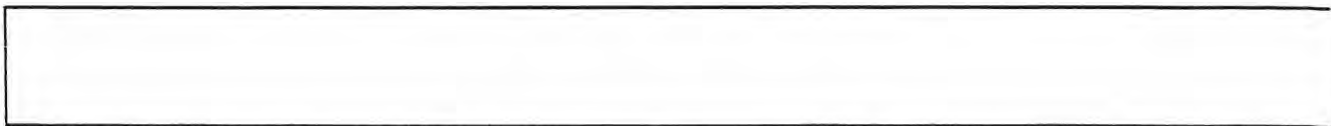


**NUCLEAR REACTOR
THEORY AND ANALYSIS
PART I**



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William R. Martin



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PREFACE

These materials are intended to accompany the University of Michigan videotape course in Nuclear Engineering entitled:

Nuclear Reactor Theory and Analysis I

Included in the materials are:

REFERENCES: We have provided a list of representative references and reading assignments intended to supplement the material covered in each lecture. Unfortunately, while there are numerous textbooks available on the subject of nuclear reactor theory, we are unaware of any textbook that covers material at a level or contemporary degree appropriate for this course. While we are preparing such a textbook, it will not be available until mid to late 1984. In the interim, we will assign specific reading assignments from the following textbooks:

- J. J. Duderstadt and L. J. Hamilton, **Nuclear Reactor Analysis** (Wiley, New York, 1976) (Covers all of the topics in both Nuclear Reactor Theory I and II at a level we believe is somewhat too advanced for these courses.)
- J. R. Lamarsh, **Introduction to Nuclear Engineering** (Addison-Wesley, Reading, Mass, 1975) (Considerably lower in level but of insufficient depth and rather dated in approach.)
- R. A. Rydin, **Nuclear Reactor Theory and Design** (University Publications, Blacksburg, VA, 1977) (Covers many of the appropriate topics but once again at a level we believe is inappropriate.)
- R. A. Knief, **Nuclear Energy Technology** (McGraw-Hill, New York, 1981) (A survey of a great many topics in nuclear engineering. Inappropriate as a text, but useful for an overview.)

We have provided reading assignments to augment each of the lectures. While not essential to the course content, these references will provide the student with additional material that may assist them in mastering the material covered in the lectures.

NOTES AND VISUAL MATERIALS: We have provided copies of all visual materials used in the videotape lectures along with comments to support these materials. These are presented in a form so that students can use them to follow the lectures and take notes in the margins. We hope to have more complete lecture notes available at a later point as the textbook on these courses nears completion. However these notes coupled with the reading assignments should be sufficient for present use.

PROBLEMS AND EXERCISES: We have included a number of problems and exercises with each lecture. We are convinced that the only

way to master the material covered by the lectures is by working such problems. Since the level and focus of the course will vary somewhat depending on the instructor and the student background, we have provided a rather wide variety of problems, ranging from simple exercises to challenging problems requiring the use of computers. The instructor will assign those problems deemed appropriate for the course (either from this set or from other sources).

LECTURE 1: Introduction to the Course

Introductions
About the Course
Course Prerequisites and Requirements
Course Outline

LECTURE 2: Review of Nuclear Physics

Radioactive Decay
Half-life
Decay Chains
Nuclear Reactions

LECTURE 3: Review of Nuclear Physics (continued)

Microscopic Cross Sections
Macroscopic Cross Sections
Mean Free Path
Beam Attenuation
Differential Scattering Cross Sections

LECTURE 4: Potential Scattering

Center of Mass Coordinates
Collision Kinematics
Differential Scattering Cross Section
S-wave Scattering

LECTURE 5: Compound Nucleus Reactions

Experimental Evidence
Bohr Model
Energetics
Binding Energy
Virtual States
Decay of Compound Nuclei

LECTURE 6: Cross Section Resonances

Review of Compound Nucleus Reactions
Breit-Wigner Cross Section
Thermal Motion and Doppler Broadening

LECTURE 7: Nuclear Fission

History and Phenomenological Description
Binding Energy Curve
Fission Energetics
Coulomb Potential Energy
Fissile, Fissionable, Fertile
Fission Cross Sections

LECTURE 8: Nuclear Fission (continued)

Fission Product Mass Yields
Fission Fragment Energy
Prompt Neutrons
Fission Neutron Spectrum
Delayed Neutrons
Energy Release from Fission

LECTURE 9: Fast vs. Thermal Reactors

Eta
Implications for Fission Chain Reaction
Fast Reactors
Thermal Reactors
Neutron Moderation
Events in a Neutron Lifetime
Multiplication Factor k

LECTURE 10: The Six-Factor Formula and Reactor Criticality

Definitions
Life Cycle
The Six-Factor Formula
Reactor Criticality
Reaction Rates and Leakage Rates
Calculation of k

LECTURE 11: Neutron Flux and Current

Reaction Rates
Neutron Number Density
Neutron Flux
Neutron Current Density

LECTURE 12: Neutron Continuity Equation

Intepretation of Current
Neutron Continuity Equation

LECTURE 13: Neutron Diffusion Equation

Review of Continuity Equation
Diffusion Approximation
Neutron Diffusion Equation
Neutron Energy Dependence
Energy Dependent Continuity Equation
Energy Dependent Diffusion Equation

LECTURE 14: Initial and Boundary Conditions

Initial Condition
Steady State Diffusion
Vacuum Boundary Condition
Partial Currents

Reflecting Boundary Condition

LECTURE 15: Solution of the Neutron Diffusion Equation

1-D Diffusion Equation
Boundary Conditions for Slab Geometry
Extrapolated Boundary Conditions
Solution for Slab Geometry

LECTURE 16: Solution of the Neutron Diffusion Equation (cont)

Solution for Slab with Reflecting Boundary
Some Numerical Comparisons

LECTURE 17: Point and Plane Source Problems

Point Source in an Infinite Medium
Mean square distance to absorption
Plane Source in an Infinite Medium

LECTURE 18: Multiregion Problems

Interface Conditions
Solution for Reflected Reactor
Effects of Reflectors

LECTURE 19: Numerical Solution of 1-D Diffusion Equation

General Mesh Structure
Finite Differencing
General Solution Strategy
Example: Bare slab reactor

LECTURE 20: Numerical Solutions (continued)

Gauss Elimination
Iterative Methods

LECTURE 21: Diffusion in Multiplying Media

The Fission Source Term
Criticality Calculations
Introduction of Multiplication Factor
The Critical Slab Problem

LECTURE 22: Criticality Calculations

The Critical Slab Problem Revisited
Criticality Condition
General Geometries

LECTURE 23: Criticality Calculations (continued)

Reactor Criticality Problem
Summary of Solutions

Reflected Reactors

LECTURE 24: Numerical Solution of Criticality Problem

1-D Slab Geometry
Finite Difference Form
Source Iteration Method

LECTURE 25: Neutron Energy Dependence

One-Speed Diffusion Model
Energy Dependence
Energy-Dependent Diffusion Theory
Energy Groups
Example: Two-Group Model

LECTURE 26: Derivation of Multigroup Diffusion Equations

Derivation of Two-Group Equations
Special Case: One-group Equations
Generalization to G Groups
Calculation of Multigroup Constants

LECTURE 27: Two-Group Diffusion Theory

Review of Two-Group Model
Analysis of Reactor Criticality
Six-Factor Formula
Collapse to One-Group Model
Modified One-Group Model

LECTURE 28: Solution of the Multigroup Diffusion Equations

Review of General Form
Strategy for Solution
Some General Comments

LECTURE 29: Generation of Multigroup Constants

Overview of MGD Calculations
Multigroup Constants
Energy Averaging
Spatial Averaging
The Task Ahead

LECTURE 30: Fast Spectrum Calculations

Neutron Slowing Down
Infinite Medium Model
Slowing Down in Hydrogen

LECTURE 31: Neutron Slowing Down (continued)

Neutron Slowing Down Density
Neutron Lethargy

Moderating Parameters

LECTURE 32: Neutron Slowing Down (One More Time...)

Slowing Down with Absorption
Nonhydrogenous Media ($A > 1$)
Inelastic Scattering

LECTURE 33: Resonance Absorption

Importance of Resonance Absorption
Example: Hydrogen + Absorber
Doppler Effect
Resonance Integrals

LECTURE 34: Resonance Integrals

General Problem
Approximations
Lattice Effects
Final Comments

LECTURE 35: Fast Spectrum Codes

The Task Before Us
Spatial Effects
MUFT-Type Codes
Group Structures

LECTURE 36: Thermal Spectrum Calculations

Neutron Thermalization
General Features of Thermal Spectra
Calculational Models

LECTURE 37: Lattice Effects

Cell Averaging
Qualitative Effects
Effects on k

LECTURE 38: Cell Homogenization

Basic Ideas
Cell-Averaged Group Constants
Detailed Procedure
More General Approaches

LECTURE 39: An Overview of Multigroup Diffusion Codes

More General Cell Calculations
Reactor Analysis Code Packages
Cross Section Libraries
Flux-Power-Reactivity Module

LECTURE 40: A Summary of the Course

Nuclear Reactor Theory
Neutron-nuclear Interactions
Neutron Diffusion
Multigroup Diffusion Theory
Neutron Slowing Down and Thermalization
Lattice Effects

LECTURE 1

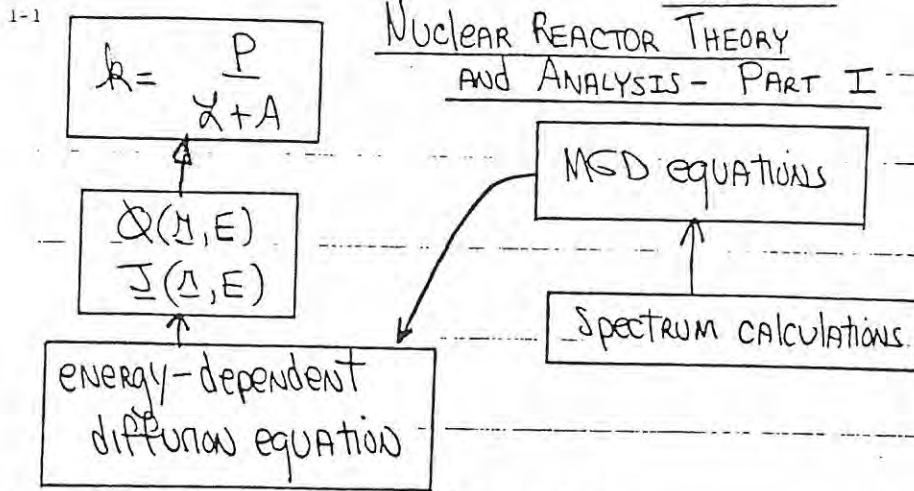
INTRODUCTION TO THE COURSE

READING ASSIGNMENT:

Duderstadt and Hamilton, Nuclear Reactor Analysis, pp. 3-8

Lamarsh, Introduction to Nuclear Engineering, pp 1-5

Nuclear Reactor Theory
AND ANALYSIS - PART I

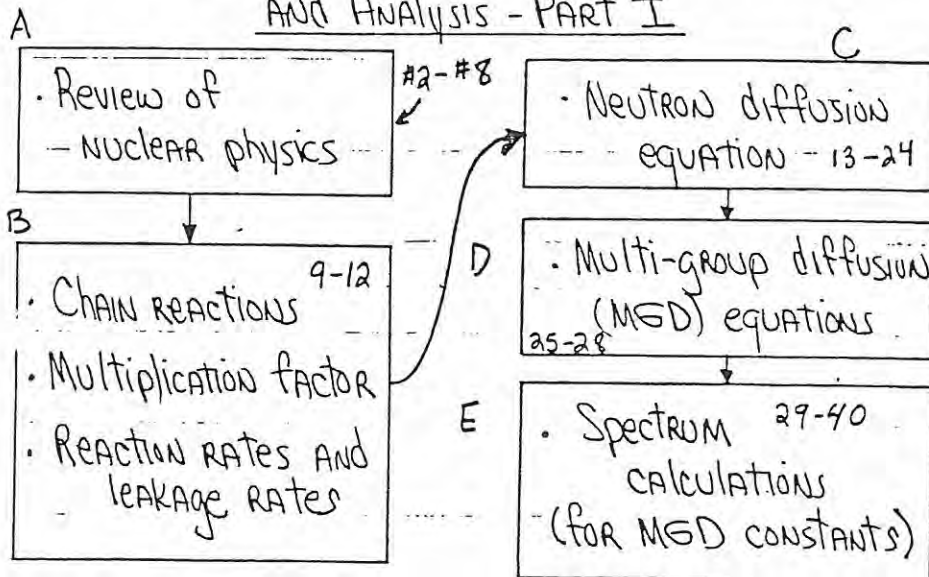


A Functional Outline of the Course.

The multiplication factor k is one important quantity to the reactor analyst. To calculate k , one needs reaction rates and leakage rates (P, A, λ). But to find them, one needs the flux and current (Φ, J). Solving the energy-dependent diffusion equation in an approximate form (the multi-group diffusion equation) will yield Φ and J . However, in order to solve the MGD equations, one needs the MGD constants, which are obtained from the spectrum calculations.

1-2

Nuclear Reactor Theory
AND ANALYSIS - PART I



A Conventional Outline of the Course

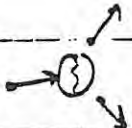
- Part A - Review
- Part B - Simple reactor concepts
- Part C - Diffusion theory - the principal model for reactor theory
- Part D - The multi-group diffusion equations (MGD) the "workhorse"
- Part E - To calculate MGD coefficients (cross sections)

Review of Nuclear Physics

- Radioactive decay $\frac{dN}{dt} = -\lambda N$ $N = \# \text{ density of nuclei}$
- Microscopic cross section σ "effective AREA"
- Macroscopic cross section $\Sigma = \sigma N$
- Elastic scattering
- Compound nucleus reactions
- Doppler broadening
- Nuclear fission

This review concerns those topics of nuclear physics of special significance to nuclear reactor theory.

CHAIN REACTIONS; etc.

- The fission chain reaction
- Significance of η $\approx \frac{\sigma_f}{\sigma_a}$ 
- Neutron history in a thermal reactor.
- Multiplication factor k $k = \epsilon p \eta f$
- 4- and 6- factor formulas
- Reaction rates and leakage rates
- Scalar flux and net current
- Neutron balance - the continuity equation

Simple reactor concepts, in particular the multiplication factor k and how one can in principle compute k given the reaction rates and leakage rates. These in turn can be computed from the flux and current, which satisfy the continuity equation.

Neutron Diffusion Equation

- The "diffusion approximation" for neutrons
- Derivation of the general time-dependent and energy-dependent diffusion equation
- The steady-state, one-speed neutron diffusion equation (fixed source)
 - Boundary conditions (vacuum & reflecting)
 - Extrapolated boundary - partial currents

The neutron diffusion equation - a model for the behavior of neutrons in a nuclear reactor.

(cont.)

- Analytical solutions
- Numerical solutions (computer)
- Diffusion equation with fission source
 - Neutron balance - multiplication factor
 - Helmholtz equation - geometric buckling
 - The critical reactor $k=1$
 - Simple reactor geometries (slab, sphere, etc.)
 - Numerical solutions (computer)

Concept of the critical reactor ($k=1$) and analytical solutions of the diffusion equation in simple geometries. One quickly finds that a computer must be utilized to solve practical problems in reactor analysis.

Multi-group Diffusion (MGD) Equations

- Energy dependence of neutrons and cross sections
- Derivation of MGD equations
- Definition of MGD constants $-\Sigma_{ag}, \nu\lambda_{fg}$
- Two-group diffusion theory
- Numerical solution of the MGD equations

MGD Equations - the "workhorse" of modern reactor analysis

An essential ingredient for the success of the MGD equations-careful calculation of the MGD constants.

Spectrum Calculations

- Generation of MGD constants
- Fast spectrum calculations
 - Slowing down
 - Resonance absorption
 - Age theory
 - Typical spectrum codes
- Thermal spectrum calculations
- Lattice calculations-heterogeneities

Spectrum Calculations - determine the constants needed to solve the MGD equations.

LECTURE 2

REVIEW OF NUCLEAR PHYSICS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 10-19.

Lamarsh, pp 6-24.

EXERCISES:

- 2.1. If the probability per unit day of a Xe-135 nucleus to decay is 1.81d^{-1} , what is the probability that the nucleus will decay within 1 day? Within 1 week?
- 2.2. Duderstadt & Hamilton, problem #2-4.
- 2.3. Duderstadt & Hamilton, problem #2-5.
- 2.4. Lamarsh, problem #2.27.
- 2.5. Lamarsh, problem #2.31.

2-1

- I. Review of Nuclear Physics
(RELEVANT TO FISSION CHAIN REACTIONS)
 - A. NUCLEAR REACTIONS
 - B. CROSS SECTIONS
 - C. NEUTRON-NUCLEAR REACTIONS
 - D. NUCLEAR FISSION
 - E. NEUTRON PROCESSES IN A
THERMAL NUCLEAR REACTOR
 - F. NEUTRON MULTIPLICATION

Present lecture - nuclear reactions and
microscopic cross sections.

2-2

- A. NUCLEAR REACTIONS
 - 1. RADIOACTIVE DECAY
 - 2. NUCLEAR COLLISIONS
- B. CROSS SECTIONS
 - 1. MICROSCOPIC
 - 2. MACROSCOPIC
 - 3. DIFFERENTIAL

A. Radioactive decay - spontaneous

disintegration of RADIOACTIVE
Nuclei

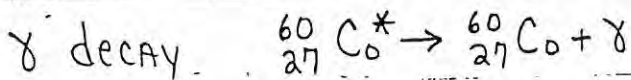
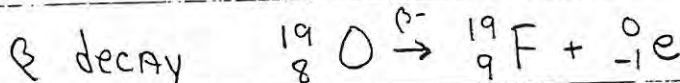
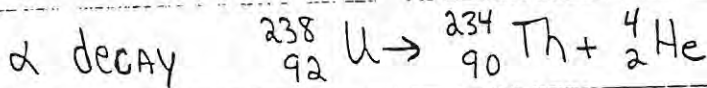
NOTATION: $\begin{matrix} A \\ Z \end{matrix} X$

A ← ATOMIC MASS (# NEUTRONS + PROTONS)
 Z ← ATOMIC NUMBER (# PROTONS)
 X ← CHEMICAL SYMBOL
 X^* ← excited STATE
 $\begin{matrix} 16 \\ 8 \end{matrix} O$

COMMON types: α decay
 β decay
 γ decay

Spontaneous disintegration - the probability of decay in a given time interval is independent of the nucleus age or its environment.

Examples:



$(E_\gamma = 58.6 \text{ keV})$

An excited nucleus can "decay" by many "modes" or "channels". The principal decay channels of interest to the nuclear engineer are α , β , and γ decay.

FUNDAMENTAL LAW

of Radioactive Decay

The probability that a nucleus will decay in a given time interval is a constant, independent of the Age of the nucleus or its surroundings. (spontaneous)

A statement of the Fundamental Law of Radioactive Decay.

2-6

Define Δt = given time interval

N = number of nuclei

constant
indep
of
The time t $\left\{ \lambda \Delta t = \text{probability that a nucleus will decay in the time interval } \Delta t \right.$

ΔN = number of nuclei which decay in the time interval Δt

Define some terms enroute to a mathematical statement (i.e., an equation) for radioactive decay.

$$\Delta N = - [\lambda \Delta t] \times [N] \quad N \downarrow \text{ as } t \uparrow$$

\uparrow probability that nucleus will decay in Δt \uparrow number of nuclei at time t

• Now take $\Delta N, \Delta t$ small,

$$dN = -\lambda N dt$$

$$\frac{dN}{N} = -\lambda dt \quad N(0) = N_0$$

$$N_0 \int_{N_0}^N \frac{dN'}{N'} = \int_0^t \lambda dt' \Rightarrow \boxed{N = N_0 e^{-\lambda(t-t_0)}} \quad N(t_0) = N_0$$

$e^{-\lambda t} = \frac{N(t)}{N_0}$ = probability that nucleus does not decay before t

$$\frac{dN}{N} = \text{probability that } dN \text{ (out of } N \text{) nuclei will decay in the time interval } dt.$$

Mean Lifetime - the average lifetime of a given type of radioactive nucleus

$$\equiv \tau$$

$\tau_i, i = 1, 2, \dots, N$ - observed lifetime

P_i = prob of lifetime τ_i

$$\tau = \sum_{i=1}^N \tau_i P_i$$

Calculation of the mean (average) lifetime for a nucleus (lifetime is terminated upon decay).

Illustrate for the fictitious case where nuclei only have specific lifetimes.

In the case of radioactive

decay of nuclei, there is

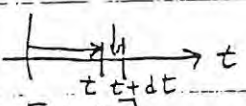
a continuum of decay times,

$$\sum_{t_i} t_i \times p_i \Rightarrow \int_0^{\infty} dt \underbrace{p(t)}_{\substack{\text{probability the} \\ \text{nucleus decays} \\ \text{in the time} \\ \text{interval} \\ (t, t+dt)}} t \quad \leftarrow \text{time of decay}$$

Must take the usual expression for an average into an integral because the lifetimes can vary continuously

$p(t)dt$ = probability the nucleus will decay in the specific time interval between t and $t+dt$.

But $p(t)dt$ = [probability the nucleus does not decay before time t] \times [probability the nucleus decays in time dt]



OR $p(t)dt = [e^{-\lambda t}] \times [\lambda dt]$

(note $\frac{N(t)}{N_0} = e^{-\lambda t}$)

If two events are independent, the probability of both occurring is the product of the probabilities.

By the Fundamental Law, the probability of decay in dt is independent of the nucleus age.

2-11

$$\text{Then } \tau = \int_0^{\infty} \underbrace{t e^{-\lambda t} \lambda}_{p(t)} dt$$

Integrate, $\tau = 1/\lambda$

\therefore MEAN lifetime = $1/\lambda$

where $\lambda =$ DECAY CONSTANT

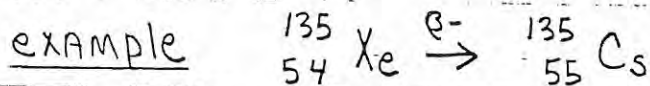
Carry out the integration to yield the mean lifetime τ .

2-12

STANDARD TERMINOLOGY

λ - "probability per unit time"

(prob/min) OR (prob/sec), etc.



$$\lambda = .0753 \text{ h}^{-1}, \tau = 13.3 \text{ hr}$$

$$\text{IN DAYS, } \lambda = 1.81 \text{ d}^{-1}, \tau = .55 \text{ d}$$

hence, "probability per day" = 1.81

Recall: λdt is the probability that the nucleus decays in the time interval dt .

λ : may be interpreted as a "probability per unit time of decay"

2-13

But probability of decay in
one day (or less) of A $^{135}_{54}\text{Xe}$
nucleus is

$$P(t \leq 1) = \int_0^1 e^{-\lambda t} \lambda dt \quad \text{where } \lambda = 1.81 \text{ d}^{-1}$$

$$= \left[-e^{-\lambda t} \right]_0^1 = 1 - e^{-1.81(1)}$$

Calculate, $P = 1 - e^{-1.81} = \boxed{.836}$

probability/day of decay = 1.81

Caution: cannot interpret $-\lambda$ as the probability for decay. Example - the xenon - 135 nucleus where $\lambda = 1.81 \text{ (days)}^{-1}$, hence the probability per unit day of decay is 1.81. This does not mean the probability of decay in one day is 1.81!!

2-14

Half-Life $\tau_{1/2}$

Time at which half of
the initial nuclei will have

decayed. Since $N(t) = N_0 e^{-\lambda t}$

$$N(\tau_{1/2}) = \frac{N_0}{2} = N_0 e^{-\lambda \tau_{1/2}}$$

$$\text{At } t = \tau_{1/2} \\ N(t) = \frac{N_0}{2}$$

$$\Rightarrow \lambda \tau_{1/2} = \ln 2$$

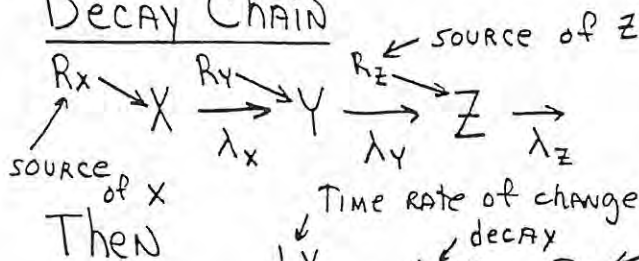
$$\ln 2 = .693$$

$$\Rightarrow \boxed{\tau_{1/2} = \ln 2 / \lambda} = \ln 2 \times \tau$$

$$\tau_{1/2} < \tau$$

A related concept - the half-life.

Decay Chain



Then

Time rate of change of X

$$\frac{dX}{dt} = -\lambda_X X + R_X$$

decay SOURCE, #/s

$$\frac{dY}{dt} = -\lambda_Y Y + R_Y + \lambda_X X$$

SOURCE

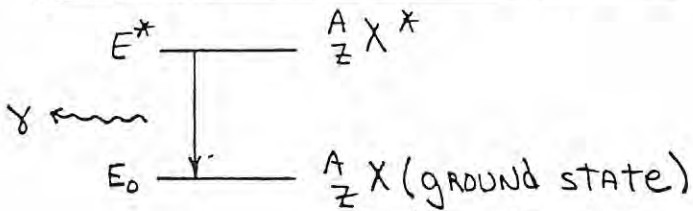
$$\frac{dZ}{dt} = -\lambda_Z Z + R_Z + \lambda_Y Y$$

term due to decay of X

Common to have complex decay chains in nuclear reactors—the "daughter" product is also radioactive with a given half-life and so is its daughter product, etc.

Simple to write out the equations - more difficult to solve them! (later)

Decay of Nuclear Excited States



γ = AVERAGE lifetime of $A/Z X^*$

E_s = excitation energy

(Definition) $= E^* - E_0$

NOTATION: Γ = "width" of excited state

$\equiv \hbar/\gamma = \hbar \lambda$ \hbar = PLANCK'S CONSTANT

Heisenberg UNCERTAINTY

The "width" of an excited state can be related to the probability of that state decaying.

Heisenberg Uncertainty Principle -

$$\Delta E \cdot \Delta t \geq \hbar$$

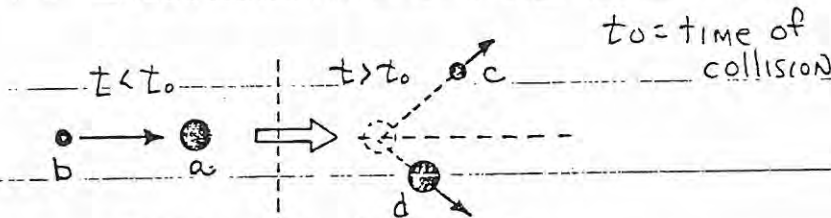
\uparrow \uparrow γ
 "width" of the energy level

$$\Gamma \gamma = \hbar$$

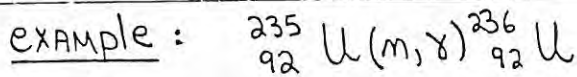
$$\Rightarrow \Gamma = \hbar / \gamma = \hbar \lambda$$

Heisenberg Principle - the product of the uncertainty in one's measurement of the energy of a given state and the uncertainty in the time at which one made the measurement is greater than or equal to a fundamental constant - Planck's constant.

2. Nuclear Collision Reactions $b + a \rightarrow c + d$



INCOMING PARTICLE \rightarrow $a(b, c) d \leftarrow$ FINAL "TARGET"
 NOTATION: $\left. \begin{array}{l} \text{INITIAL} \\ \text{"TARGET"} \end{array} \right\} a(b, c) \left. \begin{array}{l} \text{OUTGOING} \\ \text{PARTICLE} \end{array} \right\} d$



Terminology for nuclear collision reactions.

Energy change in nuclear collision reactions

$$\Delta E = \Delta m \cdot c^2 = (Q)$$

OR $Q = (\underbrace{M_a + M_b}_{\text{INITIAL MASS}} - \underbrace{M_c + M_d}_{\text{FINAL MASS}}) c^2$

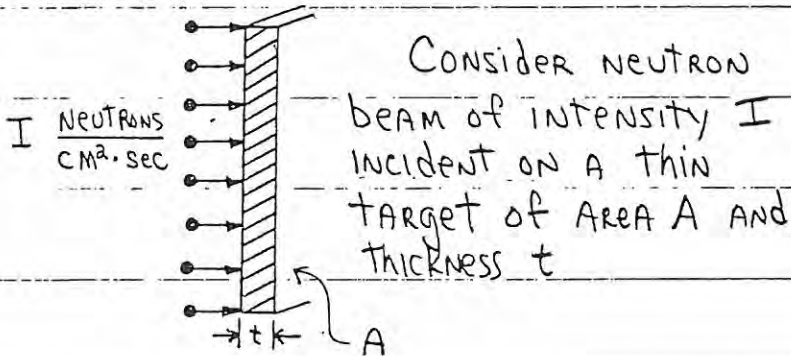
$Q > 0$ exothermic (energy released)

$Q < 0$ endothermic (energy absorbed -
must be supplied
to have reaction)

Definition of the "Q-value"

B. Cross Sections

1. Microscopic cross sections



A physical description of the microscopic cross section - a very important concept to the reactor analyst.

Experimental observation:

$$\Delta n \propto N t A I \Delta t$$

where Δn = number of reactions
in time interval Δt
 N = target nuclei density
 A = target area
 I = intensity of beam
 Δt = time interval of experiment

$$\frac{\Delta n}{\Delta t} \equiv r = \sigma I \overbrace{N t A}^{\text{volume of target}}$$

CONSTANT of proportionality TOTAL NUMBER of nuclei in target

One would naturally expect that the number of reactions observed would be proportional to the density of nuclei x thickness x area x beam intensity x duration of experiment.

Units of σ

$$\sigma = \frac{r}{I N t A} = \frac{\# \text{ REACTIONS} / s}{\frac{\# \text{ NEUTRONS}}{\text{cm}^2 \cdot s} \times \frac{\# \text{ NUCLEI}}{\text{cm}^3} \times \text{cm}^3}$$
$$= \text{cm}^2 \text{ (PER NEUTRON PER NUCLEUS)}$$

σ = "effective" AREA OF NUCLEUS per
INCIDENT NEUTRON for the
PARTICULAR REACTION TO OCCUR
"cross section"

The microscopic cross section is simply the "apparent" or "effective" area that the nucleus presents to the incoming neutron (for the particular reaction of interest to occur)

Alternatively,

$IA = \#$ NEUTRONS STRIKING
THE TARGET PER SECOND

$R = \#$ REACTIONS PER SECOND

$\frac{R}{NtA} = \text{" " " PER TARGET NUCLEUS}$
(choose one)

$$\therefore \frac{R/NtA}{IA} = \frac{\sigma I}{IA} = \frac{\sigma}{A} \cdot \text{"effective" AREA}$$

A - area of target

IS PROBABILITY A NEUTRON IN THE
BEAM WILL INTERACT WITH ^{THIS} ONE NUCLEUS

An alternate manner of interpreting the cross section - but it is still an effective interaction area.

NOTATION: $\sigma_{\alpha} =$ MICROSCOPIC CROSS
SECTION FOR SPECIFIC
REACTION " α "

examples

$\sigma_a =$ ABSORPTION CROSS SECTION
("effective" AREA FOR
NUCLEUS TO ABSORB THE
INCIDENT NEUTRON)

$\sigma_s =$ SCATTERING CROSS SECTION

$\sigma_r =$ RADIATIVE CAPTURE
CROSS SECTION

$\sigma_f =$ FISSION CROSS SECTION

One defines microscopic cross sections for many types of neutron - nuclear reactions.

LECTURE 3

REVIEW OF NUCLEAR PHYSICS (continued)

READING ASSIGNMENT:

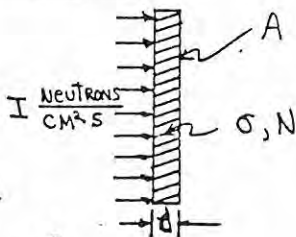
Duderstadt & Hamilton, pp 19-23, 34-39.

EXERCISES:

- 3.1. Duderstadt & Hamilton, problem #2-6.
- 3.2. Duderstadt & Hamilton, problem #2-7.
- 3.3. Duderstadt & Hamilton, problem #2-8.
- 3.4. Lamarsh, problem #3.4.
- 3.5. Lamarsh, problem #3.7.
- 3.6. Lamarsh, problem #3.9.

2. MACROSCOPIC CROSS SECTIONS

$$R = \sigma N d A I$$



R = REACTION RATE, # REACTIONS / s

σ = MICROSCOPIC CROSS SECTION, CM²

N = TARGET NUCLEI DENSITY, # NUCLEI / CM³

d = TARGET THICKNESS, CM

A = TARGET AREA, CM²

I = BEAM INTENSITY, # NEUTRONS / CM²·s

Recall our expression for the observed reaction rate (which defined σ).

3-2

$$R = \frac{R}{\text{volume}} \quad \text{volumetric REACTION RATE}$$

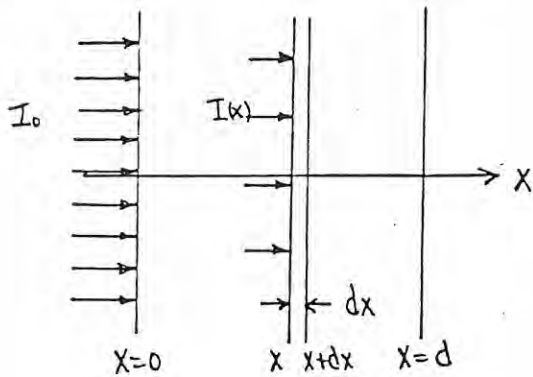
$$\text{OR } R = \frac{R}{Ad} = \underbrace{\sigma N I}_{\Sigma}$$

$$\Sigma = \sigma N \quad \text{"MACROSCOPIC CROSS SECTION"}$$

$$\text{UNITS: } \text{CM}^2 \cdot \frac{1}{\text{CM}^3} = \frac{1}{\text{CM}}$$

$$R = \Sigma I$$

Convenient to define a "macroscopic" cross section.



Define dI = portion of neutron beam $I(x)$ incident on thin slice at x which reacts in dx .

Then $-\frac{dI}{I}$ = probability that neutron at x will react in $[x, x+dx]$

Now let us consider a "thick" slab and ask the question - how will the neutron beam be attenuated in the slab due to interactions with the nuclei (as described by σ).

Recall,

$$R = \# \text{ reactions/second}$$

$$IA = \# \text{ incident neutrons/second}$$

Then $\frac{R}{IA}$ = probability incident neutron reacts in the target $\left(-\frac{dI}{I}\right)$

$$\text{OR } \frac{R}{IA} = \sigma N d \quad \uparrow \text{ thickness}$$

$$\therefore \boxed{-\frac{dI}{I} = \sigma N dx} \quad \text{for our thin target with thickness } dx$$

Equating probabilities yields a differential equation (albeit a simple one) for the beam intensity I as a function of distance x .

$$\int_{I_0}^I \frac{dI'}{I'} = -\Sigma N \int_0^x dx$$

$$\ln(I/I_0) = -\Sigma N X$$

$$I(x) = I_0 e^{-\Sigma N X}$$

exponential
ATTENUATION
of the neutron beam

Σ : physical interpretation

$$-\frac{dI}{I} = \Sigma N dx = \text{probability}$$

$$\Sigma = \text{probability per unit length}$$

Integrate the differential equation to find $I(x)$.

Average Distance to Collision

$$\bar{x} = \int_0^{\infty} x \cdot e^{-\Sigma x} \cdot \Sigma dx$$

distance \uparrow probability \uparrow probability of
the neutrons gets to x A collision in dx

$$\bar{x} = \frac{1}{\Sigma}$$

"MEAN free path"
(for the PARTICULAR
REACTION described by Σ)

$$\frac{1}{\Sigma_t}, \frac{1}{\Sigma_a}, \frac{1}{\Sigma_s}$$

Define an average distance to collision - known at the "mean free path". May have a "mean free path to absorption", or a "mean free path to fission", etc.

-7

Radioactive Decay

$$N = N_0 e^{-\lambda t}$$

λ = decay constant, $\frac{1}{s}$

N = number of nuclei remaining at time t

$\tau = \frac{1}{\lambda}$ "mean lifetime"

λ = "probability per unit time"

Neutron Attenuation

$$I = I_0 e^{-\Sigma x}$$

Σ = MACROSCOPIC CROSS SECTION, $\frac{1}{cm}$

I = intensity of NEUTRON BEAM AT distance x

MFP = $\frac{1}{\Sigma}$ "mean free path"

Σ = "probability per unit length"

Notice the similarities between radioactive decay and neutron attenuation (both are what are known as "Markov" processes - they are independent of history).

3-8

$$\Sigma_a = N \sigma_a$$

density of target nuclei

MICROSCOPIC CROSS SECTION FOR REACTION "a" WITH TARGET NUCLEUS

Σ_a = absorption cross section

Σ_f = fission cross section

EXAMPLE MACROSCOPIC CROSS SECTION FOR FISSION OF 2 MeV NEUTRON IN U-238

Can define macroscopic cross sections for many different reactions and materials. Careful - a macroscopic cross section needs both a given material number density as well as the particular reaction.

$$\sigma_f^{238} \approx .5 \text{ b} = .5 \times 10^{-24} \text{ cm}^2$$

$$N^{238} = 19.1 \frac{\text{g}}{\text{cm}^3} \times 6.02 \times 10^{23} \frac{\text{Nuclei}}{\text{mole}} \times \frac{1 \text{ mole}}{238 \text{ g}}$$

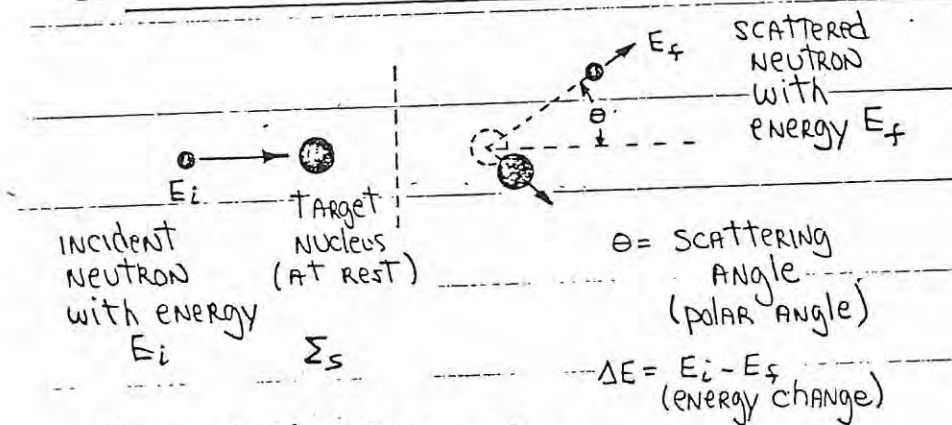
$$N^{238} = \cancel{19.1} 4.83 \times 10^{22} \text{ Nuclei/cm}^3$$

$$\Sigma_f^{238} = .0242 \text{ cm}^{-1} \text{ (2 MeV NEUTRON)}$$

$$\text{mfp} = \frac{1}{\Sigma_f^{238}} = 41.4 \text{ cm}$$

The mean free path to fission (at 2 MeV) for a 2 MeV neutron in U-238 is 41.4 cm.

3. Differential Cross Sections



FIRST: DIFFERENTIAL IN ENERGY

For a scattering reaction, one might want to know more than simply if a scattering reaction occurred. For example, one might want to know the probability that a neutron loses a given amount of energy or scatters through a given angle. Differential cross sections allow this.

Now if there were only a discrete set of allowable final energies $E_f = E_j, j = 1, 2, \dots, J$ Then one could define

$\Delta\sigma_{ij}$ = MICROSCOPIC CROSS SECTION
TO SCATTER A NEUTRON
FROM E_i TO E_j

Clearly,
$$\sigma_s(E_i) = \sum_{j=1}^N \Delta\sigma_{ij}$$

Again, let us consider a fictitious example. In this case it is clear how one would define a cross section for the particular neutron energy transfer.

Define the differential scattering cross section, $\sigma_s(E_i \rightarrow E_f)$:

$\sigma_s(E_i \rightarrow E_f) dE_f$ = MICROSCOPIC CROSS SECTION FOR A NEUTRON WITH INITIAL ENERGY E_i TO SCATTER WITH A FINAL ENERGY IN THE ENERGY RANGE dE_f ABOUT E_f .

UNITS: $\frac{\text{cm}^2}{\text{eV}}$

Real life - neutron final energy distribution is continuous. The probability of any specific final energy E_f is zero (e.g., probability of exactly $E_f = 1.7437914$ MeV). One must instead consider the probability of scattering into a range of energies (though infinitesimal) dE_f about E_f .

With $\sigma_s(E_i)$ = USUAL MICROSCOPIC SCATTERING CROSS SECTION (FOR NEUTRON of energy E_i)

Then
$$\sigma_s(E_i) = \int_0^{\infty} \sigma_s(E_i \rightarrow E_f) dE_f$$

(ANALOGY WITH DISCRETE CASE -

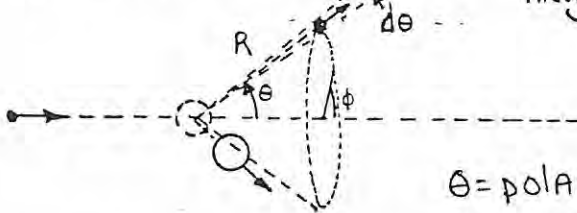
$$\Delta\sigma_{if} = \sigma_s(E_i \rightarrow E_f) dE_f$$

$$\int_0^{\infty} \iff \sum_{f=1,2,\dots,J} \Delta\sigma_{if})$$

The total cross section for scattering must be the sum (or integral) over the cross sections for scattering into all possible final energies.

Differential in Angle $\sigma_s(\theta)$

- Differential cross section for scattering into the polar angle $d\theta$ about θ : (irrespective of azimuthal angle ϕ)



θ = POLAR ANGLE
 ϕ = AZIMUTHAL ANGLE

We also need a means to define a cross section for scattering through an angle θ . Again, θ is continuous and we need to ask how many scatter into the angles $d\theta$ about θ (the annular cone defined by $d\theta$).

Define

$dN(\theta)$ = number of neutrons/second
which scatter into $d\theta$ about θ
(the cone of angles)

Then

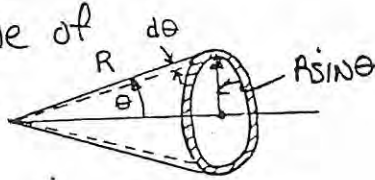
$$\begin{aligned} dN(\theta) &\propto I \quad (\text{beam intensity}) \\ &\propto A \quad (\text{area of target}) \\ &\propto d \quad (\text{thickness of target}) \\ &\propto \frac{\text{AREA OF CONE } d\theta}{\text{AREA OF SPHERE}} \quad (\text{solid angle}) \\ &\propto N \quad (\text{target nuclei density}) \end{aligned}$$

As before we expect the rate of scattered neutrons to be proportional to $I \times A \times d \times N$. However, we also want them to be scattered into $d\theta$, therefore we take the area of the cone divided by the area of the sphere as the appropriate fraction.

3-16

- But the area of the cone of angles in $d\theta$ is

$$2\pi R \sin\theta \cdot R d\theta$$



And the area of the sphere is

$$4\pi R^2$$

$$\therefore dN(\theta) \propto I N A d \left(\frac{1}{2} \sin\theta d\theta \right)$$

$$\text{OR } dN(\theta) = \underbrace{\sigma_s(E, \theta)}_{\text{PROPORTIONALITY CONSTANT}} I N A d \cdot d\theta \cdot \sin\theta$$

Standard notation to absorb the 2 into $\sigma_s(E, \theta)$ and leave $\sin\theta$ out.

- Divide by volume A_d

AND define $dR(\theta) = \frac{1}{A_d} d\mathcal{N}(\theta)$

$$dR(\theta) = IN \underbrace{\sigma_s(E, \theta) \sin\theta d\theta}$$

- COMPARE WITH OUR RESULT FOR

THE MICROSCOPIC SCATTERING
CROSS SECTION, Σ

$$R = IN \underbrace{\sigma_s(E)}$$

"EFFECTIVE AREA" FOR
NEUTRON TO SCATTER FROM NUCLEUS

Recall our previous expression for the microscopic cross section to yield an interpretation for the macroscopic cross section.

Then

$$\sigma_s(E, \theta) \sin\theta d\theta = \text{effective "AREA"}$$

for NEUTRON TO SCATTER INTO
d θ ABOUT θ

- defines $\sigma_s(E, \theta)$

$\sigma_s(E, \theta)$ } - "differential" scattering
cross section to scatter
through AN ANGLE θ INTO $d\theta$

STANDARD NOTATION

- Change of VARIABLE to
 $\mu = \cos \theta$

- Then $d\mu = -\sin \theta d\theta$
AND we CAN THEN define

$$\sigma_s(E, \mu) d\mu = \text{effective AREA} \\ \text{FOR NEUTRON TO SCATTER} \\ \text{INTO } d\mu \text{ ABOUT } \mu$$

- Note $\sigma_s(E, \mu)$ has the effective area for a neutron of energy E to scatter into $d\mu$ about μ (hence $\sigma_s(E, \mu)$ has units of area per unit cosine)

- Note we had

$$dR(\theta) = IN \sigma_s(E, \theta) \sin \theta d\theta$$

- Integrate over all θ (0 to π):

$$\int_{\text{All } \theta} dR(\theta) = R \quad \begin{array}{l} \text{NUMBER OF NEUTRONS} \\ \text{SCATTERED PER SECOND} \\ \text{(ALL ANGLES)} \end{array}$$

AND

$$\int_0^{\pi} IN \sigma_s(E, \theta) \sin \theta d\theta = IN \int_{-1}^1 \sigma_s(E, \mu) d\mu$$

Check consistency of our definitions.

• But $\sigma_s(E) = \int_{-1}^1 \sigma_s(E, \mu) d\mu$
 (integrate over all possible outgoing angles)

$\therefore R = IN \sigma_s(E)$
 $= I \Sigma_s(E)$
 (consistent with earlier definitions)

Double Differential Cross Section

$\sigma_s(E_i \rightarrow E_f, \mu) dE_f d\mu \equiv$ microscopic cross section ("effective area) for the neutron with initial energy E_i to scatter into dE_f about E_f AND $d\mu$ about μ

One might also want to know the probability (i.e., cross section) for scattering into $d\Theta$ about Θ and into the energy range dE_f about E_f .

EXAMPLE A beam of neutrons of intensity $10^{12}/\text{cm}^2\cdot\text{s}$ and energy 1 MeV is incident on a 1 cm thick slab of graphite with area 100cm^2 .

- (1) What is the rate at which neutrons are scattered?
- (2) What is the rate at which neutrons are scattered into the energy range $.8\text{ MeV} \leq E_f \leq .9\text{ MeV}$?

A simple example to illustrate cross sections.

3-24 DATA

$$\sigma_s(1\text{ MeV}) \approx 3\text{ b} \quad (1\text{ b} = 10^{-24}\text{ cm}^2)$$

$$\sigma_s(1\text{ MeV} \rightarrow E_f) = \begin{cases} 10.56\text{ b/MeV}, & .716\text{ MeV} \leq E_f \leq 1.0\text{ MeV} \\ 0, & \text{otherwise} \end{cases}$$

$$\text{Note: } \int_0^{\infty} \sigma_s(1 \rightarrow E_f) dE_f = \int_{.716\text{ MeV}}^{1.0\text{ MeV}} 10.56 dE_f = 3.0\text{ b} = \sigma_s(1\text{ MeV})$$

$$(1) \text{ SCATTER RATE} = \underbrace{\sigma_s(1\text{ MeV})}_{\Sigma_s} \times N \times A \times d \times I$$

$$\text{OR } S = (3 \times 10^{-24}\text{ cm}^2) \times N \times 100\text{ cm}^2 \times 1.0\text{ cm} \times 10^{12}/\text{cm}^2$$

$$N = 1.6 \frac{\text{g}}{\text{cm}^3} \times 6.02 \times 10^{23} / 12.01\text{ g} = 8.02 \times 10^{22}/\text{cm}^3$$

The microscopic scattering cross section for carbon is approximately 3b for a 1 MeV neutron. The differential scattering cross section for a 1 MeV neutron is also presented. Note the consistency between the total scattering cross section and the integral of the differential cross section over all final energies.

$$\therefore S = 2.41 \times 10^{13} /s \quad \# \text{ NEUTRONS SCATTERING} \\ \text{PER SECOND FROM} \\ \text{GRAPHITE} \\ \text{(1 MeV NEUTRONS)}$$

(2) The cross section for scattering into the energy range $.8 \leq E_f \leq .9$ MeV

is

$$\sigma_s (.8 \leq E_f \leq .9) = \int_{.8}^{.9} \overbrace{\sigma_s(1 \rightarrow E_f)}^{10.56} dE_f \\ = .1 \times 10.56 = 1.056 \text{ b}$$

$$\therefore S (.8 \leq E_f \leq .9 E_f) = \boxed{.848 \times 10^{13} /s}$$

To get a cross section for scattering into a given energy range, simply integrate the differential cross section over that range.

