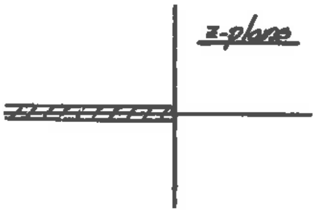
Properties:

$J_n(z)$, n integer, is an entire function of z; $Y_n(z)$ is singular at the origin



For $\nu \neq$ integer, J_ν, Y_ν, and $H_\nu^{(1)}$, $H_\nu^{(2)}$ are analytic in the z-plane cut along the negative real axis. [Each is an entire function of ν]. $J_\nu(z)$ is bounded as $z \to 0$ while $Y_\nu(z)$ diverges.

J_ν and Y_ν are linearly independent, as are $H_\nu^{(1)}$ and $H_\nu^{(2)}$.



Generating function: $$e^{\frac{x}{2}\left(u-\frac{1}{u}\right)} = \sum_{n=0}^{\infty} J_n(x)\,u^n$$

Integral representation: $$J_n(z) = \frac{1}{\pi}\int_0^\pi \cos(n\theta - z\sin\theta)\,d\theta$$

Asymptotic behavior:

$$J_\nu(z) \sim \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right), \quad |\arg z| < \pi$$

$$Y_\nu(z) \sim \sqrt{\frac{2}{\pi z}}\sin\left(z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right), \quad |\arg z| < \pi$$

$$H_\nu^{(1)}(z) \sim \sqrt{\frac{2}{\pi z}}\,e^{i\left(z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)}, \quad -\pi < \arg z < 2\pi$$

$$H_\nu^{(2)}(z) \sim \sqrt{\frac{2}{\pi z}}\,e^{i\left(z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)}, \quad -2\pi < \arg z < \pi$$

as $|z| \to \infty$

Modified Bessel Functions:

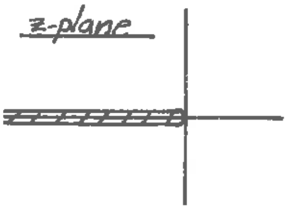
Defining Equation: $$z^2 \frac{d^2f}{dz^2} + z\frac{df}{dz} - (z^2+\nu^2)f(z) = 0$$

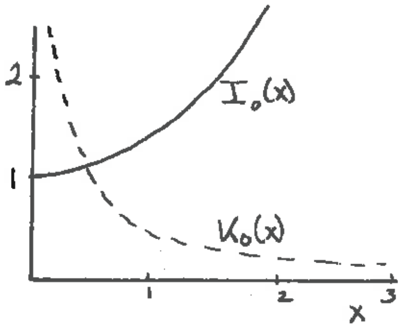
$$f(z):\ I_{\pm\nu}(z),\ K_\nu(z)$$

Representations:

$$I_\nu(z) = \left(\frac{z}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{(z^2/4)^k}{k!\,\Gamma(\nu+k+1)}\ ,\quad K_\nu(z) = \frac{\pi}{2}\ \frac{I_{-\nu}(z) - I_\nu(z)}{\sin \nu\pi}$$

Properties: Both $I_\nu(z)$ and $K_\nu(z)$ are analytic in a plane cut along the negative real axis. $I_\nu(z)$ is bounded as $z \to 0$, while $K_\nu(z)$ diverges as $z \to 0$.





F. Hypergeometric Functions:

Defining Equation: $$z(1-z)\frac{d^2f}{dz^2} + [c-(a+b+1)z]\frac{df}{dz} - abf(z) = 0$$ (Hypergeometric Equation)

$$f(z):\ F(a,b;c;z)$$

Representation: $$F(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!}$$

Habitat: This is probably the most general "named" function you will encounter in solving second order O.D.E.'s.

Properties: Series representation converges within unit circle (analytic continuations can be given for all $z \neq 1$ or ∞).

III. OTHER SPECIAL FUNCTIONS

A. Gamma Function:

Representations: $$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt\ ,\quad \mathrm{Re}\{z\} > 0$$

(can be analytically continued into LHP for $z \neq -n$, $n = 0, 1, \ldots$)

Habitat: $\Gamma(z)$ is essentially the generalization of the factorial n! for non-integer values of n. Hence it arises very frequently.

Properties: important property: $\Gamma(z+1) = z\Gamma(z)$

Other useful relations:

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi},\ \Gamma(0) = \infty,\ \Gamma(1) = 1,\ \Gamma(2) = 1,\ \Gamma(3) = 2!, \ldots$$

$$\Gamma(n+1) = n!$$

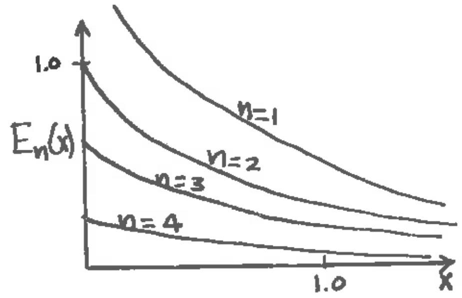
$$\Gamma(z)\Gamma(1-z) = \pi \csc \pi z$$

$$\Gamma(z) \sim e^{-z} z^{z-\frac{1}{2}} \sqrt{2\pi} \left[1 + \frac{1}{12z} + \frac{1}{288z^2} + \cdots\right],\ z \to \infty \text{ in } |\arg z| < \pi$$

Closely related is the "incomplete Gamma function"

$$\Gamma(a,x) = \int_x^\infty dt\, e^{-t} t^{a-1}$$

B. Exponential Integral:



Representation:

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t}\, dt$$

$$E_n(z) = \int_1^\infty \frac{e^{-zt}}{t^n}\, dt$$

Habitat: Solutions of the neutron transport equation in planar geometries.

Properties: $E_n(z)$ is analytic in plane cut along negative real axis.

$$E_1(z) = -\gamma - \ln z - \sum_{n=1}^{\infty} \frac{(-1)^n z^n}{n\, n!},\quad \gamma = .57721\ldots \text{ Eulers constant}$$

Other properties are tabulated in A.M.S. 55

C. Error Functions:

Representations:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$$

$$w(z) = e^{-z^2} \operatorname{erfc}(iz) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2} dt}{z-t}$$

Habitat: The erf(z) functions frequently arise in the solution of diffusion or wave equations in infinite geometries. The w(z) function arises in plasma physics, where it is denoted by

$$Z(\zeta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-t^2} dt}{t-\zeta} = i\sqrt{\pi}\, W(\zeta)$$

Properties:

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{n!\,(2n+1)}$$

Occasionally one will encounter other types of special functions--such as the elliptic integrals which occur in certain types of coordinate systems. These are really much too specialized to even define here, so we will just refer you to AMS 55.

APPENDIX E

"SOME ASSORTED FACTS ON LINEAR OPERATORS"

I. SCALAR PRODUCTS

We define the scalar product or inner product (f,g) of two functions f(x) and g(x) as

$$(f,g) \equiv \int_a^b dx\, w(x)\, f^*(x)\, g(x) \tag{E-1}$$

[here, w(x) is frequently taken as 1] where f*(x) denotes the complex conjugate of f(x). This scalar product has the properties

(i) $(f,g) = (g,f)^*$

(ii) $(af_1(x) + bf_2(x), g) = a^*(f_1,g) + b^*(f_2,g)$

(iii) $(f,f) > 0$ if $f(x) \neq 0$

[Note: Sometimes one defines a real scalar product

$$(f,g) = \int_a^b dx\, w(x)\, f(x) g(x)$$

Such a form satisfies properties (i) and (ii), but property (iii) is satisfied only for real functions. Hence, if you are going to worry about complex valuedfunctions, you are pretty much forced to use the complex form (1).]

We define the norm of a function f(x) as

$$\|f\| \equiv [(f,f)]^{1/2} \tag{E-2}$$

The norm is a real, positive number (by property (iii) above) and characterizes the "magnitude" of the function f(x).

Two functions f(x) and g(x) are said to be orthogonal if their scalar product vanishes, i.e.,

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B. Friedmann, Principles and Techniques of Applied Mathematics (John Wiley, 1956)

R. Courant and D. Hilbert, Methods of Mathematical Physics Vol. I (Interscience)

$$(f,g) = 0 \tag{E-3}$$

II. LINEAR OPERATORS

An <u>operator</u> refers to a mathematical operation by which we convert a function $f(x)$ into another function $g(x)$--i.e.,

$$A\ f(x) = g(x) \tag{E-4}$$

[In the more colorful language of linear vector spaces, an operator is "a <u>mapping</u> of a linear vector space into a linear vector space".]

EXAMPLES:

(i) differential operator $A\circ \equiv \frac{d}{dx}$, $Af = \frac{df}{dx}$

(ii) integral operator $A\circ \equiv \int_a^b dx'\,k(x,x')\circ$, $Af = \int_a^b dx'\,k(x,x')f(x')$

(iii) unit operator $A\circ \equiv 1\circ$, $Af = f(x)$

(iv) null operator $A\circ = 0\circ$, $0f = 0$

(v) displacement operator $A\circ = e^{-\alpha\frac{d}{dx}}\circ$, $Af = f(x-\alpha)$

(vi) $A\circ = (\circ)^2$, $Af = [f(x)]^2$

If $A(af + bg) = a\,Af + b\,Ag$, then we refer to A as a <u>linear</u> operator. [Note that the first five operators above are linear, while the sixth operator is a nonlinear operator.]

Notice that such operators can frequently be manipulated formally via ordinary algebra, much as one manipulates numbers or functions. However one must be very careful. In particular, note that operators are generally not <u>commutative</u>

$$A\ B\ f(x) \neq B\ A\ f(x) \tag{E-5}$$

There is one other animal, quite similar to an operator, which occasionally arises in mathematics. One refers to this mathematical operation which converts a function into a scalar as a functional $\mathcal{F}$

$$\mathcal{F}\left\{f(x)\right\} = a = \text{number} \qquad \text{(E-6)}$$

[or, if you prefer, "a mapping of a vector space into a scalar field".]

EXAMPLE: A definite integral

$$\mathcal{F}\left\{f(x)\right\} = \int_a^b dx\, f(x) \qquad = \text{number}$$

In this sense, if we fix f(x), then we can regard the scalar product of f(x) with g(x) as a functional of g(x), i.e.,

$$\mathcal{F}\left\{g(x)\right\} = (f, g) \qquad = \text{number}$$

III. LINEAR VECTOR SPACES

We have now defined the concept of an operator. Of course, such an animal is meaningless until we specify the types of functions we are going to let it act upon. For example, it makes no sense to let a differential operator d/dx act on a discontinuous function, since df/dx is not defined at the point of discontinuity.

Hence, in practice, one studies an operator A by first specifying the class or type of function upon which he will let A operate . Such classes of functions usually possess the properties of a linear vector space, defined as a set of functions closed under the operations of addition and of multiplication by a scalar and which contains a zero element. [That is, if f(x) and g(x) are any two functions (complex-valued unless otherwise specified) contained in the set V (the "linear vector space"), then

(i) f(x) + g(x) is also contained in V

(ii) [a f(x)] is contained in V for any complex scalar a

(iii) the zero function is contained in V

Examples of Linear Vector Spaces:

(i) $C^0[a,b]$: the set of all continuous functions $f(x)$ defined on the interval $x \in [a,b]$

(ii) $C^n[a,b]$: the set of all functions defined on $x \in [a,b]$ with n continuous derivatives

(iii) $L_2[a,b]$: the set of all functions $f(x)$ defined on $x \in [a,b]$ such that

$$\int_a^b dx\, |f(x)|^2 < \infty$$

[This is an example of a "Hilbert space".]

(iv) $L_p[a,b]$: the set of all functions $f(x)$ defined on $x \in [a,b]$ such that

$$\int_a^b dx\, |f(x)|^p < \infty$$

[This is an example of a "Banach space".]

Note that for studying a differential operator of order n, we usually choose a corresponding space C^{n-1}. For an integral operator, the L_p spaces are usually chosen.

The particular linear vector space or class of functions for which an operator A is defined is referred to as its domain $\mathcal{D}$. Usually, $\mathcal{D}$ will be a subspace of a larger vector space V [that is, the functions belonging to the class $\mathcal{D}$ will also belong to a more general class V.]

For instance, $A = d/dx$ is defined on the domain of all continuous functions, $D = C^0$. This class, however, is actually contained in the more general class of piecewise continuous functions P--i.e. $\mathcal{D} \subset P$.

IV. PROPERTIES OF OPERATORS

Consider now a linear operator A defined on a domain of functions $\mathcal{D}$. Then we refer to A as a <u>bounded</u> operator on this domain if

$$\frac{\|Af\|}{\|f\|} < \infty \qquad \text{for all } f(x) \in \mathcal{D} \qquad \text{(E-7)}$$

If A is bounded on $\mathcal{D}$, then we can define its norm (an operator norm) as the largest of these values

$$\|A\| = \max_{f \in \mathcal{D}} \frac{\|Af\|}{\|f\|} \qquad \text{(E-8)}$$

Let us go one step further and associate a scalar product (f,g) with any two functions f,g contained in the domain $\mathcal{D}$. Then we can define a positive definite operator as one for which

$$(f, Af) > 0 \qquad \text{for all } f \neq 0 \qquad \text{(E-9)}$$

Using the scalar product (f,g), we can now introduce the very important concept of the operator $A^\dagger$ adjoint to A. We define the adjoint $A^\dagger$ of an operator A as that operator $A^\dagger$ for which

$$(A^\dagger f, g) = (f, A g) \qquad \text{for all } f,g \in \mathcal{D}$$

Actually, it may occur in practice that $A^\dagger$ and A are defined over different domains--say $\mathcal{D}^\dagger$ and $\mathcal{D}$. Then this definition of the adjoint operator must be defined by

$$(A^\dagger f \;, g) = (f \;, A g) \qquad \text{for all } \begin{matrix} g \in \mathcal{D} \\ f \in \mathcal{D}^\dagger \end{matrix} \qquad \text{(E-10)}$$

Should

$$A^\dagger = A \qquad \text{(E-11)}$$

then we refer to the operator A as self-adjoint. Operators which are self-adjoint are very popular in mathematics--because they are easy to study--particularly with regard to their associated eigenvalue problem

$$A\psi_\lambda(x) = \lambda\psi_\lambda(x)$$

For instance, for self-adjoint operators, the eigenvalues λ are all real. Furthermore, one can make statements regarding the eigenfunctions $\psi_\lambda(x)$ --e.g., they form a complete set, etc. One reason for the preoccupation of mathematicians with self-adjoint operators concerns their role in quantum mechanics [all quantum mechanical observables correspond to self-adjoint operators].

Unfortunately, theoperators we encounter in reactor theory are usually not self-adjoint (evidence the transport operator). Moreover, the operators we must deal with aren't quite a few other things--such as bounded or compact or normal or...lots of other properties. Only very recently has the theory of such operators been investigated in detail--and frequently tends to get mixed in the muck of functional analysis.

IV. DIFFERENTIAL OPERATORS

Let's make a few more comments about the particular case of differential operators L, defined on some domain D. For such operators, we can always construct the adjoint L using integration by parts:

EXAMPLE: $L = d/dx$, $\mathcal{D} = C[a,b]$

$$(f,Lg) = \int_a^b dx\, f^*(x)\frac{dg}{dx} = f^*(b)g(b) - f^*(a)g(a) - \int_a^b dx\, \frac{df^*}{dx}g(x)$$

$$= f^*(b)g(b) - f^*(a)g(a) + \left(-\frac{df}{dx}, g\right)$$

Hence, provided $J(f,g) = f^*(b)\,g(b) - f^*(a)\,g(a) = 0$, we could identify the adjoint of L as

$$L^\dagger = -d/dx$$

How do we force $J(f,g)$ to vanish? [Here, $J(f,g)$ is sometimes referred to as the conjunct of the operator L.] For a given problem, we will be given certain boundary conditions on $g(x)$--say $g(a) = c_1$, $g(b) = c_2$.

Hence by an appropriate choice of boundary conditions to be satisfied by $f(x)$ [in this case, $f(a) = c_2^*$, $f(b) = c_1^*$] we can force $J(f,g)$ to vanish. In general, the boundary conditions we are required to place on $f(x)$ will not be the same as those we place on $g(x)$--that is, in the more abstract language developed earlier, the domain of definition of the adjoint operator $L^\dagger$, $f \in \mathcal{D}^\dagger$, will generally not be the same as the domain on which L is defined.

A couple of definitions are useful here. If

$$L = L^\dagger$$

then we refer to the operator L as being formally self-adjoint. If the domains of definition are also identical

$$L = L^\dagger \qquad \text{and} \qquad \mathcal{D} = \mathcal{D}^\dagger$$

then we refer to the operator L plus the corresponding boundary conditions as being self-adjoint.

EXAMPLE: Consider the general second order differential operator

$$Lu = a(x)\frac{d^2u}{dx^2} + b(x)\frac{du}{dx} + c(x)u(x) \qquad a, b, c \text{ real}$$

Now integration by parts yields

$$(v, Lu) = \left[a\frac{du}{dx}v^* - u\frac{d}{dx}(av^*) + buv^*\right] + (L^\dagger v, u)$$

where

$$L^\dagger v^* = \frac{d^2}{dx^2}(av^*) - \frac{d}{dx}(bv^*) + cv^*$$

Now for L to be formally self-adjoint, we require

$$L^\dagger v^* = a\frac{d^2v^*}{dx^2} + \left(2\frac{da}{dx} - b\right)\frac{dv^*}{dx} + \left(\frac{d^2a}{dx^2} - \frac{db}{dx} + c\right)v^* = Lv^*$$

or equating terms

$$2\frac{da}{dx} - b = b \quad \Rightarrow \quad \frac{da}{dx} = b$$

$$\frac{d^2a}{dx^2} - \frac{db}{dx} + c = c \quad \Rightarrow \quad \frac{d^2a}{dx^2} = \frac{db}{dx}$$

Hence the most general form of a formally self-adjoint second order differential operator (for the scalar product (1)) is

$$Lu = a(x)\frac{d^2u}{dx^2} + \left(\frac{da}{dx}\right)\frac{du}{dx} + c(x)u(x)$$

$$= \frac{d}{dx}\left(a(x)\frac{du}{dx}\right) + c(x)u(x)$$

But, of course, this is just the familiar <u>Sturm-Liouville</u> operator. [Hence you can see why the study of the Sturm-Liouville equation plays such a central role in the theory of ordinary differential equations--since it is the most general example of a second order differential operator which is formally self-adjoint. For more information, refer to Courant and Hilbert--the bible on these matters.]