LECTURE 4

POTENTIAL SCATTERING

READING ASSIGNMENT:

Duderstadt & Hamilton, pp 39-45.

Lamarsh, pp 55-58.

EXERCISES:

- 4.1. Carry out the details of the derivation of the equation relating the elastic scattering cross sections in the CM frame and the LAB frame.

$$\sigma_S(\theta_L) = \sigma_S(\theta_C) \frac{\left(\frac{1}{A} + \frac{2}{A} \cos \theta_C + 1\right)^{3/2}}{1 + \frac{1}{A} \cos \theta_C}$$

- 4.2. Verify explicitly that

$$\sigma_S(E) = \int_0^\pi \sigma_S(E \rightarrow E') dE'$$

where $\sigma_S(E \rightarrow E')$ is the differential elastic scattering cross section for a nuclide of mass A.

- 4.3. Lamarsh, problem #3.17.
4.4. Lamarsh, problem #3.18.

I. REVIEW OF NUCLEAR PHYSICS

- A. Nuclear reactions ✓
 - 1. Radioactive decay
 - 2. Nuclear collisions
- B. Cross sections ✓
 - 1. Microscopic
 - 2. Macroscopic
 - 3. Differential
- C. Neutron - nuclear reactions
 - 1. Elastic scattering
 - 2. Compound nucleus reactions

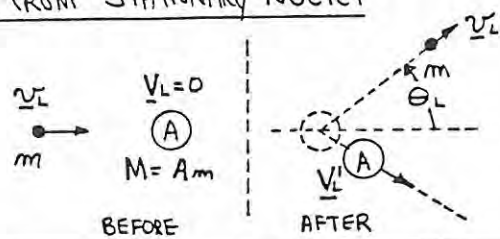
C. Neutron - nuclear reactions

- 1. Potential scattering - neutron bounces off nuclear force field - no penetration of the nucleus (billiard ball collision)
- 2. Compound nucleus formation -
 - neutron "absorbed" in nucleus
 - subsequently decays via γ , neutron, fission, etc.

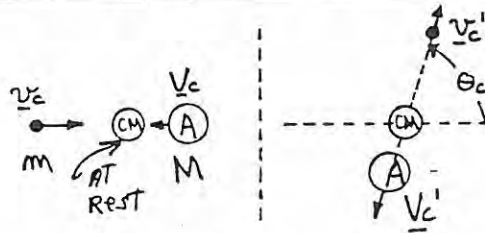
Two basic neutron - nuclear reactions of interest to the reactor analyst.

KINEMATICS OF ELASTIC SCATTERING FROM STATIONARY NUCLEI

LAB frame



CM frame



Consider a nucleus at rest with an incident neutron with velocity v_L , as measured in the laboratory (LAB) frame.

In the center-of-mass (CM), picture yourself seated on the CM, which is actually moving to the right. The reaction would then seem as shown.

Determine:

- ① Relation between θ_L and θ_c
- ② $\sigma_s(\theta_L)$ and $\sigma_s(\theta_c)$
- ③ $\sigma_s(E \rightarrow E')$

4-5 ANALYSIS

In the CM frame, velocities are relative to the velocity of the CM :

$$\underline{V}_{CM} = \text{velocity of CM}$$

Define

$$\underline{v}_L = \text{velocity of NEUTRON IN LAB}$$

$$\underline{v}_c = \text{" " " " CM}$$

$$\underline{V}_L^0 = \text{" " NUCLEUS IN LAB}$$

$$\underline{V}_c = \text{" " " " CM}$$

For now, assume the nucleus is at rest - (we will relax this assumption later).

4-6

$\underline{v}_L', \underline{v}_c', \underline{V}_L', \underline{V}_c'$ - After collision

$$\text{Position of CM} = \underline{x}_{CM} \equiv \frac{m \underline{x}_m + M \underline{x}_A}{m + M}$$

$$\text{Then velocity} = \underline{V}_{CM} = \dot{\underline{x}}_{CM} = \frac{m \underline{v}_L + M \underline{V}_L^0}{m + M}$$

$$\text{OR } \underline{V}_{CM} = \frac{1}{1+A} \underline{v}_L \quad \left(A = \frac{M}{m} \right)$$

$$\text{Then } \underline{v}_c = \underline{v}_L - \underline{V}_{CM} = \frac{A}{1+A} \underline{v}_L$$

$$\underline{V}_c = \underline{V}_L^0 - \underline{V}_{CM} = -\frac{1}{1+A} \underline{v}_L$$

\underline{v}_c and \underline{V}_c are the velocities of the neutron and nucleus relative to the CM, respectively.

Now consider kinetic energies:

$$E_L = \frac{1}{2} m v_L^2 + \frac{1}{2} M v_L^2$$

$$E_C = \frac{1}{2} m v_C^2 + \frac{1}{2} M v_C^2$$

Substitute for $v_C \neq v_L$:

$$E_C = \frac{1}{2} \mu v_L^2$$

$$\text{where } \mu \equiv \frac{mM}{m+M} \quad (\text{"Reduced MASS"})$$

$$\therefore E_C = \frac{M}{m+M} E_L = \boxed{\frac{A}{1+A} E_L}$$

(Note $E_C < E_L$ due to CM motion)

E_L = total kinetic energy before the collision

E_C = kinetic energy relative to the CM

E_{CM} = kinetic energy of the CM motion itself

$$E_L = E_C + E_{CM}$$

Conservation of Momentum AND Energy in The CM

• Total momentum in CM before collision = $m \underline{v}_C + M \underline{v}_C = \underline{P}_C$

• But $\underline{v}_C = \frac{A}{1+A} \underline{v}_L$

$$\underline{v}_C = -\frac{1}{1+A} \underline{v}_L$$

$$\therefore \underline{P}_C = \frac{(mM)}{1+A} \underline{v}_L - \frac{M}{1+A} \underline{v}_L = 0$$

(Momentum in CM frame = 0)

The momentum relative to the CM (or in the CM frame) is always zero.

Conservation of Momentum $\Rightarrow \underline{P}_c' = 0$

$$\text{OR } m\underline{v}_c' + M\underline{V}_c' = 0 \Rightarrow \underline{v}_c' = -\frac{M}{m}\underline{V}_c'$$

$$\underline{v}_c = -\frac{M}{m}\underline{V}_c$$

Conservation of Energy \Rightarrow

$$\underbrace{\frac{1}{2}m\underline{v}_c^2}_{\text{KE}} + \frac{1}{2}M\underline{V}_c^2 = \frac{1}{2}m\underline{v}_c'^2 + \frac{1}{2}M\underline{V}_c'^2$$

Now substitute

$$\underline{v}_c = -\frac{M}{m}\underline{V}_c$$

$$\underline{v}_c = -\frac{M}{m}\underline{V}_c$$

$$\underline{v}_c' = -\frac{M}{m}\underline{V}_c'$$

$$\underline{v}_c \cdot \underline{v}_c = -\left(\frac{M}{m}\underline{V}_c\right) \cdot \left(-\frac{M}{m}\underline{V}_c\right)$$

$$v_c^2 = \left(\frac{M}{m}\right)^2 V_c^2$$

INTO ABOVE EQUATION :

Conservation of energy and momentum are imposed.

$$\frac{1}{2}M(1+A)V_c^2 = \frac{1}{2}M(1+A)V_c'^2$$

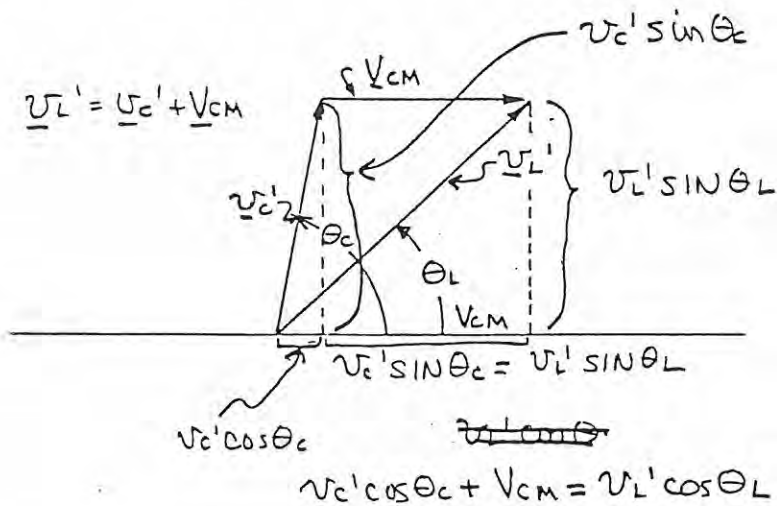
OR

$$\boxed{\begin{matrix} V_c = V_c' \\ v_c = v_c' \end{matrix}}$$

Speeds in the
CM frame are
CONSTANTS

Then after the collision, the velocity in the LAB frame can be expressed :

$$\underline{v}_L' = \underline{v}_c' + \underline{V}_{CM}$$



A diagram illustrating the relationship between the various velocities.

From the diagram

$$v_L' \sin \theta_L = v_c' \sin \theta_c$$

AND

$$v_L' \cos \theta_L = v_c' \cos \theta_c + v_{cm}$$

$$\therefore \tan \theta_L = \frac{v_c' \sin \theta_c}{v_c' \cos \theta_c + v_{cm}}$$

But $v_c' = v_c = A v_{cm}$

$$\therefore \boxed{\tan \theta_L = \frac{\sin \theta_c}{\frac{1}{A} + \cos \theta_c}} \quad \text{Relation between } \theta_c \text{ AND } \theta_L$$

Our desired relation between θ_L and θ_c -
 a consequence of the kinetics
 (conservation of energy and momentum)

Relation Between $\sigma_s(E, \theta_L)$
AND $\sigma_s(E, \theta_c)$

Recall-

$\sigma_s(E, \theta_L) \sin \theta_L d\theta_L =$ "effective AREA" for
 NEUTRON TO SCATTER INTO $d\theta_L$
 ABOUT θ_L (IN THE LAB FRAME)

A similar definition applies for $\sigma_s(E, \theta_c)$:

$\sigma_s(E, \theta_c) \sin \theta_c d\theta_c =$ "effective AREA" for
 NEUTRON WITH ENERGY E TO SCATTER
 INTO THE ANGLE $d\theta_c$ ABOUT θ_c
 (IN THE CM FRAME)

$\sigma_s(\theta_L)$ AND $\sigma_s(\theta_c)$

Since both of these are physical areas, then a measurement of them should yield the same result. Therefore, we equate them to define the relationship between the cross sections.

$$\sigma_s(\theta_c) \sin \theta_c d\theta_c = \sigma_s(\theta_L) \sin \theta_L d\theta_L$$

$$\sigma_s(\theta_L) = \sigma_s(\theta_c) \frac{\sin \theta_c}{\sin \theta_L} \left(\frac{d\theta_c}{d\theta_L} \right)$$

$$d(\tan \theta_L) = d \left(\frac{\sin \theta_c}{1 + \cos \theta_c} \right)$$

To find $\frac{d\theta_c}{d\theta_L}$, use implicit differentiation
 of the equation from Figure 4-12.

$$(1 + \tan^2 \theta_L) d\theta_L = \frac{\overbrace{\cos \theta_c \left(\frac{1}{A} + \cos \theta_c \right) + \sin^2 \theta_c}^{1 + \frac{1}{A} \cos \theta_c}}{\left(\frac{1}{A} + \cos \theta_c \right)^2} d\theta_c$$

But $1 + \tan^2 \theta_L = \frac{\left(\frac{1}{A} + \cos \theta_c \right)^2 + \sin^2 \theta_c}{\left(\frac{1}{A} + \cos \theta_c \right)^2}$ FROM (*)

$$= \frac{\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1}{\left(\frac{1}{A} + \cos \theta_c \right)^2}$$

$$\therefore \frac{\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1}{\left(\frac{1}{A} + \cos \theta_c \right)^2} d\theta_L = \frac{\frac{1}{A} \cos \theta_c + 1}{\left(\frac{1}{A} + \cos \theta_c \right)^2} d\theta_c$$

Now proceed through some tedious algebra.

$$\therefore \frac{d\theta_c}{d\theta_L} = \frac{\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1}{\frac{1}{A} \cos \theta_c + 1}$$

Substitute into

$$\sigma_s(E, \theta_L) = \sigma_s(E, \theta_c) \left(\frac{\sin \theta_c}{\sin \theta_L} \right) \left(\frac{d\theta_c}{d\theta_L} \right)$$

using (*) to find

$$\frac{\sin \theta_c}{\sin \theta_L} = \frac{\frac{1}{A} + \cos \theta_c}{\cos \theta_L}$$

$$\text{Since } \cos \theta_L = (1 + \tan^2 \theta_L)^{-\frac{1}{2}} = \frac{\frac{1}{A} + \cos \theta_c}{\left(\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1 \right)^{\frac{1}{2}}}$$

we find the desired expression:

$$\sigma_s(E, \theta_L) = \sigma_s(E, \theta_c) \frac{\left(\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1\right)^{3/2}}{1 + \frac{1}{A} \cos \theta_c}$$

OR simply

$$\sigma_s(\theta_L) = \sigma_s(\theta_c) \frac{\left(\frac{1}{A^2} + \frac{2}{A} \cos \theta_c + 1\right)^{3/2}}{1 + \frac{1}{A} \cos \theta_c}$$

(keeping in mind that the cross sections
are always functions of energy E)

Relationship between microscopic differential
scattering cross sections in LAB and CM

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

Recall

$$\sigma_s(E, \theta_c) \sin \theta_c d\theta_c = \text{"effective AREA"}$$

for neutron with energy E
to scatter into $d\theta_c$ about θ_c
(in the CM)

$$\sigma_s(E \rightarrow E') dE' = \text{"effective AREA" for}$$

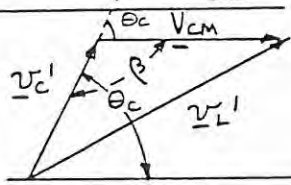
neutron of energy E to
scatter into dE' about E'

Now let us determine the differential scattering
cross section in energy.

Again, these are both physical areas that can be
measured, so we equate them.

$$\therefore \sigma_s(E \rightarrow E') = -\sigma_s(E, \theta_c) \sin \theta_c \left(\frac{d\theta_c}{dE'} \right)$$

Calculation of $\frac{d\theta_c}{dE'}$



$$\cos \beta = \cos(180^\circ - \theta_c)$$

$$v_L'^2 = v_c'^2 + v_{cm}^2 - 2v_c' v_{cm} \cos \beta$$

(LAW of COSINES)

Minus sign occurs because if θ_c increases, the final energy E' decreases.

But we found earlier:

$$v_{cm}^2 = \left(\frac{1}{1+A} \right)^2 v_L^2 \quad (v_L = 0)$$

$$v_c'^2 = v_c^2 = \left(\frac{A}{1+A} \right)^2 v_L^2$$

Substitute into LAW of COSINES,

$$v_L'^2 = \left(\frac{A}{1+A} \right)^2 v_L^2 + \left(\frac{1}{1+A} \right)^2 v_L^2 - 2 \left(\frac{A}{1+A} \right) \left(\frac{1}{1+A} \right) v_L^2 \cos \beta$$

$\cos \beta = -\cos \theta_c$
 $\cos \beta = \cos(\pi - \theta_c)$

More algebra

Then $\frac{E'}{E} = \frac{\frac{1}{2} m v_L'^2}{\frac{1}{2} m v_L^2} = \frac{v_L'^2}{v_L^2}$ ← neutron energy in LAB

OR $\frac{E'}{E} = \frac{A^2 + 2A \cos \Theta_c + 1}{(A+1)^2}$

Now define $\alpha \equiv \left(\frac{A-1}{A+1} \right)^2$

AND OBTAIN

$$E' = \left[\frac{(1+\alpha) + (1-\alpha) \cos \Theta_c}{2} \right] E$$

An important result which gives the relationship between the final energy E' and the angle of scattering (in the CM) Θ_c .

Examples

(1) $A \rightarrow \infty$ (infinitely heavy nucleus, a "brick wall")

$$\alpha \rightarrow 1$$

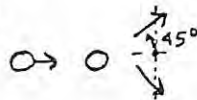
$$E' = E \quad \text{NEUTRON LOSES NO ENERGY BECAUSE NUCLEUS CANNOT RECOIL (INFINITE MASS)}$$

(2) $A=1$ ($M=m$, billiard ball collisions)

$$\alpha = \left(\frac{A-1}{A+1} \right)^2 = 0, \quad E' = \frac{1 + \cos \Theta_c}{2} E$$

$$\Theta_c = 180^\circ, \quad E' = 0 \quad (\text{incident ball stops})$$

$$\Theta_c = 90^\circ, \quad E' = \frac{1}{2} E \quad (\text{energy shared})$$



$$(3) \text{ MAXIMUM energy loss : } \Delta E_{\text{MAX}} = (E - E')_{\text{MAX}} \\ = E - E'_{\text{MIN}}$$

$$E'_{\text{MIN}} \Leftrightarrow \theta_c = -1$$

$$\therefore E'_{\text{MIN}} = \alpha E, \text{ least energy possible} \\ \text{for elastic scattering}$$

Another important result - the minimum neutron energy (in the LAB) following an elastic collision is αE , where $\alpha = \left(\frac{A-1}{A+1}\right)^2$. Note that if $A=1$, the neutron can lose all of its energy (e.g., collision with hydrogen nucleus).

$$\text{Differentiate, } E' = \left[\frac{(1+\alpha) + (1-\alpha)\cos\theta_c}{2} \right] E$$

$$\frac{dE'}{d\theta_c} = - \frac{(1-\alpha)\sin\theta_c}{2} E$$

$$\therefore \sigma_s(E \rightarrow E') = -\sigma_s(E, \theta_c) \sin\theta_c \left(\frac{2}{E(1-\alpha)\sin\theta_c} \right)$$

$$\text{OR } \sigma_s(E \rightarrow E') = \sigma_s(E, \theta_c) \frac{2}{(1-\alpha)E}$$

EXPERIMENTAL DATA: for "light" nuclei,

$\sigma_s(E, \theta_c)$ isotropic in CM

$$\text{i.e., } \sigma_s(E, \theta_c) = \frac{\sigma_s(E)}{2}$$

To find $\sigma_s(E \rightarrow E')$ we need $\frac{d\theta_c}{dE'}$, which we obtain by implicit differentiation of the equation in Figure 4-21.

$$\therefore \sigma_s(E \rightarrow E') = \sigma_s(E) \frac{1}{(1-\alpha)E}$$

Since $E'_{\text{MIN}} = \alpha E$, we can express

this concisely as

$$\sigma_s(E \rightarrow E') = \begin{cases} \sigma_s(E) \frac{1}{(1-\alpha)E} & , \alpha E \leq E' \leq E \\ 0 & , \text{otherwise} \end{cases}$$

(energy loss only, with maximum $\Delta E = (1-\alpha)E$)

LECTURE 5

COMPOUND NUCLEUS REACTIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp 23-34.

Lamarsh, pp. 24-27, 49-54.

EXERCISES:

5.1. Lamarsh, problem #3.15.

5.2. Duderstadt & Hamilton, problem #2-13.

I. REVIEW OF NUCLEAR PHYSICS

A. NUCLEAR REACTIONS

1. Radioactive decay
2. Nuclear collisions

B. CROSS SECTIONS

1. Microscopic
 2. Macroscopic
 3. Differential
-

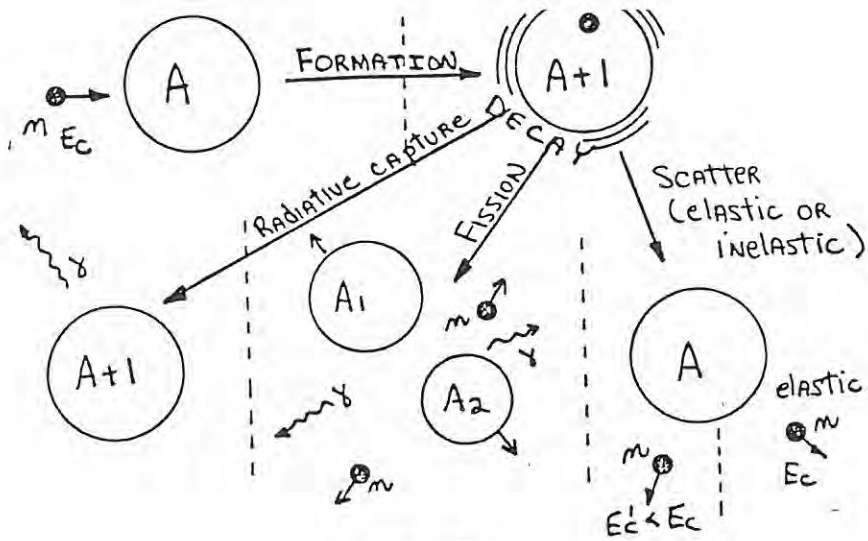
C. NEUTRON-NUCLEAR REACTIONS

1. Elastic scattering
2. Compound nucleus reactions
 - Formation
 - Decay

D. NUCLEAR FISSION

E. NEUTRON PROCESSES IN A THERMAL REACTOR

F. NEUTRON MULTIPLICATION



Schematic diagram of the compound nucleus reaction

Compound nucleus (A+1) is highly excited and decays almost instantaneously via some mode or "decay channel"

5-4

Experimental evidence

- Lifetime of excited state
Nucleus + Neutron $\approx 10^{-14}$ second
- TRAVERSAL TIME - $n \rightarrow \text{circle with } A \text{ and arrows}$
 $v \approx 10^5 \text{ cm/s}$ (A THERMAL OR "SLOW" NEUTRON)

$$d \approx 10^{-12} \text{ cm}$$

$$\Rightarrow \Delta t \approx 10^{-17} \text{ seconds}$$

The discrepancy between the time the neutron actually spends inside the nucleus and the time it would take to traverse the nucleus leads to two conclusions.

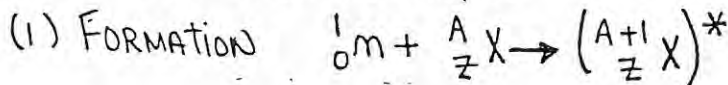
CONCLUSIONS:

1. Neutron interacts with the entire nucleus, sharing its kinetic energy and its binding energy with the nucleons
2. The compound nucleus "forgets" how it was formed (decay mode independent of formation)

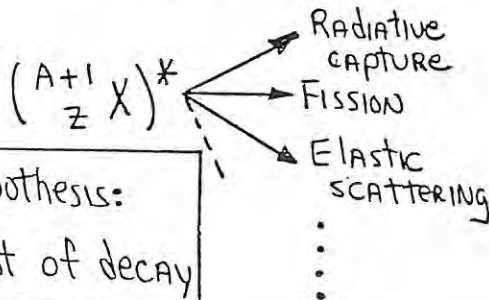
For example, the nucleus "forgets" which neutron hit the nucleus and the direction from which it came.

Bohr Model

The compound nucleus reaction occurs in two distinct steps:



(2) DECAY



Bohr independence hypothesis:
formation independent of decay

Therefore, the probability that a particular compound nucleus reaction occurs (e.g., radiative capture) is the product of the probability for formation x probability for decay via γ emission (radiative capture).

Mathematically -

$$\sigma_i(E) = \sigma_{CN}(E) \frac{\Gamma_i}{\Gamma}$$

where

$\sigma_i(E)$ = MICROSCOPIC CROSS SECTION
FOR THE i^{th} REACTION
(e.g., $i = \gamma$)

$\sigma_{CN}(E)$ = MICROSCOPIC CROSS SECTION
FOR FORMATION OF THE CN

$\frac{\Gamma_i}{\Gamma}$ = PROBABILITY THE CN NUCLEUS
DECAYS VIA THE i^{th} "CHANNEL"

Since the cross section is proportional to the probability of occurrence, this is a mathematical statement of Bohr's hypothesis.

Compound Nucleus Reaction - energetics

- NEUTRON ENERGY = $E_L = \frac{1}{2} m v_L^2$
- IF NUCLEUS AT REST, $E_C = \frac{A}{1+A} E_L$

where E_C = KINETIC ENERGY OF
NEUTRON PLUS NUCLEUS
IN THE CM FRAME

$$E_C = \frac{1}{2} m v_C^2 + \frac{1}{2} M V_C^2 \quad \left(A = \frac{M}{m} \right)$$

- $E_{CM} = E_L - E_C$ = KINETIC ENERGY OF
THE CM MOTION

Assume for the time being that the target nucleus is at rest in the LAB

Note E_C is the kinetic energy relative to an observer travelling with the CM.

CONSERVATION OF ENERGY

• The kinetic energy associated with the CM motion is conserved for all reactions

$\Rightarrow E_{CM}$ "NOT AVAILABLE"

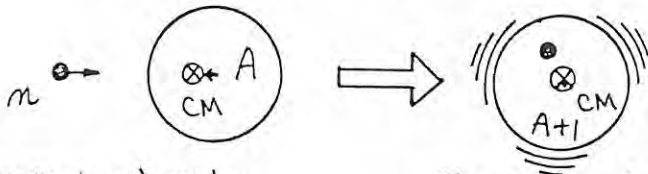
To supply reaction energy (e.g., to excite a nuclear state)

$\Rightarrow E_c =$ kinetic energy in CM is "AVAILABLE"

\therefore (CAN BE TRANSFORMED TO OTHER TYPE OF ENERGY)

Note total energy is conserved, but not kinetic energy in general. Kinetic energy may be transformed to potential energy, for example.

The compound nucleus reaction:



NEUTRON AND NUCLEUS
MOVING RELATIVE
TO CM

$$E_c = \frac{A}{1+A} E_L > 0$$

NEUTRON AND
NUCLEUS MOVING
WITH THE CM

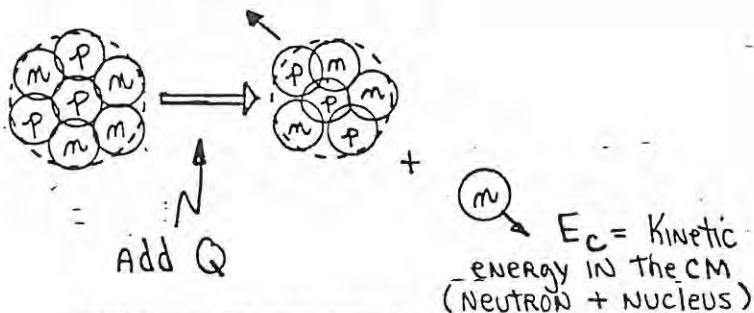
$$\Rightarrow E_{c'} = 0$$

\therefore In the compound nucleus reaction,
All of the energy available E_c
must go into excitation of $(A+1)_Z^X$ *

With respect to an observer on the CM, the neutron and nucleus are at rest after the collision. Therefore, $E_{c'} = 0$ and all available kinetic energy is transformed into excitation energy.

Binding energy

- To REMOVE A NEUTRON FROM A NUCLEUS $A+1$, need to supply energy:



Another source of excitation energy is the binding energy supplied by the incident neutron.

Recall that binding energy is the energy needed to remove a neutron from the nucleus.

- The energy Q is needed to:

(1) REMOVE THE NEUTRON

(2) SUPPLY KINETIC ENERGY E_c OF NEUTRON + FINAL NUCLEUS (RELATIVE TO CM)

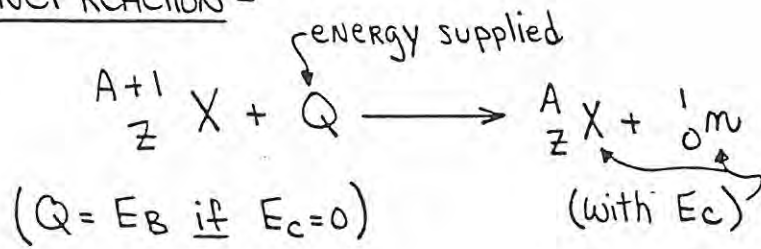
- Define

$$E_B = Q \text{ to REMOVE NEUTRON ONLY (} E_c = 0 \text{)}$$

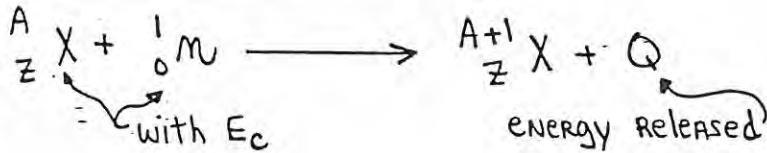
Binding energy of the last neutron

Minimum energy needed to just remove a neutron from the nucleus (no kinetic energy) is the binding energy.

Net reaction -



Reverse the reaction:



But we are concerned with adding a neutron, therefore the binding energy is released.

- How is the energy released?

Excitation energy of ${}_{Z}^{A+1}X$
(where else can it go?)

- Define $\Delta E =$ excitation energy of $({}_{Z}^{A+1}X)^*$

$$\Delta E = E_B + E_c = Q$$

“kinetic energy” available

Probability of CN Formation

QUANTUM MECHANICS: COMPOUND NUCLEUS

MORE likely to be formed

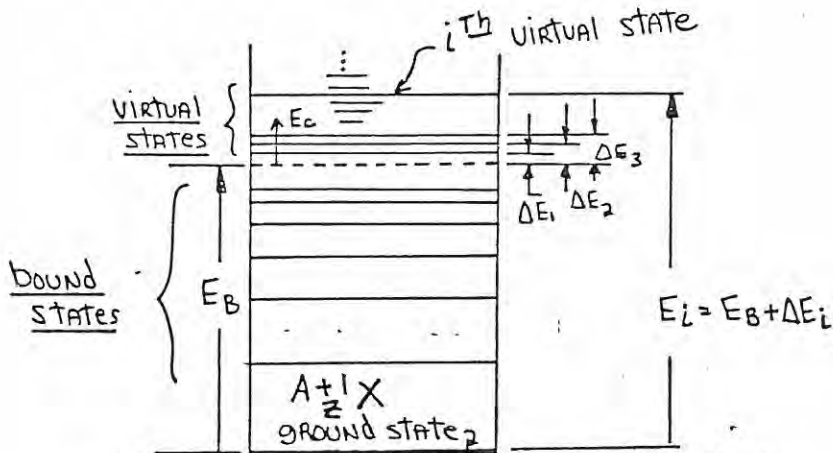
if ΔE corresponds to

AN ALLOWABLE energy level of the CN

$$\text{i.e., } \Delta E = E_B + E_c = E_i$$

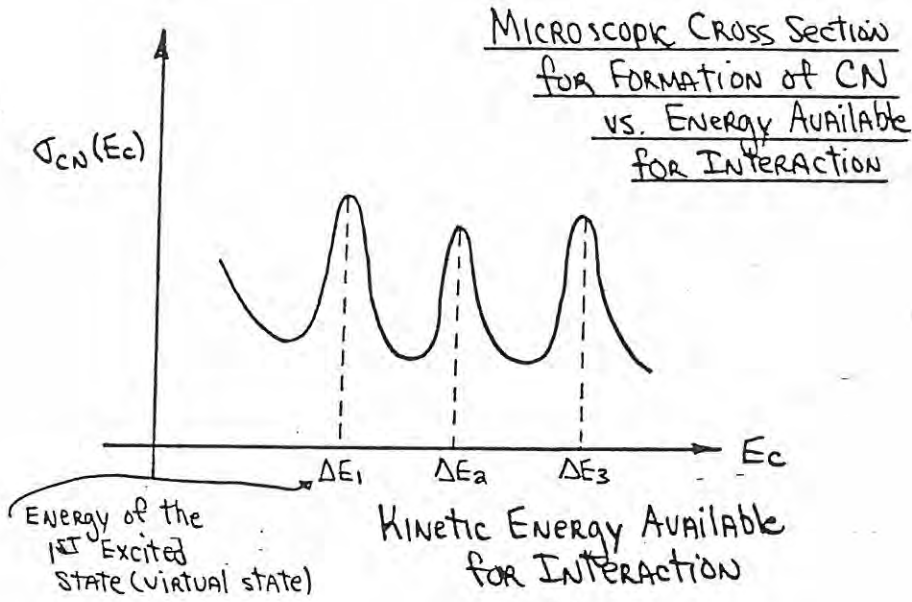
excitation
energy of
allowable state

What is the probability for compound nucleus formation?

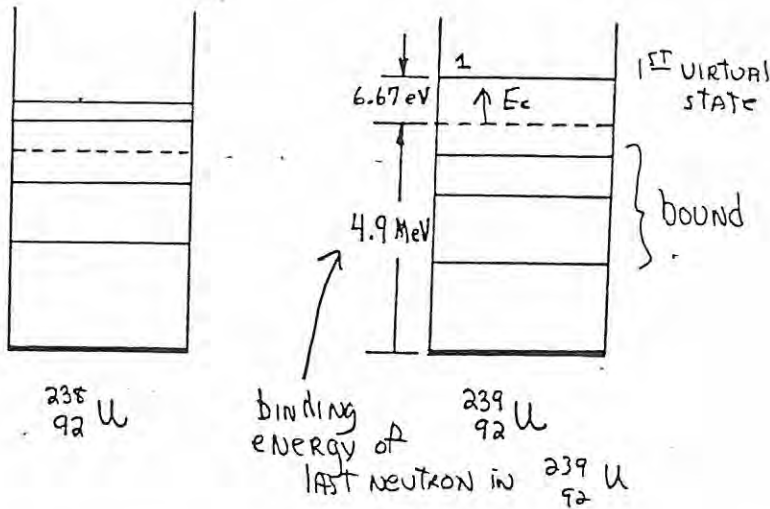
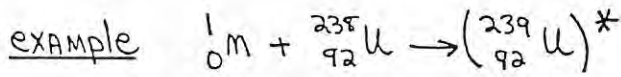


Note: if $E_i = \Delta E$ then $\Delta E_i = E_c$
 $(\begin{smallmatrix} A+1 \\ Z \end{smallmatrix} X)^*$ MUST be a VIRTUAL STATE
 $(\Delta E = E_B + E_c)$

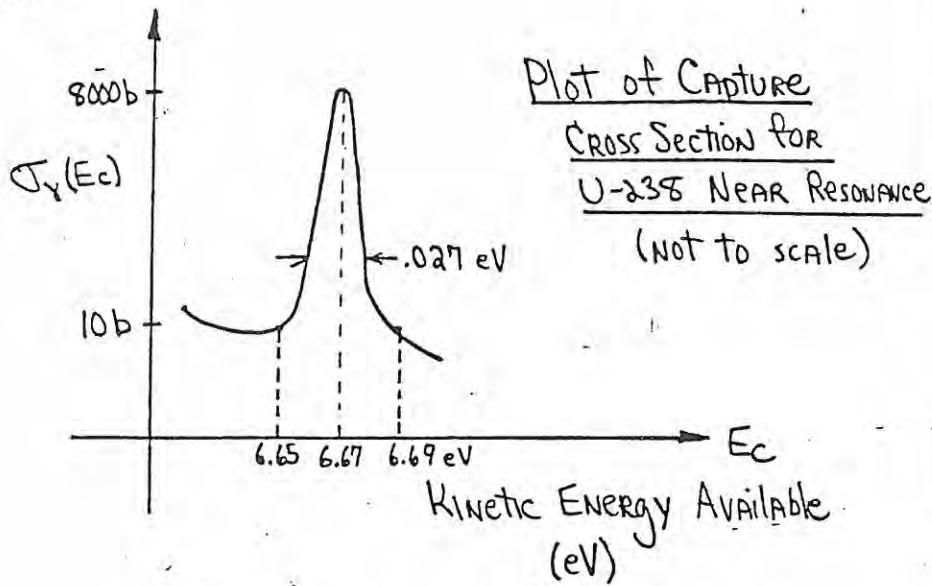
The compound nucleus must be formed with an excitation energy $\Delta E > E_B$. The amount of excitation energy in excess of E_B is simply the energy available E_c .



If model true, then we would expect the compound nucleus to be formed preferentially for $E_c = \Delta E_1$, $E_c = \Delta E_2$,etc., leading to the above type of cross section dependence.



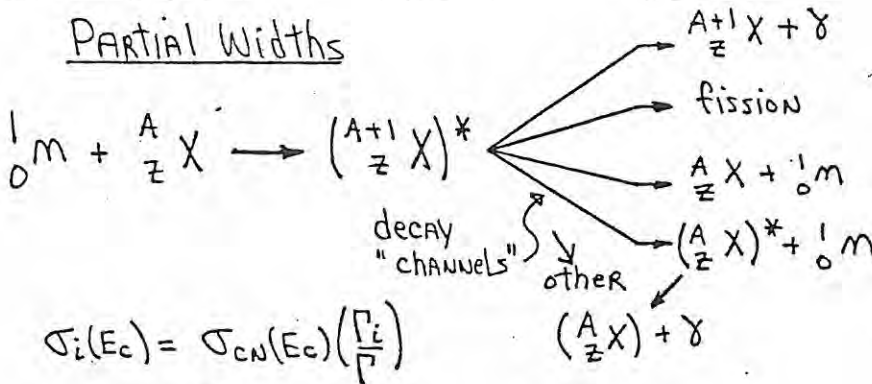
Actual example - ${}_{92}^{239}\text{U}$ has its first excited state (virtual state) at 6.67 eV above E_B .



Experimental data - "resonant" behavior of the cross section, with a peak at 6.67eV.

Decay of the Compound Nucleus

PARTIAL WIDTHS



$$\sigma_i(E_c) = \sigma_{CN}(E_c) \left(\frac{\Gamma_i}{\Gamma} \right)$$

where: $\frac{\Gamma_i}{\Gamma}$ = probability the CN decays via channel "i"

The probability of a particular decay channel is measured and tabulated in terms of the energy "width".

$\Gamma \equiv$ "width" of the excited state
 (e.g., $\Gamma = .027 \text{ eV}$ for
 $({}^{239}_{92}\text{U})^*$ at $E_c = 6.67 \text{ eV}$)

Relationship of Γ to Probability

Recall from Radioactive Decay,

$$N(t) = N_0 e^{-\lambda t}$$

$\lambda =$ decay constant (\propto probability of decay)

The "width" is actually proportional to the probability of decay.

• But $\tau =$ mean lifetime $= \frac{1}{\lambda}$

$\therefore \frac{1}{\tau} \propto$ probability of decay

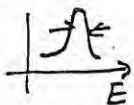
• Heisenberg Uncertainty Principle -

$$\Delta E \cdot \Delta t \approx \hbar$$

Γ τ

$$\Rightarrow \Gamma \approx \hbar / \tau$$

$$\Rightarrow \underline{\Gamma \propto \text{probability of decay}}$$



• In general,

$\Gamma_i \propto$ probability of decay
via the i^{th} channel

$$\text{AND } \Gamma = \sum_{i=1}^N \Gamma_i$$

• Γ - "total" width

Γ_i - "partial" width

e.g., Γ_γ = width for CN decay via γ

Γ_n = " " " " " " neutron

Γ_f = " " " " " " fission

Γ = total width

$$= \Gamma_\gamma + \Gamma_f + \Gamma_n + \Gamma_{n'} + \dots$$

$$\text{Clearly } \sum_j \sigma_j(E_c) = \underbrace{\sum_j \left(\frac{\Gamma_j}{\Gamma} \right)}_1 \sigma_{\text{CN}}(E_c) = \sigma_{\text{CN}}(E_c)$$

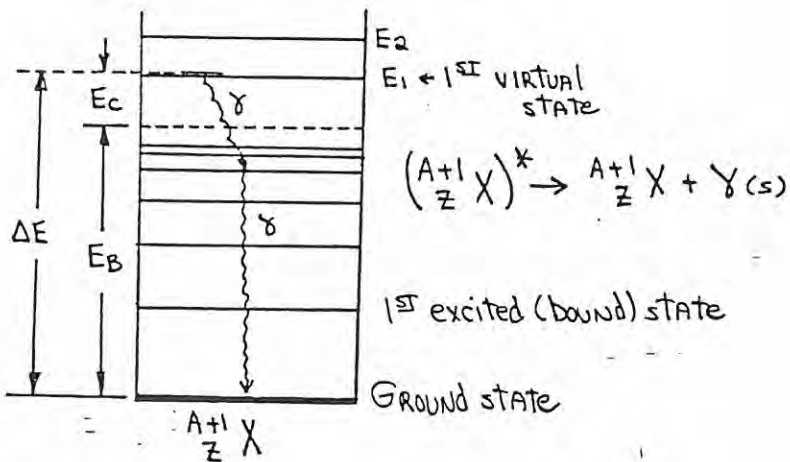
Mean lifetime for decay

via channel "i"

$$\equiv \tau_i = \hbar / \Gamma_i$$

Decay Channels $(\frac{A+1}{Z}X)^*$

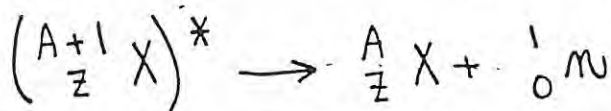
1. γ decay "RADIATIVE CAPTURE"



Radiative capture - the compound nucleus decays (eventually) to its ground state, and the neutron has been "captured"

2. Decay via Neutron Emission

a. Elastic (RESONANCE elastic scattering)

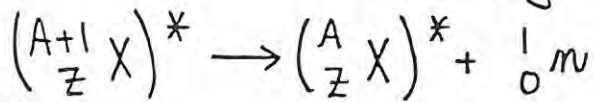


$$\boxed{E_c' = E_c} \text{ (elastic)}$$

$$A \text{ large, } E_L' = E_L$$

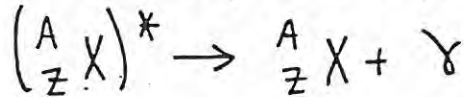
Elastic Scattering - the compound nucleus emits a neutron (a different one in general) and the kinetic energy E_c in the CM frame is conserved (note LAB energy $E_L' \approx E_L$ due to recoil of the nucleus).

b. Inelastic (RESONANCE INELASTIC SCATTERING)

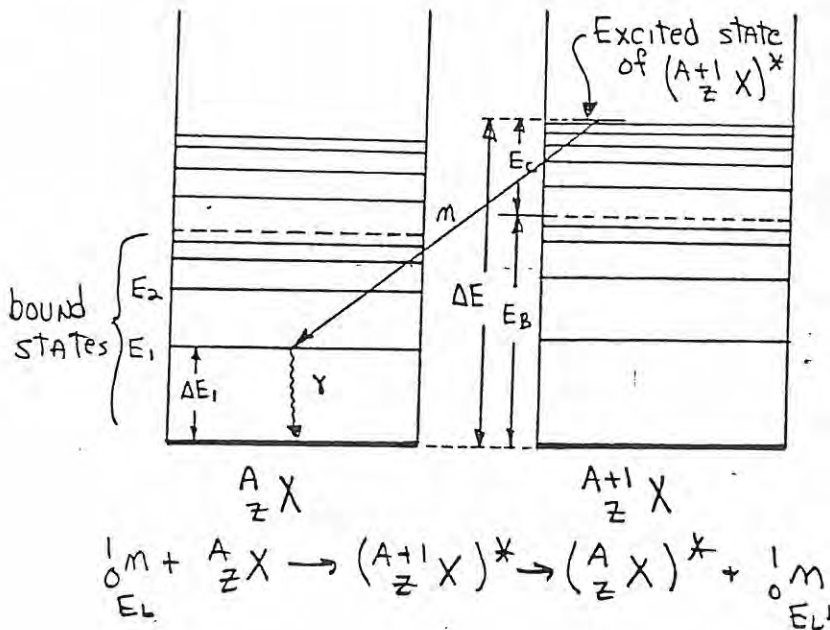


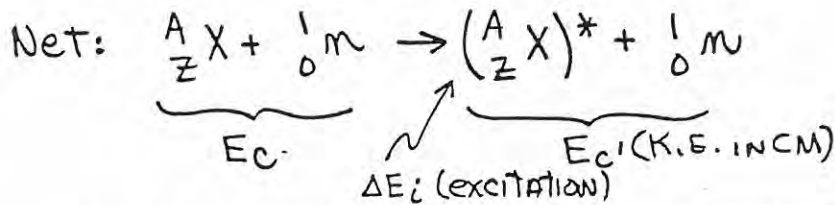
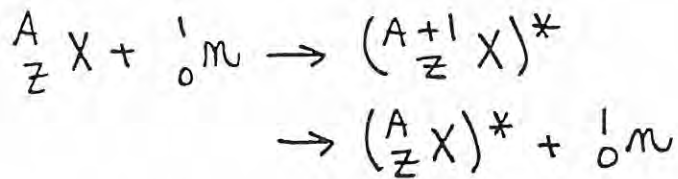
excited state
of ORIGINAL TARGET NUCLEUS

MAY have subsequent decay,



Inelastic scattering - the compound nucleus emits a neutron and the original nucleus is left in an excited state.





CONS of TOTAL ENERGY $\Rightarrow \boxed{E_c = \Delta E_i + E_{c'}}$

Note that a portion of the energy available has gone into excitation of the target nucleus.

Inelastic Scattering is
A Threshold Reaction

(REQUIRES A MINIMUM KINETIC ENERGY OF THE NEUTRON)

- Energy Balance : $E_c = \Delta E_i + E_{c'}$
- MINIMUM $E_{c'} = 0$
- MINIMUM $\Delta E_i = \Delta E_1$ excitation energy of 1st excited state

$\therefore \boxed{E_c(\text{MINIMUM}) = \Delta E_1}$ Threshold Energy

The minimum energy available is the lowest excitation energy of the target nucleus.

LECTURE 6

CROSS SECTION RESONANCES

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 45-54.

Lamarsh, pp. 59-61, 275-279.

EXERCISES:

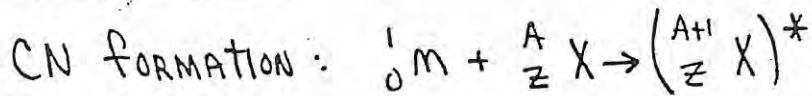
6.1. Duderstadt & Hamilton, problem #2-16.