There are lots of fascinating problems and concepts which arise in the study of differential operators* [which, of course, play the central role in most of physics]. I'll refer you to Friedmann and Courant and Hilbert for more details.

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*Integral operators rarely occur in physics--but are easy to study (in comparison to differential operators)--hence explaining the mathematician's preoccupation with them.

APPENDIX F

"AN INTRODUCTION TO MATRICES AND MATRIX ALGEBRA"

I. SOME DEFINITIONS

One defines a matrix of order (mn) to be a rectangular array of m rows and n columns

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \cdots & a_{1n} \\ a_{21} & & \vdots & \vdots \\ \vdots & & a_{ij} & \vdots \\ a_{m1} & \cdots & \cdots & a_{mn} \end{pmatrix} \qquad \text{(F-1)}$$

The matrix elements a_{ij} will be identified by subscripts denoting their row i and column j.

If the matrix has the same number of rows as columns, it is said to be a square matrix:

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \qquad \text{(F-2)}$$

A diagonal matrix has nonzero elements only along its main diagonal:

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix} \qquad \text{(F-3)}$$

A tridiagonal matrix would have nonzero elements only along its central three diagonals

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 & \cdots \\ a_{21} & a_{22} & a_{23} & 0 & \cdots \\ 0 & a_{32} & a_{33} & a_{34} & \cdots \\ \vdots & \vdots & \vdots & & \end{pmatrix} \qquad \text{(F-4)}$$

The unit matrix has only "1"'s along its diagonal:

$$\underline{\underline{I}} = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \qquad \text{(F-5)}$$

For two matrices to be equal, each of their matrix elements must be equal:

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & & \\ \vdots & & & \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & \cdots \\ b_{21} & b_{22} & \cdots & \\ \vdots & \vdots & & \end{pmatrix} = \underline{\underline{B}} \qquad \text{(F-6)}$$

The transpose of a matrix is obtained by interchanging its rows and columns:

$$[\underline{\underline{A}}^*]_{ij} = [\underline{\underline{A}}]_{ji} \qquad \text{(F-7)}$$

or

$$\underline{\underline{A}}^* = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & \cdot & & \\ a_{31} & & & \\ \vdots & & & \end{pmatrix}^* = \begin{pmatrix} a_{11} & a_{21} & a_{31} & \cdots \\ a_{12} & & & \\ a_{13} & & & \\ \vdots & & & \end{pmatrix} \qquad \text{(F-8)}$$

The determinant of a matrix is formed by taking the determinant of the elements of the matrix:

$$\det \underline{\underline{A}} \equiv |\underline{\underline{A}}| = \begin{vmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & & & \\ a_{31} & & & \\ \vdots & & & \end{vmatrix} \qquad \text{(F-9)}$$

Of course, the determinant of a matrix is a scalar--i.e., just a number.

One defines the cofactor of a square matrix for an element a_{ij} by deleting the ith row and jth column, calculating the determinant of the remaining array, and multiplying by $(-1)^{i+i}$:

$$(\mathrm{cof}\,\underline{\underline{A}})_{23} = \mathrm{cof}\begin{pmatrix} a_{11} & a_{12} & \cancel{a_{13}} & a_{14} & \cdots \\ \cancel{a_{21}} & \cancel{a_{22}} & \cancel{a_{23}} & \cancel{a_{24}} & \cdots \\ a_{31} & a_{32} & \cancel{a_{33}} & a_{34} & \cdots \\ a_{41} & a_{42} & \cancel{a_{43}} & a_{44} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} = \begin{vmatrix} a_{11} & a_{12} & a_{14} & \cdots \\ a_{31} & a_{32} & a_{34} & \cdots \\ a_{41} & a_{42} & a_{44} & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix} \qquad \text{(F-10)}$$

Using the cofactor, we can define the adjoint of a square matrix by replacing each matrix element of the matrix by its cofactor and then transposing:

$$\underline{\underline{A}}^{\dagger} = (\mathrm{cof}\,\underline{\underline{A}})^{*}$$

$$\underline{\underline{A}}^{\dagger} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}^{\dagger} = \begin{pmatrix} a_{22} & -a_{21} \\ -a_{12} & a_{11} \end{pmatrix}^{*} = \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix} \qquad \text{(F-11)}$$

If the determinant of a matrix vanishes, det($\underline{\underline{A}}$)= 0, then the matrix $\underline{\underline{A}}$ is said to be *singular*. If det($\underline{\underline{A}}$) ≠ 0, the matrix is said to *nonsingular*.

II. MATRIX ALGEBRA

Two matrices of the same order may be *added* by adding their corresponding elements (the same holds for *subtraction*):

$$\underline{\underline{A}} + \underline{\underline{B}} = \begin{pmatrix} a_{11} & a_{12} \cdots \\ a_{21} & \\ \vdots & \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} \cdots \\ b_{21} & \\ \vdots & \end{pmatrix} = \begin{pmatrix} a_{11}+b_{11} & a_{12}+b_{12} \cdots \\ a_{21}+b_{21} & \\ \vdots & \end{pmatrix} \qquad \text{(F-12)}$$

In order for *matrix multiplication* to be possible, the number of columns of the first matrix must equal the number of rows of the second matrix. One then calculates the matrix elements of $\underline{\underline{C}} = \underline{\underline{A}} \cdot \underline{\underline{B}}$ as

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \qquad \text{(F-13)}$$

or more explicitly

$$\underline{\underline{A}} \cdot \underline{\underline{B}} = \begin{pmatrix} \cancel{a_{11}} & \cancel{a_{12}} & \cancel{a_{13}} \cdots \\ a_{21} & a_{22} & a_{23} \cdots \\ a_{31} & a_{32} & a_{33} \cdots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \cancel{b_{11}} & b_{12} & b_{13} \cdots \\ \cancel{b_{21}} & b_{22} & b_{23} \cdots \\ \cancel{b_{31}} & b_{32} & b_{33} \cdots \\ \vdots & & \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} + \cdots & \\ a_{21}b_{12} + a_{22}b_{22} + \cdots & \\ & \end{pmatrix} \qquad \text{(F-14)}$$

Notice that matrix multiplication is not commutative--i.e., $\underline{\underline{A}} \cdot \underline{\underline{B}} \neq \underline{\underline{B}} \cdot \underline{\underline{A}}$ in general.

A very important matrix operation is the *inverse*, $\underline{\underline{A}}^{-1}$, which is defined by the relation

$$\underline{\underline{A}}^{-1} \cdot \underline{\underline{A}} = \underline{\underline{A}} \cdot \underline{\underline{A}}^{-1} = \underline{\underline{I}} \tag{F-15}$$

The inverse can be calculated as

$$\underline{\underline{A}}^{-1} = \frac{1}{|\underline{\underline{A}}|} \underline{\underline{A}}^{\dagger} \tag{F-16}$$

For example, consider

$$\underline{\underline{A}} = \begin{pmatrix} 2 & 1 \\ -1 & 1 \end{pmatrix}$$

Then

$$|\underline{\underline{A}}| = 3$$

while

$$\underline{\underline{A}}^{\dagger} = \begin{pmatrix} 1 & 1 \\ -1 & 2 \end{pmatrix}^{*} = \begin{pmatrix} 1 & -1 \\ 1 & 2 \end{pmatrix}$$

Hence

$$\underline{\underline{A}}^{-1} = \frac{1}{3}\begin{pmatrix} 1 & -1 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 1/3 & -1/3 \\ 1/3 & 2/3 \end{pmatrix}$$

Notice that if a matrix is singular, i.e., $\det(\underline{\underline{A}}) = 0$, then it has no inverse.

APPENDIX G

"AN INTRODUCTION TO LAPLACE TRANSFORMS"

I. MOTIVATION

Differential equations play a central role in the description of most scientific phenomena. Moreover, in many cases these phenomena can be approximately described by a particularly simple type of differential equation--namely, one with constant coefficients. In this Appendix we will try to develop one of the most powerful tools for solving such equations: the application of integral transforms, and more specifically, the use of Laplace transforms to solve differential equations.