6.2. Prove that $\Delta < 0$ in the expression

$$E_C = \frac{A}{1+A} E_L + \Delta$$

when the nucleus is moving in the same direction
as the incident neutron (an overtaking collision)

Brief Review



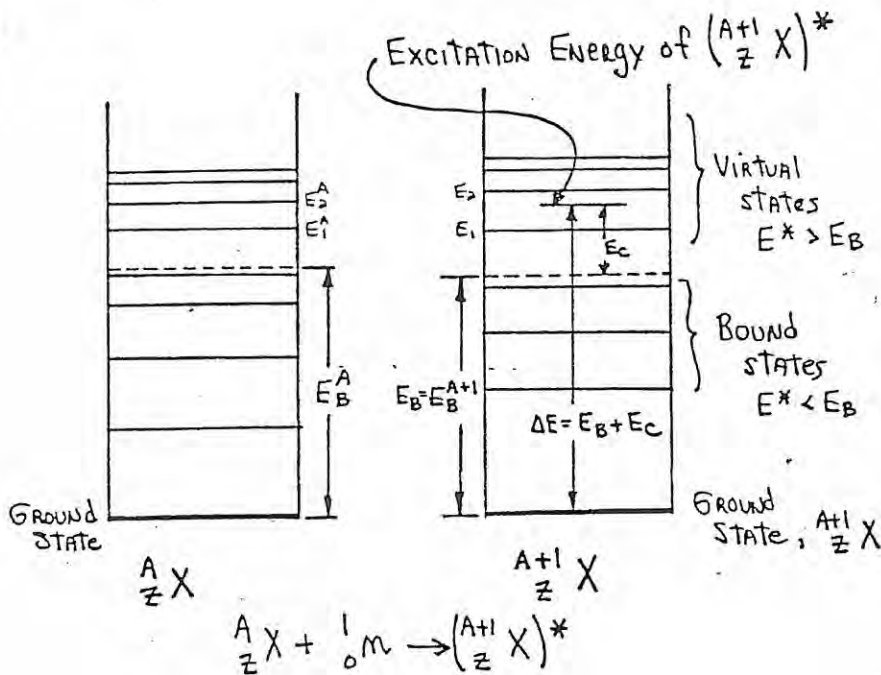
E_L = KINETIC ENERGY OF NEUTRON
IN LAB

E_C = KINETIC ENERGY OF NEUTRON +
NUCLEUS IN CM FRAME
("AVAILABLE" FOR INTERACTION)

FOR NUCLEUS AT REST,

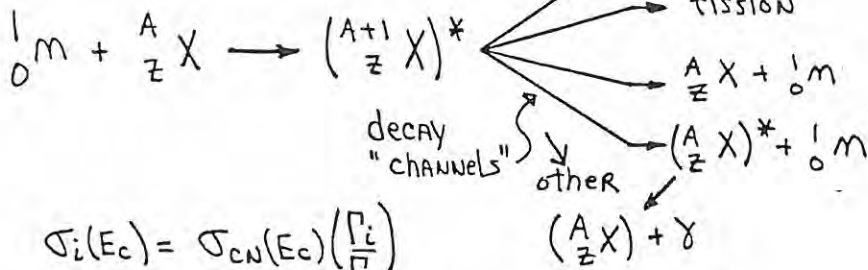
$$E_C = \frac{A}{1+A} E_L$$

6-2



Decay of the Compound Nucleus

PARTIAL WIDTHS



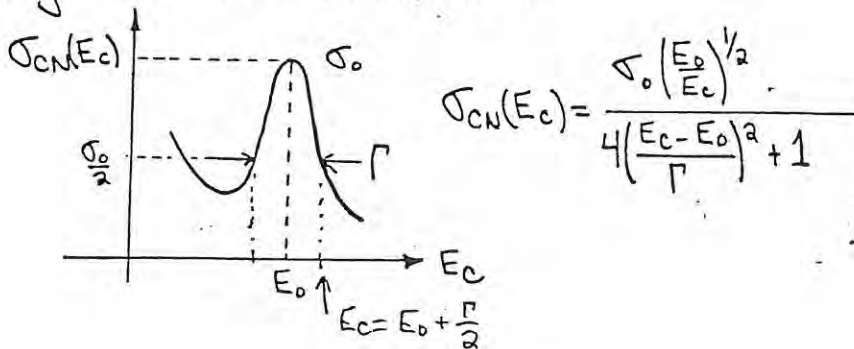
$$\sigma_i(E_c) = \sigma_{CN}(E_c) \left(\frac{\Gamma_i}{\Gamma} \right)$$

where $\frac{\Gamma_i}{\Gamma}$ = probability the CN decays via channel "i"

Energy Dependence of $\sigma_{CN}(E_c)$

NEAR AN ISOLATED RESONANCE

AT ENERGY $E_c = E_0$, THE BREIT-WIGNER SINGLE-LEVEL FORMULA. (~1936)



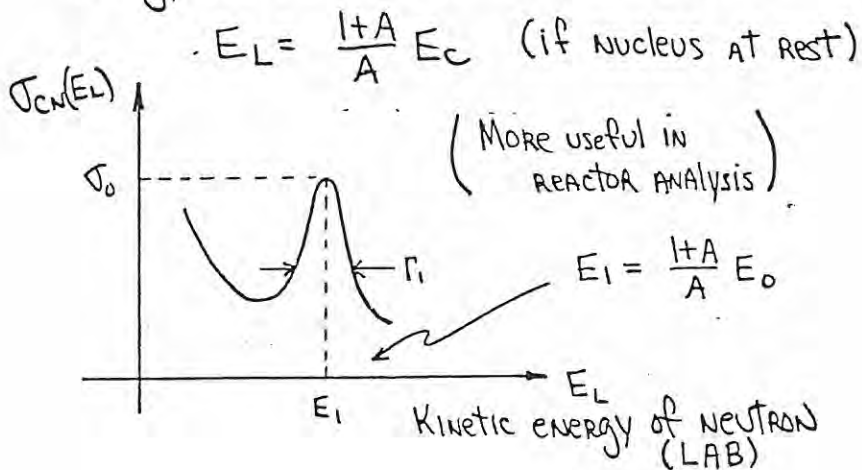
Note: $\sigma_{CN}(E_0 \pm \frac{\Gamma}{2}) = \frac{\sigma_0}{2}$
 (with $\frac{E_0}{E_c} \approx 1$)

Reactor Analysis - concerned with
 velocities measured in the
 LAB frame not the CM frame

CAN we express σ_{CN} in terms
 of the neutron LAB energy
 rather than the CM energy?

The reactor analyst would prefer to
 analyze the reactor in a reference
 frame fixed in the LAB frame (e.g.,
 reactor frame).

This curve may be plotted
 as a function of neutron
 energy (in the LAB (reactor) frame):



Simple transformation if the nuclei
 are at rest.

Actual physical situation

- Nuclei not at rest
- CONTINUAL MOTION due to their thermal energy

$$E_{th} = \text{AVERAGE thermal energy} = \frac{3}{2} k T$$

↑ Absolute temp
↑ Boltzmann

EXAMPLE: $T = 300^\circ\text{K}$

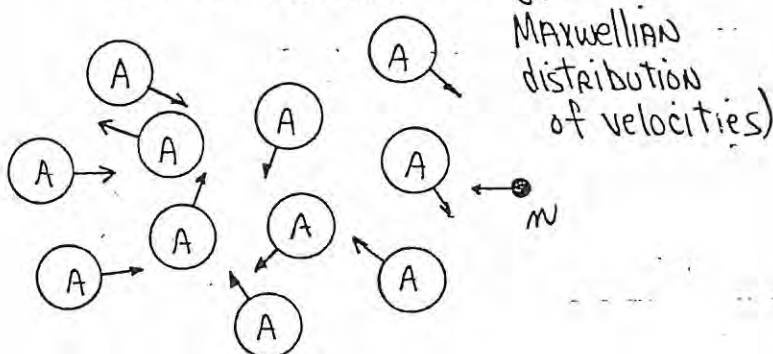
$$E_{th} = \left(\frac{3}{2}\right) (8.617 \times 10^{-5} \frac{\text{eV}}{^\circ\text{K}}) (300^\circ\text{K})$$

$$\underline{E_{th} = .039 \text{ eV}} \quad \text{AVERAGE Thermal ENERGY AT ROOM TEMP}$$

Recall the width of the ${}_{92}^{238}\text{U}$ resonance at

6.67 eV is .027 eV. The thermal motion of the nuclei is important for such sensitive behavior of the cross sections.

- Actual target may consist of a mixture of nuclei, All moving at different velocities with respect to the neutron (e.g., A



The incoming neutron sees a distribution of velocities (speeds and directions).

- What if the nuclei ARE moving?
(is it important to consider?)
- CAN we still express σ_{CN} in terms of E_L , the neutron energy in the LAB?

Note: the physical cross section is a function of E_C only

would like to express σ_{CN} in terms of the neutron kinetic energy E_L .

- Depending on the velocity of the nucleus relative to the neutron, the energy E_C MAY TAKE ON SEVERAL VALUES FOR A GIVEN E_L .

ANSWER - NO, IN GENERAL

- What now?

That is, the cross section σ_{CN} will be different for each nucleus, for the same incident neutron, because E_C will be different.

Doppler Broadening

- Idea- for a specific E_L ,
AVERAGE the cross section
 $\sigma_{CN}(E_c)$ over the expected values
of E_c

- Recall:

$E_c =$ energy of neutron +
nucleus in the CM
(OR, energy available for the reaction)

This gets us into the subject known
as "Doppler broadening"

- $E_c = \frac{1}{2} m v_c^2 + \frac{1}{2} M V_c^2$

$v_c = |\underline{v}_c|$ $\underline{v}_c =$ velocity of neutron
in the CM frame

$V_c = |\underline{V}_c|$ $A = M/mv$

- OR, $E_c = \frac{1}{2} \mu v_r^2$ $\mu = \frac{mM}{m+M} = \frac{A}{1+A}$

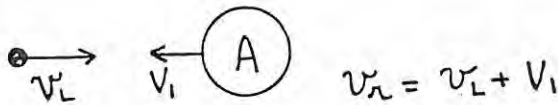
where $\underline{v}_r =$ velocity of neutron
relative to the nucleus

$$\underline{v}_r = \underline{v}_L - \underline{V}_L$$

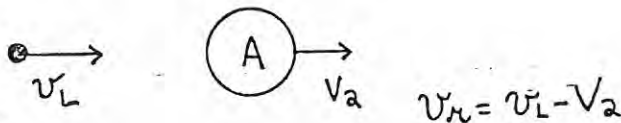
IN LAB \nearrow

Two limiting cases

Case ①



Case ②



Must have $v_L > v_2$

Let us examine how \int_{CN} would change for the two limiting cases (all other cases are bracketed by these).

Calculation of E_c $E_c = \frac{1}{2} \mu v_r^2$

Case ① $E_c = \frac{1}{2} \mu (v_L + v_1)^2$

OR $E_c = \frac{1}{2} \mu v_L^2 + \Delta_1$

where $\Delta_1 = \mu v_1 (v_L + \frac{v_1}{2})$, $\Delta_1 > 0$

Case ② $E_c = \frac{1}{2} \mu (v_L - v_2)^2$

$E_c = \frac{1}{2} \mu v_L^2 + \Delta_2$

where $\Delta_2 = -\mu v_2 (v_L - \frac{v_2}{2})$, $\Delta_2 < 0$

Note E_c is greatest for a "head on" collision and smallest for a "rear end" collision.

$$\text{Since } E_L = \frac{1}{2} m v_L^2$$

$$\text{AND } \mu = \frac{m M}{m + M}$$

$$\text{Then } \frac{1}{2} \mu v_L^2 = \frac{M}{m + M} E_L = \frac{A}{1 + A} E_L$$

$$\therefore \boxed{E_C = \frac{A}{1 + A} E_L + \Delta}$$

where Δ depends on the relative motion of the neutron and nucleus
($\Delta = 0$ if nucleus at rest)

Case ① Relative motion - approaching

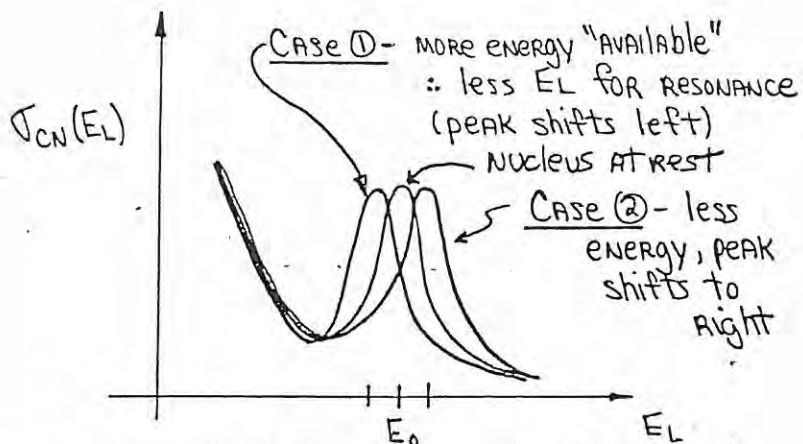
$\Delta > 0 \Rightarrow$ MORE ENERGY AVAILABLE THAN FOR CASE WITH NUCLEUS AT REST

Case ② Relative motion - away

$\Delta < 0 \Rightarrow$ less energy available

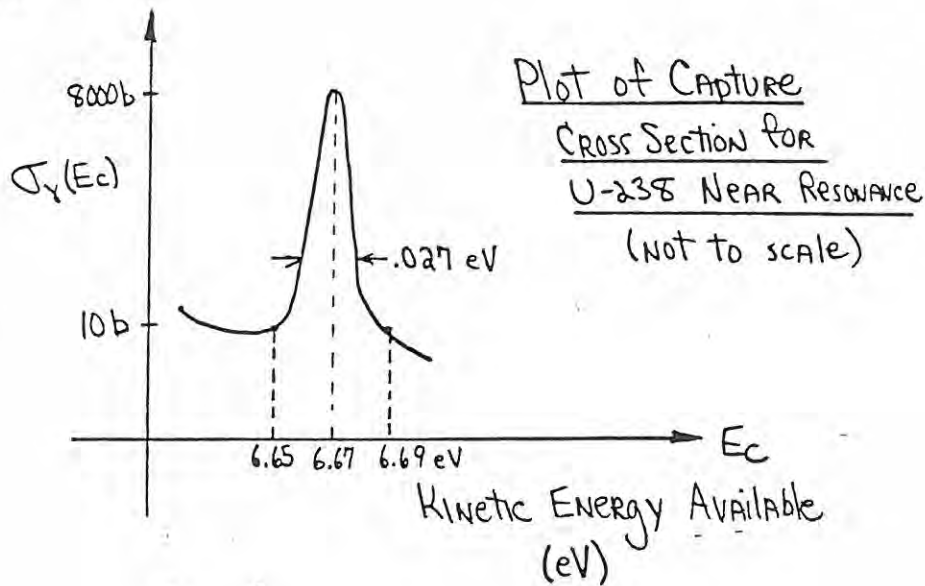
Note these two limiting cases are for the same neutron energy in the LAB frame.

FOR A GIVEN NEUTRON ENERGY E_L
 IN THE LAB (REACTOR) FRAME, THE
 ENERGY E_C WHICH CONTRIBUTES TO
 THE EXCITATION ENERGY OF THE
 COMPOUND NUCLEUS IS GREATER
 (LESS) FOR RELATIVE MOTION OF THE
 NUCLEUS TOWARD (AWAY FROM) THE
 NEUTRON THAN FOR THE CASE WHERE
 THE NUCLEUS IS AT REST



- Δ MAY BE SMALL, BUT $\sigma_{CN}(E_C)$ IS A SENSITIVE FUNCTION OF E_C NEAR A RESONANCE

SINCE THE PHYSICAL CROSS SECTION IS A FUNCTION OF E_C , NOT E_L , A HEAD ON COLLISION (CASE (1)) MEANS LESS E_L IS NEEDED FOR THE REQUIRED E_C , \therefore CURVE SHIFTS LEFT.



GOAL - find a suitable $\sigma_{CN}(E_L)$
which takes into account the
different nuclei velocities

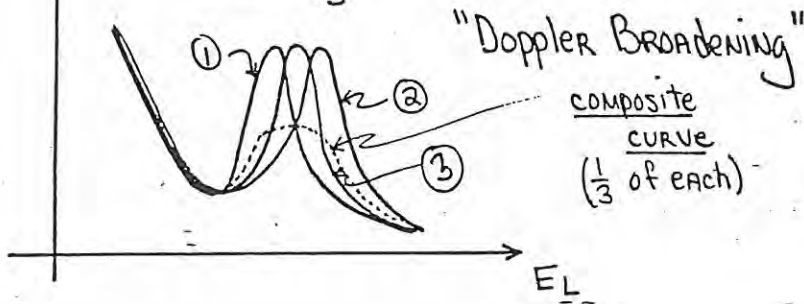
hypothetical case - A target with
3 categories of nuclei:

- ① Relative motion toward
NEUTRON
- ② Relative motion AWAY
- ③ Nucleus AT REST
(SAME AS EARLIER CASE)

So now that we know what σ_{CN} is for 3
different cases, how do we find an effective
cross section for a mixture?

SOLUTION - AVERAGE $\sigma_{CN}(E_L)$ OVER the relative abundances of these categories

- ASSUMING equal numbers, TAKE $\frac{1}{3}$ of each curve



Note how the composite (averaged) curve has "broadened".

• In practice, the cross section IS AVERAGED to preserve reaction rates

• Recall $R = \Sigma \Phi = \sigma \cdot N \cdot m \cdot v$ $1b = 10^{-24} \text{ cm}^2$

where $v =$ NEUTRON speed (cm/s)

$N =$ nuclei density (#/b.cm)

$m =$ NEUTRON density "

$\sigma =$ MICROSCOPIC CROSS SECTION (b)

$R =$ # REACTIONS / b.cm.s

The standard criterion for defining effective cross sections is to preserve reaction rates, because reaction rates can be measured and we will find later that reaction rates are of vital importance to the analyst.

- Given a distribution of \underline{v} - (LAB frame) nuclei velocities, $n(\underline{v})$

$n(\underline{v}) d^3V =$ NUMBER OF NUCLEI ^{PER UNIT VOLUME} with velocity \underline{v} in the INTERVAL $\underline{v}, \underline{v} + d^3V$

note: $\iiint_{\text{All } \underline{v}} n(\underline{v}) d^3V = N$ $n(v_x, v_y, v_z) dv_x dv_y dv_z$

- Define $\sigma(E_c) = \sigma(|\underline{v}_n|)$ \underline{v}_n - NEUTRON vel (LAB)
- $= \sigma(|\underline{v} - \underline{v}|)$

As the cross section to be AVERAGED

$n(\underline{v})$ is just a "density" in velocity as well as space.

- Then the ACTUAL REACTION RATE

is $R = \iiint_{\text{All } \underline{v}} |\underline{v}_n - \underline{v}| \sigma(|\underline{v}_n - \underline{v}|) n(\underline{v}) \rho d^3V$

- We want to define AN AVERAGE CROSS SECTION $\bar{\sigma}(v)$ THAT will yield the CORRECT REACTION RATE, i.e.,

$$R = N \cdot \bar{\sigma}(v) \cdot \rho v$$

$$\therefore \bar{\sigma}(v) = \frac{1}{N v} \iiint |\underline{v}_n - \underline{v}| \sigma(|\underline{v}_n - \underline{v}|) n(\underline{v}) d^3V$$

Velocity Distribution of Nuclei

- Assume $n(\underline{v}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-Mv^2/2kT}$

Maxwellian distribution

(characterizes velocity distribution of ideal gas molecules of mass M at temperature T in thermal equilibrium)

- Reasonable approximation for nuclei in a reactor (or other "target") at a temperature T

Average Cross Section

$\bar{\sigma}(v, T) =$ AVERAGE MICROSCOPIC CROSS SECTION FOR A NEUTRON OF speed v IN A MEDIUM OF nuclei having a Maxwellian distribution of velocities $n(\underline{v})$, the AVERAGE TAKEN TO PRESERVE REACTION RATES

Note we will get a different average at different T .

- Calculate

$$\bar{\sigma}(v, T) = \frac{1}{Nv} \left(\int \int \int_{\text{All } \underline{v}} |\underline{v} - \underline{v}'| \sigma(|\underline{v} - \underline{v}'|) n(\underline{v}') d^3v' \right)$$

Bret-Wigner

where

$$n(\underline{v}') = \left(\frac{M}{2\pi kT} \right)^{3/2} e^{-Mv'^2/2kT}$$

RESULT: (for σ_y)

$$\bar{\sigma}_y(v, T) \approx \sigma_0 \frac{\Gamma_y}{\Gamma} \left(\frac{E_0}{E} \right)^{1/2} \Psi(\beta, x)$$

↑
Tabulated function

where $x \equiv 2(E - E_0)/\Gamma$

$\beta \equiv \Gamma/\Gamma_D$

$\Gamma_D \equiv \left(\frac{4E_0 kT}{A} \right)^{1/2}$ "Doppler width"

• Note: $\Gamma_D \propto T^{1/2}$

- the "width" increases with temperature
- consistent with the physical model (nuclei may have greater velocity, hence curve will be shifted more)

LECTURE 7

NUCLEAR FISSION - ENERGETICS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp 54-62

Lamarsh, pp. 61-68.

EXERCISES:

7.1 Lamarsh, problem #3.34.

7.2 Duderstadt and Hamilton, problem #2-19.

Nuclear Fission

- History
- Phenomenological description
- Binding energy curve - significance
- Energetics
- Types of fission
- Fission products
- Energy release

7-2

Nuclear fission - history

- 1934 - Fermi and co-workers observed radioactivity after bombarding natural elements with neutrons
- explained radioactivity from neutron bombardment of natural uranium as β -decay of transuranic elements formed as a result of neutron capture

problem - decay chains not consistent with those observed with other heavy elements

Note Fermi and colleagues induced fission to occur but did not know it at the time.

1939 - HAHN AND STRASSMAN IDENTIFIED
BARIUM ($Z=56$) AS ONE OF THE
PRODUCTS OF THE NEUTRON-
URANIUM REACTION

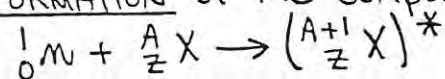
- MEITNER AND FRISCH IMMEDIATELY
PROPOSED THE FISSION MODEL,
BASED ON THE BOHR LIQUID
DROP MODEL OF THE NUCLEUS

Hahn and Strassman actually
discovered the fission reaction.

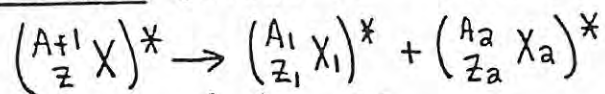
7-4

Nuclear fission - the phenomenon

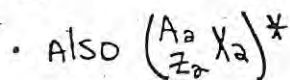
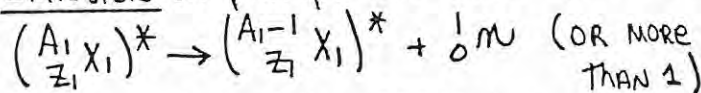
1. FORMATION of the compound nucleus



2. Scission (within 10^{-14} seconds)



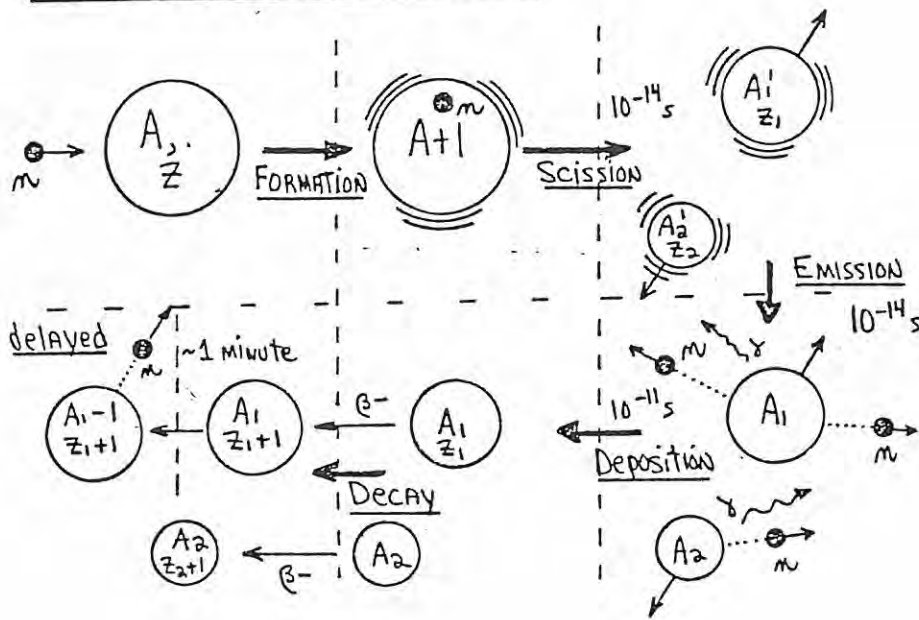
3. EMISSION of prompt neutrons (10^{-14} sec)



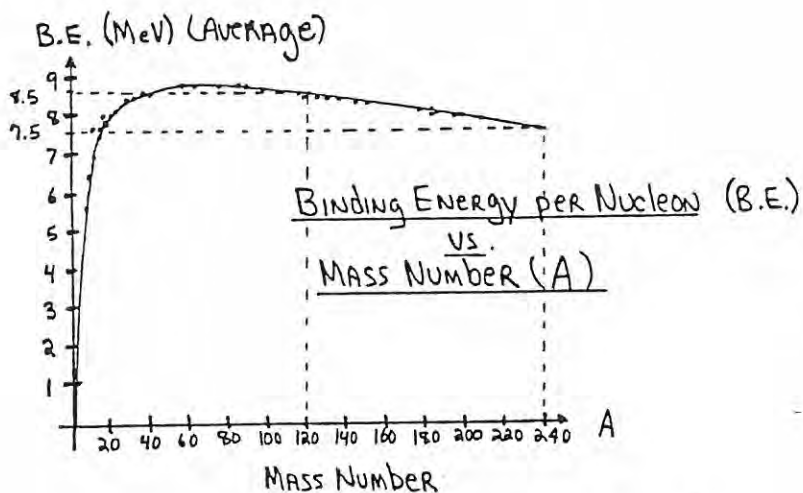
4. FISSION FRAGMENTS deposit kinetic energy (within 10^{-11} seconds)

5. FISSION FRAGMENTS AND DAUGHTER PRODUCTS CONTINUE TO DECAY (principally β and γ decay; A SMALL FRACTION emit NEUTRONS - The "delayed" NEUTRONS)

7-6 Nuclear fission - schematic



7-7



The curve of binding energy versus A indicates why fission can occur.

7-8

example: break apart nucleus with $A=240$
and recombine the nucleons into
two nuclei with $A=120$ each
(hypothetical case)

$\Delta Q_1 =$ energy needed to break
apart $A=240$ nucleus

$\Delta Q_2 =$ energy released when 2
nuclei with $A=120$ are formed.

Using plot, $\Delta Q_1 = 240 \times 7.5 \text{ MeV} = 1800 \text{ MeV}$

$\Delta Q_2 = 2 \times 120 \times 8.5 \text{ MeV} = 2040 \text{ MeV}$

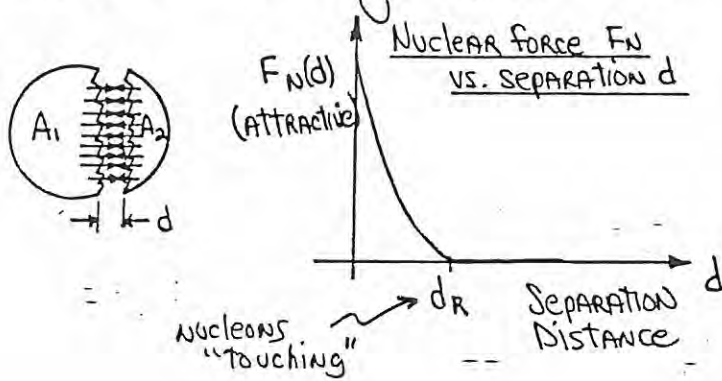
$\Delta Q = 2040 - 1800 = \boxed{240 \text{ MeV}}$ net energy release

Simple example showing that fission
is energetically possible.

Energetics (simple model)

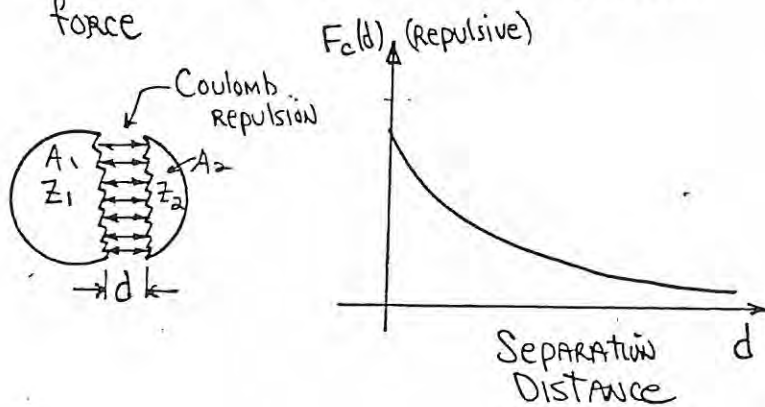
- To split ${}^A_Z X$ into ${}^{A_1}_{Z_1} X_1$ & ${}^{A_2}_{Z_2} X_2$

need to Add energy to overcome the Attractive (but short-range) Nuclear forces

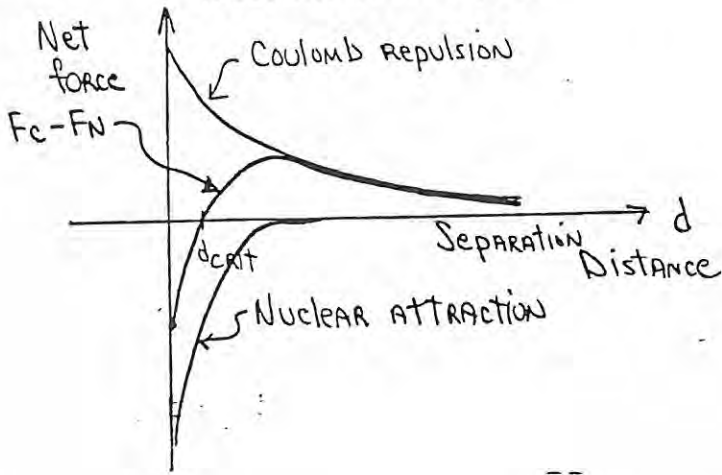


The nuclear forces "glue" the nucleus together.

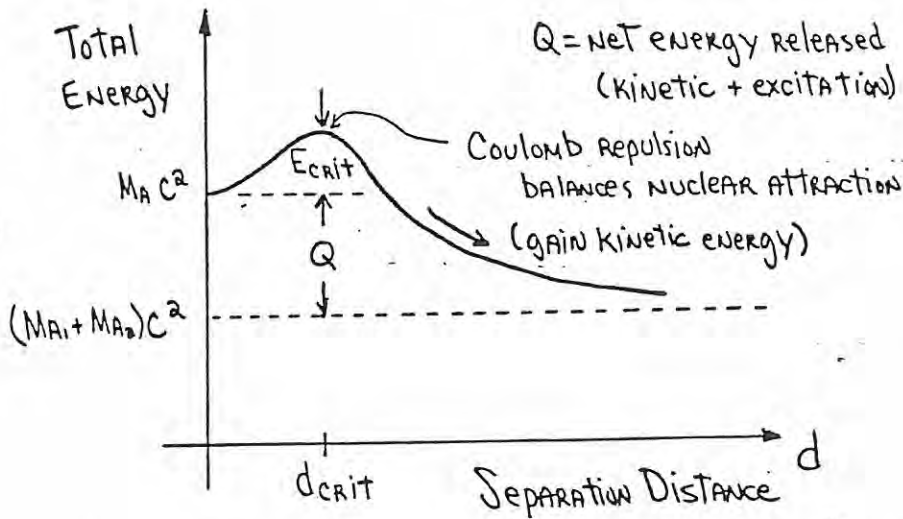
- Since A_1 and A_2 contain Z_1 and Z_2 protons, respectively, There will be a Coulomb repulsion force



- At some separation d_{crit}
The Coulomb repulsion =
NUCLEAR ATTRACTION



The short range nuclear forces decrease very rapidly.



There is a "fission barrier" that must be exceeded for the nucleus to scission.

E_{crit} - energy required to separate the fragments to the critical separation distance d_{crit}

Q - NET ENERGY RELEASE FROM THE FISSION REACTION

$$Q = 931 \frac{\text{MeV}}{\text{amu}} [M_A + M_m - M_{A_1} - M_{A_2}]$$

ACTUALLY AN AVERAGE

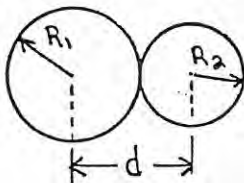
PRIOR TO NEUTRON EMISSION

A_1 and A_2 are the fission fragments prior to the emission of prompt neutrons.

Coulomb potential energy

$$V_c = \frac{Z_1 Z_2 e^2}{R_1 + R_2} \left\{ \begin{array}{l} \text{classical expression for} \\ \text{2 point charges } Z_1 \text{ and} \\ Z_2 \text{ separated by} \\ d = R_1 + R_2 \end{array} \right.$$

example Split ${}_{92}^{235}\text{U}$ into ${}_{52}^{135}\text{Te}$
And ${}_{40}^{101}\text{Zr}$



$$\begin{array}{ll} Z_1 = 52 & A_1 = 135 \\ Z_2 = 40 & A_2 = 101 \end{array}$$

The resultant energy released can be explained nicely by conventional coulomb potential energy.

• Recall $R \approx 1.4 \times 10^{-13} A^{1/3}$ (cm)

AND $r_e \equiv \frac{e^2}{m_e c^2} (\approx 2.82 \times 10^{-13} \text{ cm})$

$\therefore R \approx \frac{r_e}{2} A^{1/3} \text{ cm}$

Then $V_c = \frac{Z_1 Z_2 e^2}{R_1 + R_2} = \frac{Z_1 Z_2 e^2}{\frac{r_e}{2} [A_1^{1/3} + A_2^{1/3}]}$

OR $V_c \approx \frac{Z_1 Z_2}{A_1^{1/3} + A_2^{1/3}} \left(\frac{2e^2}{r_e} \right)$

$2 \times .511 \text{ MeV} \approx 1 \text{ MeV}$

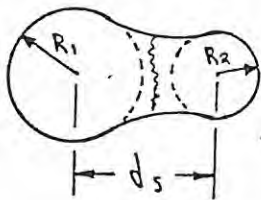
With $A_1 = 135, A_2 = 101 \Rightarrow V_c \approx 213 \text{ MeV}$

• Actual kinetic energy of fragments $\approx 168 \text{ MeV}$ calculation: $\Rightarrow 213 \text{ MeV}$

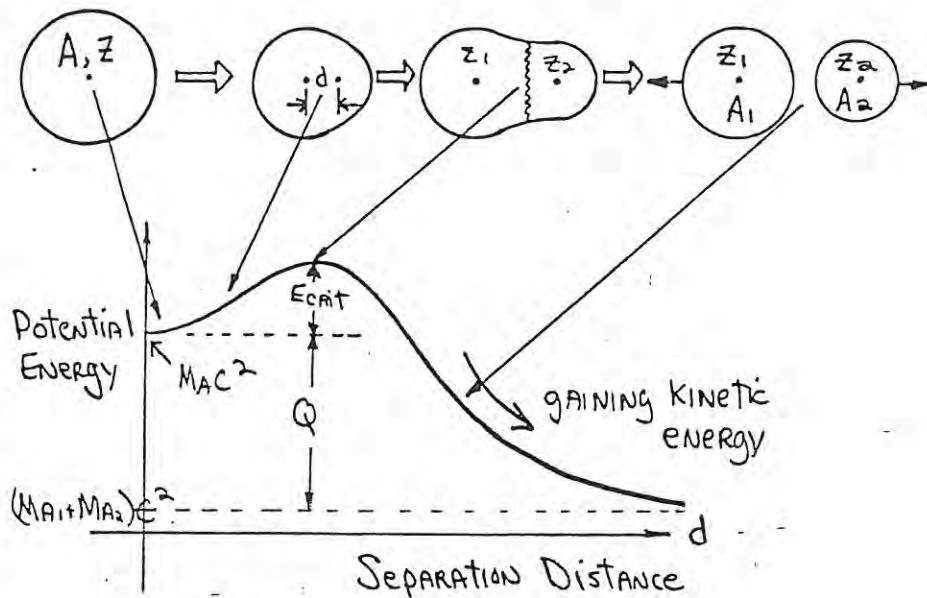
\therefore Coulomb energy at point of scission $\approx 168 \text{ MeV}$

\Rightarrow separation distance $\approx \frac{213}{168} (R_1 + R_2)$

$d_s \approx 1.27 (R_1 + R_2)$



Using the actual energy of 168 MeV, we can estimate the critical separation distance d_s .



Schematic of fission keyed to an energy diagram.

Sources of E_{crit} (Target nucleus - $\frac{A}{Z}X$)

1. Energetic γ -RAY (photo-fission)

- $E_\gamma \geq E_{crit}$, fission
 - Useful for measuring E_{crit}
 - Infrequent for nuclear reactor
- $E_{crit} \approx 6 \text{ MeV}$

2. Neutron Capture ("slow" or "thermal" neutron)

- Supplies excitation energy $E_c \approx 0$
- $= E_B$ (binding energy of last neutron)
- If $E_B \geq E_{crit}$, fission in $\frac{A+1}{Z}X$

Some possible sources of energy to overcome the fission barrier.

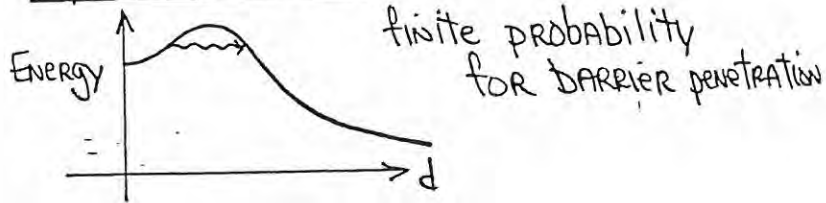
3. Neutron Capture ("Fast" Neutron)

- Supplies $E_c = \frac{A}{A+1} E_L$

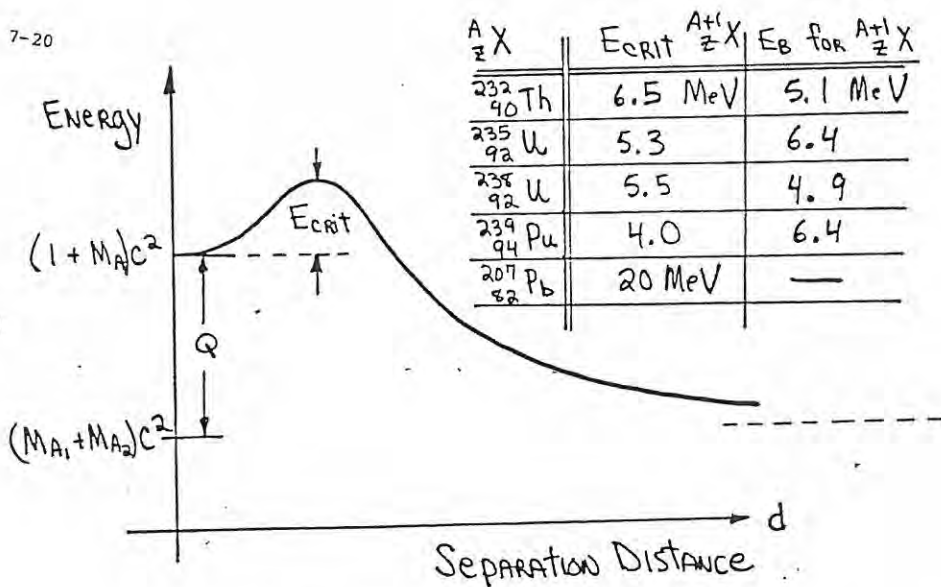
plus E_B

- $E_B + E_c \geq E_{crit} \Rightarrow$ fission

4. Spontaneous fission



7-20



Note for neutron induced fission of $\frac{A}{Z}X$, the fissioning nucleus is actually the compound nucleus $\frac{A+1}{Z}X$.

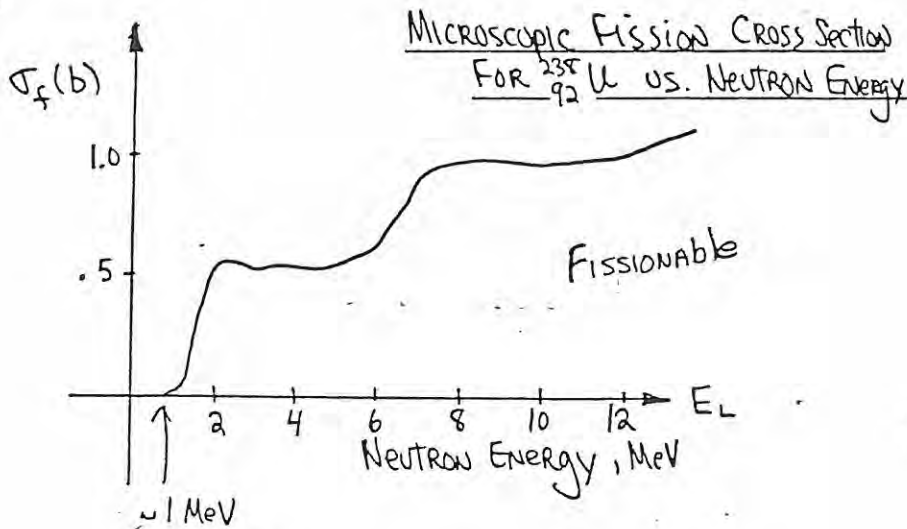
The target nucleus is defined to be fissile, fissionable, or fertile as follows:

Fissile - will fission due to capture of a thermal neutron (negligible E_c)

Fissionable - will fission due to capture of an energetic neutron (≈ 10 MeV)

Fertile - after neutron capture, the product nucleus eventually decays to a fissile nucleus

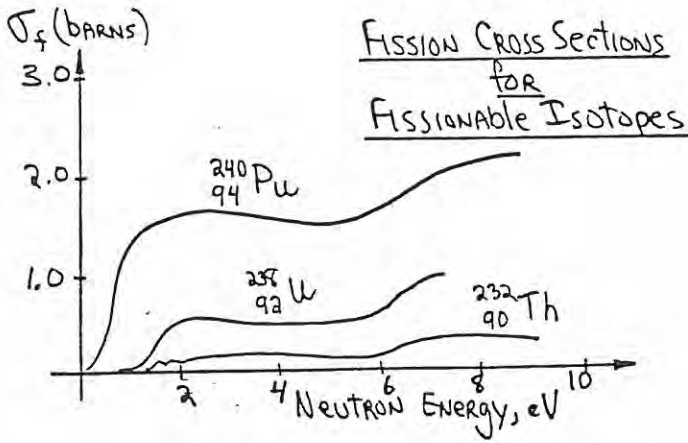
Standard terminology in the nuclear field.



Actual example - note the threshold of approximately 1 MeV for fission of

$^{238}_{92}\text{U}$.

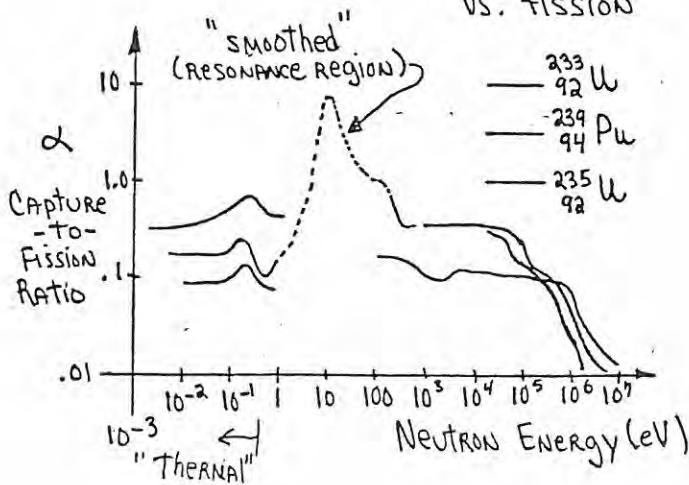
Other fissionable isotopes

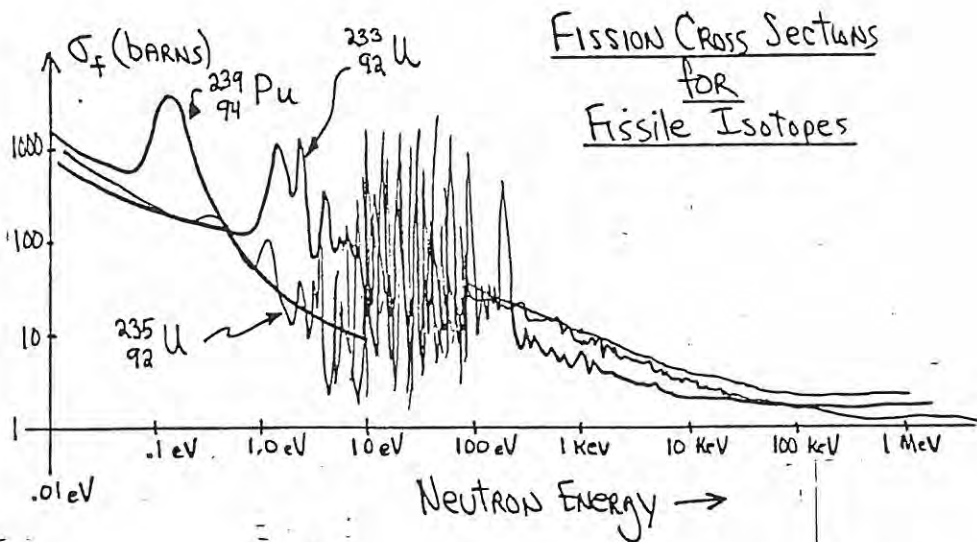


Capture-to-Fission Ratio

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

Relative probability the CN decays via γ -decay vs. fission





Products of the Fission Reaction

- FISSION FRAGMENTS
- PROMPT NEUTRONS
- DELAYED NEUTRONS
- PROMPT γ -RAYS

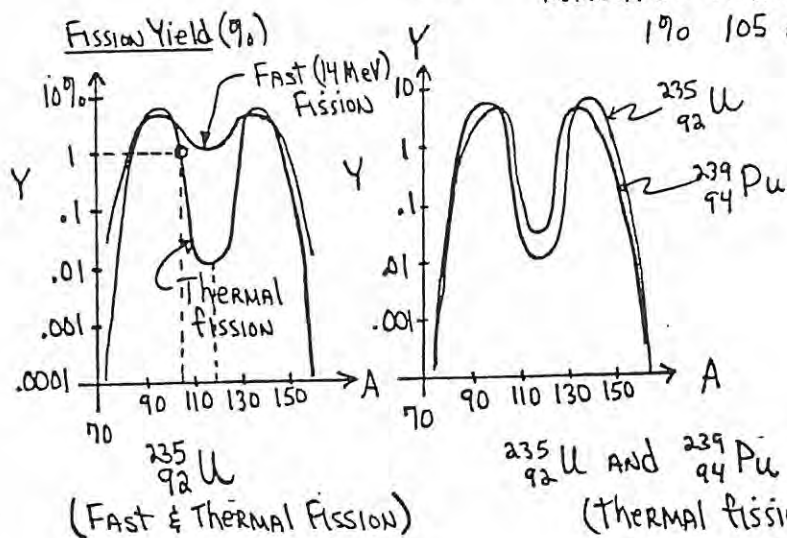
7-27

Fission Product Mass Yields

with MASS A

$$Y(A) = \frac{\text{NUMBER OF FISSION FRAGMENTS}}{\text{NUMBER OF FISSIONS}} \times 100\%$$

170 105 AND 131



Unlikely that the fissioning nucleus breaks into 2 equally massive (or nearly equal) nuclei.

7-28

Fission Fragment Energy

- E_K = kinetic energy ~ 168 MeV (80%)
- E^* = excitation energy ~ 40 MeV (20%)

E_K independent of E^* : E_K approximately same for fission of $^{235}_{92}\text{U}$ with thermal neutron or 90 MeV neutron

Also, spontaneous fission results (on the average) in one less prompt neutron

LECTURE 8

NUCLEAR FISSION - PRODUCTS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp 62-71.

Lamarsh, pp. 68-75.