The analogy between the use of transform methods to solve differential equations and the use of logarithms to simplify arithmetic operations is quite striking. Suppose we wish to multiply two complicated numbers, a and b, together. Then an easy way to do this is to use logarithms

$$a \longrightarrow \log a$$

$$a \times b \rightarrow \boxed{\text{"transform"}} \rightarrow \log a + \log b \qquad \rightarrow \boxed{\text{"invert"}} \rightarrow e^{(\log a + \log b)} = a \times b$$

That is, by first taking logs, we have simplified the original problem, reducing it to a simple sum.

This is essentially the idea behind integral transform techniques. Suppose we symbolically represent the transform operation of a function as

$$f(t) \longrightarrow \tilde{f}(s)$$

Then the idea is to transform the differential equation of interest

$$\frac{df}{dt} + \cdots \rightarrow \boxed{\text{transform}} \rightarrow s\tilde{f}(s) + \cdots \qquad \rightarrow \boxed{\text{invert}} \rightarrow f(t)$$

In this manner, the integral transform can be used to convert this differential equation into a simpler problem (frequently an algebraic equation) which can then be solved rather easily for the transformed solution. We then must somehow "invert" the transform to obtain the actual solution of interest.

EXAMPLE: Consider the very simple ordinary differential equation (familiar from reactor kinetics

$$\frac{dn}{dt} + \left(\frac{\rho}{\Lambda}\right) n(t) = 0 \,, \quad n(0) = n_0 \tag{G-1}$$

Now define the Laplace transform of n(t) as

$$\tilde{n}(s) = \int_0^\infty dt e^{-st} n(t) \equiv \mathcal{L}\{n\} \tag{G-2}$$

To transform the ordinary differential equation (1), multiply by e^{-st} and integrate over t

$$\int_0^\infty dt e^{-st} \frac{dn}{dt} + \left(\frac{\rho}{\Lambda}\right) \int_0^\infty dt e^{-st} n(t) = 0$$

or using integration by parts

$$s\tilde{n}(s) - n(0) + \left(\frac{\rho}{\Lambda}\right) \tilde{n}(s) = 0$$

But this is now just an algebraic equation which can be easily solved for

$$\tilde{n}(s) = \frac{n_0}{s + (\rho/\Lambda)} \tag{G-3}$$

We must now "invert" to find

$$n(t) = \mathcal{L}^{-1}\{\tilde{n}(s)\} \tag{G-4}$$

By noting that

$$\mathcal{L}\{e^{-at}\} = \int_0^\infty dt e^{-st} e^{-at} = \frac{1}{s+a} \Rightarrow \mathcal{L}^{-1}\left\{\frac{1}{s+a}\right\} = e^{-at}$$

we find

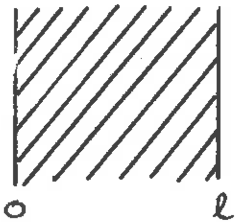
$$n(t) = n_0 \mathcal{L}^{-1}\left\{\frac{1}{s+(\rho/\Lambda)}\right\} = n_0 e^{-(\rho/\Lambda)t} \tag{G-5}$$

EXAMPLE: Integral transforms can also be applied to the solution of partial differential equations. Consider, for example, the initial value problem for a non-multiplying slab in one-speed diffusion theory

$$\frac{1}{v}\frac{\partial\Phi}{\partial t} = D\frac{\partial^2\Phi}{\partial x^2} + \Sigma_a \Phi(x,t)$$

$$\text{i.c.} \quad \Phi(x,0) = \Phi_0(x) \tag{G-6}$$

$$\text{b.c.} \quad \Phi(0,t) = \Phi(\ell,t) = 0$$



Define the Laplace transform of $\Phi(x,t)$ with respect to t by

$$\tilde{\Phi}(x,s) = \int_0^\infty dt\, e^{-st}\Phi(x,t) \tag{G-7}$$

Now multiplying (G-6) by e^{-st} and integrating over all times t, we find the transformed partial differential equation becomes

$$\frac{1}{v}\left[s\tilde{\Phi}(x,s) - \Phi(x,0)\right] = D\frac{d^2\tilde{\Phi}}{dx^2} + \Sigma_a\tilde{\Phi}(x,s)$$

Since the boundary conditions also depend on time, we must transform them to find

$$\text{b.c.} \quad \tilde{\Phi}(0,s) = \tilde{\Phi}(\ell,s) = 0$$

Hence, if we regard s only as a parameter, the application of Laplace transforms has reduced our original <u>partial</u> differential equation (G-6) to an inhomogeneous <u>ordinary</u> differential equation in x

$$D\frac{d^2\tilde{\Phi}}{dx^2} + \left(\Sigma_a - \frac{s}{v}\right)\tilde{\Phi}(x,s) = \Phi_0(x) \tag{G-8}$$

$$\text{b.c.} \quad \tilde{\Phi}(0,s) = \tilde{\Phi}(\ell,s) = 0$$

We can now solve this in any of the standard ways (e.g., eigenfunction expansions, Green's functions, etc.) to find $\tilde{\Phi}(x,s)$, and then invert to find

$$\Phi(x,t) = \mathcal{L}^{-1}\{\tilde{\Phi}(x,s)\} \tag{G-10}$$

Hence as should be apparent from these simple examples, Laplace transforms can be used to greatly simplify the solution of differential equations by

1. transforming the original differential equation
2. solving the transformed equation (which is now presumably a simpler equation such as an algebraic equation or ordinary differential equation) for the transformed solution
3. finally invert the transformed solution to obtain the desired solution of the original equation.

It is usually a straightforward task to complete the first two steps. The final step, that of inversion, can frequently be accomplished in a "cookbook" fashion by merely looking up the inverse in a table of Laplace transforms that some other fellow has had to work out. The general theory of how to perform such inversions from scratch is important, however, since the inverses of many of the functions one encounters in practice are not tabulated.

For that reason, our study of Laplace transforms will be divided into three parts: first, a look at cookbook Laplace transforms (sometimes called "operational mathematics" or Heaviside calculus), then a look at the more general theory of Laplace transforms as a subject in the theory of functions of a complex variable, and finally a brief discussion of alternative types of integral transforms (Fourier transforms, Mellin transforms, Hankel transforms, etc.)

II. COOKBOOK LAPLACE TRANSFORMS

We will now set up the recipes for solving differential equations with Laplace transforms. First, we must figure out just what types of problems we can tackle:

(i) Any differential equation (ordinary or partial) in which the variable to be transformed runs from 0 to ∞. (Such as an initial value problem in time, or a half-space problem in space.)

(ii) We will further restrict ourselves to the study of differential equations with constant coefficients (i.e., the coefficients in the equation do not depend on the variable we are transforming with respect to). This restriction can sometimes be relaxed; however we will not consider the more general problem of differential equations with variable coefficients here.

We will define the Laplace transform of a function f(t) by

$$\boxed{\tilde{f}(s) = \int_0^\infty dt\, e^{-st} f(t)} \qquad \text{(G-11)}$$

There are of course some restrictions on the type of function f(t) and the ranges of values of s for which this integral will be properly defined, but let's not worry about details at this stage of the game.

The general scheme for transforming the differential equation we are interested in solving is the same as before--namely, multiply by e^{-st} and integrate over all t, using liberal integration by parts. One then solves the resulting transformed equation and attempts to invert the solution.

To facilitate in the preparation of a table of Laplace transforms (a cookbook), one merely takes the transforms of as many different functions as possible. Several useful transforms of general functions are:[7,8]

<u>Derivatives</u>:

$$\boxed{\mathcal{L}\left\{\frac{df}{dt}\right\} = s\tilde{f}(s) - f(0)} \qquad \text{(G-12)}$$

(Recall that we obtained this by integration by parts. Further integration by parts yields

$$\boxed{\mathcal{L}\left\{\frac{d^nf}{dt^n}\right\} = s^n\tilde{f}(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - f^{[n-1]}(0)} \quad) \qquad \text{(G-13)}$$

<u>Integration</u>:

$$\boxed{\mathcal{L}\left\{\int_0^t dt' f(t')\right\} = \frac{1}{s}\tilde{f}(s)} \qquad \text{(G-14)}$$

(Proof:

$$\mathcal{L}\left\{\int_0^t dt' f(t')\right\} = \int_0^\infty dt\, e^{-st}\int_0^t dt\, f(t') = -\frac{e^{-st}}{s}\int_0^t dt' f(t')\Big|_0^\infty + \frac{1}{s}\int_0^\infty dt\, e^{-st}f(t)$$
$$= \frac{1}{s}\tilde{f}(s) \quad .)$$

<u>Differentiation by s</u>:

$$\boxed{\mathcal{L}\{t f(t)\} = -\frac{d\tilde{f}}{ds}} \qquad \text{(G-15)}$$

(Proof:

$$\frac{d\tilde{f}}{ds} = \int_0^\infty dt\, f(t)\, \frac{d}{ds}\left(e^{-st}\right) = -\int_0^\infty dt\, e^{-st}\left[t f(t)\right] \quad .)$$