EXERCISES:

8.1 Duderstadt & Hamilton, problem #2-20.

8.2 Lamarsh, problem #3.35.

Prompt Neutrons

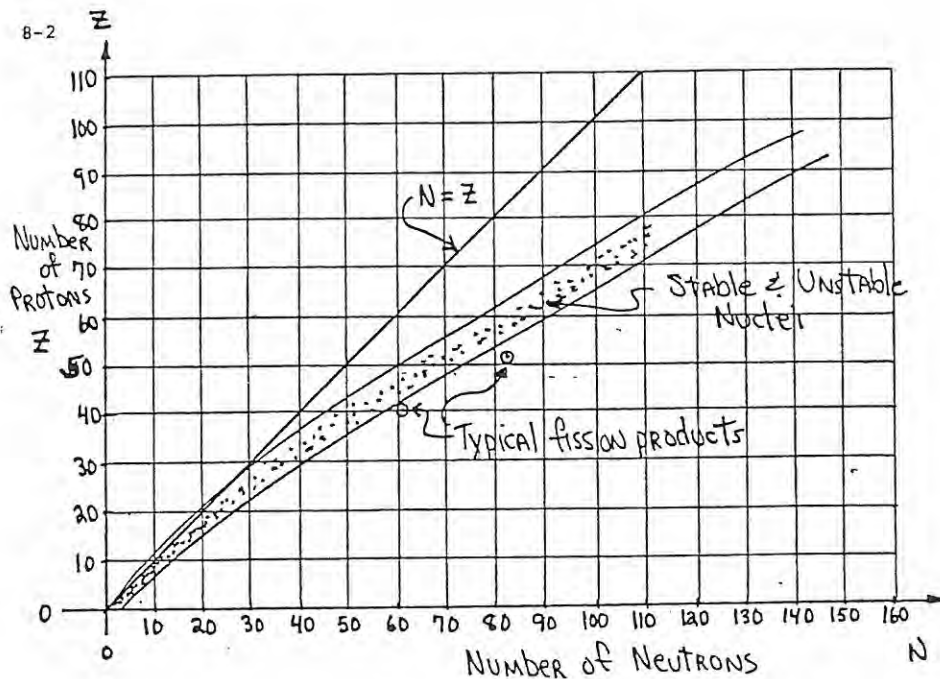
- Fission fragments "neutron rich"
- Neutrons "boil off"
within 10^{-14} seconds

Number Emitted

- Varies from fission to fission
- Define "average" number emitted
= per fission $\nu(E)$

Prompt neutrons emitted by the fission fragments almost instantaneously.

Number emitted is a function of the incident neutron energy E .



Why the fragments are neutron rich.

$\nu(E) \equiv$ AVERAGE NUMBER OF
NEUTRONS emitted per
fission due to incident
NEUTRON of energy E
(includes prompt AND delayed)

EXPERIMENTAL observation:

$$\nu(E) = \nu_0 + a E$$

\uparrow CONSTANT dependent
ON fissioning isotope

example: ${}_{92}^{235}\text{U}$

$$\nu(E) = \begin{cases} 2.43 + .065 E, & 0 \leq E \leq 1 \text{ MeV} \\ 2.35 + .150 E, & E > 1 \text{ MeV} \end{cases}$$

Fission Neutron Spectrum $\chi(E)$

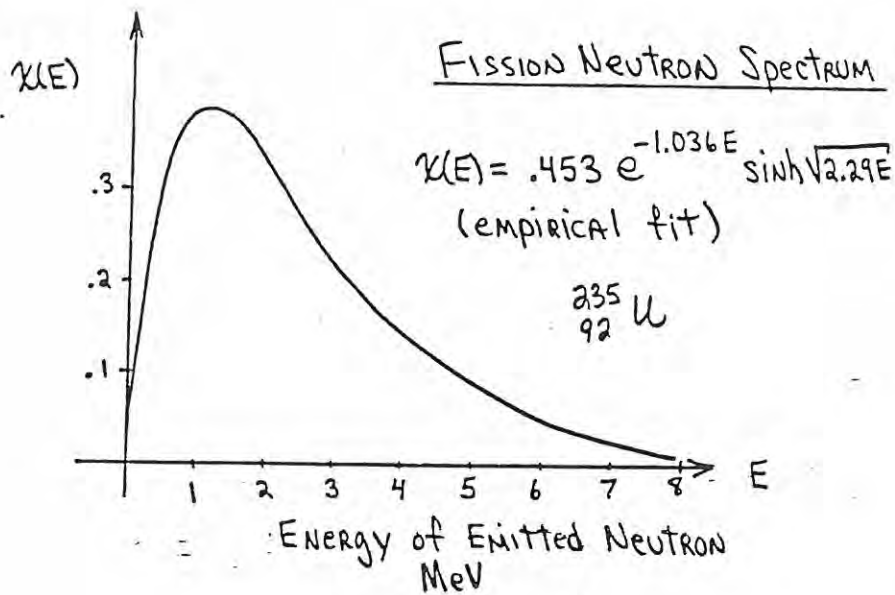
"spectrum" \leftrightarrow "energy density"

$\chi(E) dE =$ fraction of prompt neutrons
emitted with energy in dE about E

Note: (1) $\int_0^{\infty} \chi(E) dE = 1$

(2) $\int_{E_1}^{E_2} \chi(E) dE =$ fraction of prompt
neutrons with energy
 $E_1 \leq E \leq E_2$

The analyst needs to know the energy of the
prompt (and delayed) neutrons.



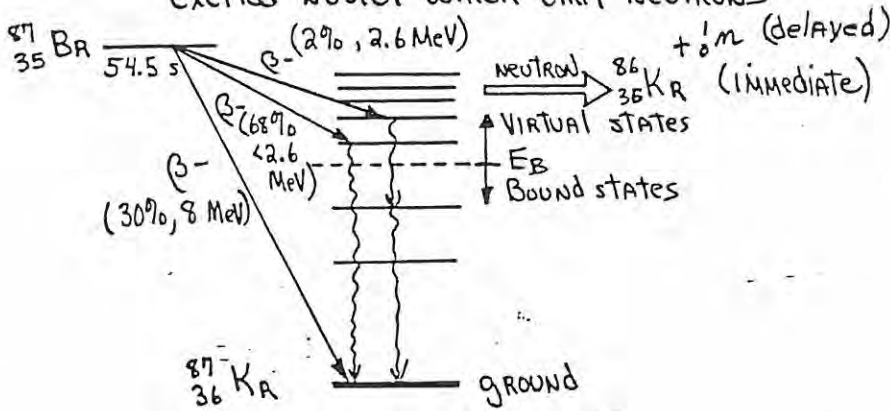
Typical fission spectrum

Observations

- $\chi(E)$ for ${}^{235}_{92}\text{U}$ similar for other fissile nuclides
- $\chi(E)$ assumed to be independent of the incident neutron energy
- Average energy = $\bar{E} \equiv \int_0^{\infty} E \chi(E) dE$
 $\bar{E} = 1.98 \text{ MeV}$
 ↑
 average energy of prompt neutron

Delayed Neutrons

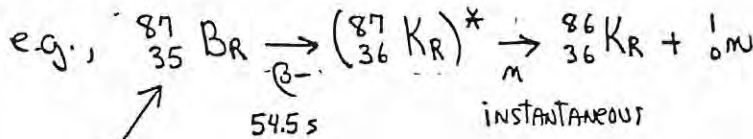
- A small fraction of fission fragments may decay to excited nuclei which emit neutrons



There is a small chance that a fission product may decay to a virtual state, which can emit a neutron.

Delayed Neutron Precursor

- The nuclide which decays to the neutron emitter



delayed neutron precursor

- Approximately 45 different precursors (all with different $\tau_{1/2}$'s)

The decay of the virtual state is instantaneous, hence the delay time is governed by the decay of the precursor.

Delayed Neutron Fraction

$$\beta = \frac{\text{NUMBER OF DELAYED FISSION NEUTRONS}}{\text{NUMBER OF PROMPT + DELAYED}}$$

Fissile nuclide	β
${}_{92}^{235}\text{U}$.0065
${}_{92}^{233}\text{U}$.0026
${}_{94}^{239}\text{Pu}$.0021

Delayed Neutron Groups

- Group precursors into classes

ACCORDING TO $\lambda_{1/2}$

- Typical: 1 delayed group (CRUDE calculations)
6 delayed groups (STANDARD)

6 groups	GROUP	$\lambda_{1/2}$	Yield, β_i/β
	1	54.5 s	.038
	2	21.8 s	.213
	3	6.0 s	.188
	4	2.23 s	.407
	5	.496 s	.129
	6	.179 s	.026

β_i = fraction of
TOTAL FISSION
NEUTRONS IN
the i th group

Energy Release from Fission

- TOTAL energy release
- Recoverable energy
(portion of the total energy release that is useful to the designer - this energy can be recovered, normally as heat energy)

8-12

Type	Energy (MeV)	%	Range	Time delay
Kinetic energy of fission frag	168	80%	<.001 cm	INSTANTANEOUS
FAST (prompt) NEUTRONS	6	3%	10-100 cm	INSTANTANEOUS
Prompt γ -rays	8	4%	100 cm	INSTANTANEOUS
Fission product β^-	8	4%	<1	delayed
Neutrinos	11 (NOT RECOVERABLE)	5%	light years	delayed
Capture γ 's	9	4%	100 cm	delayed
	210	100%		

Review of Nuclear Physics - SUMMARY

Radioactivity

$$\frac{dN}{dt} = -\lambda N$$

↑ decay constant

$$\tau = \frac{1}{\lambda} \quad \text{MEAN lifetime}$$

Cross sections

- σ - MICROSCOPIC CROSS SECTION
 - "effective AREA" per nucleus
 - for reaction with incident neutron
 - units: cm^2 (OR BARNs = 10^{-24}cm^2)

- Σ - MACROSCOPIC CROSS SECTION (cm^{-1})

$$\Sigma = \sigma N$$

↑ TARGET density
↑ MICROSCOPIC CROSS SECTION

probability
per unit length of an interaction

- MEAN free path = $\frac{1}{\Sigma}$

Average distance a neutron will travel in the target before having interaction

- $\sigma(E' \rightarrow E)$ - differential cross section (energy)

$\sigma(E' \rightarrow E) dE$ = microscopic cross section to scatter a neutron of energy E' into the energy range dE about E

- $\sigma_s(\theta)$ - differential (in angle)

$\sigma_s(\theta) \sin\theta d\theta$ = microscopic cross section for neutron to scatter into $d\theta$ about θ

(Alternatively, $\mu = \cos\theta$

$\Rightarrow \sigma_s(\mu) d\mu$)

- Kinematics of Elastic Scattering

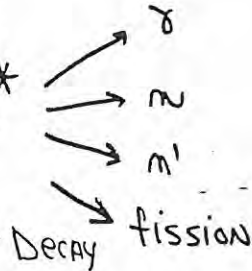
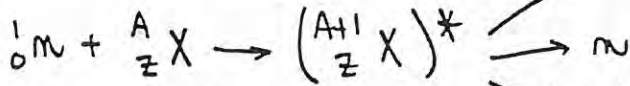
- $E_f = \frac{(1+d) + (1-d)\cos\theta_c}{2} E_i$

- OR $E_{MIN} = d E_i$ $d = \left(\frac{A-1}{A+1}\right)^2$

$$\sigma_s(E \rightarrow E') = \begin{cases} \sigma_s(E) \frac{1}{(1-\alpha)E} & , \alpha E \leq E' \leq E \\ 0 & , \text{otherwise} \end{cases}$$

(Assuming isotropic scattering in the CM)

Compound Nucleus Reactions



More likely if ΔE of $({}_{Z}^{A+1}X)^*$ corresponds to energy level

FORMATION

Decay

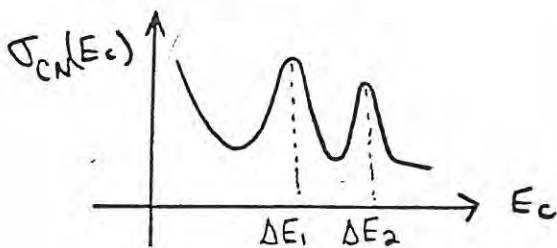
fission

$$\Delta E = E_c + E_B$$

kinetic energy available $\equiv \frac{A}{1+A} E_L$ (nucleus at rest)

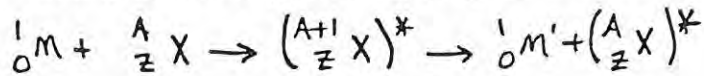
binding energy of last neutron in ${}_{Z}^{A+1}X$

Resonance reaction



- Inelastic scattering - Threshold Reaction

MINIMUM NEUTRON ENERGY
needed to leave target
nucleus in excited state:

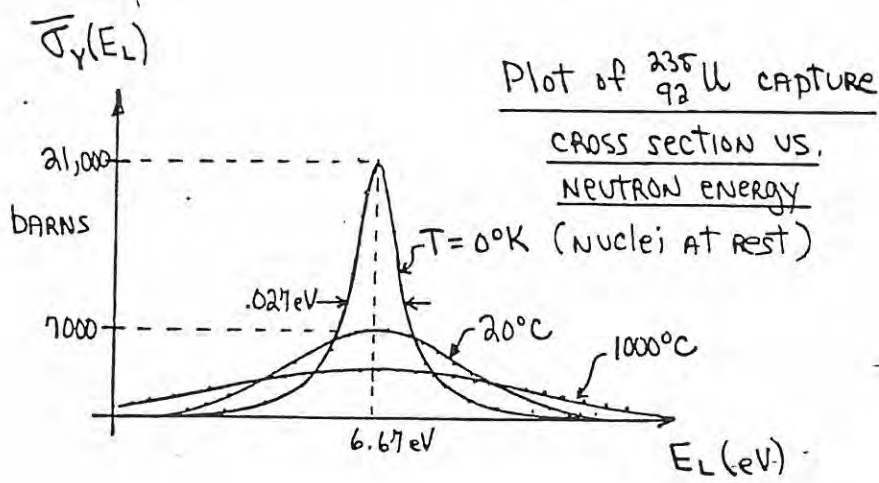


- Doppler Broadening

- Motion of nuclei effects E_c :

$$E_c = \frac{A}{1+A} E_L + \Delta$$

- $\sigma_{CN}(E_c)$ sensitive function of E_c
- Plotting σ_{CN} vs. E_L results in a shift of the curve
- Averaging $\sigma_{CN}(E_L)$ over Maxwellian distribution of the nuclei velocities broadens the curve



• Nuclear fission

- Description
- Energetics
- Fission products
- Energy release

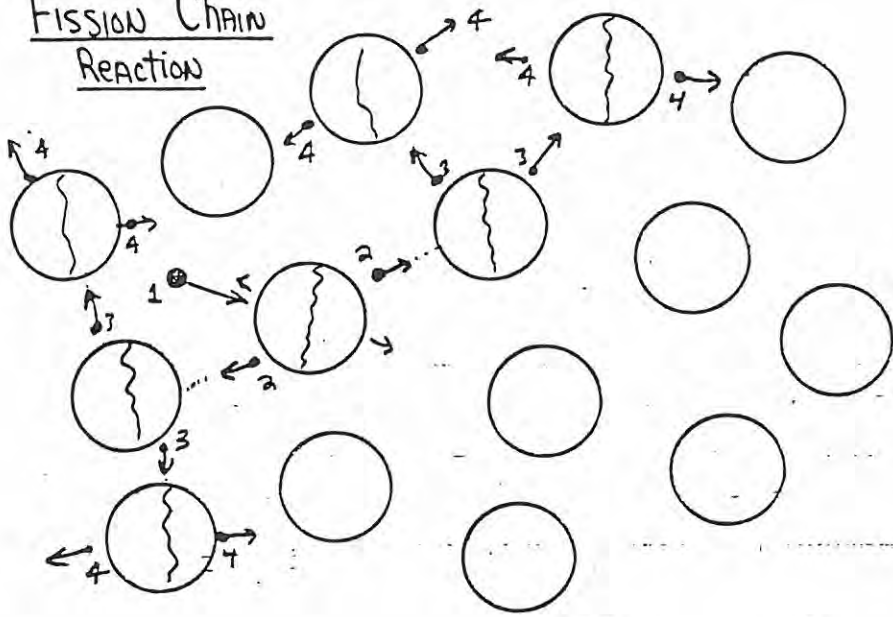
Next topics

- FISSION CHAIN REACTION
- CANDIDATE NUCLEAR FUELS
- SIGNIFICANCE OF $\eta = \nu \frac{\sigma_f}{\sigma_a}$
- TYPES OF REACTORS
 - FAST
 - THERMAL
- NEUTRON PROCESSES IN A THERMAL REACTOR

The FISSION CHAIN REACTION

- Within 10^{-14} seconds of scission
 - ↳ (ON THE AVERAGE) PROMPT NEUTRONS ARE EMITTED BY THE "NEUTRON-RICH" FISSION FRAGMENTS
- These neutrons may cause additional fissions, resulting in ν neutrons per fission

Fission Chain Reaction



NEUTRON GENERATION

- Initial neutrons entering the fissile medium - the 1ST generation

- The 1ST generation cause fissions, leading to their progeny, the 2ND generation

∴ etc.

NTH generation

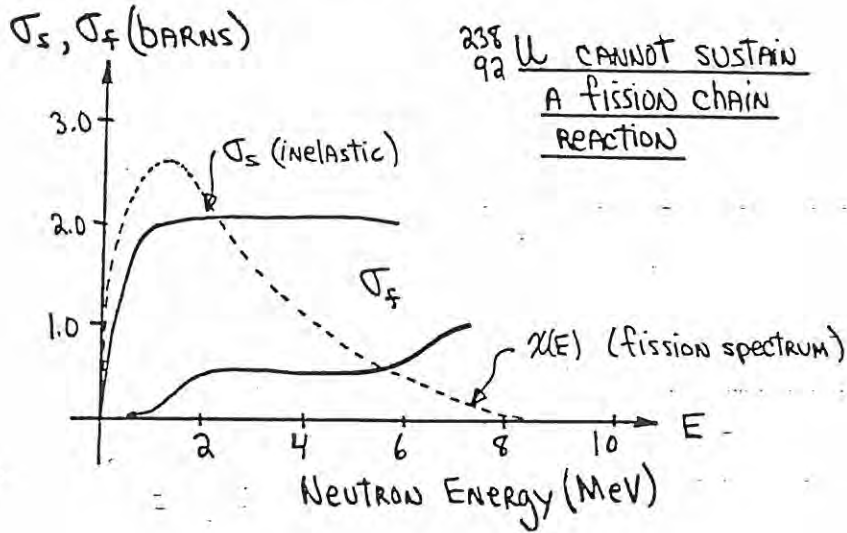
GENERATION #	Number of NEUTRONS
1	1
2	2
3	4
4	8
⋮	⋮
m	2^{m-1}

In general, will have 2^{m-1} NEUTRONS
in the m^{th} generation (only fission occurs)

Real life

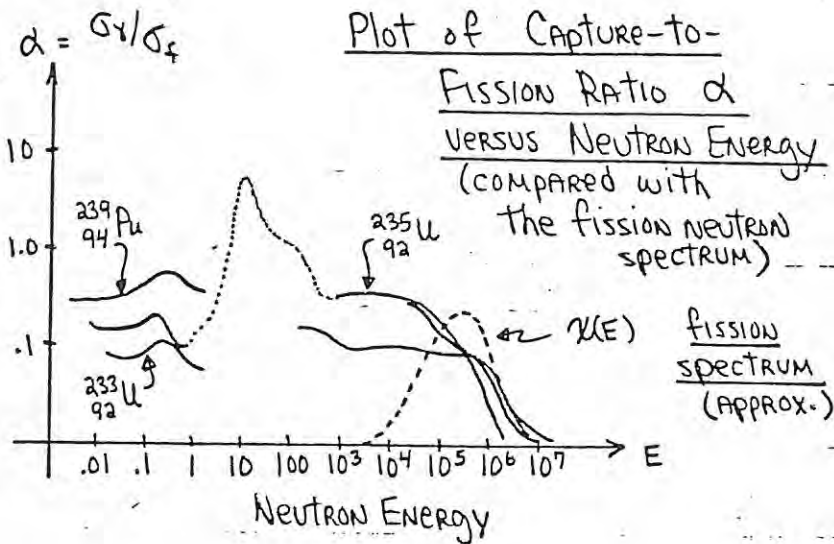
- Fissile/fissionable isotopes
also capture and scatter
neutrons in addition to fission
- Core may contain non-fissioning
materials, such as steel,
aluminum, water, etc.
- Question: can one obtain a
sustaining chain reaction with
real materials?

B-29 Pure ${}^{238}_{92}\text{U}$ (NOT NATURAL URANIUM, which
CONTAINS .71% ${}^{235}_{92}\text{U}$)



Inelastic scattering will decrease the neutron energy below the threshold, therefore ${}^{238}_{92}\text{U}$ cannot sustain a chain reaction.

B-30



LECTURE 9

FAST vs. THERMAL REACTORS

READING ASSIGNMENT:

Duderstadt and Hamilton, pp. 74-84.

Lamarsh, pp. 102-104.

EXERCISES:

- 9.1. Why isn't H_2O used as a coolant in a fast reactor?
- 9.2. The light water breeder reactor (LWBR), which recently operated for several years at the Shippingport Plant, uses the U-233/Th-232 fuel cycle. Explain how this fuel cycle might work in general terms.
- 9.3. Duderstadt & Hamilton, problem #3-2.

Today

- Continue discussion of η AND ITS IMPLICATIONS FOR CHAIN REACTIONS
- Describe fast AND thermal reactors
- • Classify types of thermal reactors
- Neutron moderation
- Multiplication factor - the "4-factor" formula

9-2

$$\eta = \nu \frac{\sigma_f}{\sigma_a} \quad \left\{ \begin{array}{l} \text{MORE SIGNIFICANT} \\ \text{PARAMETER FOR CHAIN REACTION} \end{array} \right.$$

η = AVERAGE NUMBER OF FISSION NEUTRONS EMITTED PER NEUTRON ABSORBED

$$\sigma_a = \sigma_y + \sigma_f$$

Assertion - in a medium (infinite, homogeneous) with constant $\eta = \eta_0$, then

η_0 = RATIO OF THE NUMBER OF NEUTRONS IN ONE GENERATION TO THE PREVIOUS

In order to sustain a chain reaction, need at least one neutron left over to continue.

- Start out with N_i neutrons in the i^{th} generation

- The probability of a fission

$$\frac{\sigma_f}{\sigma_f + \sigma_a}$$

$$\Rightarrow \frac{\sigma_f}{\sigma_f + \sigma_a} N_i = \# \text{ fissions which occur}$$

$$v \left[\frac{\sigma_f}{\sigma_f + \sigma_a} N_i \right] \text{ neutrons produced}$$

And will begin the $(i+1)^{\text{th}}$ generation

$$\text{Ratio} = v \frac{\sigma_f}{\sigma_a} = k \text{ gen}$$

Thus the / ratio of the number of neutrons in one generation to the next generation is k , assuming an infinite, homogeneous, fissile medium.

Implications of ν

$\nu < 1$ NO chain reaction possible.

$\nu \geq 1$ chain reaction possible

$\nu \geq 2$ breeding possible

CHAIN REACTION - NEUTRON (at least one)

FROM FISSION REACTION CAUSES ANOTHER FISSION REACTION, etc.

BREEDING - AFTER NEUTRON NEEDED FOR SUSTAINING CHAIN REACTION, HAVE ADD'L NEUTRON TO PRODUCE FISSION FUEL

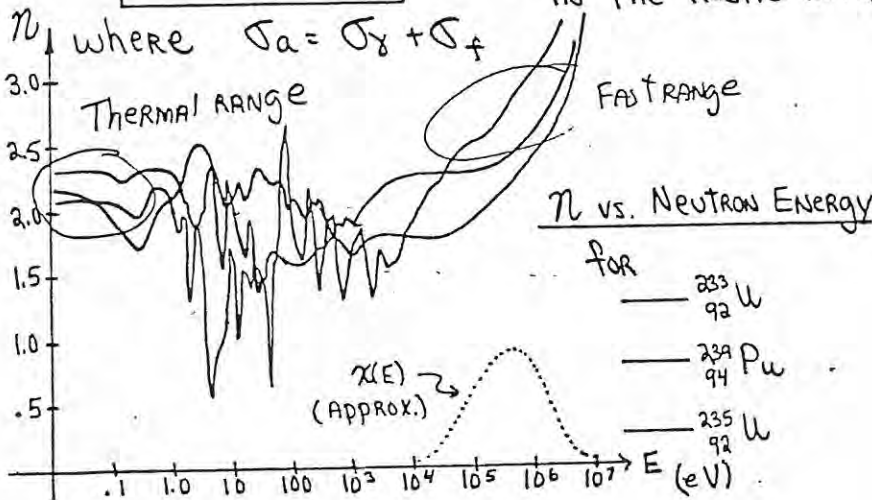
9-6 NUMBER OF NEUTRONS EMITTED PER ABSORPTION

Define

$$\nu = \nu \left(\frac{\sigma_f}{\sigma_a} \right)$$

prob of fission of the CN

NUMBER OF NEUTRONS EMITTED PER NEUTRON ABSORBED IN THE FISSION ISOTOPE



From the plot one can see why $^{239}_{94}\text{Pu}$ is a good fast breeder reactor fuel (the chain reaction is sustained primarily by fast neutrons) and $^{235}_{92}\text{U}$ a good thermal reactor fuel. Note the potential for $^{233}_{92}\text{U}$ as a thermal breeder reactor fuel.

FAST REACTOR

- FISSION CHAIN REACTION CAN BE SUSTAINED BY "FAST" NEUTRONS ONLY (i.e., CRITICAL IN A FAST SPECTRUM)
- FISSION NEUTRONS CAUSE ADDITIONAL FISSIONS ~~NEUTRONS~~ BEFORE THEY ARE SCATTERED DOWN IN ENERGY (REACTOR DESIGNER MINIMIZES MATERIALS THAT SCATTER NEUTRONS)

EXAMPLE BARE sphere of ${}_{92}^{235}\text{U}$ (A GODIVA REACTOR)

- INTRODUCES ADDITIONAL MECHANISM FOR TERMINATING THE CHAIN REACTION - LEAKAGE
- NEUTRON PRODUCTION RATE (FISSION) $\propto R^3$
- NEUTRON LEAKAGE $\propto R^2$



A neutron which leaks out cannot cause a fission.

• CRITICAL RADIUS R_c ,

production rate $>$ leakage rate

\Rightarrow CHAIN REACTION OCCUR

• CRITICAL MASS = $\frac{4}{3} \pi R_c^3 \rho_{235} = M_c$

pure U-235, $R_c = 8.7 \text{ cm}$

$M_c = 5.2 \text{ kg}$

Thermal Reactor

• Most fissions are induced by thermal (slow) neutrons ($< 1 \text{ eV}$)

• Curve of η vs. E FAST - 10^6 eV
 in the thermal range ($E \leq .6 - 1.0 \text{ eV}$)
 indicates chain reaction possible for

${}_{92}^{233}\text{U}$, ${}_{92}^{235}\text{U}$, ${}_{94}^{239}\text{Pu}$ (principal fissile isotopes)

- Problem - fission neutrons are emitted with $E \sim 1 \text{ MeV} = 10^6 \text{ eV}$
- fissions are caused by neutrons with energy $E \sim 1 \text{ eV}$

The neutrons emitted in fission must have their energy reduced by a factor of 10^7 in order to cause a fission to sustain the chain reaction.

We need a means for slowing down the neutrons.

Neutron Moderator

- Necessary to slow down, or moderate, the neutrons in a thermal reactor
- Water (H_2O) - an excellent moderator due to the presence of hydrogen

$$\text{MINIMUM final energy} = E_{\text{min}} = \alpha E_i$$

$$\text{where } \alpha = \left(\frac{A-1}{A+1}\right)^2 \quad A=1 \text{ for hydrogen!}$$

A neutron can lose all of its energy in one collision with hydrogen (not very likely, but possible).

Thermal Reactor - Types

LWR (light water reactor)

Moderator

H₂O

CANDU (CANADA deuterium URANIUM REACTOR)

D₂O heavy water

HTGR (high temperature GAS REACTOR)

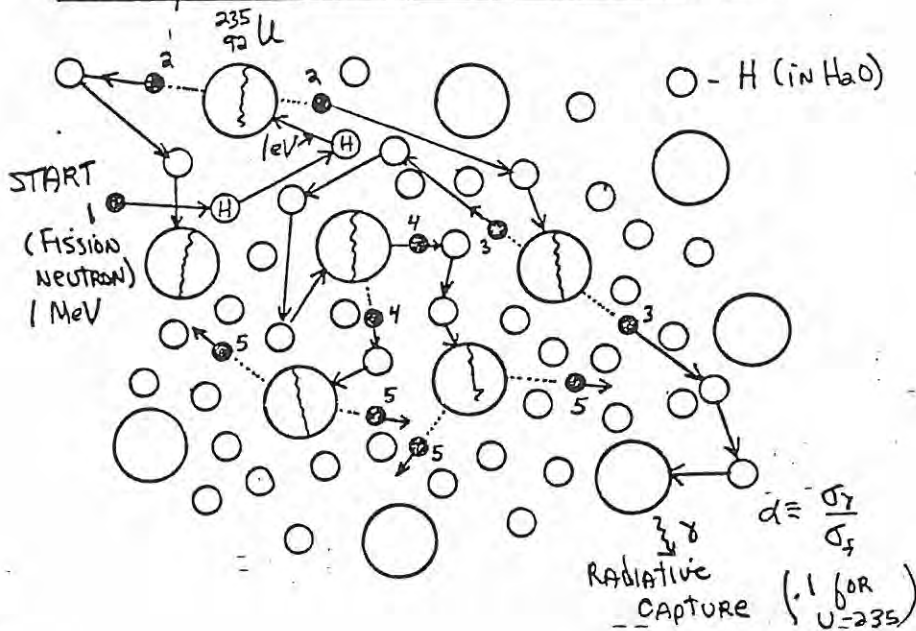
• graphite
 ${}^{12}_6\text{C}$
 A=12

coolant is helium

Neutron History in A Thermal Reactor

- Thermal neutron causes fission
- Fission neutrons emitted (energetic) 1-2 MeV
- Neutrons moderated to thermal energies (<1eV)
- Cause more fissions

9-15 HISTORY OF NEUTRON IN A THERMAL REACTOR



9-16

COMPLICATIONS (FOR THERMAL REACTOR)

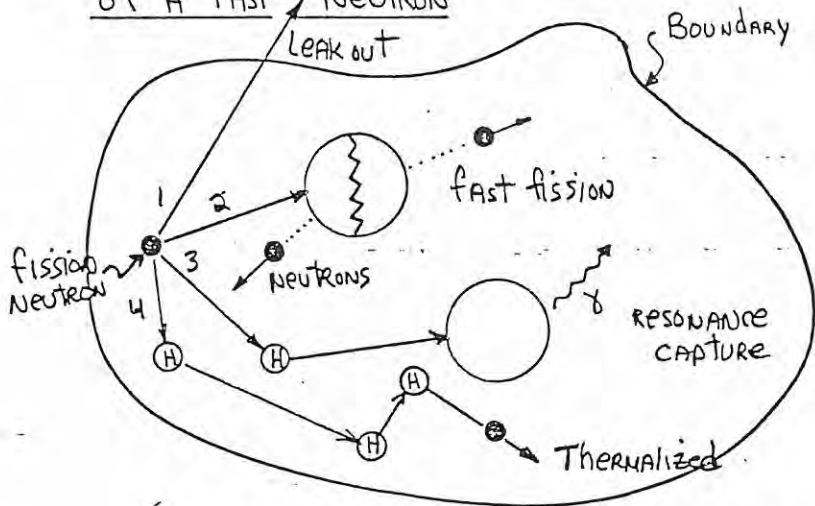
- SOME FAST NEUTRONS (FROM FISSION) MAY CAUSE FISSIONS (FAST FISSIONS)
- SOME FAST NEUTRONS MAY LEAK OUT OF THE REACTOR
- SOME NEUTRONS MAY BE ABSORBED (IN RESONANCES) WHILE SLOWING DOWN
- THERMAL NEUTRONS MAY :

- (i) LEAK out
- (ii) Be absorbed in NON-fuel (JUNK)
- (iii) Be absorbed in fuel, hence captured, $\alpha = \frac{\sigma_c}{\sigma_f} \neq 0$ OR CAUSING A THERMAL fission thus leading to 2 fission neutrons

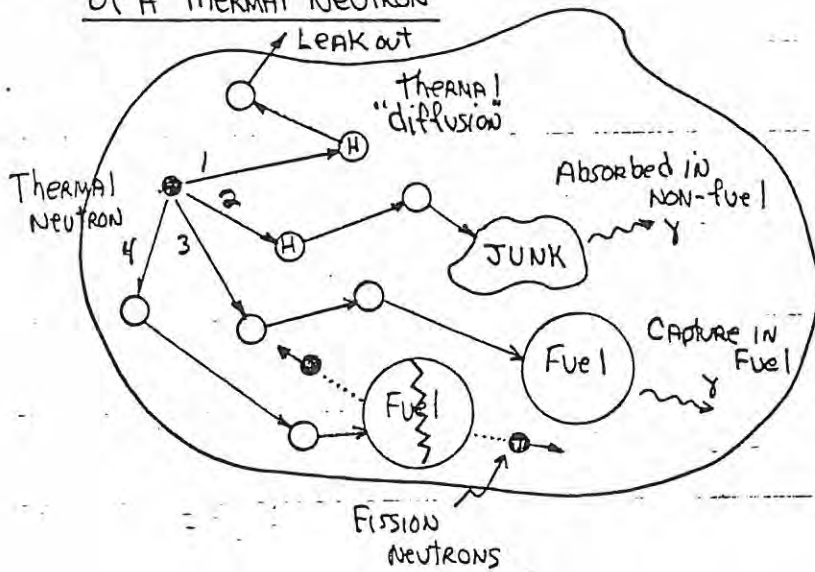
Realistic Neutron Life Diagram -

- Includes all of the above possibilities
- (Break into 2 diagrams, one for FAST neutrons and one for THERMAL neutrons)

9-18 Events in the Life of a Fast Neutron



Events in the Life of a Thermal Neutron



Multiplication Factor k

$k \equiv$ ratio of the number of fast (or fission) neutrons in one generation to the number in the previous generation

example - if there are N fission neutrons in one generation and the multiplication factor is k , there will be kN fission neutrons in the next generation

Calculation of the Multiplication Factor (the "4-factor" formula)

- Define appropriate expressions for each of the possible events in the life cycle of the neutron (fast and thermal)
- Combine to calculate k

FAST NEUTRON EVENTS

FAST FISSION FACTOR ϵ

$\epsilon \equiv$ the INCREASE IN the
NUMBER OF FISSION NEUTRONS
DUE TO FAST FISSIONS

e.g., $\epsilon = 1.00$ NO FAST FISSIONS
 $\epsilon = 1.02$ 2% OF THE FISSION
NEUTRONS ARE EMITTED
AFTER A FAST FISSION

We will now define several quantities.
Later we will say something about calculating them.

- FAST NON-LEAKAGE PROBABILITY P_{FNL}

$P_{FNL} \equiv$ probability that a fast neutron will not leak out of the system

- RESONANCE ESCAPE PROBABILITY p

$p \equiv$ probability that a fast neutron will successfully slow down to thermal energy (hence escaping the resonances)

The resonance escape probability is conditional on the neutron not leaking out. That is, the probability that a neutron that does not leak out will successfully slow down.

Thermal Neutron Events

- THERMAL NON-LEAKAGE PROBABILITY P_{TNL}

$P_{TNL} \equiv$ probability that a thermal neutron will NOT leak out of the system

- THERMAL UTILIZATION f

$f \equiv$ probability that a thermal neutron is absorbed in fuel versus non-fuel (JUNK)

Note f is conditional on the neutron not leaking out.

• Eta η

$\eta \equiv$ NUMBER OF FISSION
NEUTRONS PRODUCED
PER ABSORPTION
IN THE FUEL

$$\sigma_a = \sigma_f + \sigma_r$$

$$\eta = \nu \frac{\sigma_f}{\sigma_f + \sigma_r}$$

$$= \nu \frac{1}{1 + \alpha}$$

$\alpha \neq 0$

e.g., for fuel with a single
isotope, ${}^{235}_{92}\text{U}$ (100%)

$$\eta = \nu \frac{\sigma_f}{\sigma_a}$$

CONSISTENT
WITH OUR
EARLIER DEFINITION

Eta is property of the fuel.

LECTURE 10

The Six-Factor Formula and Reactor Criticality

READING ASSIGNMENT:

Duderstadt and Hamilton, pp 84-88, 89-99 (skim).

Lamarsh, pp. 108-116, 116-152 (optional)

EXERCISES:

10.1. Duderstadt & Hamilton, problem #3-3.

10.2. Duderstadt & Hamilton, problem #3-6.

10.3. Duderstadt & Hamilton, problem #3-8.

Today

- Describe the neutron life cycle
IN A THERMAL REACTOR
- Formal calculation of k
(the "4 factor" formula)
- Criticality
- Reaction rates and leakage rates

Previous Lecture

- Defined the
multiplication factor k

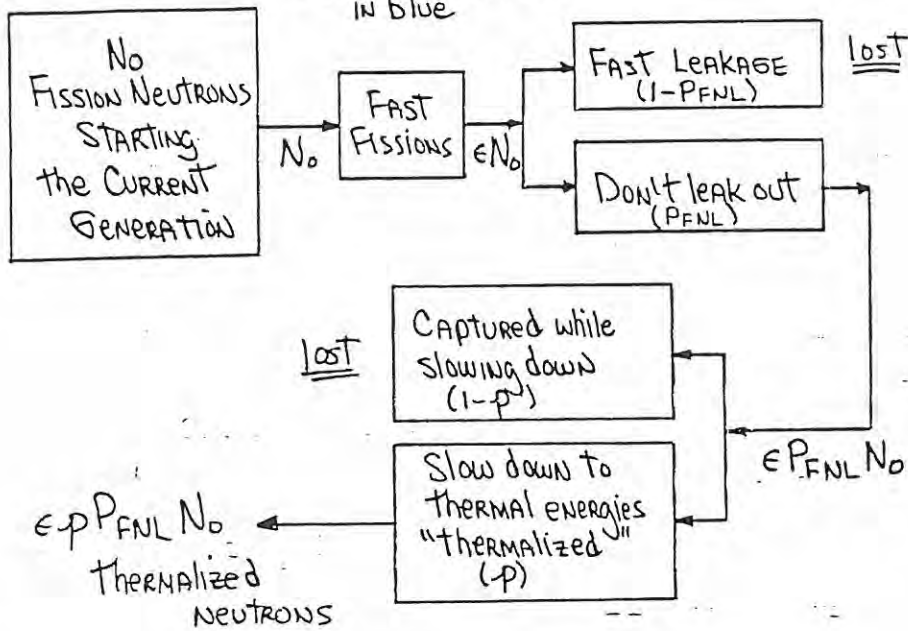
k = ratio of the number of
fast (or fission) neutrons
in one generation to the
number in the previous
generation

- Noted that we need to consider MANY physical phenomena in a THERMAL reactor:

- 6 physical factors
- Moderation
 - Fast fission
 - Resonance capture
 - Thermal absorption in non-fuel and fuel
 - Leakage (fast \neq thermal)

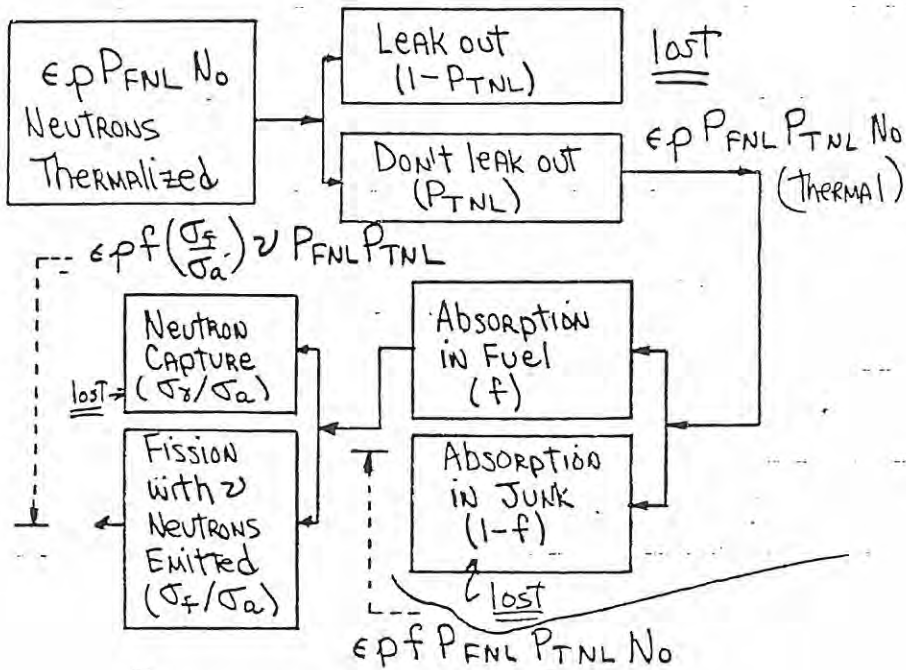
- Definitions (for calculation of k in a Thermal reactor)
 - ϵ "fast fission factor"
 - P_{FNL} "fast non-leakage probability"
 - p "resonance escape probability"
 - P_{TNL} "thermal non-leakage probability"
 - f "thermal utilization"
 - η "eta"

NOTATION : (probability)
 • NUMBER OF NEUTRONS IN BLUE



Calculate the number of neutrons at each stage of the neutron life history.

Have $\epsilon p P_{FNL} N_0$ neutrons which successfully reach thermal energies.

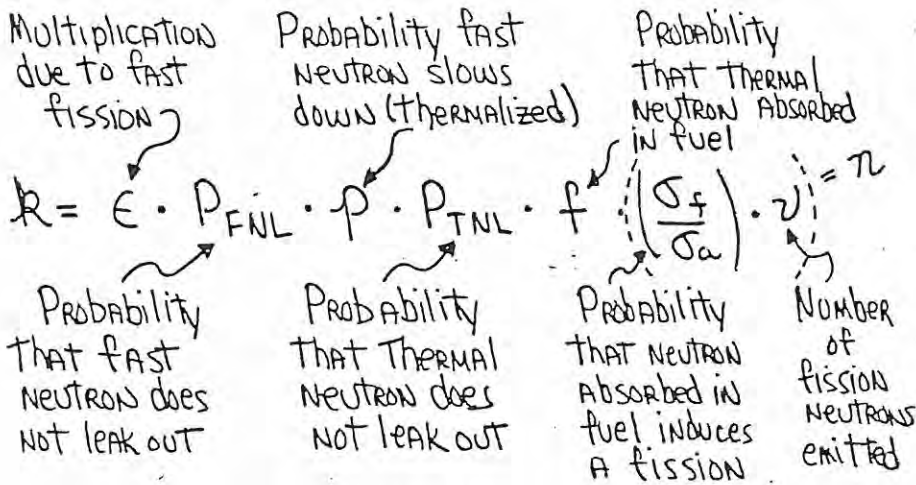


- Number of neutrons at start of generation = N_0
- Number of fission neutrons at end of generation (actually starting the next generation) = $N_0 \epsilon p f \eta P_{FNL} P_{TNL}$
 "6-factor" $\left(\nu \frac{\sigma_f}{\sigma_a} \right)$
 "4-factor" $P_{FNL} = P_{TNL} = 1.0$

Multiplication Factor = $\epsilon p \eta f P_{FNL} P_{TNL}$

k "6-factor" "4-factor" $P_{FNL} = P_{TNL} = 1.0$

SUMMARY



$k = \epsilon p \eta f P_{FNL} P_{TNL}$

• Define

P_{NL} = non-leakage probability
(probability that any
neutron, fast or thermal,
will not leak out)

$$P_{NL} = P_{FNL} \cdot P_{TNL}$$

k_{∞} = multiplication factor for
an "infinite" medium, i.e.,
where leakage is zero

$$k_{\infty} = \epsilon p \eta f$$

($P_{NL} = 1.0$) infinite medium
multiplication factor

$$k = k_{\infty} P_{NL}$$

Significance of k

$$k = \frac{\text{Number in a generation}}{\text{Number in the previous}}$$

λ = "mean neutron lifetime"
(e.g., the time for one generation)

- N_0 FISSION NEUTRONS
AT $t=0$

• What is $N(t)$?

NUMBER OF GENERATIONS = t/l

- Each generation results in a multiplication of k

$$\Rightarrow N(t) = N_0 \underbrace{[k \cdot k \cdot k \dots k]}_{t/l \text{ times}} = N_0 [k]^{t/l}$$

EXAMPLE

$k = 1.001$ "modest" mult factor

$l \approx 10^{-4}$ seconds (typical lifetime for
A prompt neutron in
A thermal ~~reaction~~
reactor)

If 1 neutron at $t=0$

How many at $t=1$ second?

$$N(1 \text{ second}) = N_0 (1.001)^{1/10^{-4}} = (1.001)^{10^4}$$

$$= 22,000$$

Control the reactor?

Seems unlikely that one could control a reactor that increases its power level by a factor of 22,000 in one second!

- CONCLUSION - NEUTRON POPULATION
TO SENSITIVE TO MULTIPLICATION
FACTOR

How CAN ONE CONTROL
A REACTOR?

We have ignored:

- (1) Delayed neutrons
(will INCREASE "effective" k).
- (2) Feedback effects (Doppler feedback,
MODERATOR feedback, etc.)

Real reactors can be controlled (as we know) and the primary reason is delayed neutrons.

TERMINOLOGY

$k < 1$ "SUB-CRITICAL"

$k = 1$ SUSTAINED CHAIN
REACTOR

"CRITICAL REACTOR"

$k > 1$ "SUPER-CRITICAL REACTOR"

Reactor Designer-

- Design the reactor to REMAIN CRITICAL for the duration of the operating cycle (1-2 years)
- Design the reactor so that it CAN ALWAYS be shutdown ($k < 1$)
CAN MAKE (e.g., insert rods)
- Design the reactor to produce the specified amount of energy over the operating cycle

- All of these tasks require knowledge of the multiplication factor k
- How can one calculate the multiplication factor?

$$k = \epsilon p \eta f P_{NL} P_{TL}$$

"6-factor"

MUST ACCOUNT FOR :

- (1) Fast fissions (e.g., ${}^{238}_{92}\text{U}$)
- (2) Fast leakage
- (3) Resonance Absorption (and other absorption mechanisms)
- (4) Slowing down (moderation)
- (5) Thermal leakage
- (6) Thermal absorption (capture + fission)
- (7) Spatial "diffusion" of fast and thermal neutrons

REACTION RATES
AND LEAKAGE RATES

\mathcal{R} REACTION
RATE
(#/CM³.S)

- Fast fission rate = $\mathcal{R}_{FF} \left(\frac{\# \text{ FAST FISSIONS}}{\text{SECOND}} \right)$
- Fast leakage rate = $\mathcal{L}_F \left(\frac{\# \text{ FAST NEUTRONS LEAKING}}{\text{SECOND}} \right)$
- Resonance absorption rate = $\mathcal{R}_{RA} \left(\frac{\# \text{ ABSORBED}}{\text{SECOND}} \right)$
- Slowing down rate = $\mathcal{R}_{SD} \left(\frac{\# \text{ SLOWING DOWN}}{\text{SECOND}} \right)$

Now let us define some reaction rates and leakage rates, with which we can calculate the factors appearing in the 6 factor formula for k.

- Thermal leakage rate = λ_T (#/second)
 - Thermal absorption rate
IN FUEL = R_{AF} (#/second)
 - Thermal absorption rate
IN JUNK = R_{AJ} (#/second)
(NON-FUEL)
 - $\eta = \nu \frac{\sigma_f}{\sigma_a}$ property of the FUEL
(KNOWN)
- (ALSO ASSUME ν SAME FOR FAST OR THERMAL FISSION)

Calculation of k

- ϵ Number of fission neutrons produced from both fast and thermal fissions
- $$\epsilon = \frac{\text{Number of fission neutrons produced from both fast and thermal fissions}}{\text{Number of fission neutrons produced from thermal fissions}}$$

$$\frac{\# \text{ fast fissions}}{\text{second}} = \frac{\nu R_{FF} + \nu R_{TF}}{\nu R_{TF}} = \boxed{\frac{R_{FF} + R_{TF}}{R_{TF}}}$$

Note we said ϵ gives the increase in the fission neutron population due to fast fission and $\epsilon = 1$ means no fast fission.