<u>Complex translation</u>:

$$\boxed{\mathcal{L}\{e^{at}f(t)\} = \tilde{f}(s-a)} \qquad \text{(G-16)}$$

(Proof:

$$\int_0^\infty dt\, e^{at}e^{-st}f(t) = \int_0^\infty dt\, e^{-(s-a)t}f(t) = \tilde{f}(s-a) \quad .)$$

<u>Real translation</u>:

$$\boxed{\mathcal{L}\{f(t-a)\Theta(t-a)\} = e^{-as}\tilde{f}(s)} \qquad \text{(G-17)}$$

where $\Theta(t)$ is the step function, $\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}$

Several examples of more specific transform pairs are:

$f(t)$	$\tilde{f}(s) = \mathcal{L}\{f(t)\}$
e^{-at}	$\frac{1}{s+a}$
$\frac{t^n}{n!}$	$\frac{1}{s^{n+1}}$
$\sin \omega t$	$\frac{\omega}{s^2+\omega^2}$

$\cos\omega t$	$\frac{s}{s^2+\omega^2}$
$1(t)$	$\frac{1}{s}$
$\delta(t)$	1

Several other very useful relations[7,8] are

Convolution Theorem:

$$\boxed{\mathcal{L}\left\{\int_0^t d\tau f(t-\tau)g(\tau)\right\} = \tilde{f}(s)\tilde{g}(s)} \qquad \text{(G-18)}$$

(This result is useful for relating the inverse of the product of two transformed functions.)

Initial Value Theorem:

$$\boxed{\lim_{t\to 0} f(t) = \lim_{s\to\infty} s\tilde{f}(s)} \qquad \text{(G-19)}$$

Final Value Theorem:

$$\boxed{\lim_{t\to\infty} f(t) = \lim_{s\to 0} s\tilde{f}(s)} \qquad \text{(G-20)}$$

There are a number of reasonably complete tables of such transform pairs.[7,8] After obtaining the transformed solution, one can then turn to such tables in an effort to locate the desired inverse. However in many cases it will be necessary to proceed with a direct inversion calculation. Hence we will now develop the general theory of Laplace transforms and their inverses.

III. THE GENERAL THEORY OF LAPLACE TRANSFORMS

Consider the class of all functions f(t) such that

1) f(t) is defined and continuous for all $t \geq 0$ except for a finite number of points.

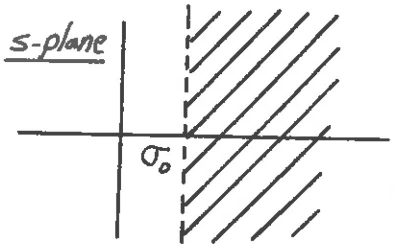
2.) $\int_0^T |f(t)|\, dt$ exists for every $T > 0$ (absolutely integrable over any finite interval).

3.) $\int_0^\infty e^{-\sigma t}|f(t)|\,dt < \infty$ for some real number σ.

We can then define the Laplace transform of f(t) by

$$\tilde{f}(s) = \mathcal{L}\{f(t)\} = \int_0^\infty e^{-st} f(t)\,dt \quad \text{for} \quad \mathrm{Re}\{s\} > \sigma. \tag{G-21}$$

One can prove that this definition is unique (i.e., f(t) uniquely implies $\tilde{f}(s)$ and vice versa). Further, if we denote σ_0 to be the greatest lower bound of the set of all σ such that condition (3) is satisfied, then one can show that

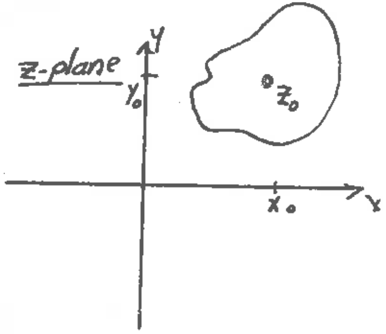


THEOREM: The Laplace transform $\tilde{f}(s)$ is an <u>analytic</u> function of the complex variable s for all s such that $\mathrm{Re}\{s\} > \sigma_0$.

(Here, σ_0 is referred to as the "abscissa of convergence".)

We have given a rigorous definition of the Laplace transform $\tilde{f}(s)$ of any admissible function f(t). Our task is now to invert this definition to obtain a formula for f(t) in terms of $\tilde{f}(s)$. There are several ways to proceed--all of which rely on the theory of functions of a complex variable. Hence, let's first lay a little background.

A Review of the Theory of Functions of a Complex Variable:[1,2,3]

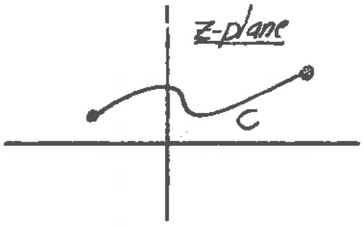


Consider a function f(z) of a complex variable $z = x + iy$. Then we say that f(z) is "analytic" at a point $z = z_0$ if df/dz exists for all z in some neighborhood of z_0. (Frequently one uses the words "regular" or "holomorphic" in place of "analytic".) A necessary condition for the analyticity of a function $f(z) = u(x,y) + iv(x,y)$ at z_0 is that it satisfy the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \quad \text{at } x = x_0,\ y = y_0 \tag{G-22}$$

If f(z) is analytic for all finite z, then we say it is an "entire" function.

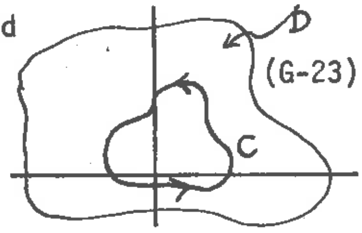
One can also talk about integrals of functions of a complex variable. However, unlike real integrals, one must now specify the path of integration, e.g.,



$$\int_C f(z)\,dz$$

The most important theorem concerning such integrals is the following (Cauchy Integral Theorem):

THEOREM: Consider a function f(z) which is analytic in a domain D. Then if C is a simple closed curve in D,



$$\oint_C f(z)\,dz = 0 \tag{G-23}$$

This theorem plays a very fundamental role in the theory of functions of a complex variable. A related theorem is

THEOREM: (Cauchy Integral Formula)

$$f(z) = \frac{1}{2\pi i}\oint_C \frac{f(\xi)\,d\xi}{\xi - z} \tag{G-24}$$

where z is inside C and f(z) is analytic on and inside C.

Thus far we have been discussing functions which are analytic. But the most interesting functions are ones which exhibit nonanalytic behavior--that is, possess "singularities". We will limit our immediate attention to functions which are nonanalytic only at certain discrete points, i.e., possess "isolated singularities" or "isolated singular points" (i.s.p.)

EXAMPLES:

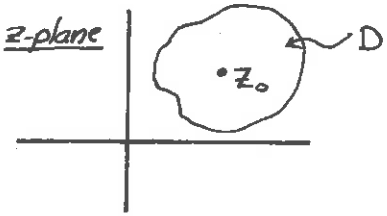
(i) $f(z) = (z - z_0)^{-1}$ $z = z_0$ is an i.s.p.

(ii) $f(z) = 1/\sin(1/z)$ $z = 1/n\pi$ are i.s.p. for $n = \pm 1, \pm 2, \ldots$ (Note however that the origin $z = 0$ is not an i.s.p.)

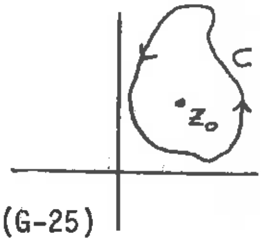
(iii) $f(z) = \log z$ $z = 0$ is not an i.s.p.

To classify such isolated singularities, one considers power series expansions about the point of interest. If $f(z)$ is analytic at and in some neighborhood of a point z_0, then one can use the usual <u>Taylor series</u> expansion

$$f(z)=\sum_{n=0}^{\infty} \frac{1}{n!} f^{[n]}(z_0)\,(z-z_0)^n$$



Suppose, however, that $f(z)$ has an i.s.p. at $z = z$, but is analytic in some neighborhood of z_0. Then one must use an alternative type of expansion, a so-called "Laurent series"



$$f(z)= \frac{a_{-N}}{(z-z_0)^N} + \frac{a_{-N+1}}{(z-z_0)^{N-1}} + \cdots + \frac{a_{-1}}{(z-z_0)} + a_0 + a_1(z-z_0) + \cdots \qquad \text{(G-25)}$$

where

$$a_n = \frac{1}{2\pi i}\oint_C \frac{f(z)\,dz}{(z-z_0)^{n+1}}$$

Such an expansion can actually be used to classify thenature of the singularity at $z = z_0$. To this end, consider the expansion (25)

$$f(z)= \frac{a_{-N}}{(z-z_0)^N} + \frac{a_{-N+1}}{(z-z_0)^{N-1}} + \cdots + \frac{a_{-1}}{(z-z_0)} + a_0 + a_1(z-z_0) + \cdots \qquad \text{(G-25')}$$

The leading term of the Laurent expansion (25) about z_0 determines the type of singularities at z_0. If the leading term is

$\frac{a_{-1}}{(z-z_0)}$,	then we say that $f(z)$ has a "pole" at $z = z_0$
$\frac{a_{-N}}{(z-z_0)^N}$,	" " " " " " " "pole of order N"
$N=\infty$,	" " " " " " " "essential singularity"
$a_n(z-z_0)^n$,	then $f(z)$ is analytic at z_0, and $z = z_0$ is a zero of order n.

A further definition of considerable use is the "residue" of an i.s.p., defined to be the coefficient a_{-1} of the $(z - z_0)^{-1}$ term in the Laurent expansion. This is denoted by

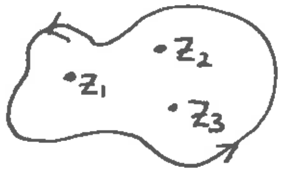
$$\operatorname*{Res}_{z=z_0}\{f(z)\} = a_{-1} \tag{G-26}$$

From its definition (26) and (25), one can give an alternative expression for the residue of a function at a pole of order N

$$\operatorname*{Res}_{z=z_0}\{f(z)\} = \lim_{z\to z_0} \frac{1}{(N-1)!}\frac{d^{N-1}}{dz^{N-1}}\left[(z-z_0)^N f(z)\right] \tag{G-27}$$

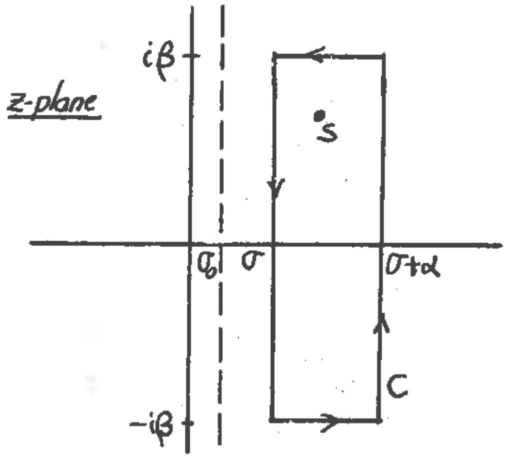
With these definitions, we can state a final theorem involving complex integration:

RESIDUE THEOREM: Let C be a simple closed curve and let f(z) be analytic on and within C except at the points $z_1, z_2, \ldots, z_m$, all of which lie inside C. Then



$$\oint_C f(z)dz = 2\pi i \sum_{j=1}^{m} \operatorname*{Res}_{z=z_j}\{f(z)\} \tag{G-28}$$

Let's return now to construct the inversion formula for Laplace transforms. Since $\tilde{f}(s)$ is analytic for Re $\{s\} > \sigma_0$, suppose we apply Cauchy's formula (24) to the contour C as shown



$$\tilde{f}(s) = \frac{1}{2\pi i}\oint_C \frac{\tilde{f}(z)dz}{z-s}$$

where C is a simple closed curve surrounding s and lying in the half-plane $\operatorname{Re}\{z\} > \sigma_0$. We expect that as $\alpha, \beta \to \infty$, keeping σ fixed, all but the vertical path through σ will vanish. Thus let $\alpha, \beta \to \infty$. Then if the contributions from the two horizontal sides and the vertical side at Re $\{s\} = \sigma + \alpha$ vanish in the limit, we have

$$\tilde{f}(s) = -\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\tilde{f}(z)dz}{z-s} \ , \quad Re\{s\} > \sigma, \ \sigma > \sigma_0$$

But

$$\mathcal{L}\{f(t)\} = \tilde{f}(s)$$

Hence we can formally write

$$f(t) = \mathcal{L}^{-1}\{\tilde{f}(s)\} = -\frac{1}{2\pi i}\mathcal{L}^{-1}\left\{\int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\tilde{f}(z)dz}{z-s}\right\}$$

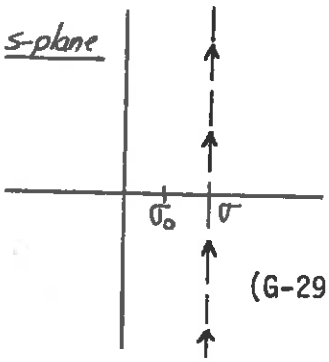
$$= -\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \tilde{f}(z)\,\mathcal{L}^{-1}\left\{\frac{1}{z-s}\right\}dz$$

But from p. 2, we know $\mathcal{L}\{\frac{1}{z-s}\} = -e^{zt}$. Hence

$$f(t) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \tilde{f}(z)e^{zt}dz$$

Thus our proposed inversion formula is

$$f(t) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} e^{st}\tilde{f}(s)ds \tag{G-29}$$



This formula, called the "Bromwich inversion formula" for Laplace transforms, can be verified in a more rigorous fashion by cleaning up the steps in our heuristic derivation.

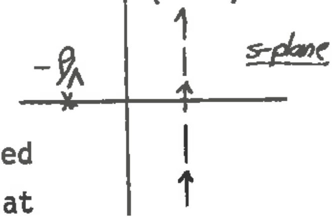
Thus we have now developed an explicit formula for the inverse of a Laplace transform. But the Bromwich inversion formula is obviously a rather complicated beast, involving as it does a contour integration in the complex s-plane. Hence we must now turn to a discussion of how one utilizes this formula in practice. Let's proceed by way of an example:

EXAMPLE: Consider the very simple ordinary differential equation (1) we solved earlier. Recall we found

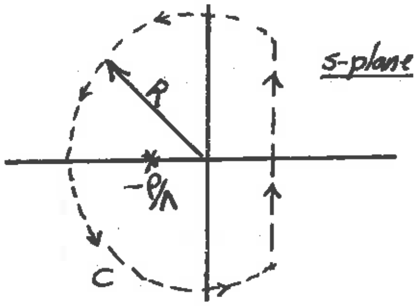
$$\tilde{n}(s) = \frac{n_0}{s+(\rho/\Lambda)} \tag{G-3}$$

Let's now try to apply the inversion formula (29) to find n(t)

$$n(t) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\, e^{st}\frac{n_0}{s+(\rho/\Lambda)} \tag{G-30}$$



Now we recall from its definition (2), $\tilde{n}(s)$ is only defined for Re $\{s\} > \sigma_0$. But in solving for $\tilde{n}(s)$, we now find that $\tilde{n}(s)$ as given by (3) is in fact defined and analytic for all s, with the exception of an isolated pole at $s = -\rho/\Lambda$. We can now use this information in the following way. Consider the closed contour C as shown. Since $\tilde{n}(s)$ is analytic, except for a pole in C, we can use the residue formula (28) to find



$$\oint_C \tilde{n}(s)e^{st}ds = 2\pi i \operatorname*{Res}_{s=-\rho/\Lambda}\{\tilde{n}(s)e^{st}\} = 2\pi i n_0 e^{-(\rho/\Lambda)t} \tag{G-31}$$

Now it is straightforward to verify that as $R \to \infty$, the contributions from the circular part of the contour C vanish, leaving

$$\lim_{R\to\infty}\oint_C \tilde{n}(s)e^{st}ds = \int_{\sigma-i\infty}^{\sigma+i\infty} ds\,\tilde{n}(s)e^{st} \tag{G-32}$$

Thus using (30), we find

$$n(t) = \frac{1}{2\pi i}\left[2\pi i\, n_0 e^{-(\rho/\Lambda)t}\right] = n_0 e^{-(\rho/\Lambda)t} \tag{G-33}$$

which agrees with our earlier inversion.

This same procedure can be used to evaluate the inversion integral (29) in more complicated cases:

1. First determine the analytic properties of $\tilde{f}(s)$ in the left half s-plane. (This is referred to as "analytic continuation".)

2. Using this information, construct a closed contour about all of the singularities of $\tilde{f}(s)$ in the left half plane, and use the residue theorem to evaluate the integral about this closed contour. ("contour deformation")
3. Take the curved portion of the contour path to infinity to reduce the contour integral to the form given by the original Bromwich formula (29).