• $P_{FNL} = 1 - P_{FL}$ ^{= prob of leakage}

$$P_{FNL} = 1 - \frac{\text{Number of fast neutrons which leak out}}{\text{Number which leak out plus the number which don't}}$$

$$= 1 - \frac{\mathcal{L}_F}{\mathcal{L}_F + \underbrace{R_{FF} + R_{RA} + R_{SD}}_{\text{NUMBER THAT DON'T LEAK OUT}}}$$

$$P_{FNL} = \frac{R_{FF} + R_{RA} + R_{SD}}{\mathcal{L}_F + R_{FF} + R_{RA} + R_{SD}}$$

• P probability that a fast neutron slows down (escaping resonance absorption)

$$P = \frac{\text{Number of fast neutrons which slow down}}{\text{Number which slow down plus the number absorbed}}$$

$$= \frac{R_{SD}}{R_{SD} + R_{RA}}$$

• f Thermal utilization

$$f = \frac{\text{NUMBER OF THERMAL NEUTRONS ABSORBED IN FUEL}}{\text{TOTAL NUMBER OF THERMAL NEUTRONS ABSORBED (IN FUEL OR JUNK)}}$$

$$= \frac{R_{AF}}{R_{AF} + R_{AJ}}$$

• P_{TNL} (similar to expression for P_{FNL})

$$P_{TNL} = \frac{R_{AF} + R_{AJ}}{R_{AF} + R_{AJ} + \lambda_T}$$

$$k = \epsilon p \eta f P_{FNL} P_{TNL}$$

↑
KNOWN
(physical data)

CAN BE CALCULATED
PROVIDING WE KNOW
REACTION RATES AND
LEAKAGE RATES

How do we calculate reaction rates and leakage rates? The rest of this course is devoted to this topic.

Alternative Expression for k

Define (FAST AND THERMAL)

A = TOTAL NEUTRON ABSORPTION RATE

λ = " " " LEAKAGE "

P = " " " PRODUCTION "

Then we assert

$$k = \frac{P}{\lambda + A} \quad \left(\frac{\text{production}}{\text{loss}} \right)$$

We can define an alternative expression for k based on neutron balance.

Now prove that both k 's are equal.

P = RATE AT WHICH FISSION NEUTRONS PRODUCED (ALL NEUTRONS PRODUCED MUST BE FISSION NEUTRONS IF NO SOURCE IS PRESENT)

$\lambda + A$ = RATE AT WHICH FISSION NEUTRONS ARE LOST (REMEMBER - THERMAL NEUTRONS begin AS FISSION NEUTRONS)

Then we have

N_0 = NUMBER OF FISSION NEUTRONS ENTERING CURRENT GENERATION

$N = P\lambda$ ← production rate
 ← TIME FOR ONE GENERATION
 IS THE NUMBER OF
 FISSION NEUTRONS IN THE
next generation

$$\therefore k = \frac{P\lambda}{N_0}$$

But $(\lambda + A)\lambda = N_0$ (All fission neutrons
 IN CURRENT generation
 ARE EITHER absorbed
 OR lost via leakage)

$$\therefore k = \frac{P}{\lambda + A} \text{ged}$$

LECTURE 11

NEUTRON FLUX AND CURRENT

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 103-107.

Lamarsh, pp. 156-158.

EXERCISES:

11.1. Duderstadt & Hamilton, problem #4-2.

11.2. The unusual situation exists wherein 3 directed beams intersect at right angles throughout an infinite medium. Assume the beams have intensities ϕ_1 , ϕ_2 and ϕ_3 neutrons/cm²·s and are directed along the +x, +y, and +z axes, respectively -

- (a) What is the scalar flux?
- (b) What is the net current?

REACTION RATES AND LEAKAGE RATES - FLUX AND CURRENT

PREVIOUS lecture

$$k = \epsilon p \eta f P_{FNL} P_{TNL}$$

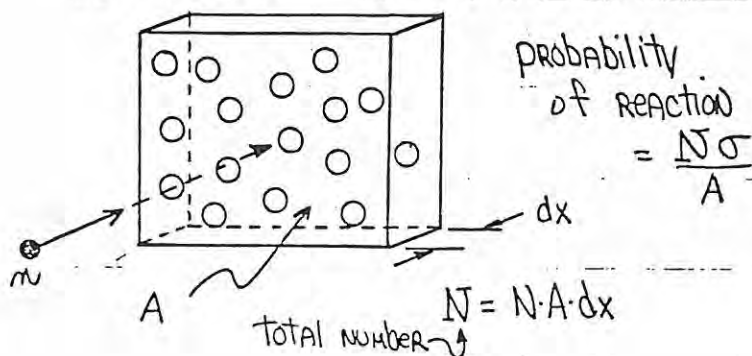
- CAN express the "6 factors" in terms of reaction rates (R) and leakage rates (L)
- Today - define neutron flux ϕ and neutron current \underline{J}

If ϕ and \underline{J} are known, then the R's and L's can be calculated.

11-2 Microscopic Cross Sections

σ = MICROSCOPIC CROSS SECTION for the reaction (e.g., σ_x, σ_f , etc.)

σ = "effective area" of the nucleus for the reaction to occur



$$I \frac{\text{NEUTRONS}}{\text{CM}^2 \cdot \text{s}}$$

$I \cdot A = \#$ NEUTRONS INCIDENT
ON THE TARGET
PER SECOND

$$\text{TOTAL NUMBER OF REACTIONS/SEC} \\ = \mathcal{R} = I \cdot A \cdot \left[\frac{\sigma \cdot N \cdot A \cdot dx}{A} \right]$$

REACTION RATE (TOTAL) \uparrow PROB OF REACTION

$$R = \text{VOLUMETRIC REACTION RATE} \\ = \frac{\mathcal{R}}{A \cdot dx} = I \cdot \sigma \cdot N = \boxed{I \cdot \Sigma} \leftarrow \begin{array}{l} \text{MACROSCOPIC} \\ \text{CROSS SECTION} \\ \text{\#/CM}^2 \cdot \text{s} \end{array}$$

Review of material from Lecture 3.

$$R = I \cdot \Sigma$$

$\uparrow \sigma N$

\uparrow target nuclei number
nuclei/cm³

cm²
(b = 10⁻²⁴ cm²)

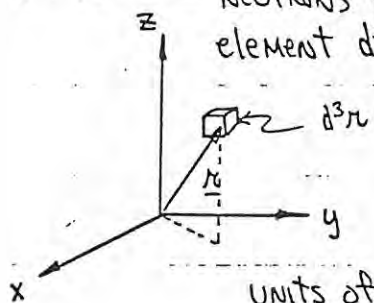
$R = I \cdot \Sigma$ - generalize
to the case
where the neutrons
are travelling in
arbitrary directions

For example, the center of a reactor core.

Definitions

1. Neutron number density $n(\underline{r})$

$n(\underline{r}) d^3r \equiv$ expected number of
neutrons in the volume
element d^3r at \underline{r}



generalization:

$$n(\underline{r}, t) - \#/\text{cm}^3$$

at time t

units of $n(\underline{r})$: $\#/\text{cm}^3$

Similar to a nuclei number density.

2. Neutron scalar flux

$$\Phi(\underline{r}) \equiv v n(\underline{r}) \text{ (speed } \times \text{ density)}$$

where v = speed of the neutrons

(assume for now all neutrons

have the same speed -

relax this assumption later)

$$\text{units: } \left(\frac{\text{cm}}{\text{s}}\right) \cdot \left(\frac{\#}{\text{cm}^3}\right) = \frac{\#}{\text{cm}^2 \cdot \text{s}}$$

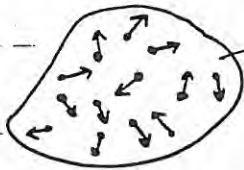
CAUTION: $\Phi(\underline{r})$ has no directional significance
(unlike other "fluxes", e.g., \mathbf{q})

One cannot emphasize too strongly this note of caution! Let us now examine a physical definition for Φ that brings out its non-directional nature.

ϕ - convenient for
calculating reaction rates

Physical significance -

consider the small volume ΔV which contains neutrons with velocity v (speed) and density n_0



Total number
of neutrons
in $\Delta V =$
 $n_0 \Delta V$

The neutron density is constant (i.e., $n(\underline{r}) = n_0$ neutrons/cm³)

Let us now tabulate the total distance travelled by all of the neutrons in ΔV in the time interval Δt .

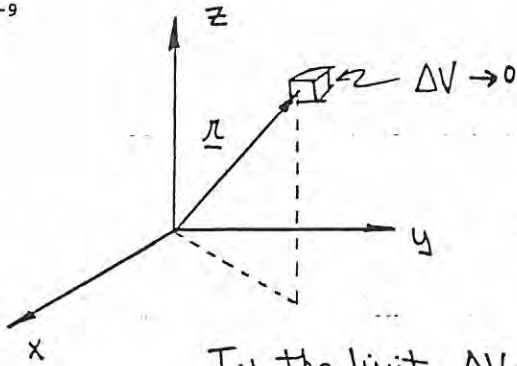
• In the time interval Δt , each neutron in ΔV travelled a distance $v \Delta t$

• Then the total distance D travelled by neutrons in ΔV during the time interval Δt ,

$$D = [n \cdot \Delta V] [v \cdot \Delta t]$$

• Then $\phi = n v = \frac{D}{\Delta V \cdot \Delta t}$ } total distance traversed by neutrons per cm³ per second

ϕ is the rate per unit volume per unit time that path length is traversed by neutrons.



In the limit $\Delta V \rightarrow 0$

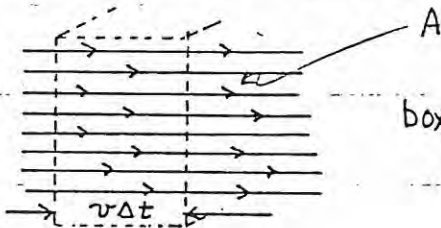
$\phi(\underline{r}) =$ path length density
per unit time at \underline{r}

"SCALAR flux"

"NEUTRON flux"

We are interested in path length traversed by the neutrons because we know the interaction probability is Σ , which is a probability per unit length.

Calculate ϕ for a Parallel
Beam of Neutrons with
Intensity I neutrons
 $\text{cm}^2 \cdot \text{s}$



box - AREA A
- length $v\Delta t$

- In the time Δt ,
 $IA\Delta t$ neutrons enter
The box

11-11

$I \cdot A \cdot \Delta t = \# \text{ of neutrons}$
in the box

$A \cdot v \cdot \Delta t = \text{volume of box}$

Neutron density = $\frac{I \cdot A \cdot \Delta t}{A \cdot v \cdot \Delta t}$

$$m = \frac{I}{v}$$

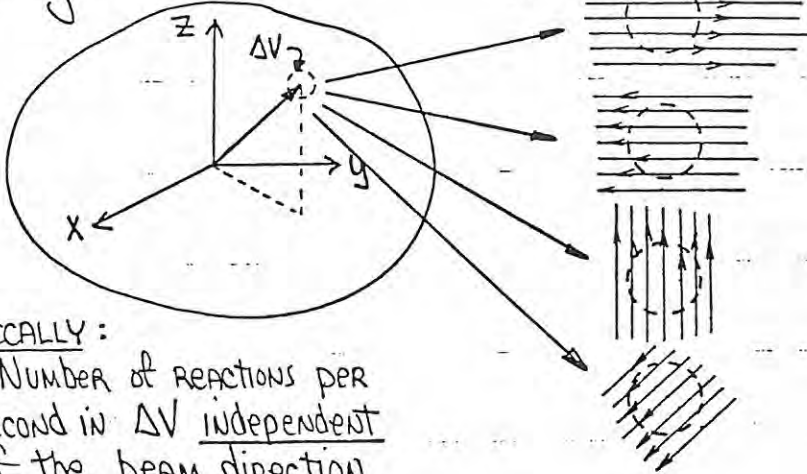
$$\phi = m v = I$$

$\boxed{\phi = I}$ for a parallel beam
(special case)

This is a special case - do NOT view this as the physical situation which defines ϕ . It just happens that the scalar flux for a directed beam is just the beam intensity.

11-12

Consider some arbitrary target

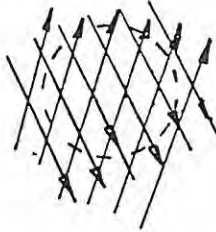
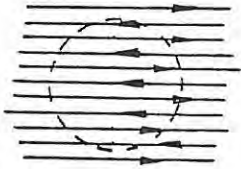
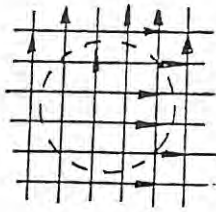
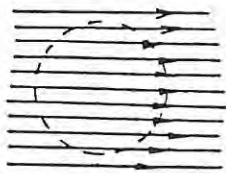


PHYSICALLY:

Number of reactions per second in ΔV independent of the beam direction
(same intensity)

Note that the nuclei do not care from which direction the neutrons are coming.

11-13

 $\Delta V \rightarrow$ 

Number of reactions in $\Delta V \propto$ to the rate at which neutron path length is swept out in ΔV (per second)

11-14

Conclusion

- Generalize the expression for reaction rate due to parallel beam

$$R = \Sigma I$$

$$R = v \underbrace{m}_{\phi} \Sigma$$

To the general case where the neutrons are travelling in arbitrary directions:

$$R = \Sigma \phi$$

volumetric reaction rate (#/cm³.s)

Key Ideas - $\Phi(\underline{x})$

- $\Phi(\underline{x})$ NOT A "true" flux because it has NO directional significance
- $\Phi(\underline{x}) = v M(\underline{x})$
- Useful for reaction rates
 - $R = \Sigma \Phi$
- Physical significance - rate at which neutron path length swept out per cm³ per second

Do not view Φ as a heat flux or other type of flux, which carry the connotation of a certain quantity crossing a unit area per unit time. Specifying a unit area implies a directional nature.

Neutron Current \underline{J}

operational definition



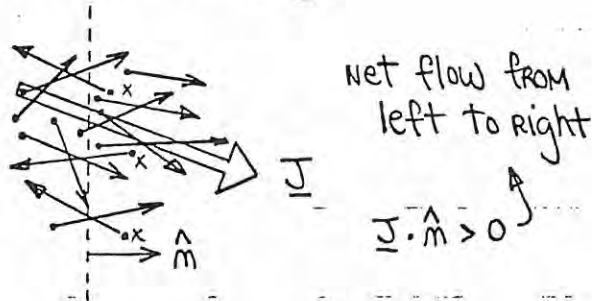
$\underline{J} \cdot \hat{n} A =$ NET NUMBER OF NEUTRONS CROSSING THE AREA A PER SECOND, where

$\hat{n} =$ NORMAL to the AREA A

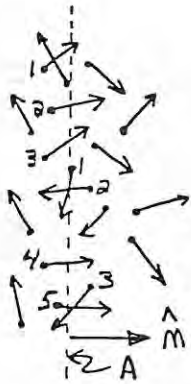
AND $+$ CORRESPONDS TO CROSSING IN THE DIRECTION DEFINED BY \hat{n}

The net current \underline{J} does carry directional information because it specifies the direction of the net flow as well as the net magnitude.

\underline{J} is a vector expressing the directional dependence of the flow of neutrons (similar to the flow of heat described by \underline{q})



If the net flow is in the direction defined by \hat{n} , it is positive.



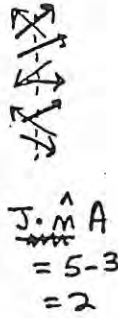
- In time Δt , neutron travels distance indicated
- Number crossing from left to right in the time $\Delta t = \underline{5}$
- Number crossing from right to left in the time $\Delta t = \underline{3}$

Net number crossing left to right $\equiv 5 - 3 = 2$

An example illustrating the concept of net flow.

• Then $\underline{J} \cdot \hat{m} = \frac{2}{A \cdot \Delta t}$

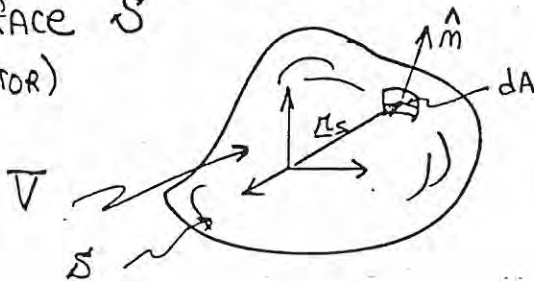
- Note that if you only know \underline{J} , you only have information concerning the net flow of neutrons across a given surface. Nothing may be inferred concerning composition of \underline{J} (number going left-to-right vs. up-to-down, etc.)



$$\begin{aligned} \underline{J} \cdot \hat{m} A \\ = 5 - 3 \\ = 2 \end{aligned}$$

Knowing that 2 net particles crossed from left to right, we have no idea if the numbers traveling left and right were 10 and 8, or 100 and 98, or whatever.

- \underline{J} is useful because we can calculate leakage rates
- Let $\underline{J}(\underline{r})$ be the (known) neutron current as a function of \underline{r} in a volume V bounded by a surface S (our reactor)



- Net leakage ($\frac{\text{NEUTRONS}}{\text{SECOND}}$)
Through the elemental
AREA dA is

$$\underline{J}(\underline{r}_s) \cdot \hat{m}_s dA$$

where

$$\underline{J}(\underline{r}_s) = \text{NET CURRENT AT } \underline{r}_s$$

$$\hat{m}_s = \text{OUTWARD NORMAL TO } dA$$

This is just our previous definition of \underline{J} .

Total leakage through S :

$$\mathcal{L} = \oint_S \underline{J}(\underline{r}_s) \cdot \hat{m}_s dA$$

NEUTRONS/s CROSSING
the SURFACE FROM
the INSIDE (leaking out)

Integrate over all elemental areas comprising S .

LECTURE 12

NEUTRON CONTINUITY EQUATION

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 149-152.

Lamarsh, pp. 158-161.

EXERCISES:

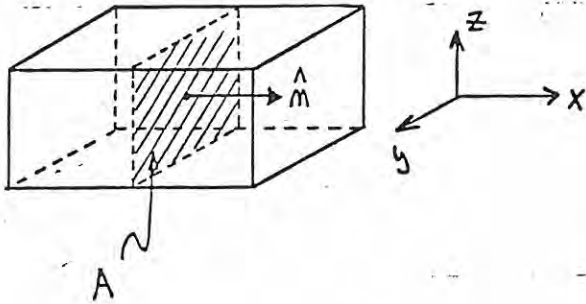
12.1. Duderstadt & Hamilton, problem #4-9.

12.2. Lamarsh, problem #5.1.

12.3. Lamarsh, problem #5.2.

Examples

- Assume $\phi(\underline{r}) = \phi_0$ (constant)
inside a volume V



12-2

1. How many neutrons cross the shaded area A per unit time?

(a) $\phi_0 \cdot A$

(b) Zero

(c) CANNOT determine ✓

2. If the net current in the box, \underline{J} , is a constant

$$\underline{J} = \underline{J}_0 = J_0 \hat{e}_x$$

(a) Calculate the net number of neutrons crossing from left to right. (in time Δt)

$$\underline{J}_0 \cdot \hat{m} A = J_0 \cdot A \cdot \Delta t$$

$$\hat{m} = \hat{e}_x$$

$$\underline{J}_0 = J_0 \hat{e}_x$$

(b) Net number from right to left? $- J_0 A \Delta t$

(c) Total number crossing A in any direction?

CANNOT determine

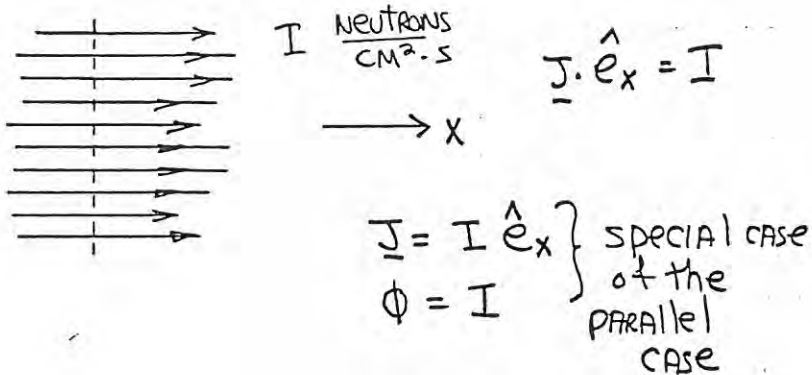
We only know the net number crossing A.

• Assume we have two collections of neutrons described by ϕ_1 and \underline{J}_1 and ϕ_2 and \underline{J}_2 . What is the total ϕ and \underline{J} if they are combined?

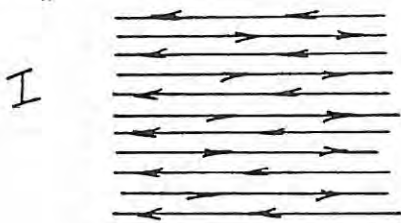
$$\phi = \phi_1 + \phi_2 \quad (\text{Algebraic Addition})$$

$$\underline{J} = \underline{J}_1 + \underline{J}_2 \quad (\text{vector Addition})$$

- What is \underline{J} and ϕ for a ^{PARALLEL} BEAM of intensity I travelling in the x -direction?



- What is \underline{J} and ϕ for two opposing beams, each of intensity I ?



$$\phi = \phi_1 + \phi_2 = I + I = 2I$$

$$\underline{J} = \underline{J}_1 + \underline{J}_2 = I \hat{e}_x - I \hat{e}_x = 0$$

$I \text{ NEUTRONS/CM}^2 \cdot \text{s}$

$$\underline{J}_1 = I \hat{e}_x$$

$$\underline{J}_2 = -I \hat{e}_x$$

$$\phi = 2I$$

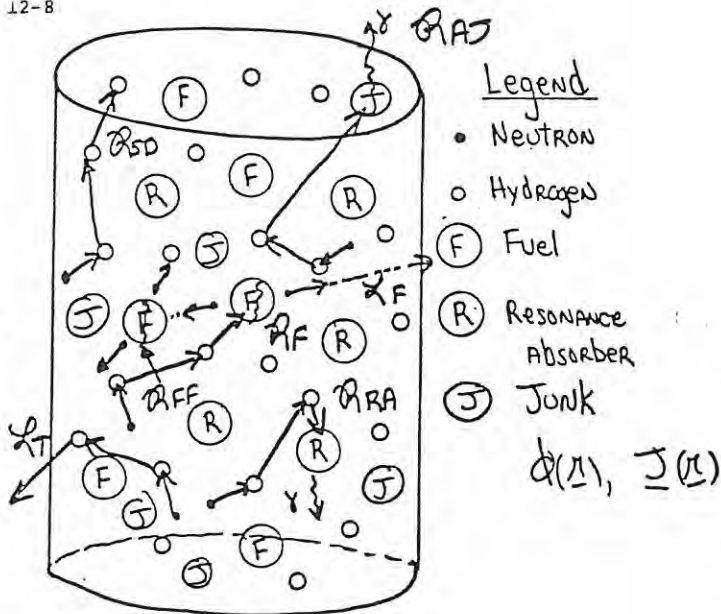
$$\underline{J} = 0 \quad (\text{NOTE THAT A KNOWLEDGE OF ONLY } \underline{J} \text{ DOES NOT SAY MUCH})$$

$\Phi(\underline{r})$ - calculate
REACTION RATES

$\underline{J}(\underline{r})$ - calculate
leakage RATES

- We can then calculate k
- How do we calculate $\Phi(\underline{r})$, $\underline{J}(\underline{r})$?

It seems we have a never-ending spiral of definitions - but now we are in a position to derive an equation relating ϕ and \underline{J} .



- NEUTRON SCALAR FLUX $\Phi(\underline{r})$
 - NEUTRON NET CURRENT $\underline{J}(\underline{r})$
- } sufficient to calculate the REACTION RATES & leakage rates

$$\mathcal{L}_F = \oint_S \underline{J} \cdot \hat{n} dA$$

EXAMPLE

- Absorption rate in the FUEL \underline{J} for FAST NEUTRONS

$$R_{AF} = \int_{\text{REACTOR}} \underbrace{\sum_a^F(\underline{r}) \Phi(\underline{r})}_{\text{VOLUMETRIC REACTION RATE}} d^3r \quad \left(\frac{\text{ABSORPTIONS}}{\text{SECOND}} \right)$$

NEUTRON DIFFUSION EQUATION

- Describes the spatial VARIATION of the NEUTRON flux $\Phi(\underline{r})$
- CAN determine $\underline{J}(\underline{r})$ FROM $\Phi(\underline{r})$ ("diffusion approximation")
- Determine REACTION RATES R AND leakage rates \mathcal{L}
- Include energy and time dependence later

Derivation of the Diffusion Equation

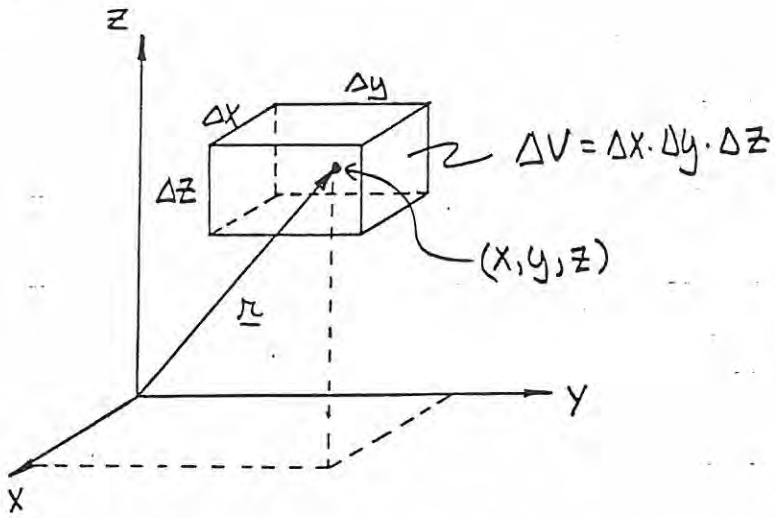
- The "continuity" equation (one-speed) neutron balance
- The diffusion approximation $\underline{J} = \underline{J}(\phi)$
- The one-speed diffusion equation
- Include energy dependence

Neutron Continuity Equation

- Statement of
NEUTRON BALANCE
- Derivation - consider the balance of neutrons (i.e., production and loss) for an elemental volume ΔV

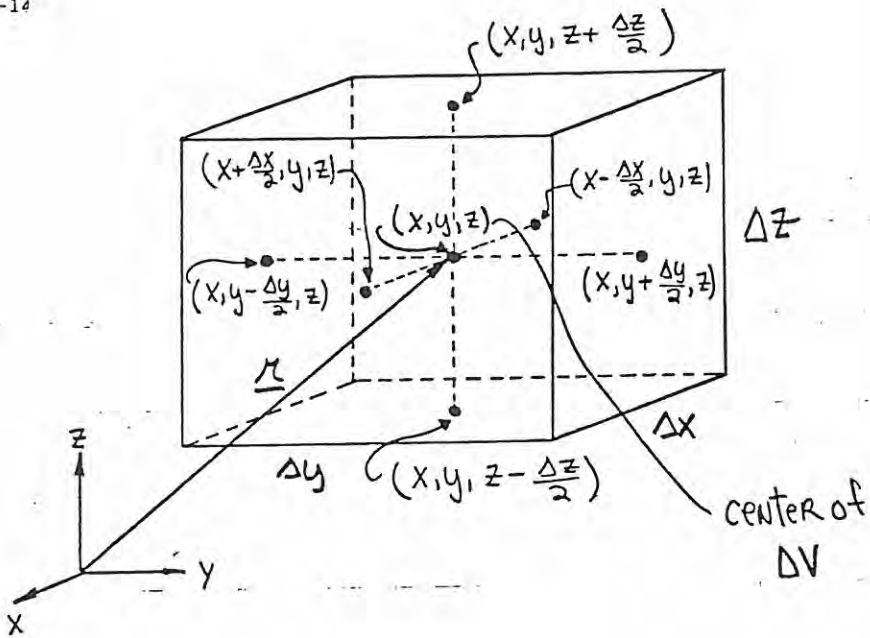
Neutron balance means the balance of neutron loss and neutron gain.

12-13



Consider neutron balance for the elemental volume $\Delta V = \Delta x \cdot \Delta y \cdot \Delta z$ which is centered at x, y, z and has sides $\Delta x, \Delta y, \Delta z$.

12-14



NEUTRON BALANCE IN ΔV

Define $N(t)$ = TOTAL NUMBER OF
NEUTRONS IN ΔV
AT TIME t

Then at time $t + \Delta t$,

$$N(t + \Delta t) = N(t) + \overset{\textcircled{1}}{\# \text{ NEUTRONS PRODUCED}}$$

- $\overset{\textcircled{2}}{\# \text{ NEUTRONS ABSORBED}}$

- $\overset{\textcircled{3}}{\# \text{ NEUTRONS LEAKED}}$

$$N(t + \Delta t) = N(t) + \textcircled{1} - \textcircled{2} - \textcircled{3}$$

N is the total number, not the density.

TERM $\textcircled{1}$ NEUTRONS PRODUCED IN ΔV

Define $S(\underline{r}, t) \equiv$ RATE AT WHICH
NEUTRONS ARE
PRODUCED IN ΔV
(# produced/cm³.s)

(e.g., $S(\underline{r}, t) = \Sigma_f(\underline{r}) \phi(\underline{r}, t)$
FOR A FISSION SOURCE)

- Then the number of neutron produced in ΔV during the time interval Δt :

$$\textcircled{1} = \text{production} = \boxed{S(\underline{r}, t) \cdot \Delta V \cdot \Delta t} \quad \textcircled{1}$$

Term ② # Neutrons absorbed
in ΔV during Δt

Definition of reaction rate:

$$\Sigma_a(\underline{r}) \phi(\underline{r}, t) = \# \text{ neutrons absorbed/cm}^3 \cdot \text{s}$$

$$\therefore \textcircled{2} = \# \text{ absorbed} = \boxed{\Sigma_a(\underline{r}) \phi(\underline{r}, t) \cdot \Delta V \cdot \Delta t} \quad \textcircled{2}$$

Term ③ Neutrons leaked out of ΔV (in Δt)

Recall

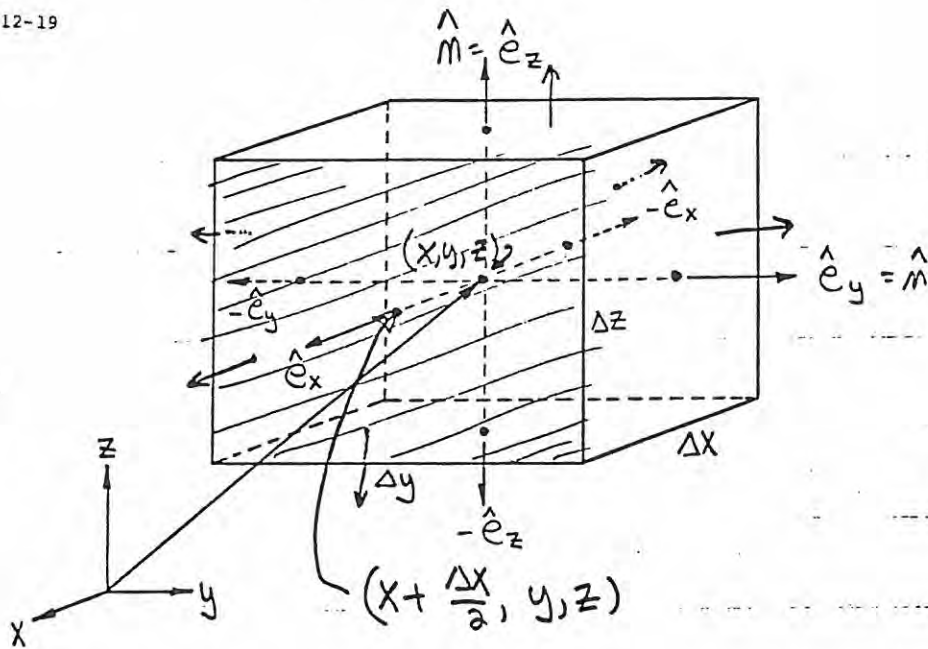
$$\underline{J} \cdot \hat{m} A = \text{net number of neutrons crossing the area } A \text{ per second}$$

$$\underline{J} \cdot \hat{m} A < 0 \leftarrow \text{in-leakage}$$

$$\underline{J} \cdot \hat{m} A > 0 \text{ out-leakage}$$

$$\hat{m} = \text{unit outer normal}$$

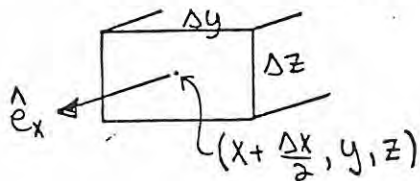
So far the terms have been easy because of our previous definitions. We now need a little algebra, however.



+ X face

$$\bar{J}(x + \frac{\Delta x}{2}, y, z) \cdot \hat{e}_x \cdot \overbrace{\Delta y \cdot \Delta z}^A \cdot \Delta t$$

= NET NUMBER OF NEUTRONS
CROSSING THE +X FACE IN THE
TIME INTERVAL Δt (FROM INSIDE TO
OUTSIDE)



-X face

Net number crossing the -X
face in the time Δt

$$\underline{J}(x - \frac{\Delta x}{2}, y, z) \cdot \underbrace{[-\hat{e}_x]}_{\hat{m}} \cdot \underbrace{\Delta y \cdot \Delta z}_A \cdot \Delta t$$

(\hat{m} for the
-X face)

(from inside to outside due to
our definition of \hat{m})

 $\pm y, \pm z$ faces

• Leakage across $\oplus y$ faces

$$\underline{J}(x, y \oplus \frac{\Delta y}{2}, z) \cdot \underbrace{[\oplus \hat{e}_y]}_A \cdot \Delta x \cdot \Delta z \cdot \Delta t$$

• Leakage across $\pm z$ faces

$$\underline{J}(x, y, z \pm \frac{\Delta z}{2}) \cdot \underbrace{[\pm \hat{e}_z]}_A \cdot \Delta x \cdot \Delta y \cdot \Delta t$$

Add to find the
Total leakage from ΔV :

③ = Total leakage from ΔV

$$\begin{aligned} \textcircled{3} &= \left[\bar{J}\left(x + \frac{\Delta x}{2}, y, z\right) - \bar{J}\left(x - \frac{\Delta x}{2}, y, z\right) \right] \cdot \hat{e}_x \cdot \Delta y \cdot \Delta z \cdot \Delta t \\ &+ \left[\bar{J}\left(x, y + \frac{\Delta y}{2}, z\right) - \bar{J}\left(x, y - \frac{\Delta y}{2}, z\right) \right] \cdot \hat{e}_y \cdot \Delta x \cdot \Delta z \cdot \Delta t \\ &+ \left[\bar{J}\left(x, y, z + \frac{\Delta z}{2}\right) - \bar{J}\left(x, y, z - \frac{\Delta z}{2}\right) \right] \cdot \hat{e}_z \cdot \Delta x \cdot \Delta y \cdot \Delta t \end{aligned}$$

We have determined all of
the terms in the neutron
balance expression:

$$N(t + \Delta t) = N(t) + \textcircled{1} - \textcircled{2} - \textcircled{3} \quad (*)$$

Now note

$$N(t) = m(\underline{r}, t) \cdot \Delta V$$

$$N(t + \Delta t) = m(\underline{r}, t + \Delta t) \cdot \Delta V$$

• Divide eq. (*) by $\Delta V \cdot \Delta t$:

$$\frac{m(\underline{r}, t + \Delta t) - m(\underline{r}, t)}{\Delta t} = S(\underline{r}, t) - \sum_a(\underline{r}) Q(\underline{r}, t)$$

$$- \frac{[\underline{J}(x + \frac{\Delta x}{2}, y, z) - \underline{J}(x - \frac{\Delta x}{2}, y, z)] \cdot \hat{e}_x}{\Delta x}$$

$$- \frac{[\underline{J}(x, y + \frac{\Delta y}{2}, z) - \underline{J}(x, y - \frac{\Delta y}{2}, z)] \cdot \hat{e}_y}{\Delta y}$$

$$- \frac{[\underline{J}(x, y, z + \frac{\Delta z}{2}) - \underline{J}(x, y, z - \frac{\Delta z}{2})] \cdot \hat{e}_z}{\Delta z}$$

• Now take the limits

$$\Delta x \rightarrow 0 \quad \Delta z \rightarrow 0$$

$$\Delta y \rightarrow 0 \quad \Delta t \rightarrow 0$$

Noting

$$\frac{\partial m}{\partial t} \equiv \lim_{\Delta t \rightarrow 0} \frac{m(\underline{r}, t + \Delta t) - m(\underline{r}, t)}{\Delta t}$$

$$\frac{\partial J_x}{\partial x} \equiv \lim_{\Delta x \rightarrow 0} \frac{J_x(x + \frac{\Delta x}{2}, y, z) - J_x(x - \frac{\Delta x}{2}, y, z)}{\Delta x}$$

$$(J_x \equiv \underline{J} \cdot \hat{e}_x)$$

These are just the first year calculus definitions of partial derivatives.

$$\frac{\partial M}{\partial t} = S(\underline{r}, t) - \Sigma_a(\underline{r})\Phi(\underline{r}, t) - \nabla \cdot \underline{J}(\underline{r}, t)$$

$$\text{where } \nabla \cdot \underline{J} \equiv \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}$$

Now using $\Phi(\underline{r}, t) = v M(\underline{r}, t)$,

$$\frac{1}{v} \frac{\partial \Phi}{\partial t} + \nabla \cdot \underline{J}(\underline{r}, t) + \Sigma_a(\underline{r})\Phi(\underline{r}, t) = S(\underline{r}, t)$$

Neutron Continuity Equation
(one-speed)

This is the one-speed neutron continuity equation. No approximations have been made to date - it is essentially EXACT (within the one-speed approximation)

- Continuity equation - 1 equation
- How many unknowns - 4

$$\Phi(\underline{r}), \underline{J}(\underline{r})$$

$$\underline{J} = J_x \hat{e}_x + J_y \hat{e}_y + J_z \hat{e}_z$$

- "Diffusion Approximation"

$$\underline{J} \approx \underline{J}(\phi)$$

should be \hat{e}_z

1 equation for ϕ alone
(diffusion equation)

Predicament - the neutron continuity equation has 4 unknown. We need some way to relate ϕ and \underline{J} , which will be done with the diffusion approximation in the next few lectures.

LECTURE 13

NEUTRON DIFFUSION EQUATION

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 152-153.

Lamarsh, pp. 161-163.

EXERCISES:

13.1. Lamarsh, problem #5.3.

13.2. Lamarsh, problem #5.16.

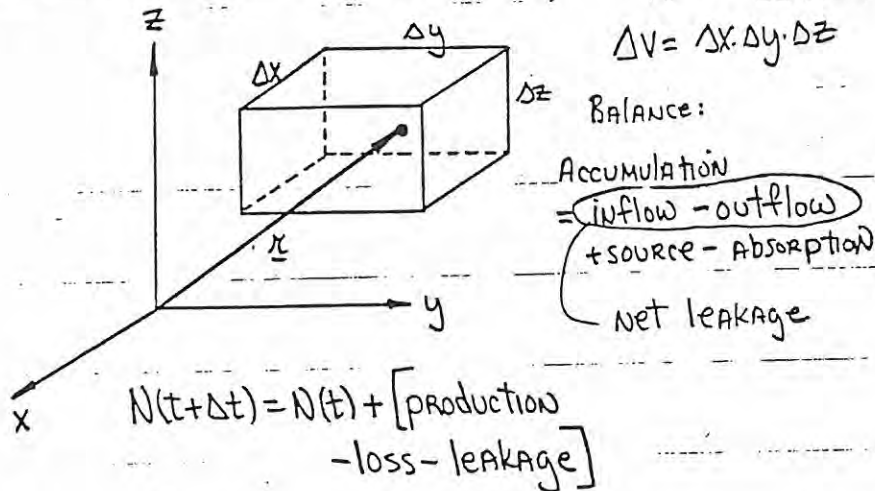
Previous Lecture

- Reaction rates & leakage rates
- Need $\Phi(\underline{r})$, $\underline{J}(\underline{r})$
- Neutron Continuity Equation relates $\Phi(\underline{r})$ to $\underline{J}(\underline{r})$
- Cannot solve

Today $\underline{J} = \underline{f}(\Phi)$ "diffusion approximation"

- Neutron diffusion equation

13-2

Neutron Continuity Equation

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{J} + \Sigma_a(\underline{r}) \phi(\underline{r}, t) = S(\underline{r}, t)$$

NEUTRON CONTINUITY EQUATION (1-speed)

Notes: ① Expresses neutron balance

② Essentially exact:

(i) ONE speed (relax this today)

(ii) NO NEUTRON-NEUTRON INTERACTIONS $n \sim 10^8 - 10^9$ (neutrons/cm³)

(iii) IGNORE NEUTRON DECAY

(iv) IGNORE FLUCTUATIONS $N \sim 10^{18} - 10^{19}$

$$\tau \sim 13 \text{ sec}$$

$$\lambda \sim 10^{-5} \text{ sec}$$

OUR DILEMMA:

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{J} + \Sigma_a \phi = S$$

(1 equation)

Unknowns: $\phi(\underline{r}, t)$

$$\underline{J}(\underline{r}, t) = J_x \hat{e}_x + J_y \hat{e}_y + J_z \hat{e}_z$$

Possible remedy:

Model - relates \underline{J} to ϕ

e.g., $\underline{J} = \underline{f}(\phi)$

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{f}(\phi) + \Sigma_a \phi = S$$

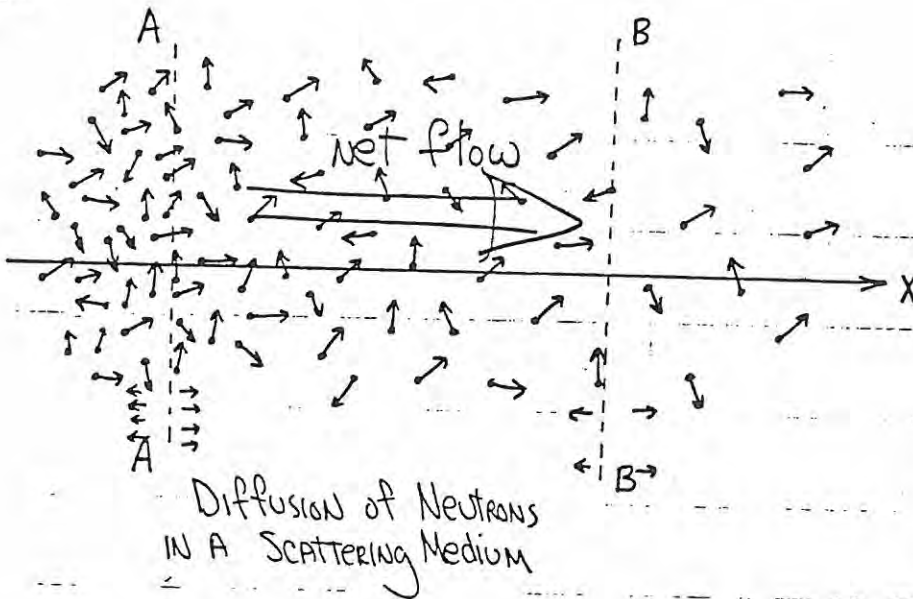
The Diffusion Approximation

• Model yielding $\underline{J} = \underline{f}(\phi)$

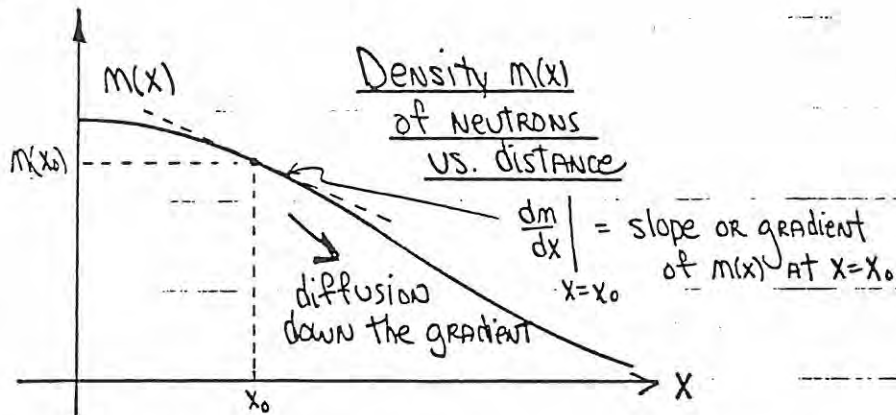
• Physical model :

Neutrons tend to diffuse
from regions of high neutron
density to regions of low
neutron density

(Fick's LAW)



There is a net flow from A to B due to the fact
the concentration is higher at A.



Fick's Law: net flow \propto
concentration gradient

Fick's law is a mathematical statement of the observation that for many physical situations, the net flow is proportional to the concentration gradient (flow is down the gradient)

• Net flow \propto density gradient
 $= \nabla m$ (Fick's Law)

• Net flow $\propto \underline{J}$

$$\underline{J} \propto -\nabla m$$

• $\phi = m v$

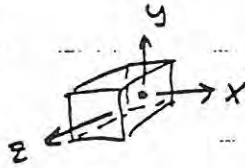
$$\underline{J} = -D \nabla \phi$$

diffusion
constant

13-9

$$\underline{J} \equiv J_x \hat{e}_x + J_y \hat{e}_y + J_z \hat{e}_z$$

$$\nabla \phi \equiv -\frac{\partial \phi}{\partial x} \hat{e}_x + \frac{\partial \phi}{\partial y} \hat{e}_y + \frac{\partial \phi}{\partial z} \hat{e}_z$$



$$\therefore J_x = -D \frac{\partial \phi}{\partial x}$$

$$J_y = -D \frac{\partial \phi}{\partial y}$$

$$J_z = -D \frac{\partial \phi}{\partial z}$$

same D for
all directions
 $D = D(\underline{r})$

In general, $D = D(\underline{r})$

AND $\underline{J}(\underline{r}) = -D(\underline{r}) \nabla \phi(\underline{r})$

Isotropic material - expect the same diffusion coefficient D for all directions.

13-10

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Sigma_a \phi + \nabla \cdot \underline{J} = S(\underline{r}, t)$$

$$\underline{J}(\underline{r}, t) = -D(\underline{r}) \nabla \phi(\underline{r}, t)$$

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(\underline{r}) \nabla \phi(\underline{r}, t)$$

$$+ \Sigma_a(\underline{r}) \phi(\underline{r}, t) = S(\underline{r}, t)$$

Neutron Diffusion Equation

1 equation

1 unknown $\phi(\underline{r}, t)$

Simply substitute the expression for the net current into the continuity equation.

Observations

- Basic assumption - diffusion model
- valid for scattering media ("diffusing" media)
- not valid for:
 - strong absorbers
 - voids
 - localized sources
 - near boundaries

Energy Dependence

- Thermal reactor -
 - neutrons "born" with energies in the MeV range and slow down to the eV (and smaller) energy range
 - total energy range $\approx 10 \text{ MeV to } .01 \text{ eV} - 10^7 \text{ eV} \rightarrow 10^{-2} \text{ eV}$

We have been ignoring an important characteristic of the neutrons.

Definitions

$$n(\underline{r}, E, t) d^3r dE \leftarrow \text{energy "volume"}$$

= NUMBER OF NEUTRONS
IN THE VOLUME d^3r
ABOUT \underline{r} AND WHICH
HAVE ENERGY IN THE
RANGE dE ABOUT E

$$\Phi(\underline{r}, E, t) = v n(\underline{r}, E, t)$$

where $v = \sqrt{\frac{2E}{m}} \leftarrow \text{NEUTRON MASS}$

Density per unit volume and per unit energy.

Note: $\Phi(\underline{r}, E, t) dE$

is the rate at
which path length
is swept out per
 cm^3 per second at
 \underline{r} AND time t by

NEUTRONS IN THE ENERGY
RANGE dE ABOUT E

USUAL DEFINITION
OF ϕ
(1-speed)

$$\Phi(\underline{r}, t) = \int_0^{\infty} \Phi(\underline{r}, E, t) dE$$

TOTAL \rightarrow

Generalize concept of ϕ to distinguish path length
traversed by neutrons of different energy (need
because $\Sigma(E)$).