This scheme is straightforward provided one only has isolated singularities to worry about (as will be the case with ordinary differential equations with constant coefficients). However, more general types of singularities arise in the case of partial differential equations. Consider the example below:

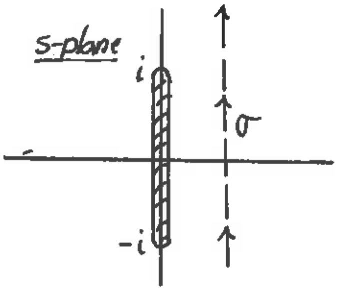
EXAMPLE: Suppose we try to invert

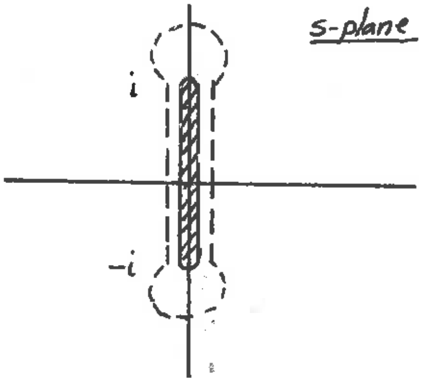
$$\tilde{f}(s) = \frac{1}{\sqrt{1+s^2}} \tag{G-34}$$

Then using the inversion formula (29), we wish to study

$$f(t) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\, e^{st}\frac{1}{\sqrt{1+s^2}} \tag{G-35}$$

Our first task is to identify the singularities of $\tilde{f}(s)$ in the complex s-plane. In this case, however, we note $\tilde{f}(s)$ must be defined very carefully since it is a multiple-valued function. In particular, $\tilde{f}(s)$ has branch point singularities at $s = \pm i$. We will define $\tilde{f}(s)$ to be a single-valued function by drawing in the branch cut as shown. Hence $\tilde{f}(s)$ is analytic, with the exception of all s on this cut.





If we now apply Cauchy's theorem, we can deform the Bromwich contour about the cut as shown. Then letting $s = i\beta$ on the cut, we find (35) becomes

$$f(t) = \frac{1}{\pi}\int_{-1}^{+1}\frac{e^{i\beta t}\,d\beta}{\sqrt{1-\beta^2}}$$

Letting $\beta = \sin\phi$, we find

$$f(t)=\frac{1}{\pi}\int_{-\pi/2}^{\pi/2}\frac{e^{it\sin\varphi}\cancel{\cos\varphi}\,d\varphi}{\cancel{\cos\varphi}} = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} e^{it\sin\varphi}\,d\varphi = J_0(t)$$

where $J_0(t)$ is a Bessel function of zeroth order.

To summarize and integrate these ideas, let's consider in detail the solution of a typical boundary value problem in partial differential equations using Laplace transforms:

EXAMPLE: Consider the problem given by

$$\frac{\partial^2\phi}{\partial x^2} - \frac{1}{\alpha^2}\frac{\partial\phi}{\partial t} = \delta(t - x/c) \quad , \quad \propto x<\infty, \; 0<t<\infty \tag{G-36}$$

with initial condition: $\phi(x,0)=0 \quad , \quad 0<x<\infty$

and boundary condition: $\phi(0,t)=0 \quad , \quad t>0$

(Such a problem would arise in the determination of the time-dependent neutron flux resulting from a source moving with speed c in a semi-infinite medium.)

Step 1: First we define the Laplace transform with respect to time t

$$\tilde{\phi}(x,s) \equiv \int_0^\infty dt\, e^{-st}\phi(x,t) \tag{G-37}$$

Now Laplace transform the differential equation and boundary conditions, noting that

$$\mathcal{L}\left\{\frac{\partial\phi}{\partial t}\right\} = s\tilde{\phi}(x,s) - \phi(x,0) = s\tilde{\phi}(x,s)$$

$$\mathcal{L}\{\delta(t-x/c)\} = \int_0^\infty dt\, e^{-st}\delta(t-x/c) = e^{-sx/c}$$

$$\mathcal{L}\left\{\frac{\partial^2\phi}{\partial x^2}\right\} = \frac{d^2\tilde{\phi}}{dx^2}$$

Thus our transformed equation becomes an inhomogeneous ordinary differential equation

$$\frac{d^2\tilde{\Phi}}{dx^2} - \frac{s}{\alpha^2}\tilde{\Phi}(x,s) = e^{-sx/c} \tag{G-38}$$

with boundary conditions $\tilde{\Phi}(0,s) = 0$

$\tilde{\Phi}(x,s)$ finite for all x

Step 2: We now must solve the transformed equation. Since this is an inhomogeneous equation, we seek both a homogeneous and particular solution

$$\tilde{\Phi}(x,s) = \tilde{\Phi}_{hom}(x,s) + \tilde{\Phi}_{part}(x,s)$$

The homogeneous solution obeying the boundary conditions is

$$\tilde{\Phi}_{hom}(x,s) = A e^{-\sqrt{s}\,x/\alpha}$$

For the inhomogeneous solution, try $\tilde{\Phi}_{part}(x,s) = B(s)e^{-sx/c}$ and substitute into (38) to find

$$B(s) = \frac{c^2}{s(s-c^2/\alpha^2)}$$

Thus our general transformed solution to (38) is

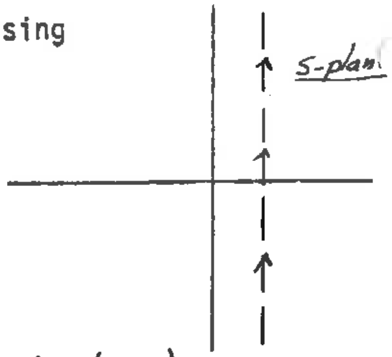
$$\tilde{\Phi}(x,s) = Ae^{-\sqrt{s}x/\alpha} + \frac{c^2}{s(s-c^2/\alpha^2)}e^{-sx/c}$$

Now applying the boundary condition $\tilde{\Phi}(0,s) = 0$ implies

$$A = -\frac{c^2}{s(s-c^2/\alpha^2)}$$

Hence the transformed solution becomes

$$\tilde{\Phi}(x,s) = \frac{c^2}{s(s-c^2/\alpha^2)}\left[e^{-sx/c} - e^{-\sqrt{s}\,x/\alpha}\right] \tag{G-39}$$



Step 3: We must now invert this transformed solution, using the inversion formula (29)

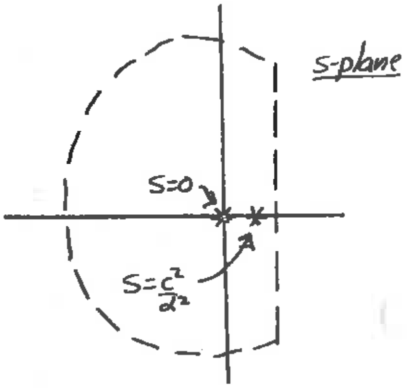
$$\phi(x,t)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\, e^{st}\,\tilde{\phi}(x,s)$$

For convenience, we will break this up into two parts

$$\phi(x,t)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{st}c^2e^{-sx/c}}{s(s-c^2/\alpha^2)}-\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{st}c^2e^{-\sqrt{s}x/\alpha}}{s(s-c^2/\alpha^2)}\equiv\phi_1(x,t)+\phi_2(x,t)$$

and invert each separately. Consider first

$$\phi_1(x,t)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{st}c^2e^{-sx/c}}{s(s-c^2/\alpha^2)}$$



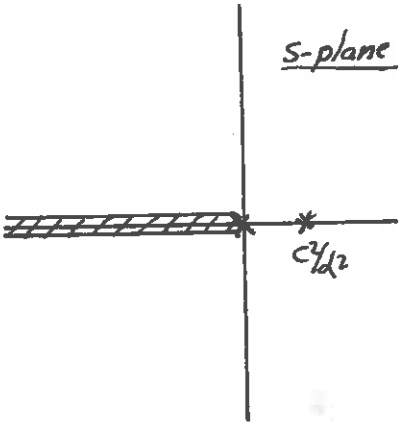
This has two poles in the s-plane as indicated. Hence by completing the contour in the LHP and using the residue theorem, we find

$$\phi_1(x,t)=\left[\frac{-c^2}{c^2/\alpha^2}+\frac{c^2e^{c^2/\alpha^2(t-x/c)}}{c^2/\alpha^2}\right]\Theta(t-x/c)$$

$$=-\alpha^2\left[1-e^{+c^2/\alpha^2(t-x/c)}\right]\Theta(t-x/c)$$

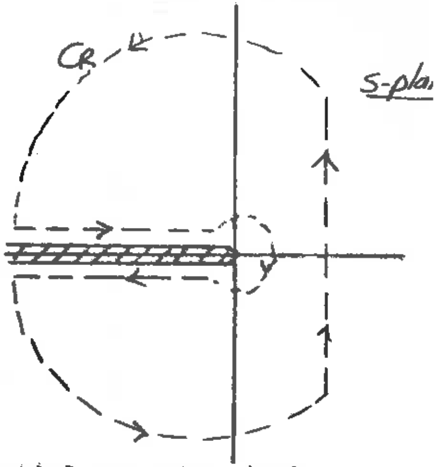
Now consider

$$\phi_2(x,t)=-\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{+st}c^2e^{-\sqrt{s}x/\alpha}}{s(s-c^2/\alpha^2)}$$



This inversion will be more complicated since $e^{-\sqrt{s}x/\alpha}$ has a branch point at the origin. We will define the branch cut to be along the negative real axis as shown.

Then by completing the contour into the LHP as shown, and letting $C_R \to \infty$, we find a contribution from the branch cut as well as contributions from the simple poles at $s = 0$ and $s = c^2/\alpha^2$



$$\phi_2(x,t) = \alpha^2\left[1 - e^{c^2/\alpha^2 t - cx/\alpha^2}\right] + \frac{1}{2\pi i}\int_{\text{cut}} ds \frac{e^{st} c^2 e^{-\sqrt{s}\, x/\alpha}}{s(s - c^2/\alpha^2)}$$

$$= \alpha^2\left[1 - e^{c^2/\alpha^2 (t - x/c)}\right] - \frac{1}{\pi}\int_0^\infty d\xi \frac{e^{-\xi t} c^2 \sin\sqrt{\xi}\, x/\alpha}{\xi(\xi + c^2/\alpha^2)}$$

Thus the final solution to the original partial differential equation (36) becomes

$$\phi(x,t) = -\alpha^2\left[1 - e^{c^2/\alpha^2 (t - x/c)}\right]\Theta(t - x/c)$$

$$+ \alpha^2\left[1 - e^{c^2/\alpha^2 (t - x/c)}\right] - \frac{1}{\pi}\int_0^\infty d\xi \frac{e^{-\xi t} c^2 \sin\sqrt{\xi}\, x/\alpha}{\xi(\xi + c^2/\alpha^2)}$$

IV. OTHER TYPES OF INTEGRAL TRANSFORMS

A. The Fourier Transform[4,5]

Consider a function f(x) defined for all $-\infty < x < \infty$ such that

$$\int_{-\infty}^{\infty} dx\, |f(x)| < \infty \qquad \text{(G-40)}$$

Then we define the Fourier transform of f(x) by

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{ikx} f(x) \qquad \text{(G-41)}$$

The inverse of this transform is given by

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, e^{-ikx} F(k) \qquad \text{(G-42)}$$

Fourier transforms find application to differential equations in which one of the variables ranges between $-\infty$ and ∞. The procedure for applying Fourier transforms is essentially identical to that we have outlined for Laplace transforms. Once again, contour integration in the complex k-plane can be used to invert the transformed solution.

EXAMPLE: Consider the simple ordinary differential equation

$$\frac{d^2\phi}{dx^2} - \kappa^2\phi(x) = \delta(x) \quad , \qquad -\infty < x < \infty$$

where, as boundary conditions, we will demand $\phi(x) \to 0$ as $|x| \to \infty$.

Now define the Fourier transform of $\phi(x)$ as

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{ikx} \phi(x).$$

Hence multiplying by e^{ikx} and integrating, one finds

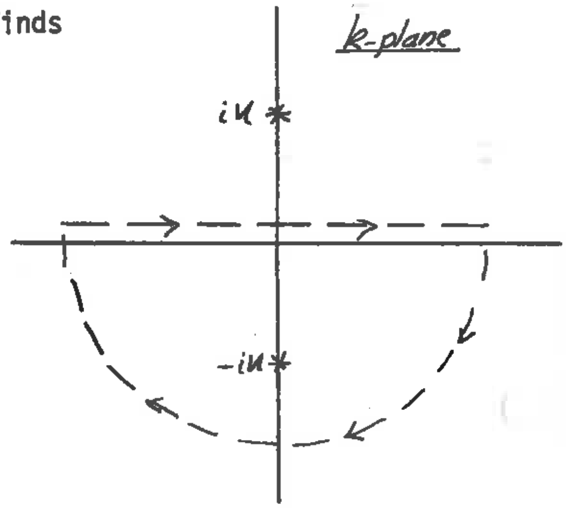
$$-(k^2+\kappa^2)\,\Phi(k) = \frac{1}{\sqrt{2\pi}}$$

Hence the transformed solution is just

$$\Phi(k) = \frac{-1/\sqrt{2\pi}}{k^2+\kappa^2}$$

Thus we can invert to obtain

$$\phi(x) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \frac{e^{-ikx}}{k^2+\kappa^2}$$



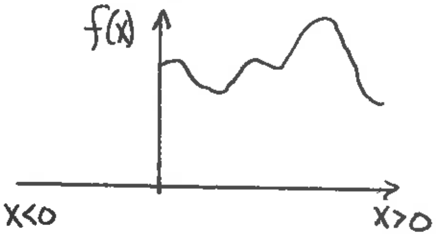
Notice that the integration path runs along the real axis of the complex k-plane. If we identify the poles of $\Phi(k)$ as $k = \pm i\kappa$, then for $x > 0$ we can complete the contour into the lower half plane, and evaluate the residue at $k = -i\kappa$ to find

$$\phi(x) = \frac{2\pi i}{2\pi} \operatorname*{Res}_{k=-i\kappa} \left\{ \frac{e^{-ikx}}{k^2+\kappa^2} \right\} = \frac{e^{-\kappa x}}{2\kappa} \quad , \quad x > 0 .$$

For $x < 0$, the contour can be completed in the upper half plane to find

$$\phi(x) = \frac{e^{\kappa x}}{2\kappa} \quad , \quad x < 0 .$$

There is a very direct connection between Fourier and Laplace transforms. (In fact, this relationship is frequently used to "derive" the Laplace transform inversion formula (29).) Remember that the Laplace transform applies to functions defined over the range 0 to ∞. Hence suppose we consider the Fourier transform of a function f(x) which is zero for all $x < 0$



$$F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,e^{ikx}f(x)=\frac{1}{\sqrt{2\pi}}\int_{0}^{\infty}dx\,e^{ikx}f(x)$$

or letting -s = ik

$$F(k)=\frac{1}{\sqrt{2\pi}}\int_{0}^{\infty}dx\,e^{-sx}f(x)=\frac{1}{\sqrt{2\pi}}\tilde{f}(s) \qquad \text{(G-43)}$$

The inverse is then given by

$$f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,e^{-ikx}F(k)=\frac{1}{\sqrt{2\pi}}\int_{+i\infty}^{-i\infty}\left(-\frac{1}{i}\right)ds\,e^{sx}\left[\frac{1}{\sqrt{2\pi}}\tilde{f}(s)\right] \qquad \text{(G-44)}$$

$$=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}ds\,e^{sx}\tilde{f}(s)$$

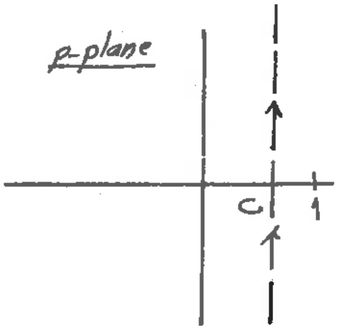
which is the usual Bromwich inversion formula (29) (if we note that from (40), $\sigma = 0$). Hence we can easily consider Laplace transforms to be merely a special case of Fourier transforms.

Suppose we consider the related question: If we know the Laplace transform $\tilde{f}(s)$ of a function, can we then determine its Fourier transform F(k)? In general, the answer to this question is no, since the inversion formula (29) only yields f(x) for $x > 0$, and the Fourier transform requires a knowledge of f(x) for all x such that $-\infty < x < \infty$. (In certain cases, knowledge of $\tilde{f}(s)$ is sufficient to imply F(k), but we shall not discuss these here.)

B. Mellin Transforms[4,5]

There are numerous other types of integral transforms which prove useful in the study of differential equations. One such animal is the Mellin transform, defined for some function f(r) as

$$F_m(p) = \int_0^\infty dr\, f(r)\, r^{p-1} \tag{G-45}$$



The inverse transform is

$$f(r) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} r^{-p} F_m(p)\, dp \tag{G-46}$$

where $0 < c < 1$. Such a transform is useful for polar coordinates--e.g., for equations such as

$$r \frac{\partial}{\partial r}\left(r \frac{\partial \psi}{\partial r} \right) + \frac{\partial^2 \psi}{\partial \theta^2} = 0$$

Then if we define

$$\Psi_m(p) = \int_0^\infty dr\, \psi(r)\, r^{p-1}$$

we can transform this equations to find

$$\frac{d^2 \Psi_m}{d\theta^2} + p^2 \Psi_m(\theta) = 0$$

which is just a simple ordinary differential equation for the transformed solution.

C. Hankel Transforms

Yet another transform is the Hankel transform defined for a function f(r) by

$$F_H(\rho) = \int_0^\infty dr\, r\, f(r)\, J_0(\rho r) \tag{G-47}$$

The inverse is

$$f(r) = \int_0^\infty d\rho\, F_H(\rho)\, J_0(\rho r) \tag{G-48}$$

where $J_0(\rho r)$ is the Bessel function of zero order. This transform is useful for problems involving cylindrical coordinates such as

$$\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r}\frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} = 0$$

The Hankel transform of this equation is just

$$\frac{d^2\Phi_H}{dz^2} - \rho^2\,\Phi_H(z) = 0$$

There are numerous other types of integral transforms one can use to attack differential equations. In fact, one can actually "derive" the integral transform most useful for treating a given equation directly from the form of this equation itself. This latter scheme is very closely connected with the ideas of Green's functions and eigenfunction expansions. The discussion of this very interesting subject will be deferred.

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