Reaction rates

- Total absorption rate

$$R = \iiint_V \Sigma_a(\mathbf{r}) \Phi(\mathbf{r}) d^3r$$

$$\Phi(\mathbf{r}) = \int_0^{\infty} \Phi(\mathbf{r}, E) dE$$

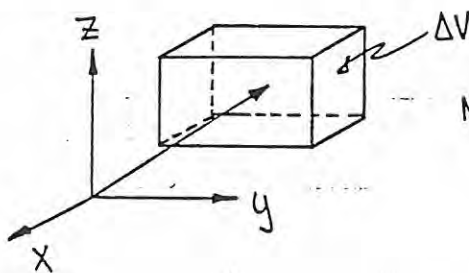
- Absorption rate of neutrons in the energy range dE

$$R_{dE} = \iiint_V \Sigma_a(\mathbf{r}) \Phi(\mathbf{r}, E) dE d^3r$$

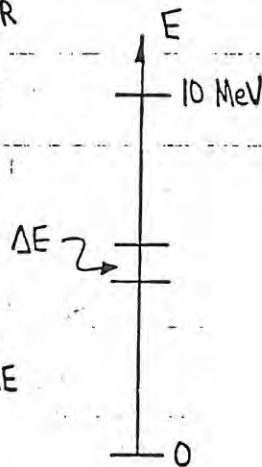
$$= dE \iiint_V \Sigma_a(\mathbf{r}) \Phi(\mathbf{r}, E) d^3r$$

Energy-dependent Continuity Equation

- Express neutron balance for the neutrons in ΔV which ^{also} have energy in the range ΔE



NEUTRONS IN
 ΔV AND ΔE



NEUTRON BALANCE

NEUTRONS IN ΔV WITH ENERGY IN ΔE AT TIME t

$$N_{\Delta E}(t + \Delta t) = N_{\Delta E}(t) + \textcircled{1} - \textcircled{2} - \textcircled{3} - \textcircled{4} + \textcircled{5}$$

where

$\textcircled{1} =$ NUMBER OF NEUTRONS PRODUCED IN ΔV WITH ENERGY IN ΔE

SCATTER OUT OF ΔE (STILL IN ΔV)

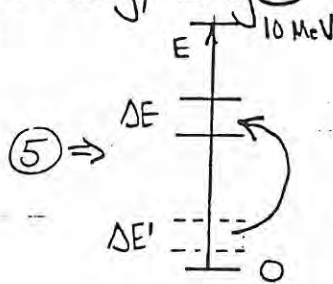
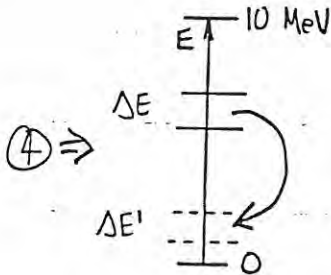
$\textcircled{2} =$ NUMBER OF NEUTRONS IN $\Delta V \cdot \Delta E$ ABSORBED

SCATTER INTO ΔE

$\textcircled{3} =$ NUMBER IN $\Delta V \cdot \Delta E$ WHICH LEAK OUT

$\textcircled{4} =$ NUMBER OF NEUTRONS IN ΔV WHICH SCATTER OUT OF ΔE INTO SOME OTHER ENERGY RANGE

$\textcircled{5} =$ NUMBER OF NEUTRONS IN ΔV WHICH SCATTER INTO ΔE FROM SOME OTHER ENERGY RANGE



Individual terms become:

$$N_{\Delta E}(t + \Delta t) = M(\mu, E, t + \Delta t) \cdot \Delta V \cdot \Delta E \quad \text{by definition}$$

$$N_{\Delta E}(t) = M(\mu, E, t) \cdot \Delta V \cdot \Delta E$$

$$\textcircled{1} = S(\mu, E, t) \cdot \Delta V \cdot \Delta E \cdot \Delta t$$

(by definition of $S(\mu, E, t)$)

$$\textcircled{2} = \sum_a \alpha_a(\mu, E) \cdot \Phi(\mu, E, t) \cdot \Delta V \cdot \Delta E \cdot \Delta t$$

(note: $\Phi(\mu, E, t) \equiv v M(\mu, E, t)$)

$\textcircled{3}$ = similar to earlier (one-speed) term except multiply by ΔE

TERM $\textcircled{4}$ Outscatter

Assume that ΔE is small enough that if a neutron with energy in ΔE undergoes a scattering collision, it will be removed from ΔE ($\Delta E \rightarrow 0$) (up- or down-scatter)

Then

$$\textcircled{4} = (\Sigma_s(\mu, E) \Phi(\mu, E, t) \Delta E) \Delta V \cdot \Delta t$$

Term ⑤ INSCATTER

Recall definition of the differential scattering cross-section:

$\sigma_s(E' \rightarrow E) dE$ = microscopic cross section for a neutron with energy E' to scatter into the energy range dE about E

- Then by definition of reaction rate, $\Sigma \phi$

$$[\Sigma_s(E' \rightarrow E) \cdot \Delta E] \cdot [\Phi(\mu, E', t) \cdot \Delta E'] \cdot \Delta V \cdot \Delta t$$

is the number of neutrons which scatter from the energy range $\Delta E'$ into the energy range ΔE

- The total number scattered into ΔE is the summation over all of the $\Delta E'$

$$\begin{aligned} \textcircled{5} &= \sum_{\text{All } j} \left\{ \Sigma_s(\mu, E_j \rightarrow E) \cdot \Delta E \cdot \Phi(\mu, E_j, t) \cdot \Delta E_j \cdot \Delta V \cdot \Delta t \right\} \\ &= \Delta V \cdot \Delta t \cdot \Delta E \sum_j \Sigma_s(\mu, E_j \rightarrow E) \Phi(\mu, E_j, t) \Delta E_j \end{aligned}$$

Combine Terms

$$\begin{aligned} N(\mu, E, t + \Delta t) \cdot \Delta V \cdot \Delta E \\ = N(\mu, E, t) \cdot \Delta V \cdot \Delta E + \textcircled{1} - \textcircled{2} - \textcircled{3} \\ - \textcircled{4} + \textcircled{5} \end{aligned}$$

• Divide by $\Delta V \cdot \Delta E \cdot \Delta t$

• Take the limits

$$\begin{aligned} \Delta x \rightarrow 0 & \quad \Delta t \rightarrow 0 \\ \Delta y \rightarrow 0 & \quad \Delta E \rightarrow 0 \text{ (actually } \Delta E_j) \\ \Delta z \rightarrow 0 & \end{aligned}$$

• Note

$$\lim_{\Delta E_j \rightarrow 0} \sum_j \Sigma_s(\mu, E_j \rightarrow E) \Phi(\mu, E_j, t) \Delta E_j = \int_0^\infty \Sigma_s(\mu, E' \rightarrow E) \Phi(\mu, E', t) dE'$$

(RIEMANN SUM)

FINAL Result

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{J}(\underline{r}, E, t) + \overset{\Sigma_t = \Sigma_a + \Sigma_s}{\Sigma_t(\underline{r}, E)} \phi(\underline{r}, E, t)$$

$$= S(\underline{r}, E, t) + \underbrace{\int_0^{\infty} \Sigma_s(\underline{r}, E' \rightarrow E) \phi(\underline{r}, E', t) dE'}_{\text{INSCATTER}}$$

Energy-dependent neutron
continuity equation

Looks the same as the one-speed equation except for the inscatter integral term. We still have the same problem - 1 equation in 4 unknowns.

LECTURE 14

INITIAL AND BOUNDARY CONDITIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 153-157.

Lamarsh, pp. 161-163.

EXERCISES:

- 14.1. If the original core were rectangular, can the "1/4 core" in slide 14-23 be made a "1/8 core" using symmetry? What if the original core were square?

FINAL Result

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{J}(\underline{r}, E, t) + \overset{\Sigma_t = \Sigma_a + \Sigma_s}{\Sigma_t(\underline{r}, E)} \phi(\underline{r}, E, t)$$

$$= S(\underline{r}, E, t) + \int_0^{\infty} \underbrace{\Sigma_s(\underline{r}, E' \rightarrow E)}_{\text{INSCATTER}} \phi(\underline{r}, E', t) dE'$$

Energy-dependent neutron
continuity equation

This equation is essentially exact - but it cannot be solved without an auxiliary equation relating ϕ and \underline{J} (i.e., Fick's Law).

Energy-dependent Diffusion
Equation

- Assume Fick's Law is valid for neutrons at a given energy E

$$\underline{J}(\underline{r}, E) = -D(\underline{r}, E) \nabla \phi(\underline{r}, E)$$

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(\underline{r}, E) \nabla \phi(\underline{r}, E, t) + \Sigma_t(\underline{r}, E) \phi(\underline{r}, E, t)$$

$$= S(\underline{r}, E, t) + \int_0^{\infty} \Sigma_s(\underline{r}, E' \rightarrow E) \phi(\underline{r}, E', t) dE'$$

INITIAL CONDITIONS &
BOUNDARY CONDITIONS

(NEUTRON DIFFUSION EQUATION)

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D \nabla \phi + \Sigma_a \phi(\underline{r}, t) = S(\underline{r}, t)$$

1ST order derivative

IN TIME - $\frac{\partial \phi}{\partial t}$

$D \neq D(\underline{r})$

2ND order in space

$$-\nabla \cdot D \nabla \phi = -D \nabla^2 \phi = -D \left[\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right]$$

• 1ST order derivative -

• The system "evolves" IN TIME FROM SOME INITIAL CONFIGURATION (AT $t=0$)
e.g.

• To solve, we need to specify the INITIAL CONFIGURATION, e.g.

$$M_0(\underline{r}) \equiv M(\underline{r}, 0)$$

OR $\phi_0(\underline{r}) \equiv \phi(\underline{r}, 0)$ INITIAL CONDITIONS

Best to visualize the situation physically, in order to calculate the state of a system at some time t , we must know the original state.

A Steady-State Situation
(No Time-dependence)

$$\Phi(\underline{r}, t) = \Phi(\underline{r})$$

$$S(\underline{r}, t) = S(\underline{r})$$

$$\boxed{-\nabla \cdot D(\underline{r}) \nabla \Phi(\underline{r}, t) + \Sigma_a(\underline{r}) \Phi(\underline{r}, t) = S(\underline{r})}$$

one-speed, steady-state
neutron diffusion equation

2nd order derivative

$$-\nabla \cdot D(\underline{r}) \nabla \Phi$$

(e.g., heat conduction equation)

• Boundary value problem:

$\Phi(\underline{r}_s)$ ON S } combination
OR $\nabla \Phi \cdot \hat{n}_s$ ON S } of these two

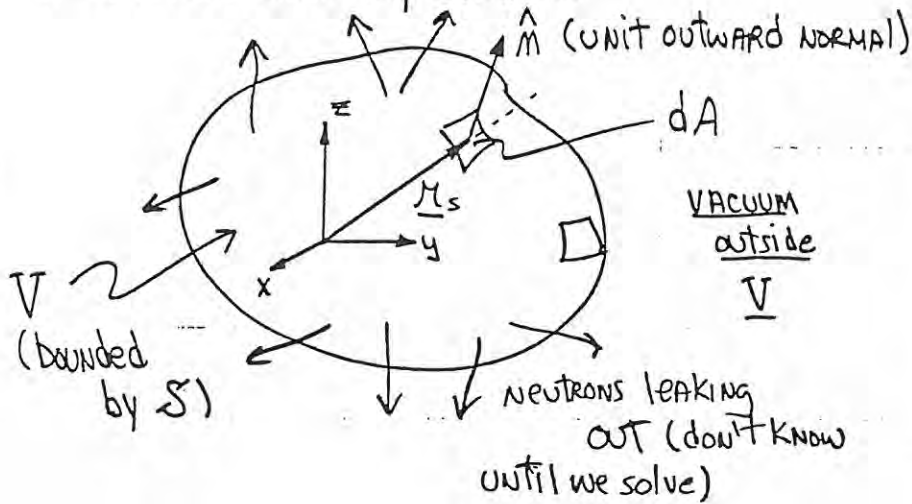
$$-\nabla \cdot D(\underline{r}) \nabla \Phi + \Sigma_a(\underline{r}) \Phi(\underline{r}) = S(\underline{r})$$

IN V

Boundary conditions are a little harder to motivate.

BOUNDARY CONDITIONS

1. VACUUM BOUNDARY CONDITION



The vacuum boundary condition would correspond to an isolated reactor.

• Physical boundary condition

- NO NEUTRONS ENTERING V

• MATHEMATICS

- Do not know $\phi(\mathcal{M}_S)$ ON S

- Do not know $\underline{J} \cdot \hat{\mathcal{M}}_S$ ON S

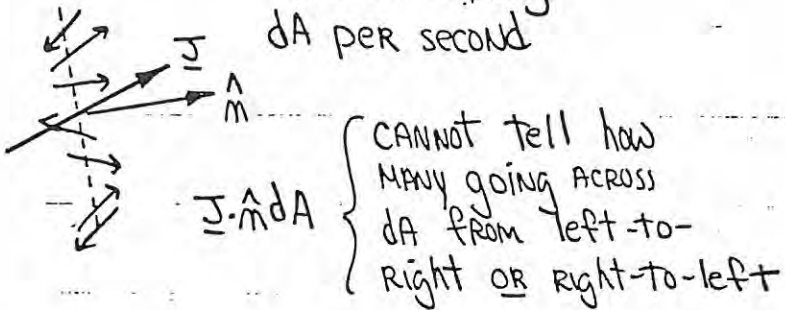
$$= \underbrace{\text{net leakage from } S}_{?} - \underbrace{\text{leakage in}}_{0}$$

Our boundary condition specifies a directional quantity, therefore the flux ϕ cannot be specified. Also, it does not represent a net flow but rather an actual flow in one direction (zero flow inward).

PARTIAL CURRENTS

$\underline{J}(\underline{n})$ - calculate net flow of neutrons

$\underline{J} \cdot \hat{n} dA =$ - net number of neutrons crossing dA per second

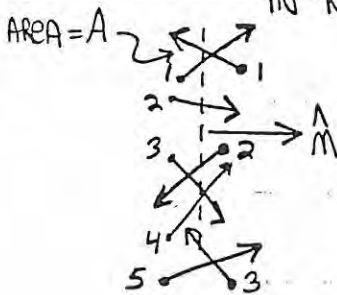


This concept of partial current will allow us to pose the vacuum boundary condition in a mathematical way.

Define

$J_+ A =$ NUMBER OF NEUTRONS (per second) CROSSING A GIVEN SURFACE IN THE DIRECTION DEFINED AS POSITIVE BY \hat{n}

$J_- A =$ NUMBER PER SECOND CROSSING IN NEGATIVE DIRECTION



$$J_+ A = \underline{5}$$

$$J_- A = \underline{3}$$

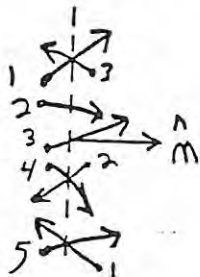
J_+ = PARTIAL CURRENT IN
the $+\hat{n}$ direction

J_- = PARTIAL CURRENT IN
the $-\hat{n}$ direction

NOTE

J_+ AND J_- CANNOT BE DEFINED
WITHOUT SPECIFYING THE
PARTICULAR SURFACE (i.e., \hat{n})

J_+ , J_- ARE MEANINGLESS w/o \hat{n}



$$J_+ A = 5$$

$$J_- A = 3$$

$$\underline{J} \cdot \hat{n} A = (J_+ - J_-) A$$

$$= 5 - 3 = 2$$

- Assume we know J_+ and J_- for the above surface

- By definition of $\underline{J} \cdot \hat{n}$,

$$\underline{J} \cdot \hat{n} = \overset{\text{left-to-right}}{J_+} - \overset{\text{right-to-left}}{J_-}$$

Net \uparrow

Reasonable Assumption:

$$\phi \propto J_+ + J_-$$

$$\phi = C (J_+ + J_-)$$

↑ CONSTANT

$$\underline{J} \cdot \hat{m} = J_+ - J_-$$

CAN WE CALCULATE C?

Remember, ϕ is the total rate at which path length is traversed. Therefore, seems reasonable to add the partial currents (which are each positive).

- IN AN ISOTROPIC FLUX
(WHERE AN EQUAL NUMBER
OF NEUTRONS IS TRAVELLING
IN EACH DIRECTION)
ONE CAN SHOW

$$J_+ = J_- = \frac{nv}{4} = \frac{\phi}{4}$$

(NOW IT DOESN'T MATTER WHAT
THE ORIENTATION OF \hat{m} IS - CAN
YOU SEE WHY?)

∴ for an isotropic flux,

$$\phi = 4J_+ = 4J_-$$

$$\phi = \frac{2(J_+ + J_-)}{1} = C$$

AND if we ASSUME the SAME
CONSTANT C for GENERAL
CONFIGURATIONS of NEUTRONS,

$$\phi = 2(J_+ + J_-)$$

Also $\underline{J} \cdot \hat{m} = J_+ - J_-$

Solve for J_+ , J_-

$$J_+ = \frac{\phi}{4} + \frac{1}{2} \underline{J} \cdot \hat{m}$$

$$J_- = \frac{\phi}{4} - \frac{1}{2} \underline{J} \cdot \hat{m}$$

NEUTRON
PARTIAL
CURRENTS

J_{\pm} = NEUTRON PARTIAL CURRENTS

(VALID for systems NEAR-

isotropic i.e.g., valid

for diffusion theory)

This derivation is a little artificial -
it should really be derived using the quantity
known as the angular flux, which appears in the
transport equation. But this is beyond the scope
of this text.

VACUUM BOUNDARY CONDITION (revisited)

- Physical condition - NO NEUTRONS ENTERING V FROM THE VACUUM

- Pose as follows:

- Set the INWARD-directed PARTIAL CURRENT equal to zero

- Total number of neutrons entering V will be zero

Now we have a physical quantity that corresponds to our boundary condition.

Convention: \hat{M}_s UNIT OUTWARD NORMAL
TO S AT \underline{r}_s

$$J_+(\underline{r}_s) = \frac{\phi(\underline{r}_s)}{4} + \frac{1}{2} \underline{J}(\underline{r}_s) \cdot \hat{M}_s$$

$$J_-(\underline{r}_s) = \frac{\phi(\underline{r}_s)}{4} - \frac{1}{2} \underline{J}(\underline{r}_s) \cdot \hat{M}_s$$

$$J_-(\underline{r}_s) = 0 \text{ for } \underline{r}_s \in S'$$

diffusion theory:

$$\underline{J}(\underline{r}_s) = -D(\underline{r}_s) \nabla \phi(\underline{r}_s) \Big|_{\underline{r} = \underline{r}_s}$$

Then the VACUUM boundary condition becomes:

$$\boxed{\frac{\phi(\underline{r}_s)}{4} - \frac{1}{2} D(\underline{r}_s) \nabla \phi \cdot \hat{m}_s = 0} \quad \begin{array}{l} J_n = 0 \\ \text{ON } S \end{array}$$

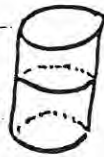
$\underline{r} = \underline{r}_s \quad \text{for } \underline{r}_s \in S$

in practice: $\phi(\tilde{\underline{r}}_s) = 0$ approx. b.c.

We will discuss $\phi(\tilde{\underline{r}}_s) = 0$ later.

2. Reflecting boundary condition

- Generally employed to account for symmetry
- "MIRROR IMAGE"
- Reduce size of problem domain by taking advantage of problem symmetry

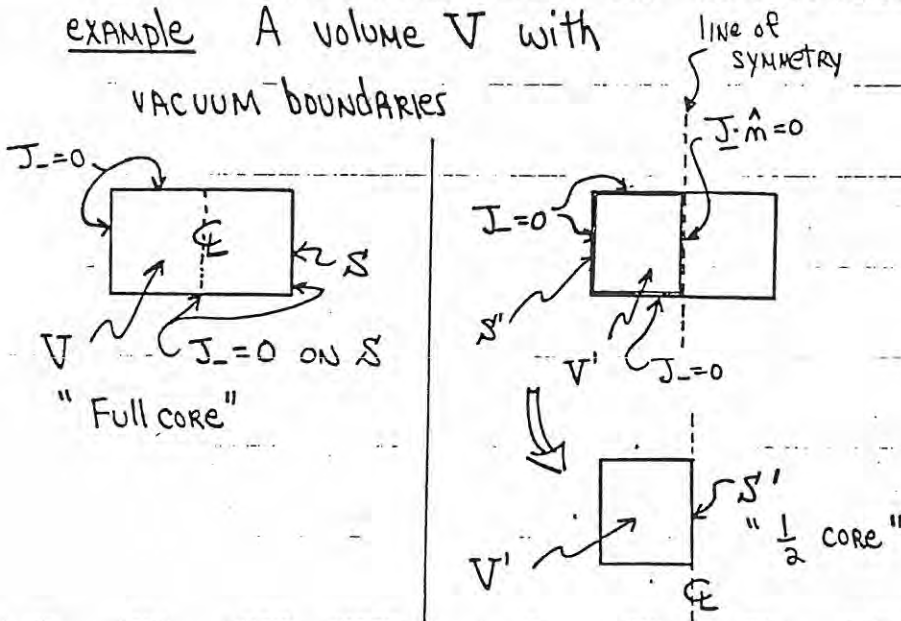


The neutrons do not actually reflect - the boundary condition makes the solution appear as such.

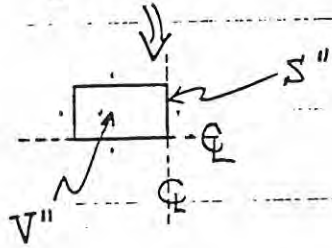
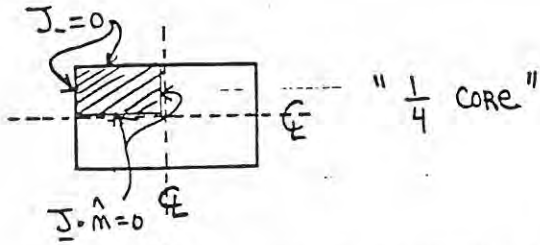
- Symmetry boundary
 - ⇒ identical configuration on either side
 - ⇒ No preference for neutron flow across the boundary
 - ⇒ $\underline{J} \cdot \hat{m} = 0$ ($J_+ = J_-$)

(if $J_+ \neq J_-$, then boundary could not be a symmetry boundary)

example A volume V with VACUUM BOUNDARIES



Symmetry has reduced the "full-core" problem to a "half-core" problem, which is at least half as expensive to solve (on a computer).



problem domain (the region over which the diffusion equation is solved) is reduced by a factor of 4 by using symmetry

Reflecting?

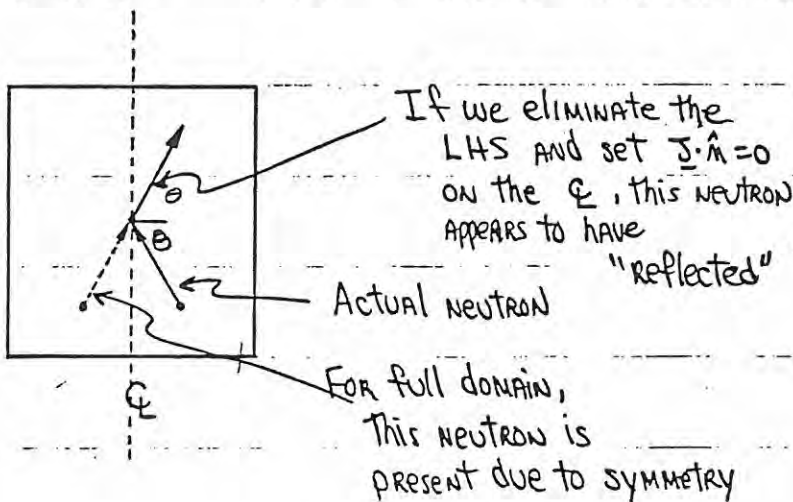


Illustration of why we call a symmetry boundary a reflecting boundary.

The 1-D Diffusion Equation

general-

$$-\nabla \cdot D(\underline{r}) \nabla \phi(\underline{r}) + \Sigma_a(\underline{r}) \phi(\underline{r}) = S(\underline{r})$$

$$\underline{r} \in V$$

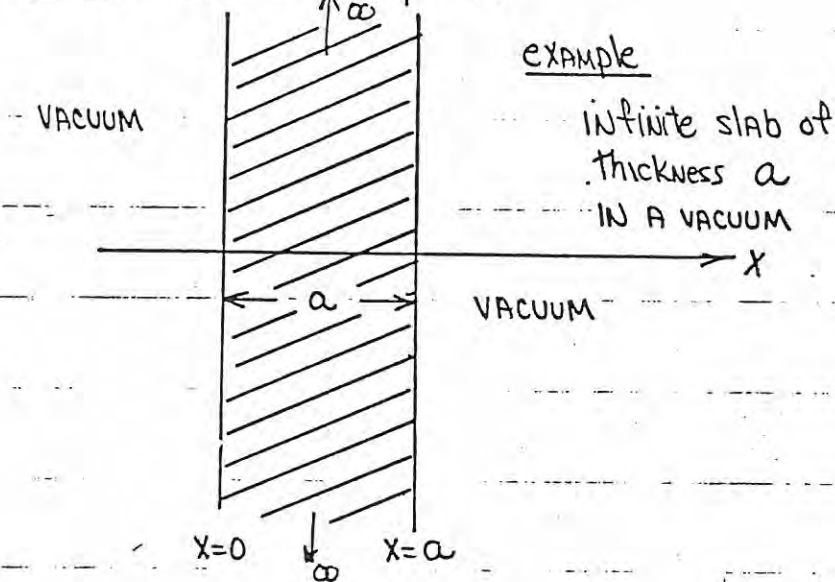
with b.c.

$$\underline{J} \cdot \underline{n}_s = 0 \text{ for } \underline{r}_s \in S \text{ (VACUUM b.c.)}$$

$$\text{OR } -\underline{J} \cdot \underline{\hat{m}}_s = 0 \text{ for } \underline{r}_s \in S \text{ (REFLECTING b.c.)}$$

$$\text{(OR COMBINATION, } S = S_V + S_R)$$

1-D (infinite in y & z)



LECTURE 15

SOLUTION OF THE NEUTRON DIFFUSION EQUATION

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 157-160.

Lamarsh, pp. 163-170.

EXERCISES:

15.1 Duderstadt & Hamilton, problem #5-8

15.2 Duderstadt & Hamilton, problem #5-9

The 1-D Diffusion Equation

general-

$$-\nabla \cdot D(\underline{x}) \nabla \phi(\underline{x}) + \Sigma_a(\underline{x}) \phi(\underline{x}) = S(\underline{x})$$

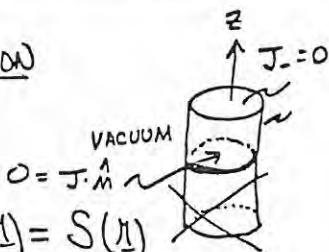
$$\underline{x} \in V$$

with b.c.

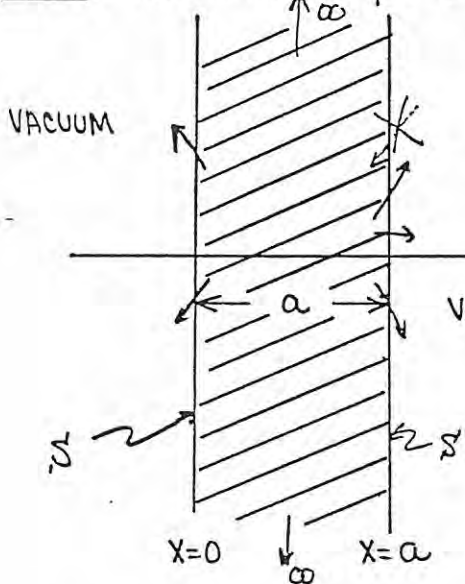
$$J \cdot \hat{n}_s = 0 \text{ for } \underline{x}_s \in S \text{ (VACUUM b.c.)}$$

$$\text{OR } \underline{J} \cdot \hat{n}_s = 0 \text{ for } \underline{x}_s \in S \text{ (REFLECTING b.c.)}$$

$$\text{(OR COMBINATION, } S = S_V + S_R)$$



1-D (infinite in y & z)



example

infinite slab of thickness a IN A VACUUM

$$J_n = 0 \text{ ON } S$$

Infinite up and down and in and out of the paper.

$$\Sigma_a(\underline{r}) = \Sigma_a(x)$$

$$D(\underline{r}) = D(x)$$

$$\Phi(\underline{r}) = \Phi(x)$$

$$S(\underline{r}) = S(x)$$

$S(x) dV = \# \text{ neutrons produced in } dV$

$$dV = A dx$$

$$-\nabla \cdot D(x) \nabla \Phi(x) = - \left[\frac{\partial}{\partial x} D(x) \frac{\partial \Phi}{\partial x} + \frac{\partial}{\partial y} D(x) \frac{\partial \Phi}{\partial y} + \frac{\partial}{\partial z} D(x) \frac{\partial \Phi}{\partial z} \right]$$

$$= - \frac{\partial}{\partial x} D(x) \frac{\partial \Phi}{\partial x}$$

The cross sections are functions only of x .

$$- \frac{d}{dx} D(x) \frac{d\Phi}{dx} + \Sigma_a(x) \Phi(x) = S(x)$$

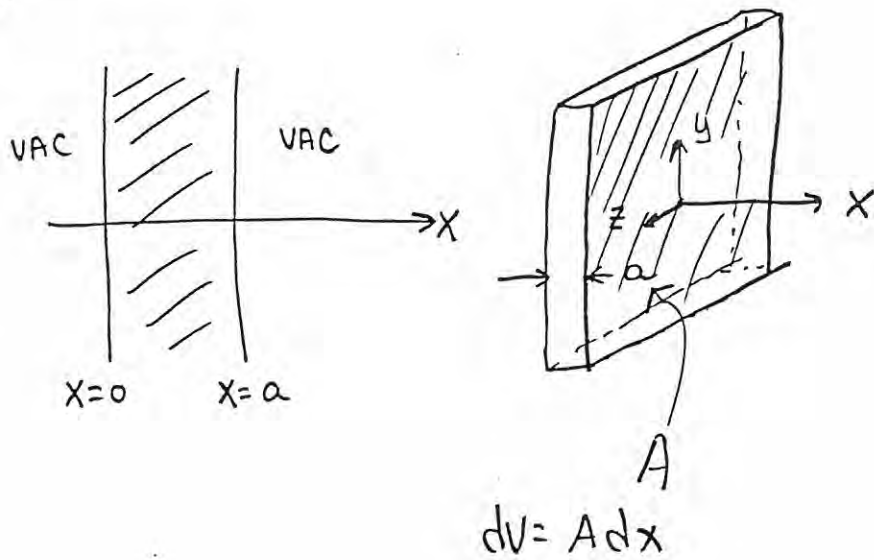
$$0 \leq x \leq a$$

$\Phi(x) = \text{SCALAR flux (SAME AS } \Phi(\underline{r}))$

$$\underbrace{\Sigma_a(x) \Phi(x)}_{dV} \cdot A dx = \# \text{ REACTIONS/SECOND}$$

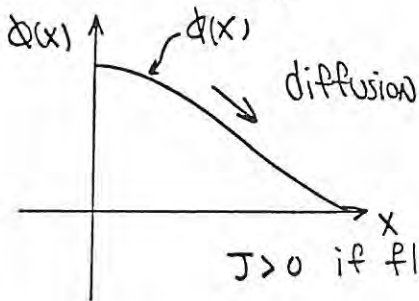
IN THE VOLUME
 $dV = A dx$, where
 A IS THE AREA OF
 $dV \perp$ TO \hat{e}_x

A is simply the area of a representative portion of the slab.



Net current $J(x)$

$$J(x) = -D(x) \frac{d\phi}{dx}$$



$$\begin{aligned} \vec{J} &= -D \nabla \phi = -D \frac{\partial \phi}{\partial x} \hat{e}_x \\ &= -D(x) \left[\frac{\partial \phi}{\partial x} \hat{e}_x + \frac{\partial \phi}{\partial y} \hat{e}_y + \frac{\partial \phi}{\partial z} \hat{e}_z \right] \end{aligned}$$

(from region of high neutron "concentration" to low)

$J > 0$ if flow is in $+x$ direction

$J(x) \cdot A =$ net number of neutrons crossing the area A (\perp to \hat{e}_x) per second

PARTIAL CURRENTS

$J_{\oplus}(x) \equiv$ NUMBER OF NEUTRONS
PER SECOND CROSSING
A UNIT AREA \perp TO
THE X-AXIS, GOING
IN THE $\oplus X$ DIRECTION

$J_{-}(x) \equiv$ SAME, BUT TRAVELLING IN
THE $-X$ DIRECTION

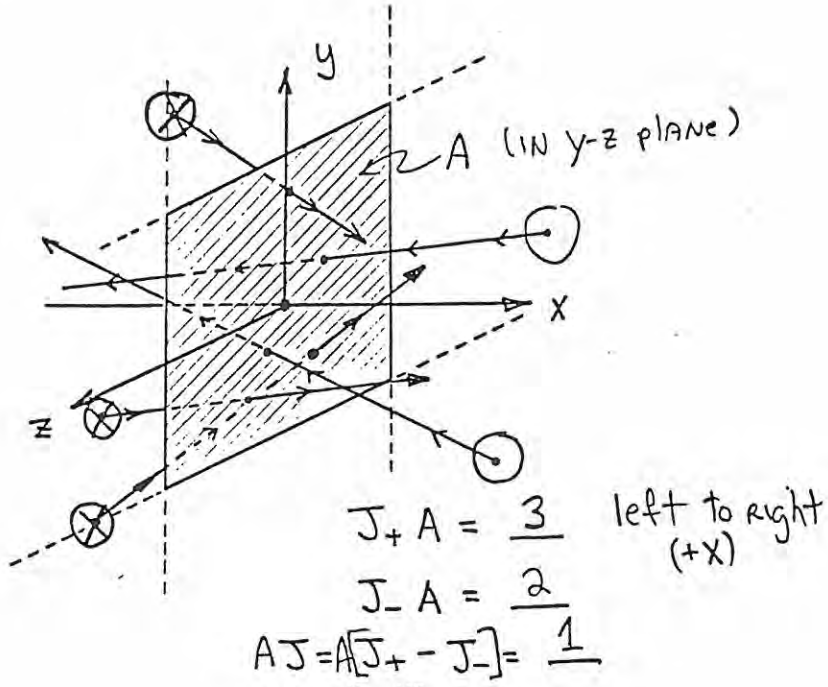
$$J_{+}(x) = \frac{1}{4} \phi(x) + \frac{1}{2} J(x) \quad \text{or} \quad J_{+}(x) = \frac{\phi}{4} + \frac{J \cdot x}{2}$$

$$J_{-}(x) = \frac{1}{4} \phi(x) - \frac{1}{2} J(x)$$

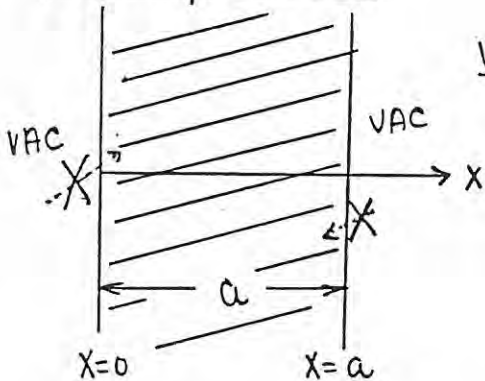
Since $J(x) = -D(x) \frac{d\phi}{dx}$

$$\text{Then } J_{+}(x) = \frac{1}{4} \phi(x) - \frac{1}{2} D(x) \frac{d\phi}{dx}$$

$$J_{-}(x) = \frac{1}{4} \phi(x) + \frac{1}{2} D(x) \frac{d\phi}{dx}$$



BOUNDARY CONDITIONS



INWARD PARTIAL CURRENT AT $x=0$

VACUUM b.c.

$$\left. \begin{aligned} J_+(0) &= 0 \\ J_-(a) &= 0 \end{aligned} \right\}$$

slight difference compared with general case (due to definition of J_{\pm} for 1-D)

$$-\frac{d}{dx} D(x) \frac{d\phi}{dx} + \Sigma_a(x) \phi(x) = S(x) \quad (0 \leq x \leq a)$$

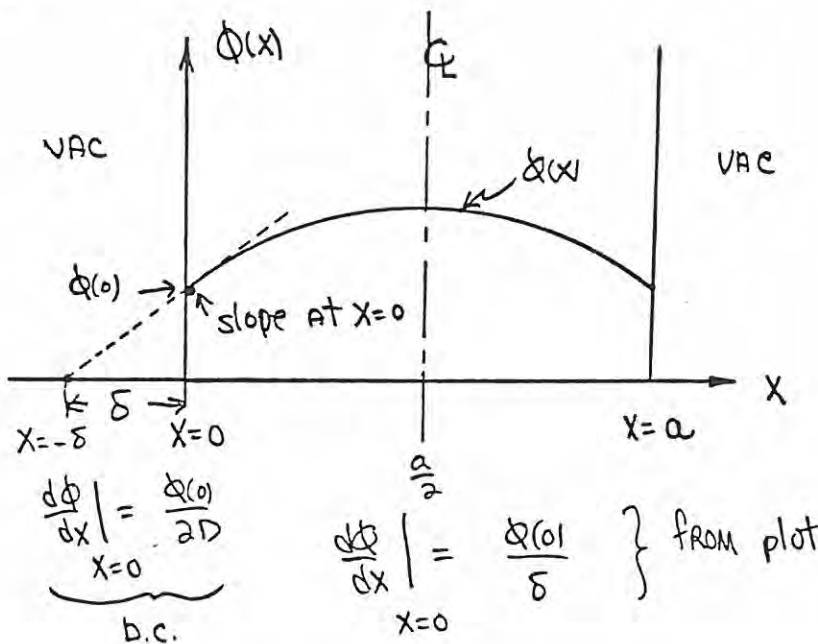
$$J_+(0) = 0$$

$$\frac{1}{4} \phi(0) - \frac{1}{2} D \left. \frac{d\phi}{dx} \right|_{x=0} = 0$$

$$\left. \frac{d\phi}{dx} \right|_{x=0} = \frac{\phi(0)}{2D}$$

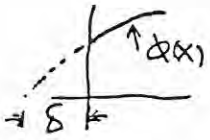
relation between

$$\left. \frac{d\phi}{dx} \right|_{x=0} \neq \phi(0)$$



What if we were to extrapolate the solution along a line with the same slope as at the boundary? It would go to zero at some distance δ .

CAUTION - $\Phi(x)$ NOT ACTUALLY = 0
AT $x = -\delta$



- ONLY SOLVING FOR $\Phi(x)$ INSIDE THE REGION $0 \leq x \leq a$
- ^{LINEAR} EXTRAPOLATION OF THE INTERIOR SOLUTION RESULTS IN $\Phi = 0$ AT $x = -\delta$ (MATHEMATICALLY)

AN APPROXIMATE BOUNDARY CONDITION (the "extrapolated" end point)

- Replace the ACTUAL VACUUM BOUNDARY CONDITION AT $x=0$, $J_+(0) = 0$

$$\frac{1}{4} \Phi(0) - \frac{1}{2} D \left. \frac{d\Phi}{dx} \right|_{x=0} = 0$$

with a zero flux condition
at the "extrapolated boundary"
 $\Phi(-\delta) = 0$

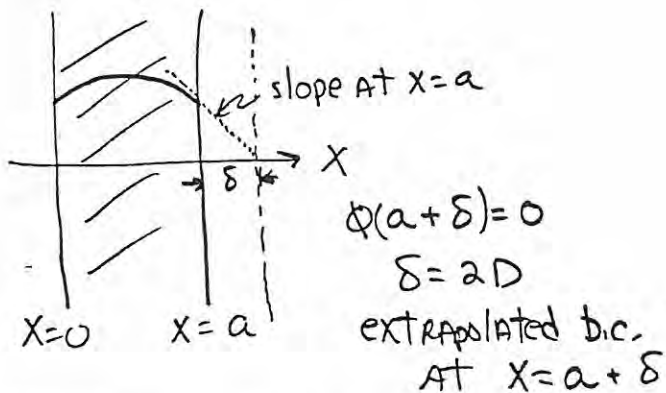
Mathematically

• Replacing the physical boundary condition of no entering neutrons

$$J_+(0) = \frac{1}{4} \phi(0) - \frac{1}{2} D \left. \frac{d\phi}{dx} \right|_{x=0} = 0$$

with the "extrapolated" boundary condition

$$\phi(-\delta) = 0$$



(replaces $J_-(a) = 0$, or $\frac{1}{4} \phi(a) + \frac{1}{2} D \left. \frac{d\phi}{dx} \right|_{x=a} = 0$)

- The problem domain is extended to $x = -\delta$ and the diffusion equation is solved over the extended domain: $-\delta \leq x \leq a + \delta$ ($0 \leq x \leq a$)
- The solution in the region $-\delta \leq x \leq 0$ and $a \leq x \leq a + \delta$ is meaningless. One only uses the solution in $0 \leq x \leq a$. (interior solution)

This is an approximate boundary condition.

NOTATION: $\tilde{a} = a + \delta$ $\delta = 2D$

extrapolated boundary physical boundary

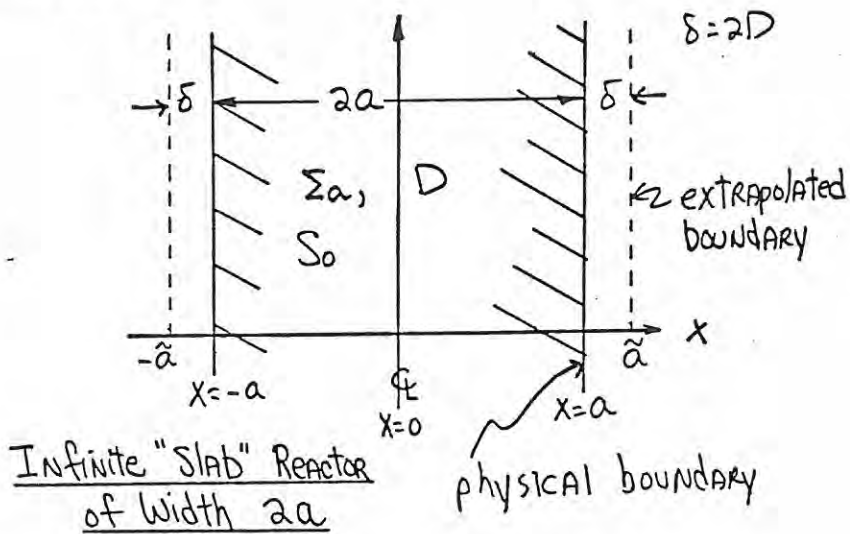
$\phi(\tilde{a}) = 0$ extrapolated boundary condition } APPROX. FOR THE VACUUM B.C.

Solutions To the 1-D
Neutron Diffusion Equation
 (1-speed ; steady-state)

- (1) Slab reactor of width $2a$ ($-a \leq x \leq a$)
 with $S(x) = S_0$ AND $\phi(\tilde{a}) = 0$
extrapolated boundary conditions (AT $x = \pm \tilde{a}$)
- (2) Same except reflecting boundary
 condition AT $x=0$ ($0 \leq x \leq a$)
- (3) Same except VACUUM boundary
 condition AT $x=a$ $J_-(a) = 0$

15-20

Problem (1)



equation

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = S_0 \quad (i)$$

$$-\tilde{a} \leq x \leq \tilde{a}$$

boundary conditions

$$\phi(-\tilde{a}) = 0 \quad (ii)$$

$$\phi(\tilde{a}) = 0 \quad (iii)$$

steps1. Divide eq.(i) by $-D$,

$$\frac{d^2\phi}{dx^2} - \frac{\Sigma_a}{D} \phi(x) = -\frac{S_0}{D} \quad (iv)$$

2. Define the "diffusion

length" L ,

$$L^2 = D/\Sigma_a$$

$$-\tilde{a} \leq x \leq \tilde{a}$$

AND express (iv) AS

$$\boxed{\frac{d^2\phi}{dx^2} - \frac{1}{L^2} \phi(x) = -\frac{S_0}{D}} \quad (v)$$

3. The general solution to (v) subject to the boundary conditions (ii) and (iii) may be obtained from the homogeneous solution and a particular solution

$$\Phi(x) = \Phi_h(x) + \Phi_p(x)$$

4. homogeneous solution $\Phi_h(x)$

$$\frac{d^2\Phi_h}{dx^2} - \frac{1}{L^2}\Phi_h(x) = 0 \quad - \text{hom eq}$$

$$\Phi_h(x) = A e^{x/L} + B e^{-x/L}$$

5. PARTICULAR SOLUTION $\Phi_p(x)$

$$\Phi_p(x) = S_0/\Sigma a \quad (\text{try it!})$$

Then

$$\Phi(x) = A e^{x/L} + B e^{-x/L} + \frac{S_0}{\Sigma a}$$

6. Apply boundary conditions

$$\Phi(-\tilde{a}) = Ae^{-\tilde{a}/L} + Be^{+\tilde{a}/L} + \frac{S_0}{\Sigma_a} = 0$$

$$\Phi(\tilde{a}) = Ae^{+\tilde{a}/L} + Be^{-\tilde{a}/L} + \frac{S_0}{\Sigma_a} = 0$$

Subtract,

$$A(e^{-\tilde{a}/L} - e^{+\tilde{a}/L}) = +B(e^{+\tilde{a}/L} - e^{-\tilde{a}/L})$$

$$\text{OR } A = B$$

$$\text{Then } A = \frac{1}{e^{+\tilde{a}/L} + e^{-\tilde{a}/L}} \left(-\frac{S_0}{\Sigma_a} \right)$$

7. Since $\cosh\left(\frac{x}{L}\right) = \frac{1}{2}(e^{x/L} + e^{-x/L})$

we obtain

$$\Phi(x) = \frac{S_0}{\Sigma_a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

$$x = \pm \tilde{a} : \Phi = 0$$

SOLUTION OF THE NEUTRON DIFFUSION EQUATION (cont.)

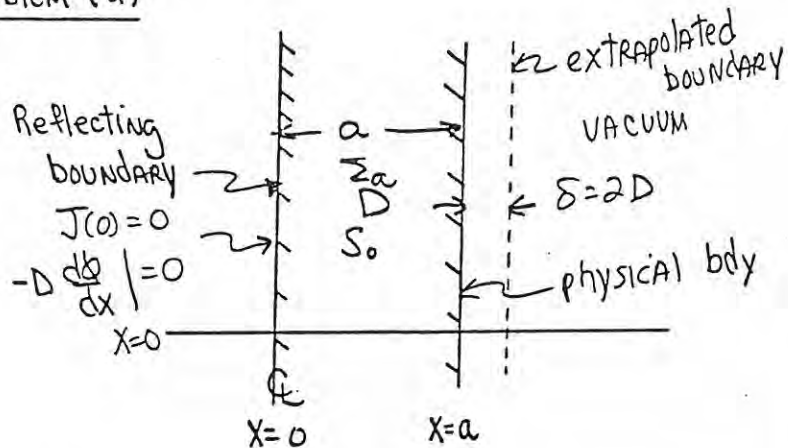
READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 160-162.

Lamarsh, pp. 170-171.

EXERCISES:

16.1. Lamarsh, problem #5.6

Problem (2)

Now compare the previous problem with the current one which takes advantage of symmetry to eliminate half of the problem domain.

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = S_0$$

$$0 \leq x \leq \tilde{a}$$

b.c.

$$\phi(\tilde{a}) = 0 \quad (\text{extrapolated})$$

$$-D \left. \frac{d\phi}{dx} \right|_{x=0} = 0 \quad (\text{reflecting, zero current, symmetry})$$

Now we have a reflecting boundary condition at $x = 0$.

GENERAL solution

$$\phi(x) = Ae^{x/L} + Be^{-x/L}$$

+ S_0/Σ_a

$$\phi(\tilde{a}) = Ae^{\tilde{a}/L} + Be^{-\tilde{a}/L} + \frac{S_0}{\Sigma_a} = 0$$

$$\left. \frac{d\phi}{dx} \right|_{x=0} = \left[\frac{1}{L} Ae^{x/L} - \frac{1}{L} Be^{-x/L} \right]_{x=0}$$

$$= \frac{1}{L} (A - B) = 0$$

$$\boxed{A = B}$$

$$\phi(x) = \frac{S_0}{\Sigma_a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

identical to problem (1) solution

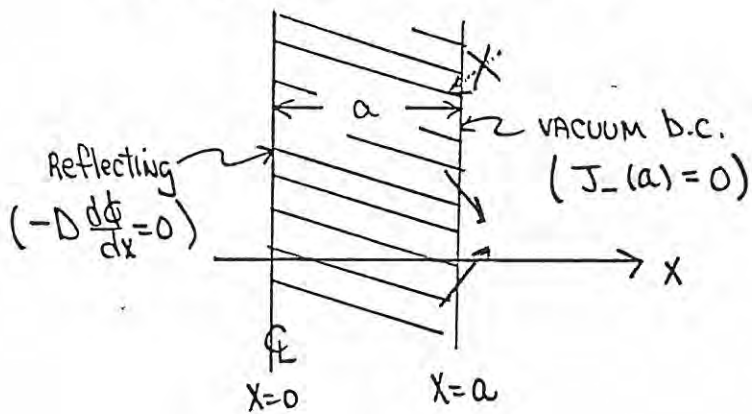
Notes: • ANALYSIS (ALGEBRA)

simplified slightly
with reflecting b.c.

- complicated reactors: exploiting SYMMETRY \Rightarrow fraction of the work

Saves work because computers must be used to solve complicated geometries. Eliminating half of the problem domain will result in at least half and probably less than half the computer effort.

Prob. (3) Slab reactor with VACUUM
 b.c. AT $x = a$ (NOT
 extrapolated b.c. AT $x = \tilde{a}$)



Now we compare the earlier solution obtained with the approximate boundary condition with the solution for vacuum boundary condition.

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = S_0$$

$$0 \leq x \leq a$$

(NOT \tilde{a})

b.c.

$$x=0: -D \left. \frac{d\phi}{dx} \right|_{x=0} = 0 \quad \text{SYMMETRY}$$

$$x=a: J_-(a) = \frac{\phi(a)}{4} + \frac{D}{2} \left. \frac{d\phi}{dx} \right|_{x=a} = 0$$

Sufficient to find
 A AND B

Solution

$$\Phi(x) = Ae^{x/L} + Be^{-x/L} + \frac{S_0}{\Sigma a}$$

The reflecting b.c. At
 $x=0 \Rightarrow \underline{A=B}$

$$\therefore \Phi(x) = C \cosh\left(\frac{x}{L}\right) + \frac{S_0}{\Sigma a}$$

$$\frac{d\Phi}{dx} = \frac{1}{L} C \sinh\left(\frac{x}{L}\right) \quad (C=2A)$$

Substitute into $J_-(a)=0$:

$$\frac{1}{4} \left[\overbrace{C \cosh\left(\frac{a}{L}\right)}^{\Phi(a)} + \frac{S_0}{\Sigma a} \right] \quad J_-(a) = \frac{\Phi(a)}{4} + \frac{D}{2} \left. \frac{d\Phi}{dx} \right|_{x=a}$$

$$+ \left(\frac{D}{2}\right) \left[\frac{1}{L} C \sinh\left(\frac{a}{L}\right) \right] = 0$$

$$\therefore C = \frac{-S_0/\Sigma a}{\cosh\left(\frac{a}{L}\right) + 2 \frac{D}{L} \sinh\left(\frac{a}{L}\right)} \quad \left. \frac{d\Phi}{dx} \right|_{x=a}$$

$$\therefore \Phi(x) = \frac{S_0}{\Sigma a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{a}{L}\right) + 2 \frac{D}{L} \sinh\left(\frac{a}{L}\right)} \right]$$

SUMMARY

- 1.
- EXTRAPOLATED
- boundary condition AT
- $x = \tilde{a}$

$$\tilde{\Phi}(x) = \frac{S_0}{\Sigma a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

- 2.
- VACUUM
- boundary condition AT
- $x = a$

$$\Phi(x) = \frac{S_0}{\Sigma a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{a}{L}\right) + \frac{2D}{L} \sinh\left(\frac{a}{L}\right)} \right]$$

16-10

$\tilde{\Phi}(x) \approx \Phi(x)$? (within the interior)

$$\cosh\left(\frac{\tilde{a}}{L}\right) \approx \cosh\left(\frac{a}{L}\right) + 2 \frac{D}{L} \sinh\left(\frac{a}{L}\right) \quad ?$$

$$\tilde{a} \approx a, \text{ if } a + 2D \approx a$$

$$1 + \frac{2D}{a} \approx 1$$

$$\frac{D}{a} \ll 1$$

$$\frac{a}{L} \gg 1 : \cosh\left(\frac{a}{L}\right) \approx \sinh\left(\frac{a}{L}\right)$$

$$\text{Expand } \cosh\left(\frac{\tilde{a}}{L}\right) = \cosh\left(\frac{a}{L}\right) \cosh\left(\frac{2D}{L}\right) + \sinh\left(\frac{a}{L}\right) \sinh\left(\frac{2D}{L}\right)$$

$$= \cosh\left(\frac{a}{L}\right) \left[1 + \frac{1}{2} \left(\frac{2D}{L}\right)^2 + \mathcal{O}\left(\frac{2D}{L}\right)^4 \right]$$

$$+ \sinh\left(\frac{a}{L}\right) \left[\frac{2D}{L} + \frac{1}{6} \left(\frac{2D}{L}\right)^3 - \mathcal{O}\left(\frac{2D}{L}\right)^5 \right]$$

$$= \cosh\left(\frac{a}{L}\right) + \left[\sinh\left(\frac{a}{L}\right) \right] \left(\frac{2D}{L}\right) \quad \checkmark$$

$$+ \left[\cosh\left(\frac{a}{L}\right) \right] \frac{1}{2} \left(\frac{2D}{L}\right)^2 + \sinh\left(\frac{a}{L}\right) \left[\frac{2D}{L}\right]$$

For both of these $\rightarrow 0$, need

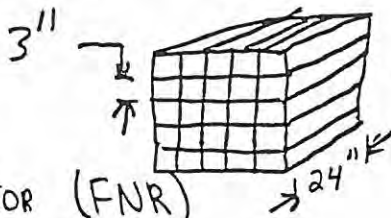
$$\left(\frac{a}{L}\right) \ll 1$$

$$\left(\frac{D}{L}\right) \ll 1$$

$$\begin{aligned} \text{RHS} &\approx \cosh\left(\frac{a}{L}\right) \left[1 + 2\frac{D}{L}\right] \\ &\approx \cosh\left(\frac{\tilde{a}}{L}\right) \approx \cosh\left(\frac{a}{L}\right) \quad ? \end{aligned}$$

$$\left. \begin{array}{l} \frac{D}{L} \ll 1 \\ \frac{a}{D} \gg 1 \end{array} \right\} \text{conditions for } \tilde{\phi} \approx \phi$$

Numerical Examples

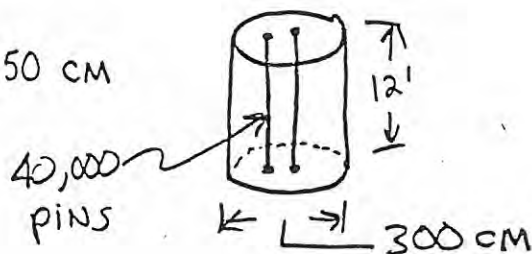


- Ford Nuclear Reactor (FNR)
(University of Michigan)

$$\tilde{a} \approx 20 \text{ cm}$$

- Commercial Pressurized Water Reactor (PWR)

$$\tilde{a} \approx 150 \text{ cm}$$



Cross sections (1 group)

$$D \approx 1.2 \text{ cm} \quad \left. \begin{array}{l} \\ \Sigma_a \approx .02 \text{ cm}^{-1} \end{array} \right\} \text{SAME FOR FNR \& PWR}$$

$$L = \sqrt{D/\Sigma_a} \approx 7.75 \text{ cm}$$

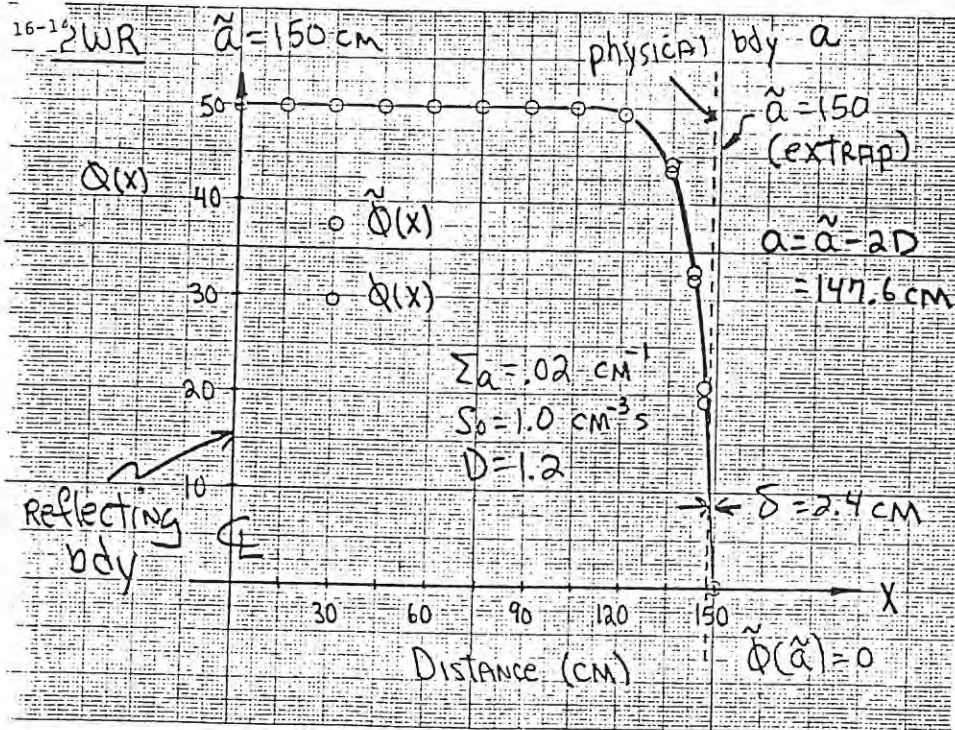
Volometric source

$$S_0 = 1.0 \text{ NEUTRONS/cm}^3 \cdot \text{sec}$$

$$\tilde{a} = 20 \text{ cm} \\ 150 \text{ cm}$$

$$\tilde{\Phi}(x) = 50 \left[1 - \frac{\cosh(x/7.75)}{\cosh(\tilde{a}/7.75)} \right]$$

$$\Phi(x) = 50 \left[1 - \frac{\cosh(x/7.75)}{\cosh\left(\frac{a}{7.75}\right) + 0.31 \sinh\left(\frac{a}{7.75}\right)} \right]$$



16-17 150 cm

$\Phi(x)$ solved for $0 \leq x \leq a$

$\tilde{\Phi}(x)$ " " $0 \leq x \leq \tilde{a}$

"Throw" away the $\tilde{\Phi}(x)$

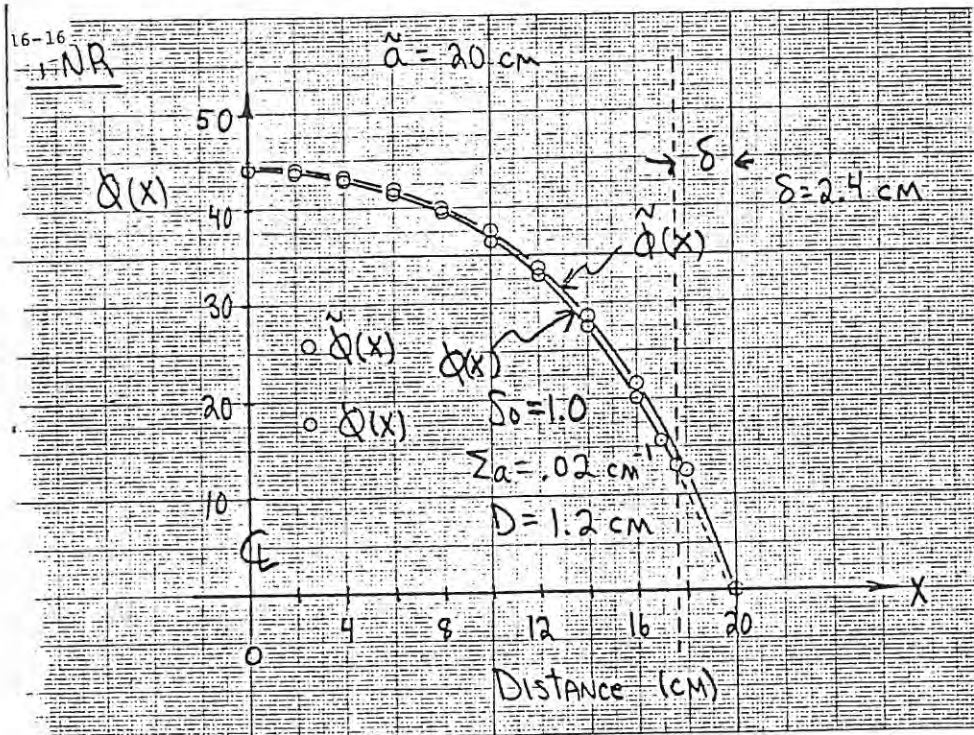
in $a \leq x \leq \tilde{a}$

$\Phi(x) \approx \tilde{\Phi}(x)$ in $0 \leq x \leq a$

$$\frac{a}{L} = \frac{147.6}{7.75} \approx 19 \Rightarrow \frac{a}{L} \gg 1$$

$$\frac{D}{L} = \frac{1.2}{7.75} = .155 \ll 1$$

} expect $\tilde{\Phi}(x) \approx \Phi(x)$



$$\frac{a}{L} = \frac{17.6}{7.75} \approx 2 \quad \frac{a}{L} \not\ll 1$$

$$\frac{D}{L} = .155 \quad \frac{D}{L} \ll 1 \quad \checkmark$$

Do not expect excellent agreement with FUR

$$\text{AT } X=16, \quad \frac{\tilde{Q}(16)}{Q(16)} = \frac{21.57}{20.16} = 1.07 \quad (7\% \text{ ERROR})$$

$$X=0, \quad \frac{\tilde{Q}(0)}{Q(0)} = \frac{44.28}{43.99} = 1.007 \quad (.7\% \text{ ERROR})$$

Comments on the Extrapolated Boundary

1. Excellent approximation for "large" reactors $\frac{a}{L} \gg 1$ width \gg "diffusion length"
2. Questionable for "small" reactors (but then - so is diffusion theory)
3. $\tilde{Q}(X)$ (with extrapolated b.c.) should only be used inside the reactor, $X \leq a$ (not \tilde{a})

4. The extrapolation distance

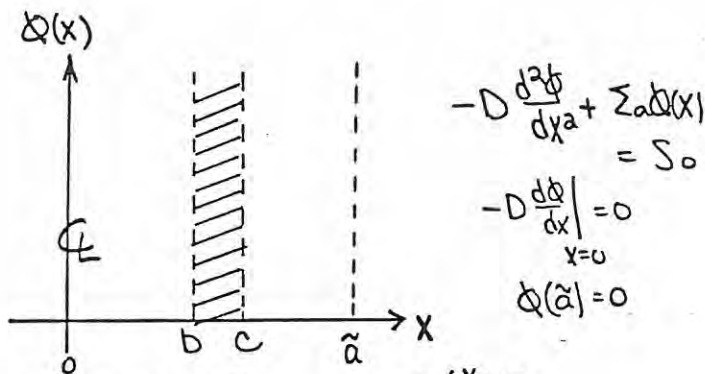
$$\delta = 2D \quad (\text{diffusion theory})$$

is often replaced by a

"TRANSPORT-CORRECTED" $\tilde{a} = a + 2.13D$
extrapolation distance

$$\boxed{\delta = 2.13D} \quad \text{FROM TRANSPORT THEORY}$$

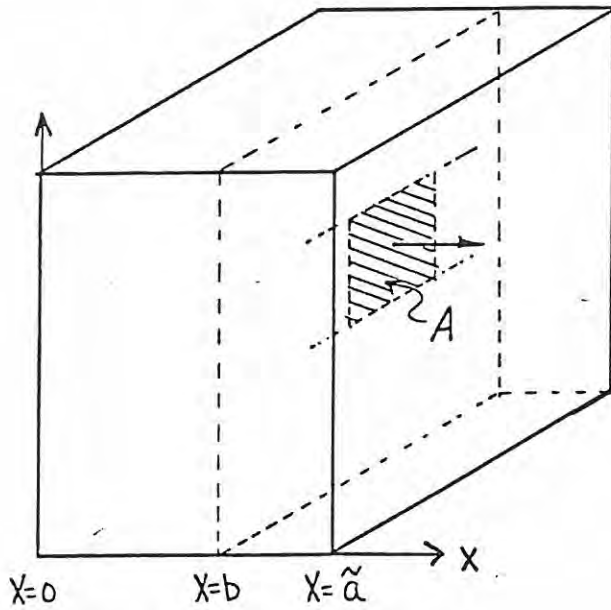
5. Remember- the extrapolated boundary is a fictitious boundary



$$\phi(x) = \frac{S_0}{\Sigma_a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

$$J(x) = -D \frac{d\phi}{dx} = \left(\frac{D}{L}\right) \frac{S_0}{\Sigma_a} \left[\frac{\sinh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

Using the calculated flux $\phi(x)$ and current $J(x)$, let us find some reaction rates in the region $b \leq x \leq c$.



In the region $b \leq x \leq c$,

- (1) What is the Absorption rate,
 ASSUMING A CROSS SECTIONAL
 AREA A ?

$$\text{Absorption rate} = \int_V \Sigma_a(x) \phi(x) dV$$

" "
 $A dx$

$$R_A = A \int_b^c \Sigma_a \phi(x) dx$$

$$R_P = R_A + Q$$

LECTURE 17

POINT SOURCE AND PLANE SOURCE PROBLEMS

READING ASSIGNMENT:

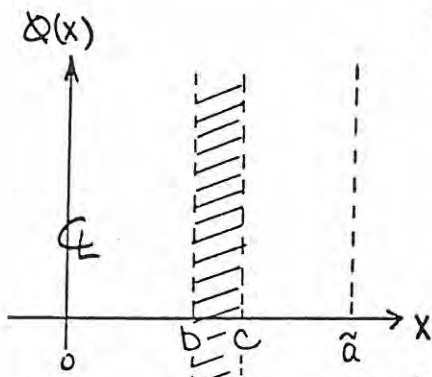
Duderstadt and Hamilton, pp. 162-166.

EXERCISES:

- 17.1. Duderstadt and Hamilton, problem #5-7
- 17.2. Duderstadt and Hamilton, problem #5-10

17-1

LECTURE 17



$$-D \frac{d^2 \phi}{dx^2} + \sum_a \phi(x) = S_0$$

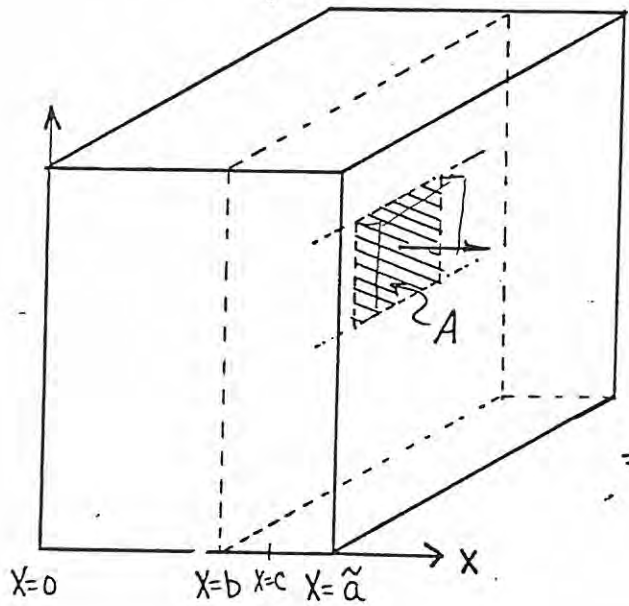
$$-D \frac{d\phi}{dx} \Big|_{x=0} = 0$$

$$\phi(\tilde{a}) = 0$$

$$\phi(x) = \frac{S_0}{\sum_a} \left[1 - \frac{\cosh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

$$J(x) = -D \frac{d\phi}{dx} = \left(\frac{D}{L}\right) \frac{S_0}{\sum_a} \left[\frac{\sinh\left(\frac{x}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

17-2



Volume
of the
Region
= (c-b) A

In the region $b \leq x \leq c$,

(1) What is the Absorption rate,
ASSUMING A CROSS SECTIONAL
AREA A ?

$$\text{Absorption rate} = \int_V \Sigma_a(x) \phi(x) dV$$

"
 $A dx$

$$R_A = A \int_b^c \Sigma_a \phi(x) dx$$

$$R_P = R_A + \dots \quad \text{verify explicitly}$$

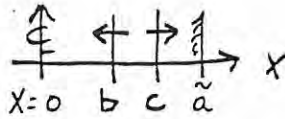
$$R_A = A \Sigma_a \int_b^c \left(\frac{S_0}{\Sigma_a} \right) \left[1 - \frac{\cosh(\frac{x}{L})}{\cosh(\frac{a}{L})} \right] dx$$

$$R_A = A S_0 (c-b) - \frac{A S_0 L}{\cosh(\frac{a}{L})} \left[\sinh(\frac{c}{L}) - \sinh(\frac{b}{L}) \right]$$

(a) What is the production rate?

$$R_P = A \int_b^c S_0 dx = A S_0 (c-b)$$

(3) What is the net leakage
out of the region
at $x=b$?



$$\begin{aligned} \chi_b &= -J(b) \cdot A \\ &= -\left(\frac{S_0}{\Sigma_a}\right) \left(\frac{D}{L}\right) \frac{\sinh\left(\frac{b}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \cdot A \end{aligned}$$

(4) What is the net leakage
out of the region at $x=c$?

$$\begin{aligned} \chi_c &= +J(c) \cdot A \\ &= \left(\frac{S_0}{\Sigma_a}\right) \left(\frac{D}{L}\right) \frac{\sinh\left(\frac{c}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \end{aligned}$$

In (3), note the net leakage out at $x=b$ is negative, indicating the net flow is actually in at $x=b$. On the other hand, the net leakage out at $x=c$ is positive, as it has to be.

SUMMARY

$$R_p = A S_0 w \Rightarrow w = c - b$$

$$R_A = A S_0 w - \frac{A S_0 L}{\cosh\left(\frac{\tilde{a}}{L}\right)} \left[\sinh\left(\frac{c}{L}\right) - \sinh\left(\frac{b}{L}\right) \right]$$

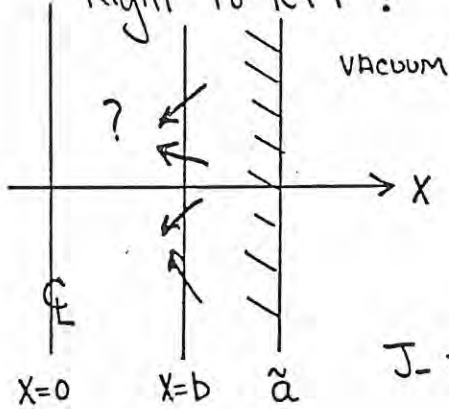
$$\chi_b = \left(\frac{S_0}{\Sigma_a}\right) \left(\frac{D}{L}\right) A \left[\frac{\sinh\left(\frac{b}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

$$\chi_c = +\left(\frac{S_0}{\Sigma_a}\right) \left(\frac{D}{L}\right) A \left[\frac{\sinh\left(\frac{c}{L}\right)}{\cosh\left(\frac{\tilde{a}}{L}\right)} \right]$$

Since $L^2 \equiv D/\Sigma_a$, $R_p = R_A + \chi_b + \chi_c$

Neutron balance!

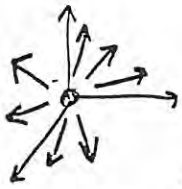
(5) How many neutrons per second cross the area A at $x=b$ from right to left?



$J_-(b) \cdot A = \text{total}$
 number crossing
 per second from
 right to left

$$J_- = \left(\frac{\phi(b)}{4} - \frac{J(b)}{2} \right)$$

Point Source in an
Infinite Homogeneous Medium



So neutrons per second are emitted at the origin ($r=0$) (uniformly in all directions)

$$-\nabla \cdot D(r) \nabla \phi(r) + \Sigma_a(r) \phi(r) = S(r) + \text{boundary conditions (?)}$$

Let us now try spherical symmetry.

$$D(\underline{r}) = D$$

$$\Sigma_a(\underline{r}) = \Sigma_a$$

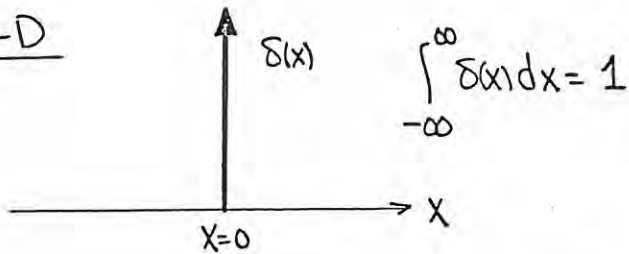
$$S(\underline{r}) = S_0 \delta(\underline{r}) \leftarrow \text{The point source emits } S_0 \text{ neutrons/second}$$

$$\delta(\underline{r}) d^3r = \# \text{ of neutrons emitted PER SECOND IN } d^3r \text{ ABOUT } \underline{r}$$

$$\iiint_{\text{All space}} S_0 \delta(\underline{r}) d^3r = S_0 \Rightarrow \iiint_{\text{All space}} \delta(\underline{r}) d^3r = 1$$

A point source is a mathematical artifice that is quite convenient and represents some physical situations nicely.

1-D



$$\delta(\underline{r}) = \delta(x) \cdot \delta(y) \cdot \delta(z)$$

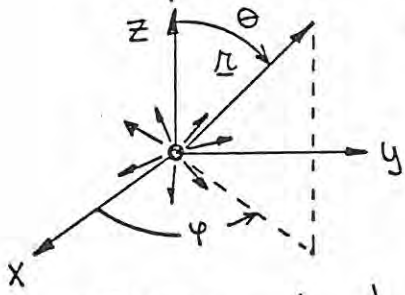
$$\iiint \delta(\underline{r}) d^3r = \int_{-\infty}^{\infty} \delta(x) dx \int_{-\infty}^{\infty} \delta(y) dy \int_{-\infty}^{\infty} \delta(z) dz$$

$\begin{matrix} \text{"} & \text{"} & \text{"} \\ 1 & 1 & 1 \end{matrix}$

$$\iiint S_0 \delta(\underline{r}) d^3r = S_0$$

The total source strength (# neutrons emitted/second) is S_0 .

- Solution $\Phi(\underline{r})$ CAN ONLY depend on r



$$\Phi(\underline{r}) = \Phi(r, \theta, \varphi)$$

symmetry

\Rightarrow

(spherical symmetry)

$$\nabla^2 \Phi(\underline{r}) = \frac{1}{r^2} \frac{d}{dr} r^2 \Phi(r)$$

$$-\nabla^2 \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d\Phi}{dr} + \Sigma_a \Phi(r) = S(r)$$

$$\text{where } S(r) = S_0 \delta(r)$$

note: $\delta(r) = 0, r \neq 0$

hence $\delta(r) = 0$ everywhere
except at the origin.

solution method: solve the homogeneous equation ($S(r) = 0$) and account for the point source with a boundary condition

Solve:

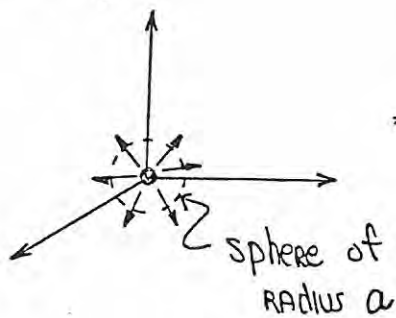
$$-\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d\phi}{dr} + \frac{\Sigma_a}{D} \phi(r) = 0, \quad r > 0$$

subject to AN appropriate
BOUNDARY CONDITION AT $r=0$
to account for the point source

BOUNDARY CONDITION

note - the source emits S_0
NEUTRONS PER SECOND

Consider a sphere
of radius a AT
the origin:



$$J(r) = \frac{\text{Net CURRENT}}{\text{AT } r}$$

$$\Rightarrow J(r) \cdot 4\pi r^2 = \underline{\text{net}} \\ \text{NUMBER OF NEUTRONS} \\ \text{CROSSING SPHERICAL} \\ \text{SURFACE AT } r \\ \text{PER SECOND}$$

↙ NET CURRENT

$$\lim_{a \rightarrow 0} J(a) \cdot 4\pi a^2 = S_0$$

↑ AREA ↑ SOURCE STRENGTH

(NET NUMBER OF NEUTRONS LEAVING THE "SURFACE" OF THE SOURCE PER SECOND IS EQUAL TO THE SOURCE STRENGTH)

BOUNDARY CONDITION:

$$\lim_{r \rightarrow 0} \left[4\pi r^2 J(r) - D \frac{d\phi}{dr} \right] = S_0$$

{ ACCOUNTS FOR THE POINT SOURCE OF STRENGTH S_0 AT THE ORIGIN

As you squeeze down around the origin, the net current leaving must be the source strength.

Second boundary condition:

NO NEUTRONS AT $r = \infty$

(FINITE SOURCE, INFINITE MEDIUM, $\Sigma_a > 0$)

$$\Rightarrow \phi(r) = 0 \text{ AT } r = \infty$$

SUMMARY

$$\text{Solve } -\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\phi}{dr} \right) + \frac{1}{L^2} \phi(r) = 0 \quad r > 0$$

$$\text{subject to } \lim_{r \rightarrow 0} 4\pi r^2 \cdot J(r) = 0$$

$$\phi(r) = \frac{1}{r} \cdot v$$

$$\lim_{r \rightarrow \infty} \phi(r) = 0$$

Steps

1. Guess A solution

$$\Phi(r) = A \frac{e^{-r/L}}{r} + \frac{B e^{r/L}}{r} \quad \text{TRY IT!}$$

2. Apply boundary conditions

$$\bullet \lim_{r \rightarrow \infty} \Phi(r) = 0 \Rightarrow B = 0$$

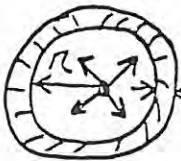
$$\therefore \Phi(r) = A \frac{e^{-r/L}}{r}$$

$$\bullet \lim_{r \rightarrow 0} 4\pi r^2 \nabla \Phi(r) = S_0$$

Application RMS distance to absorptionWhat is the (average distance)²

that a neutron emitted by the point source will diffuse before being absorbed?

define $p(r)dr \equiv$ probability that a neutron emitted at $r=0$ will be absorbed in the shell $r, r+dr$



17-19

$$J(r) = -D \frac{d\phi}{dr} \quad \phi(r) = A \frac{e^{-r/L}}{r}$$

$$= DA \left[\frac{1}{L} e^{-r/L} + \frac{1}{r^2} e^{-r/L} \right]$$

$$\therefore \lim_{r \rightarrow 0} 4\pi r^2 \cdot J(r) =$$

$$4\pi DA \lim_{r \rightarrow 0} e^{-r/L} \left[\frac{1}{L} r^2 + 1 \right]$$

\downarrow \downarrow
 1 0

$$= 4\pi DA = S_0$$

$$A = \frac{S_0}{4\pi D}$$

$$\phi(r) = \frac{S_0}{4\pi D r} e^{-r/L}$$

17-20

- Then the AVERAGE SQUARE distance to absorption MAY be expressed:

$$\text{AVERAGE } \langle r^2 \rangle = \int_0^{\infty} r^2 p(r) dr$$

probability neutron
is absorbed in
 $r, r+dr$

- # NEUTRONS absorbed per second in $r, r+dr = \Sigma_a \phi(r) 4\pi r^2 dr$
- # NEUTRONS emitted per second = S_0

$$\begin{aligned} \therefore p(r)dr &= \frac{\# \text{ Absorbed in } r, r+dr}{\# \text{ emitted at } r=0} \\ &= \frac{\sum_a \Phi(r) 4\pi r^2 dr}{S_0} \end{aligned}$$

$$\text{Since } \Phi(r) = \frac{S_0}{4\pi D r} e^{-r/L}$$

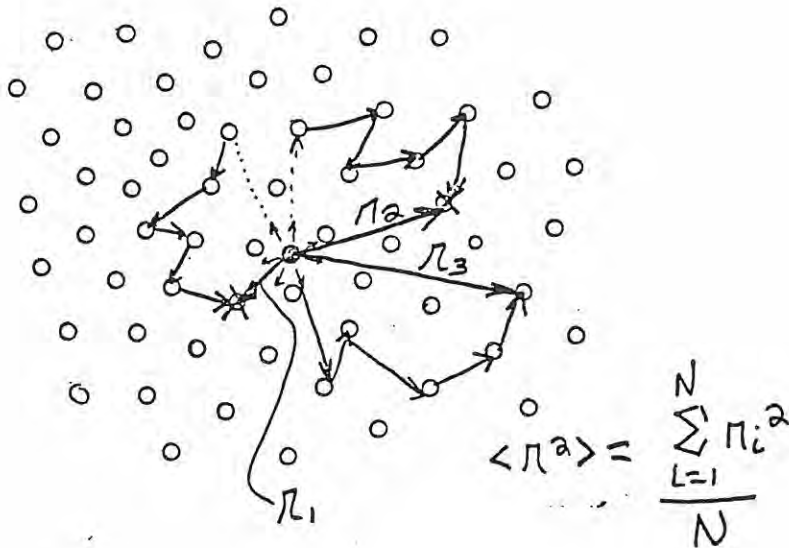
$$p(r)dr = \frac{r}{L^2} e^{-r/L} dr$$

$$\therefore \langle r^2 \rangle = \int_0^{\infty} \frac{r^3}{L^2} e^{-r/L} dr = 6L^2$$

$$\begin{aligned} \therefore \text{RMS distance to absorption} \\ &= [\langle r^2 \rangle]^{1/2} = \sqrt{6} L \end{aligned}$$

$L \propto$ distance which a neutron will diffuse (on the average) from its birth to its point of absorption

"diffusion length"

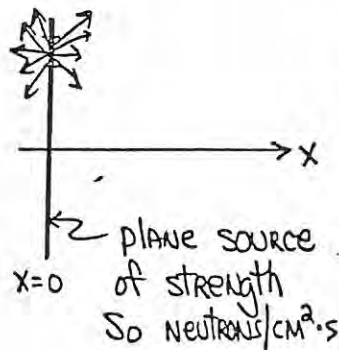
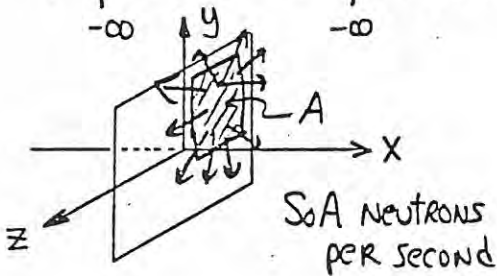


PLANE SOURCE IN

AN INFINITE MEDIUM (S_0 NEUTRONS/ $\text{cm}^2 \cdot \text{s}$)

$S(x) = S_0 \delta(x)$ DIRAC DELTA FUNCTION

$$\int_{-\infty}^{\infty} S(x) dx = S_0 \int_{-\infty}^{\infty} \delta(x) dx = 1$$



$$D(\eta) = D$$

$$\Sigma_a(\eta) = \Sigma_a$$

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = S_0 \delta(x)$$

$$-\infty < x < \infty$$

boundary conditions:

(i) No neutrons at infinity

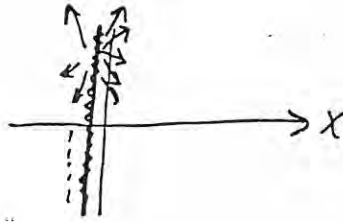
$$\lim_{|x| \rightarrow \infty} \phi(x) = 0$$

(ii) Replace plane source with boundary condition at $x=0$

Same as before, if we approach the source plane, the net current must equal the source strength.

$$\lim_{x \rightarrow 0^+} J(x) = \frac{S_0}{2}$$

$$\lim_{x \rightarrow 0^-} J(x) = -\frac{S_0}{2}$$



By symmetry we know

$$\phi(x) = \phi(-x)$$

\therefore solve only for $x > 0$:

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = 0 \quad x > 0$$

$$\lim_{x \rightarrow \infty} \phi(x) = 0$$

$$\lim_{x \rightarrow 0} J(x) = S_0/2$$

17-27

Steps (note $x > 0$)

1. Solve homogeneous equation

$$\Phi(x) = Ae^{-x/L} + Be^{+x/L}$$

2. Apply boundary conditions

$$(i) \lim_{x \rightarrow \infty} \Phi(x) = 0$$

$$\Rightarrow B = 0 \quad \therefore \Phi(x) = Ae^{-x/L}$$

$$(ii) \lim_{x \rightarrow 0} J(x) = S_0/2$$

17-28

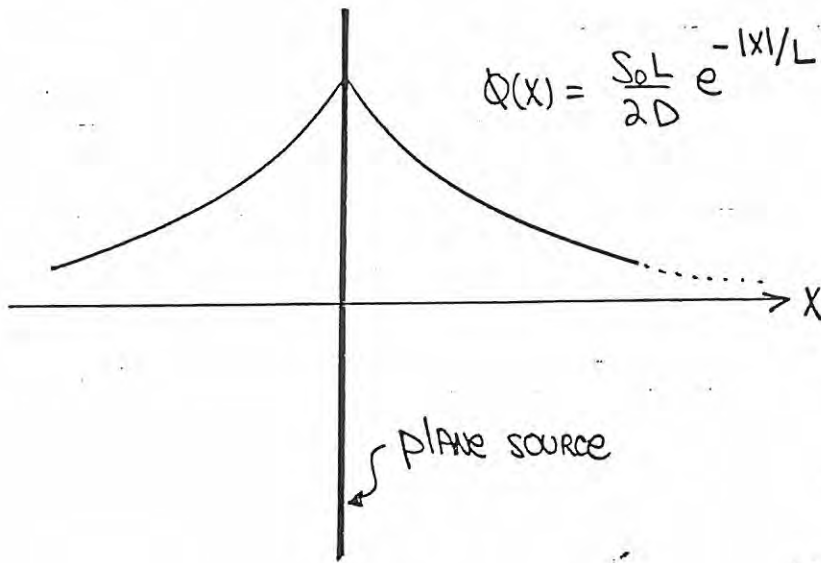
$$J(x) = -D \frac{d\Phi}{dx} = \frac{DA}{L} e^{-x/L}$$

$$\lim_{x \rightarrow 0} J(x) = \frac{DA}{L} = \frac{S_0}{2}$$

$$\therefore A = \frac{S_0 L}{2D}$$

$$\Phi(x) = \frac{S_0 L}{2D} e^{-x/L} \quad x > 0$$

$$\Phi(x) = \frac{S_0 L}{2D} e^{x/L} \quad x < 0$$



LECTURE 18

Multiregion Problems

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 176-182.

EXERCISES:

- 18.1. Duderstadt & Hamilton, problem #5-8
- 18.2. Duderstadt & Hamilton, problem #5-9
- 18.3. The matrix A for a typical computer problem is, for N=4,
($\Delta = 1/4$)

$$A = \begin{pmatrix} \Sigma_a + \frac{2D}{h^2} & -\frac{D}{h^2} & 0 \\ -\frac{D}{h^2} & \Sigma_a + \frac{2D}{h^2} & -\frac{D}{h^2} \\ 0 & -\frac{D}{h^2} & \Sigma_a + \frac{2D}{h^2} \end{pmatrix} \\
 = \begin{pmatrix} 33 & -16 & 0 \\ -16 & 33 & -16 \\ 0 & -16 & 33 \end{pmatrix}$$

and the systems of equations to be solved is

$$\begin{pmatrix} 33 & -16 & 0 \\ -16 & 33 & -16 \\ 0 & -16 & 33 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Solve by hand (calculator) this system of equations in 4 different ways:

- (1) Directly by LU decomposition

$$\underline{\phi} = \begin{pmatrix} .084922 \\ .11265 \\ .084922 \end{pmatrix} \quad (\text{answer})$$

- (2) Jacobi method

- (3) Gauss-Seidel

- (4) SOR (with $W = 1.5$)

For the last 3 methods, carry thru the calculations up to $\underline{\phi}^{(3)}$ given

$$\underline{\phi}^{(0)} = \text{initial guess} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

- (5) Using the actual solution $\underline{\phi}$ from part (1) (LU method gives exact solution to precision carried in calculations), calculate the final relative error vector $\underline{\epsilon}$ for each of the iterative methods, where

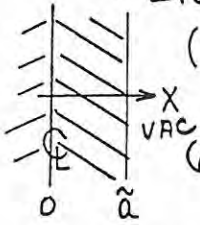
$$\underline{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{pmatrix} \quad \underline{\phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} \quad (\text{from (1) above})$$

And

$$\epsilon_i = \left| \frac{\phi_i - \phi_i^{(3)}}{\phi_i} \right|$$

Solutions to the 1-D Diffusion Equation

• Infinite slab



(i) Extrapolated b.c.

$$\tilde{a} = a + 2D, \phi(\tilde{a}) = 0$$

(ii) Vacuum b.c.

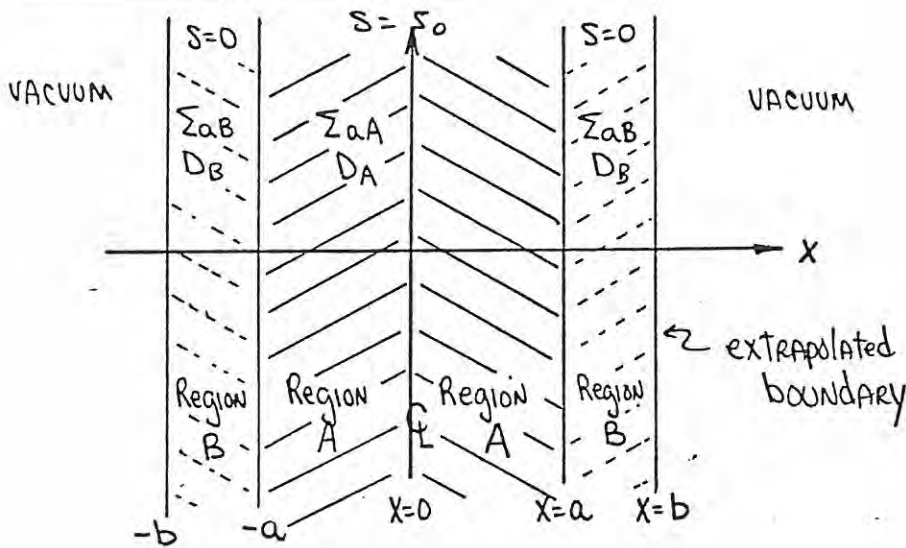
$$J_-(a) = 0$$

• Infinite medium

(i) Point source at $x=0$ $L = \sqrt{6 [k/\Sigma_a]^{1/2}}$

(ii) Plane source at $x=0$

Multi-Region Reactor



Examine now a multi-region reactor, such as a reactor core surrounded by a reflector. Assume a uniform source inside the core and no source in the reflector.

Interface condition

Solve the diffusion equation
in both regions A and B:

$$-D_A \frac{d^2 \phi_A}{dx^2} + \Sigma_A \phi_A(x) = S_A(x) \stackrel{= S_0}{}, \quad 0 \leq x \leq a$$

$$-D_B \frac{d^2 \phi_B}{dx^2} + \Sigma_B \phi_B(x) = S_B(x) \stackrel{= 0}{}, \quad a \leq x \leq b$$

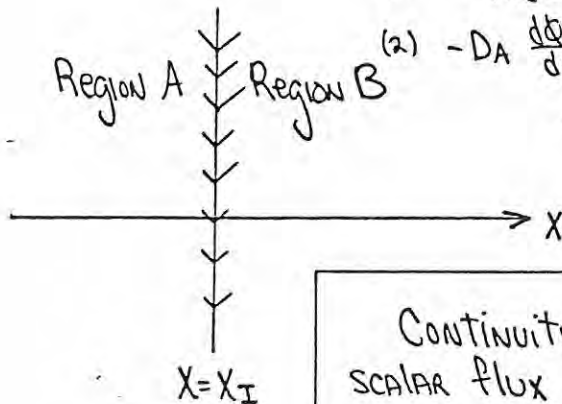
boundary conditions: $\phi_B(b) = 0$ (extrapolated b.c.)

$$-D_A \left. \frac{d\phi_A}{dx} \right|_{x=0} = 0 \quad (\text{symmetry})$$

The diffusion equation must be satisfied in each region separately.

Impose interface conditions

AT $x = x_I$



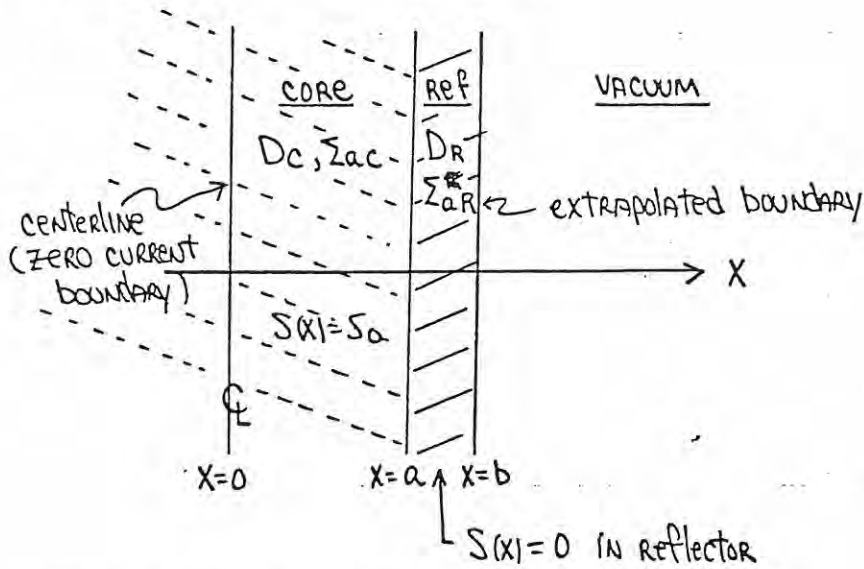
$$(1) \quad \phi_A(x_I) = \phi_B(x_I)$$

$$(2) \quad -D_A \left. \frac{d\phi_A}{dx} \right|_{x=x_I} = -D_B \left. \frac{d\phi_B}{dx} \right|_{x=x_I}$$

Continuity of the
SCALAR flux $\phi(x)$ AND
NORMAL CURRENT $\underline{j} \cdot \hat{m}$ AT
The interface

The first interface condition simply expresses the continuity of neutron flux. The second expresses the continuity of neutron flow across a surface, hence continuity of normal current. Mathematically, the original equation has the highest derivative - $\nabla \cdot D\nabla\phi$ and the second condition is needed to allow the derivative to be defined.

Example - Reflected Reactor



The zero current boundary at $x=0$ accounts for the symmetry. There will also be a reflector from $x = -a$ to $x = -b$, but we are eliminating the domain $x < 0$ by using the symmetry b.c.

Equations

$$(1) -D_c \frac{d^2 \phi_c}{dx^2} + \Sigma_{ac} \phi_c(x) = S_0, \quad 0 \leq x \leq a$$

$$(2) -D_R \frac{d^2 \phi_R}{dx^2} + \Sigma_{aR} \phi_R(x) = 0, \quad a \leq x \leq b$$

Boundary conditions

$$(i) -D_c \left. \frac{d\phi_c}{dx} \right|_{x=0} = 0 \quad (ii) \phi_R(b) = 0$$

Interface conditions

$$(iii) \phi_c(a) = \phi_R(a) \quad (iv) -D_c \left. \frac{d\phi_c}{dx} \right|_{x=a} = -D_R \left. \frac{d\phi_R}{dx} \right|_{x=a}$$

Summary of the resultant equation, boundary conditions, and interface conditions.

Solution method $e^{x/L}, e^{-x/L}$

$$\cosh\left(\frac{x}{L}\right) = \frac{1}{2} [e^{x/L} + e^{-x/L}]$$

$$\sinh\left(\frac{x}{L}\right) = \frac{1}{2} [e^{x/L} - e^{-x/L}]$$

PARTICULAR
SOLUTION

CORE

$$\Phi_c(x) = \underbrace{A \cosh\left(\frac{x}{L_c}\right) + B \sinh\left(\frac{x}{L_c}\right)}_{\text{homogeneous solution}} + \frac{S_0}{\Sigma a c}$$

$$-D_c \frac{d\Phi_c}{dx} \Big|_{x=0} = 0 \Rightarrow B = 0$$

$$\begin{aligned} \cosh(0) &= 1 \\ \sinh(0) &= 0 \end{aligned}$$

$$\therefore \Phi_c(x) = A \cosh\left(\frac{x}{L_c}\right) + \frac{S_0}{\Sigma a c}$$

Assume exponential solutions, or more conveniently assume cosh and sinh solutions (since they are linear combinations of the exponentials). $B=0$ for core region because derivative of $\sinh x$ is $\cosh x$, which is greater than zero.

Reflector $\Phi_R(b) = 0$

\sinh, \cosh

$$\Phi_R(x) = B \sinh\left(\frac{x-b}{L_R}\right)$$

$$\Phi_c(x) = A \cosh\left(\frac{x}{L_c}\right) + \frac{S_0}{\Sigma a}$$

$$(iv) -D_A \frac{A}{L_c} \sinh\left(\frac{a}{L_c}\right) = -D_R \frac{B}{L_R} \cosh\left(\frac{x-b}{L_R}\right)$$

$$B = a A$$

Since $\sinh(0) = 0$, we find reflector solution by inspection.

$$\text{where } \alpha = \left(\frac{L_R}{L_C} \right) \frac{\sinh\left(\frac{a}{L_C}\right)}{\cosh\left(\frac{a-b}{L_R}\right)} \left(\frac{D_A}{D_B} \right) \left(\frac{D_C}{D_R} \right)$$

$$\text{Then (iii)} \Rightarrow \phi_C(a) = \phi_R(a)$$

$$A \cosh\left(\frac{a}{L_C}\right) + \frac{S_0}{\Sigma a} = \alpha A \sinh\left(\frac{a-b}{L_R}\right)$$

$$\therefore A = \frac{-S_0/\Sigma a}{\cosh\left(\frac{a}{L_C}\right) - \alpha \sinh\left(\frac{a-b}{L_R}\right)}$$

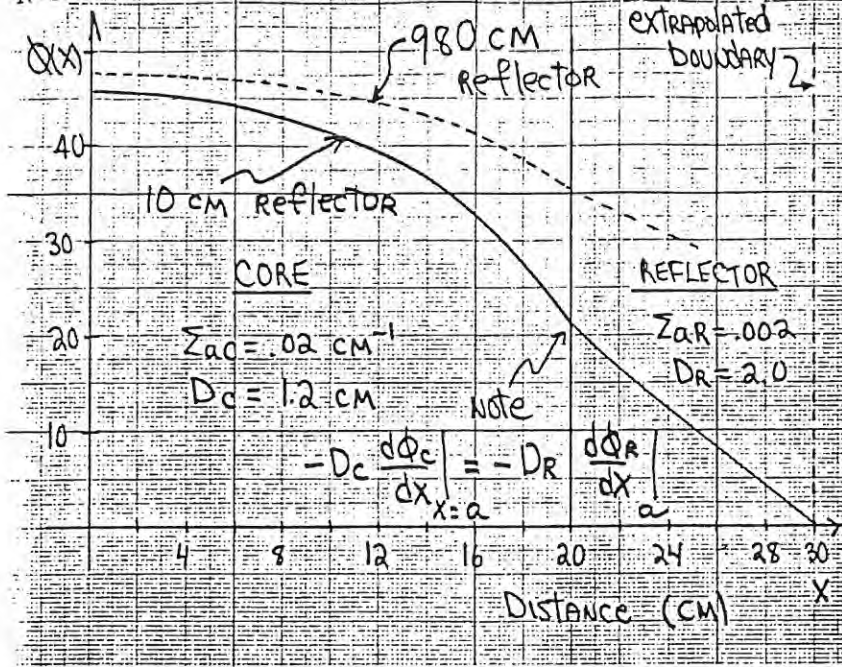
A little algebra and we find the constant A (verify on your own).

Final solution

$$\phi_C(x) = \left(\frac{S_0}{\Sigma a} \right) \left[1 - \frac{\cosh(x/L_C)}{\cosh\left(\frac{a}{L_C}\right) - \alpha \sinh\left(\frac{a-b}{L_R}\right)} \right]$$

$$\phi_R(x) = \frac{-\alpha(S_0/\Sigma a)}{\cosh\left(\frac{a}{L_C}\right) - \alpha \sinh\left(\frac{a-b}{L_R}\right)} \sinh\left(\frac{x-b}{L_R}\right)$$

$$\text{where } \alpha = \left(\frac{L_R}{L_C} \right) \frac{\sinh\left(\frac{a}{L_C}\right)}{\cosh\left(\frac{a-b}{L_R}\right)} \left(\frac{D_C}{D_R} \right)$$



We have plotted the solution for two different reflectors. Note how the thicker reflector increases the flux in the core. Let us now relate this behavior to the leakage probability.

Define

l = leakage probability

l = probability that a neutron emitted by the source within the core leaks out of the core

$$l = \frac{\text{net leakage from core}}{\text{production rate in core}} = \frac{J(a) \cdot A_{\text{REA}}}{S_0 \cdot a \cdot A_{\text{REA}}}$$

The overall leakage probability for the core is simply the average probability that a neutron "born" in the core eventually leaks out.

$$l = \frac{J(a)}{S_0 \cdot a}$$

$$a = 20.0 \text{ cm - CORE}$$

$$S_0 = 1.0 \text{ NEUTRONS/CM}^3 \cdot \text{s}$$

$$L_R = (D_R / \Sigma_{aR})^{1/2} = 31.6 \text{ cm}$$

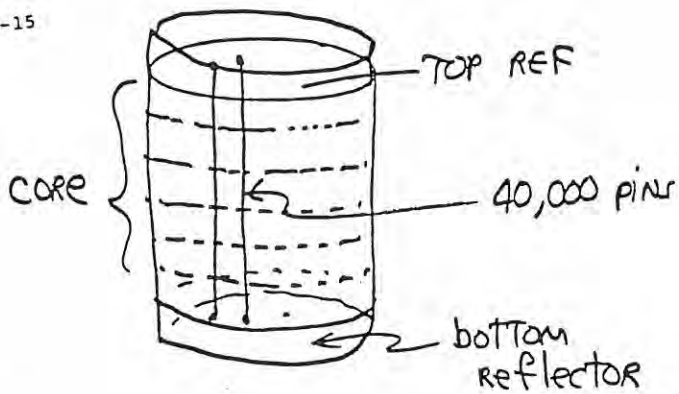
Reflector thickness (b-a)		leakage probability J_l (x100%)
10 cm	$\frac{1}{3}$	22%
30	~ 1	13.7%
80	$\sim 2\frac{1}{2}$	11.3%
160	~ 5	11.2%
980	~ 32	11.2%
∞		11.2%

CONCLUSIONS: - Reflector Thickness

~ 3 to 4 diffusion lengths
is essentially "infinite"
AS FAR AS THE CORE
IS CONCERNED

- INCREASE in Reflector Thickness
 \Rightarrow decrease in leakage
probability OR INCREASE
in non-leakage probability
 $P_{FNL} \uparrow \Rightarrow k \uparrow$

A reflector will generally increase the multiplication factor for a core.



ANALYTICAL SOLUTIONS- NOT USEFUL
FOR PRACTICAL CALCULATIONS
DIGITAL COMPUTER

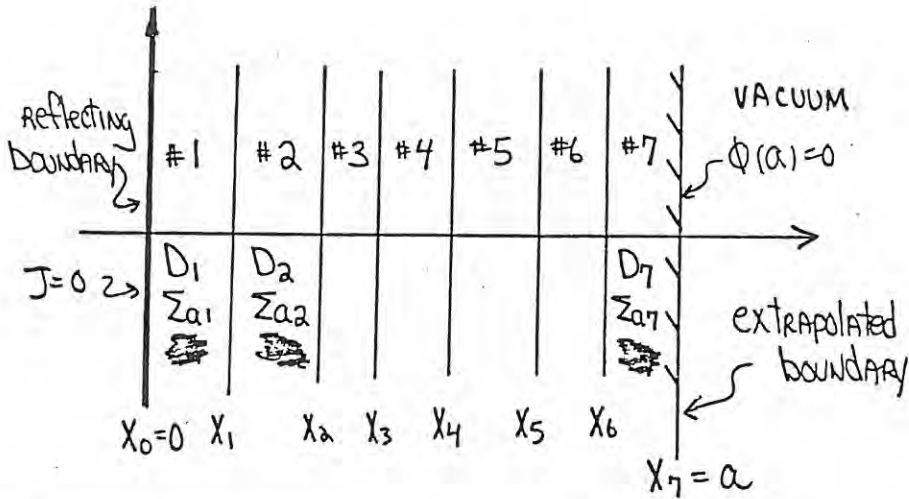
Now we have expended sufficient time examining analytical solutions to the diffusion equation. The home exercises will provide you with additional practice in solving the diffusion equation. However, eventually the engineer is faced with solving the diffusion equation for a realistic configuration, such as a commercial pressurized water reactor.

- Fuel enrichments different
- WATER CHANNELS
- NON-UNIFORM DEPLETION
- CONTROL RODS, BURNABLE POISON, etc.

NOT HOMOGENEOUS

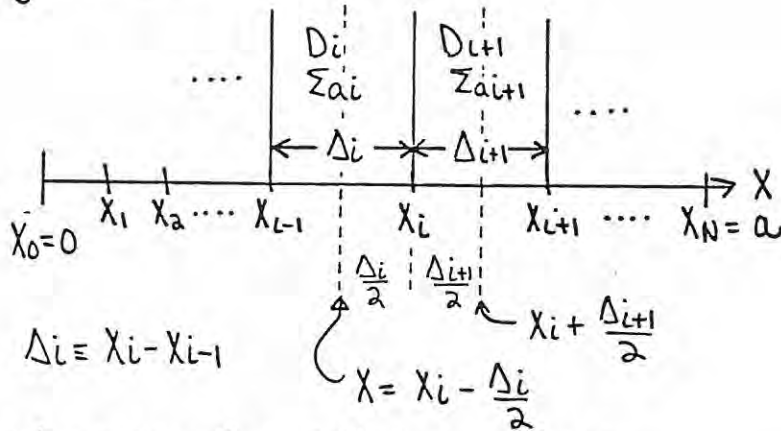
Now the task is much too difficult for analytical solutions. One is forced to resort to a computer to solve most, if not all, of the realistic reactor analysis problems commonly encountered by the nuclear analyst.

Numerical Solution of The 1-D Diffusion Equation



The basic idea of any computational method is to DISCRETIZE the equations to be solved by superimposing a computational mesh over the analytical domain.

general mesh structure



$$\Delta_i = x_i - x_{i-1}$$

$$x = x_i - \frac{\Delta_i}{2}$$

goal: solve the diffusion equation over each mesh (cell) $i, i=1, 2, \dots, N$ subject to boundary and interface conditions

The particular numerical scheme that we will examine in some detail employs the above characteristic mesh structure.

Solve

$$-D \frac{d}{dx} D(x) \frac{d\phi}{dx} + \Sigma_a(x) \phi(x) = S(x) \quad (1)$$

$$0 \leq x \leq a$$

subject to

$$\phi(a) = 0$$

$$-D \left. \frac{d\phi}{dx} \right|_{x=0} = 0$$

$$x=0$$

AND $\phi(x)$, $-D \frac{d\phi}{dx}$ CONTINUOUS
AT THE INTERFACES x_i , $i=1, 2, \dots, N-1$.

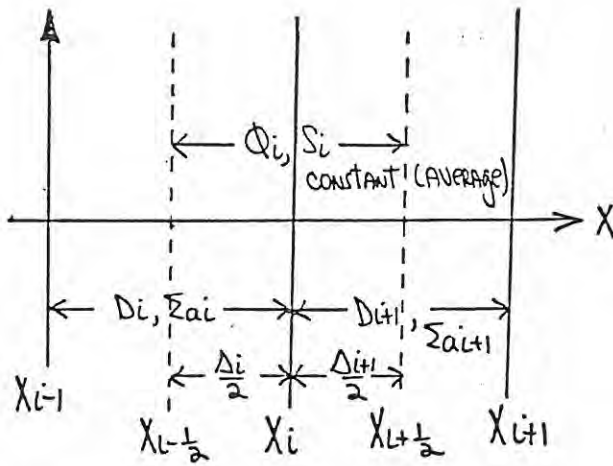
• Define $\boxed{\phi_i \equiv \phi(x_i)}$ AND

ASSUME ϕ_i CONSTANT OVER THE
INTERVAL $x_i - \frac{\Delta_i}{2}$ TO $x_i + \frac{\Delta_{i+1}}{2}$

• Define $S_i =$ AVERAGE SOURCE OVER
THE INTERVAL $x_i - \frac{\Delta_i}{2}$ TO $x_i + \frac{\Delta_{i+1}}{2}$:

$$S_i \equiv \frac{1}{\frac{\Delta_i}{2} + \frac{\Delta_{i+1}}{2}} \int_{x_i - \frac{\Delta_i}{2}}^{x_i + \frac{\Delta_{i+1}}{2}} S(x) dx$$

Since the source is known (assumed to be known) we can readily define S_i as indicated. Note we have DISCRETE values for the unknown flux $\phi(x)$ - these will be the unknown to be solved for



"cell-edges" scheme: fluxes Φ_i ARE defined ON the edges of the cells

This particular mesh structure is characteristic of a class of finite difference methods for the neutron diffusion equation known as "cell-edges" schemes. They are embodied in such codes as PDQ, a well-known computer code for solving the multi-dimensional neutron diffusion equation.

• Integrate Eq. (1) from

$$X = X_i - \frac{\Delta_i}{2} \quad \text{to} \quad X = X_i + \frac{\Delta_{i+1}}{2}$$

$$\int_{X_i - \frac{\Delta_i}{2}}^{X_i + \frac{\Delta_{i+1}}{2}} \left[-\frac{d}{dx} D(x) \frac{d\phi}{dx} + \Sigma_a(x)\phi(x) \right] dx = \int_{X_i - \frac{\Delta_i}{2}}^{X_i + \frac{\Delta_{i+1}}{2}} S(x) dx$$

A typical step in deriving a finite difference approximation is to integrate the differential equation over each of the mesh intervals. Let us consider each of the three terms separately.

TERM ③ (easiest)

$$\textcircled{3} = S_i \left(\frac{\Delta_i}{2} + \frac{\Delta_{i+1}}{2} \right)$$

by definition of S_i

$$\begin{aligned} \text{TERM ②} \\ \textcircled{2} = \int_{x_i - \frac{\Delta_i}{2}}^{x_i + \frac{\Delta_{i+1}}{2}} \Sigma_a(x) \Phi(x) dx &= \int_{x_i - \frac{\Delta_i}{2}}^{x_i} \Sigma_{ai} \Phi_i dx \\ &+ \int_{x_i}^{x_i + \frac{\Delta_{i+1}}{2}} \Sigma_{a_{i+1}} \Phi_i dx \end{aligned}$$

Term (3) is the easiest because of our previous definition of S_i . Term (2) has to be broken into 2 integrals because $\Phi(x)$ is discontinuous at $x = x_i$ (recall our definition of Φ_i)

$$\textcircled{2} = \left(\Sigma_{ai} \frac{\Delta_i}{2} + \Sigma_{a_{i+1}} \frac{\Delta_{i+1}}{2} \right) \Phi_i$$

TERM ① LEAKAGE TERM

$$\begin{aligned} \textcircled{3} &= \int_{x_i - \frac{\Delta_i}{2}}^{x_i + \frac{\Delta_{i+1}}{2}} - \frac{d}{dx} \left(D(x) \frac{d\Phi}{dx} \right) dx \\ &= - D(x) \frac{d\Phi}{dx} \Big|_{x=x_i - \frac{\Delta_i}{2}}^{x=x_i + \frac{\Delta_{i+1}}{2}} \end{aligned}$$

The leakage term is always the problem term, whether for this simple 1-D diffusion equation or a multi-dimensional "transport" equation.

LECTURE 19

NUMERICAL SOLUTION OF 1-D DIFFUSION EQUATION

READING ASSIGNMENT:

Duderstadt and Hamilton, pp. 183-185.

EXERCISES:

- 19.1. Write a computer code to solve the 1-D diffusion equation in slab geometry

$$-\frac{d}{dx} D(x) \frac{d\phi(x)}{dx} + \Sigma_a(x) \phi(x) = S(x)$$

subject to extrapolated boundary conditions

at $x = \tilde{a} = a + 2D$,

$$\phi(\pm \tilde{a}) = 0$$

This problem should be done in the following steps

1. Read in as input data the following:
 - (a) The number of mesh intervals N
 - (b) The extrapolated width of the slab, $2\tilde{a}$
 - (c) D , Σ_a , and S
2. Write out the input data as a check
3. Compute the source vector S_i , $i = 1, 2, \dots, N-1$
(note S_i is defined with respect to the centered mesh)

EXERCISES (cont'd)

4. Compute the matrix elements

$$A_{ij}, \quad \begin{array}{l} i = 1, 2, \dots, N-1 \\ j = 1, 2, \dots, N-1 \end{array}$$

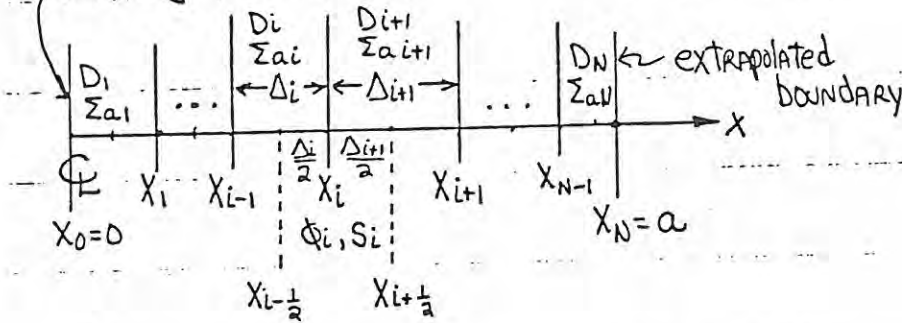
5. Solve for the flux vector ϕ_i , $i = 1, 2, \dots, N-1$ where

$$\underline{\underline{A}} \underline{\underline{\phi}} = \underline{\underline{S}}$$

You may use a solution algorithm of your choice.

NUMERICAL Solution of the 1-D Diffusion Equation

reflecting boundary



$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} dx \left[\textcircled{1} \frac{d}{dx} D(x) \frac{d\phi}{dx} + \textcircled{2} \Sigma_a(x) \phi(x) = \textcircled{3} S(x) \right]$$

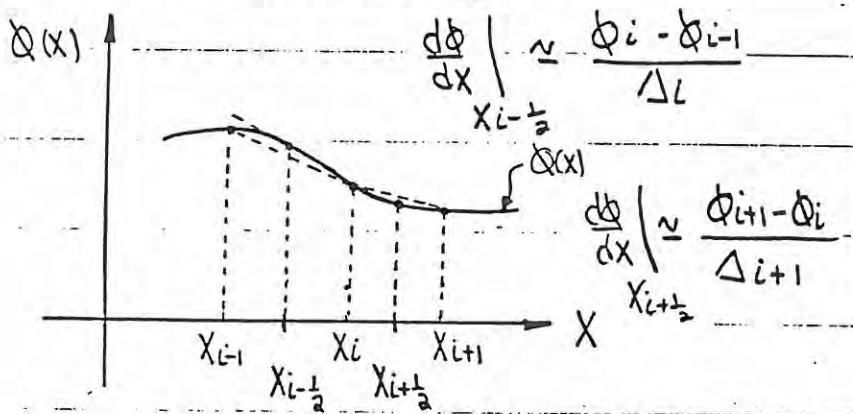
$$\textcircled{3} = S_i \left(\frac{\Delta_i}{2} + \frac{\Delta_{i+1}}{2} \right)$$

$$\textcircled{2} = \left(\Sigma_{ai} \frac{\Delta_i}{2} + \Sigma_{ai+1} \frac{\Delta_{i+1}}{2} \right) \phi_i$$

Term ①

$$\begin{aligned} \textcircled{1} &= \int_{x_L - \frac{\Delta_i}{2}}^{x_i + \frac{\Delta_{i+1}}{2}} \left[-\frac{d}{dx} (D(x) \frac{d\phi}{dx}) \right] dx \\ &= -D(x) \frac{d\phi}{dx} \Big|_{x_L - \frac{\Delta_i}{2}}^{x_i + \frac{\Delta_{i+1}}{2}} \end{aligned}$$

Approximation of a Derivative by a Finite Difference



Now we come to the first numerical approximation - we will replace the derivative term by a "finite difference", which is simply an algebraic approximation to the derivative.

$$\begin{aligned} \textcircled{1} &= -D(x) \left. \frac{d\phi}{dx} \right|_{x_{i+1/2}} + D(x) \left. \frac{d\phi}{dx} \right|_{x_{i-1/2}} \\ &\approx -D_{i+1} \left(\frac{\phi_{i+1} - \phi_i}{\Delta_{i+1}} \right) + D_i \left(\frac{\phi_i - \phi_{i-1}}{\Delta_i} \right) \end{aligned}$$

Collect terms $\textcircled{1} + \textcircled{2} + \textcircled{3}$

We have two derivatives to approximate in term (11), and we use the above definition of a finite difference.

$$\begin{aligned}
 & -D_{i+1} \left(\frac{\phi_{i+1} - \phi_i}{\Delta x_{i+1}} \right) + D_i \left(\frac{\phi_i - \phi_{i-1}}{\Delta x_i} \right) \\
 & + \left(\sum a_i \frac{\Delta x_i}{2} + \sum a_{i+1} \frac{\Delta x_{i+1}}{2} \right) \phi_i \\
 & \textcircled{2} \rightarrow = S_i \left(\frac{\Delta x_i}{2} + \frac{\Delta x_{i+1}}{2} \right) \textcircled{3} \quad (1)
 \end{aligned}$$

This integration can be performed
 for $i=1, 2, \dots, N-1$ (INTERNAL)
 (NOT $i=0$ OR $i=N$)
 BOUNDARY NODES

The integration of the diffusion equation over a typical mesh cell can be repeated for all similar mesh cells—those mesh cells in the interior. The boundary cells need special treatment.

BOUNDARIES

$x=a$ Extrapolated bdy

$\phi(a) = 0$ - desire this

$\phi_N \equiv \phi(x_N) = \phi(a) = 0$

$\boxed{\phi_N = 0}$

$x=0$ ZERO CURRENT

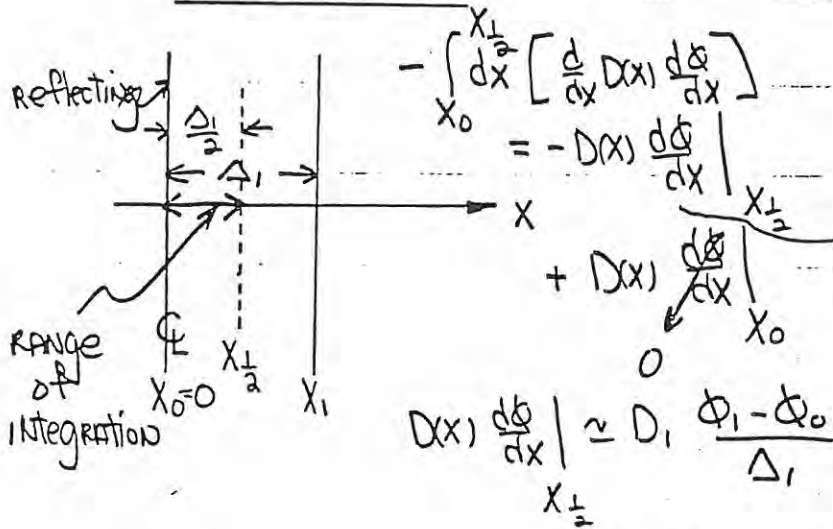
$\left. \frac{d\phi}{dx} \right|_{x=0} = 0$

$x=0$

The extrapolated boundary condition is easily implemented because the fluxes are defined at the mesh corners. We simply set the approximate flux on the boundary equal to zero.

Integration Path

for the 1st cell



For boundary conditions other than zero flux (extrapolated b.c.), the finite difference approximation is best derived by integrating the diffusion equation over the boundary mesh cell.

equation ($i=0$)

$$-D_1 \frac{\phi_1 - \phi_0}{\Delta_1} + \sum a_i \phi_0 \frac{\Delta_i}{2} = S_0 \frac{\Delta_1}{2}$$

• Now have equations

for $i=0, 1, \dots, N$

$$\phi_N = 0$$

• Define $\Delta_{ii} \equiv \frac{\Delta_i}{2} + \frac{\Delta_{i+1}}{2}$ length of path of integration

$$\sum a_{ii} \equiv \frac{\sum a_i \Delta_i + \sum a_{i+1} \Delta_{i+1}}{\Delta_i + \Delta_{i+1}}$$

There is a separate equation for the first cell, many similar equations for the interior cells, and a simple equation for the last cell ($\phi_N = 0$). For convenience define the coefficients as shown.

REARRANGE Eq. (1) : a_{ii} ← for the INTERNAL nodes

$$-\frac{D_i}{\Delta_i \Delta_{ii}} \phi_{i-1} + \left[\frac{D_i}{\Delta_i \Delta_{ii}} + \frac{D_{i+1}}{\Delta_{i+1} \Delta_{ii}} + \sum a_{ii} \Delta_{ii} \right] \phi_i$$

$$a_{ii-1} \frac{-\frac{D_i}{\Delta_i \Delta_{ii}} \phi_{i-1}}{a_{ii+1}} + \frac{D_{i+1}}{\Delta_{i+1} \Delta_{ii}} \phi_{i+1} = S_i \Delta_{ii} \quad (2)$$

$$i = 1, 2, \dots, N-1$$

$$a_{ii-1} = -\frac{D_i}{\Delta_i \Delta_{ii}}$$

$$a_{ii} = \frac{D_i}{\Delta_i \Delta_{ii}} + \frac{D_{i+1}}{\Delta_{i+1} \Delta_{ii}} + \sum a_{ii}$$

$$a_{ii+1} = -\frac{D_{i+1}}{\Delta_{i+1} \Delta_{ii}}$$

Defining some additional terms, we obtain the system of equations for the fluxes ϕ_i

Equation (2) becomes

$$a_{ii-1} \phi_{i-1} + a_{ii} \phi_i + a_{ii+1} \phi_{i+1} = S_i$$

$$i = 1, 2, \dots, N-1$$

Also

$$\phi_N = 0$$

And

$$a_{00} \phi_0 + a_{01} \phi_1 = S_0$$

where $a_{00} = \sum a_{00} + 2D_1/\Delta_1^2$

$$a_{01} = -2D_1/\Delta_1^2$$

- Equation for ϕ_{N-1} :

$$a_{N-1,N-2}\phi_{N-2} + a_{N-1,N-1}\phi_{N-1} + \cancel{a_{N-1,N}\phi_N} = S_{N-1}$$

• Have N equations in N unknowns

$$\phi_0, \phi_1, \phi_2, \dots, \phi_{N-1}$$

System of ordinary differential equations \Rightarrow system of algebraic equations

COMPUTER!

We have approximated the original set of ordinary differential equations (the diffusion equation over each mesh) by a set of algebraic equations.

$$\begin{array}{rcl} a_{00}\phi_0 + a_{01}\phi_1 & = & S_0 \\ a_{10}\phi_0 + a_{11}\phi_1 + a_{12}\phi_2 & = & S_1 \\ a_{21}\phi_1 + a_{22}\phi_2 + a_{23}\phi_3 & = & S_2 \\ \vdots & & \vdots \\ a_{N-1,N-2}\phi_{N-2} + a_{N-1,N-1}\phi_{N-1} & = & S_{N-1} \end{array}$$

3-point difference equations

$$\underline{A} \underline{\phi} = \underline{S}$$

Arrange the system of equations in matrix form.

where

$$\underline{A} = \begin{bmatrix} a_{00} & a_{01} & 0 & \dots & 0 \\ a_{10} & a_{11} & a_{12} & 0 & \dots \\ 0 & a_{21} & a_{22} & a_{23} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & \dots & 0 & a_{N-1, N-2} & a_{N-1, N-1} \end{bmatrix}$$

N x N
MATRIX
banded

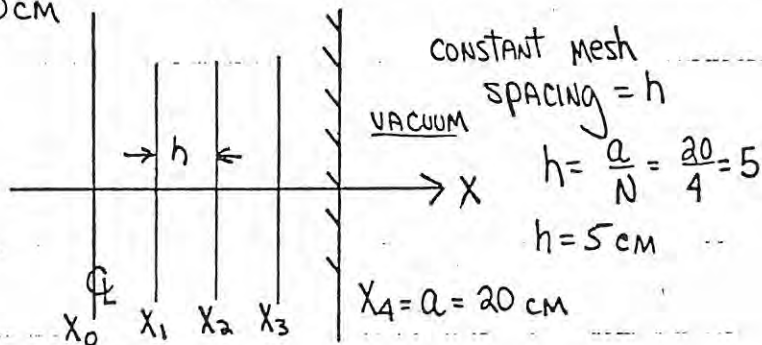
$$\underline{\Phi} = \begin{bmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{N-1} \end{bmatrix} \quad \underline{S} = \begin{bmatrix} S_0 \\ S_1 \\ \vdots \\ S_{N-1} \end{bmatrix}$$

N-vector

Can see that the matrix is tridiagonal.

EXAMPLE: BARE slab reactor (FNR)

$$\left. \begin{array}{l} \Sigma_a = .02 \text{ cm}^{-1} \\ D = 1.2 \text{ cm} \\ S = 1.0 \text{ cm}^{-3} \text{ s}^{-1} \\ a = 20 \text{ cm} \end{array} \right\} \text{constant} : 0 \leq x \leq a$$



Let us now go back to our FNR configuration which we solved analytically.

$$a_{ii} = \sum a + \frac{2D}{h^2} = .116 \quad \Delta ii = h, \Delta i = h$$

$$a_{ii-1} = a_{ii+1} = -\frac{D}{h^2} = -.048 \quad \sum a_{ii} = \sum a$$

$$a_{00} = .116$$

$$a_{01} = -\frac{2D}{h^2} = -.096$$

$$\sum c_i = 1.0$$

$$.116 \phi_0 - .096 \phi_1 = 1.0$$

$$-.048 \phi_0 + .116 \phi_1 - .048 \phi_2 = 1.0$$

$$-.048 \phi_1 + .116 \phi_2 - .048 \phi_3 = 1.0$$

$$-.048 \phi_2 + .116 \phi_3 = 1.0$$

Solve for $\phi_0, \phi_1, \phi_2, \phi_3$.

Assume a uniform mesh of 4 intervals.

MATRIX NOTATION

$$\begin{pmatrix} .116 & -.096 & 0 & 0 \\ -.048 & .116 & -.048 & 0 \\ 0 & -.048 & .116 & -.048 \\ 0 & 0 & -.048 & .116 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

A

Solve for $\phi_0, \phi_1, \phi_2, \phi_3$
(fluxes at cell edges)

The resultant 4 x 4 system of equations is easily solved by methods (hopefully) taught in an introductory calculus sequence. However, what if there were 100 equations or 1,000,000 equations (1,000,000 x 1,000,000 matrix!) It is worth discussing the computer methods for solving such systems.

Solution Methods 3 banded

The TRIDIAGONAL MATRIX \underline{A}
CAN be represented AS follows:

$$\underline{A} = \begin{bmatrix} a_0 & b_0 & & & & & \\ c_1 & a_1 & b_1 & & & & \\ & c_2 & a_2 & b_2 & & & \\ & & c_3 & a_3 & b_3 & & \\ & & & & & \ddots & \\ & & & & & & b_{N-2} \\ & & & & & & c_{N-1} & a_{N-1} \end{bmatrix}$$

a_i = DIAGONAL element
IN i^{th} ROW

Tridiagonal matrices are especially easy to solve
(or "invert").

where

$$\begin{aligned} a_0 &= a_{00} \\ b_0 &= a_{01} \\ a_i &= a_{ii}, \quad i=1, 2, \dots, N-1 \\ b_i &= a_{i,i+1}, \quad i=1, 2, \dots, N-2 \\ c_i &= a_{i,i-1}, \quad i=1, 2, \dots, N-1 \end{aligned}$$

FORMAL solution

$$\underline{A}^{-1} \underline{A} \underline{\phi} = \underline{A}^{-1} \underline{S}$$

$$\underline{I} \underline{\phi} = \underline{A}^{-1} \underline{S}$$

↑ INVERSE OF \underline{A}

$$\underline{A}^{-1} \underline{A} = \underline{I}$$

$$\underline{I} \underline{\phi} = \underline{\phi}$$

CAREFUL!

Careful when someone mentions "inverting"
a matrix. Very seldom does one actually calculate an
inverse matrix. One does not need the actual inverse
although the formal solution might imply that that is
the case.

$$\underline{\underline{A}} \underline{\underline{A}}^{-1} = \underline{\underline{A}}^{-1} \underline{\underline{A}} = \underline{\underline{I}}$$

$$\underline{\underline{I}} = \begin{pmatrix} 1 & 0 & 0 & \text{---} & 0 \\ 0 & 1 & 0 & \text{---} & 0 \\ 0 & 0 & 1 & \text{---} & 0 \\ & 0 & & 1 & 0 \\ & & & & 0 & 1 \end{pmatrix}$$

$$\underline{\underline{I}} \underline{\underline{\phi}} = \underline{\underline{\phi}}$$

$$\underline{\underline{\phi}} = \underline{\underline{A}}^{-1} \underline{\underline{S}}$$

↑ "NEVER" SOLVE
FOR $\underline{\underline{A}}^{-1}$, ONLY FOR
 $\underline{\underline{\phi}}$

LECTURE 20

NUMERICAL SOLUTIONS (cont.)

GAUSS ELIMINATION AND ITERATIVE METHODS
TO SOLVE $\underline{A} \underline{x} = \underline{b}$

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 188-193.

EXERCISES:

20.1 Run your code for the following configuration

$$\begin{aligned} N &= 5 \\ a &= 18 \text{ cm} & 2a &= 16 \text{ cm} \\ \sum a &= 1.0 \text{ cm}^{-1} & \Rightarrow 2\tilde{a} &= 20 \text{ cm} \\ D &= 1.0 \text{ cm} \\ S &= 1.0 / \text{cm}^3 \cdot \text{sec} \end{aligned}$$


20.2 Repeat for $N = 10$

20.3 Plot the $N = 5$ and $N = 10$ solutions on a graph along with the analytic solution

$$\phi(x) = \frac{S}{\sum a} \left(1 - \frac{\cosh x/L}{\cosh \tilde{a}/L} \right)$$

or
$$\phi(x) = 1.0 - \frac{\cosh x}{\cosh 10}$$

GAUSS ELIMINATION Solution Method #1

- CAN add or subtract equations or multiples of equations without changing the solution 
- Idea - eliminate terms below the MAIN diagonal by adding multiples of equations together. The subsequent system of equations will be easier to solve.

Gauss elimination is just a systematic procedure for solving a set of algebraic equations by adding and subtracting multiples of equations. It is basically what one would do if faced with 2 or 3 equations to solve.

20-2

FORWARD ELIMINATION -

- eliminate the matrix elements below the diagonal, forming an UPPER TRIANGULAR MATRIX

$$\underline{A}' \underline{\Phi} = \underline{S}'$$

where $\underline{A}' = \begin{pmatrix} a_0' & b_0' & & 0 \\ & a_1' & b_1' & \\ & & \ddots & \ddots \\ 0 & & a_{N-2}' & b_{N-2}' \\ & & & a_{N-1}' \end{pmatrix}$

The systematic procedure has 2 basic steps -- (1) forward elimination and (2) back substitution. This approach is readily implemented on a computer (hence the reason for its popularity).

FORWARD elimination

$$\begin{aligned} \left(\frac{c_1}{a_0}\right) \times [a_0 \phi_0 + b_0 \phi_1 + 0 + \dots] &= S_0 & (0) \\ \boxed{c_1 \phi_0} + a_1 \phi_1 + b_1 \phi_2 &= S_1 & (1) \\ c_2 \phi_1 + a_2 \phi_2 + b_2 \phi_3 &= S_2 & (2) \end{aligned}$$

eliminate this term
by adding $(-\frac{c_1}{a_0}) \times \text{Eq. (0)}$

to Eq. (1):

$$\left[a_1 - \left(\frac{c_1}{a_0}\right)b_0\right] \phi_1 + b_1 \phi_2 = S_1 - \left(\frac{c_1}{a_0}\right)S_0 \quad (1')$$

" a'_1

The details of the steps will now be presented. We leave the 1st equation alone and eliminate ϕ_0 from the second equation. Then ϕ_1 from the third, etc.

So now we have

$$\begin{aligned} a'_0 \phi_0 + b'_0 \phi_1 &= S_0 & (0) \\ \left(-\frac{c_2}{a'_1}\right) \times [a'_1 \phi_1 + b'_1 \phi_2] &= S'_1 & (1') \\ \boxed{c_2 \phi_1} + a_2 \phi_2 + b_2 \phi_3 &= S_2 & (2) \\ & \vdots & \vdots \end{aligned}$$

Eliminate by multiplying
Eq. (1') by $-\frac{c_2}{a'_1}$ and adding
to Eq. (2):

$$\left[a_2 - \left(\frac{c_2}{a'_1}\right)b'_1\right] \phi_2 + b_2 \phi_3 = S_2 - \left(\frac{c_2}{a'_1}\right)S'_1 \quad (2')$$

- This may be continued until the last term below the diagonal (C_{N-1}) is eliminated.
- The general expressions are

$$a_0' = a_0$$

$$a_i' = a_i - \left(\frac{C_i}{a_{i-1}'} \right) b_{i-1} \quad i=1, 2, \dots, N-1$$

$$s_0' = s_0$$

$$s_i' = s_i - \left(\frac{C_i}{a_{i-1}'} \right) s_{i-1}'$$

The student is urged to carry out the algebraic steps leading to these expressions.

Backward substitution

- We can immediately solve the last equation for ϕ_{N-1} :

$$a_{N-1}' \phi_{N-1} = s_{N-1}'$$

$$\therefore \phi_{N-1} = \frac{1}{a_{N-1}'} s_{N-1}'$$

- The next equation is then solved:

$$a_{N-2}' \phi_{N-2} + b_{N-2} \phi_{N-1} = s_{N-2}'$$

$$\phi_{N-2} = \frac{1}{a'_{N-2}} [S'_{N-2} - b_{N-2} \phi_{N-1}]$$

↑ already calculated

etc. Through ϕ_0

• General expression

$$\phi_i = \frac{1}{a'_i} [S'_i - b_i \phi_{i+1}]$$

$$i = N-2, N-3, N-4, \dots, 0$$

Again, the student should verify the algebra.

EXAMPLE FNR Reactor (DARE)

$$\underline{A} \underline{\phi} = \underline{S} \quad \text{where} \quad \underline{S} = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}, \quad \underline{\phi} = \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix}$$

$$\underline{A} = \begin{pmatrix} .116 & -.096 & 0 & 0 \\ \textcircled{-.048} & .116 & -.048 & 0 \\ 0 & \textcircled{-.048} & .116 & -.048 \\ 0 & 0 & \textcircled{-.048} & .116 \end{pmatrix}$$

↑ UNKNOWN

Forward elimination yields

$$\underline{A}' \underline{\phi} = \underline{S}'$$

where

$$\underline{A}' = \begin{pmatrix} .116 & -.096 & 0 & 0 \\ 0 & .07628 & -.048 & 0 \\ 0 & 0 & .08579 & -.048 \\ 0 & 0 & 0 & .08915 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix}$$

$$\underline{S}' = \begin{pmatrix} 1.0 \\ 1.414 \\ 1.890 \\ 2.057 \end{pmatrix}$$

$$\underline{A}' \underline{\phi} = \underline{S}'$$

$$.08915 \phi_3 = 2.057$$

$$\therefore \phi_3 = \frac{2.057}{.08915} = \underline{23.08}$$

$$.08579 \phi_2 - .048 \phi_3 = 1.890$$

$$\phi_2 = 34.94$$

The solution is

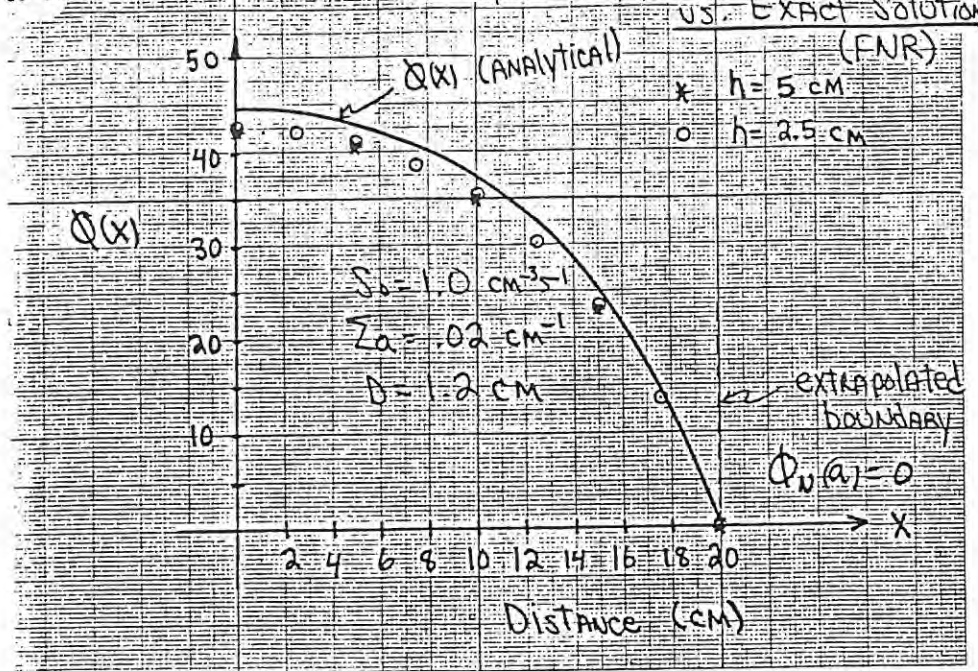
	EXACT*	% difference
0cm $\phi_0 = 42.16$	44.28	4.8%
5cm $\phi_1 = 40.52$	42.75	5.2%
10cm $\phi_2 = 34.94$	37.37	6.5%
15cm $\phi_3 = 23.08$	25.27	8.7%

$$* \text{ FROM } \phi(x) = 50 \left[1 - \frac{\cosh(x/L)}{\cosh(20/L)} \right]$$

$$\text{where } L = \sqrt{\frac{1.2}{.02}} = 7.75 \text{ cm}$$

Note that even with this fairly crude numerical mesh, the relative error is less than 7%.

COMPARISON OF FINITE DIFFERENCE

Iterative Methods toSolve $\underline{A} \underline{\Phi} = \underline{S}$

$$\underline{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1N} \\ a_{21} & a_{22} & & & \\ \vdots & & \ddots & & \vdots \\ a_{N1} & a_{N2} & \dots & \dots & a_{NN} \end{pmatrix}$$

Divide $\underline{A} = \underline{D} + \underline{B}$

where $\underline{D} =$ DIAGONAL PART of \underline{A}

$\underline{B} =$ REST of \underline{A}

Gauss elimination has its drawbacks, including a large number of computations (multiplications, divisions, etc.) which can be expensive for large problems (e.g., 10,000 unknowns) and can require a large amount of computer memory. An alternative is iterative methods.

$$\underline{A} \underline{\phi} = \underline{S} \quad \text{original system}$$

$$\underline{A} = \underline{D} + \underline{B}$$

$$\underline{\phi}^{(0)} = \begin{pmatrix} | \\ | \\ | \end{pmatrix}$$

$$\underline{D} \underline{\phi}^{(m)} = \underline{S} - \underline{B} \underline{\phi}^{(m-1)}$$

• Guess a solution $\underline{\phi}^{(0)}$

$$\underline{D} \underline{\phi}^{(1)} = \underline{S} - \underline{B} \underline{\phi}^{(0)}$$

solve for $\underline{\phi}^{(1)}$

$$\underline{D} \underline{\phi}^{(2)} = \underline{S} - \underline{B} \underline{\phi}^{(1)}$$

⋮

The idea of all iterative methods is to solve a simpler equation (or set of equations) several times, hoping that the solutions will approach the true solution (i.e., converge to the true solution)

m^{th} iteration

$$\underline{D} \underline{\phi}^{(m)} = \underline{S} - \underline{B} \underline{\phi}^{(m-1)}$$

MATRIX x VECTOR
MULTIPLICATION

STOP? $\underline{\phi}^{(m)}$ AND $\underline{\phi}^{(m-1)}$ AGREE
WITHIN SOME PRECISION
(METHOD HAS CONVERGED)

Advantage

- Must solve

$$\underline{D} \underline{\phi}^{(m)} = \underline{Q}^{(m)} = \underline{S} - \underline{B} \underline{\phi}^{(m-1)}$$

where $\underline{Q}^{(m)} = \underline{S} - \underline{B} \underline{\phi}^{(m-1)}$

effective source for m^{th} iteration

$$\begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \quad \begin{matrix} \phi_1 = q_1/a_1 \\ \phi_2 = q_2/a_2 \\ \vdots \end{matrix}$$

$\underline{D} \quad \quad \quad \underline{\phi} \quad \quad \quad \underline{Q}$

Example FNR

$$\underline{A} \underline{\phi} = \underline{S}$$

$$\begin{pmatrix} .116 & -.096 & 0 & 0 \\ -.048 & .116 & -.048 & 0 \\ 0 & -.048 & .116 & -.048 \\ 0 & 0 & -.048 & .116 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

Rewrite with $\underline{A} = \underline{D} + \underline{B}$ for

The m^{th} iteration :

$$\underline{D} \underline{\Phi}^{(m)} = \underline{S} - \underline{B} \underline{\Phi}^{(m-1)}$$

$$\underbrace{\begin{pmatrix} .116 & 0 & 0 & 0 \\ 0 & .116 & 0 & 0 \\ 0 & 0 & .116 & 0 \\ 0 & 0 & 0 & .116 \end{pmatrix}}_{\underline{D}} \begin{pmatrix} \Phi_0^{(m)} \\ \Phi_1^{(m)} \\ \Phi_2^{(m)} \\ \Phi_3^{(m)} \end{pmatrix} = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

$$- \underbrace{\begin{pmatrix} 0 & -.096 & 0 & 0 \\ -.048 & 0 & -.048 & 0 \\ 0 & -.048 & 0 & -.048 \\ 0 & 0 & -.048 & 0 \end{pmatrix}}_{\underline{B}} \begin{pmatrix} \Phi_0^{(m-1)} \\ \Phi_1^{(m-1)} \\ \Phi_2^{(m-1)} \\ \Phi_3^{(m-1)} \end{pmatrix}$$

Initial guess

$$\underline{\Phi}^{(0)} = \begin{pmatrix} \Phi_0^{(0)} \\ \Phi_1^{(0)} \\ \Phi_2^{(0)} \\ \Phi_3^{(0)} \end{pmatrix} \quad \text{eg., } \underline{\Phi}^{(0)} = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

$$\text{Then } \underline{B} \underline{\Phi}^{(0)} = \begin{pmatrix} -.096 \\ -.096 \\ -.096 \\ -.048 \end{pmatrix} \quad \underline{B} = \begin{pmatrix} 0 & -.096 & 0 & 0 \\ -.048 & 0 & -.048 & 0 \\ 0 & -.048 & 0 & -.048 \\ 0 & 0 & -.048 & 0 \end{pmatrix}$$

$$\text{And } \underline{Q}^{(1)} = \underline{S} - \underline{B} \underline{\Phi}^{(0)} = \begin{pmatrix} 1.096 \\ 1.096 \\ 1.096 \\ 1.048 \end{pmatrix}$$

$$\underline{D} = \underline{\Phi}^{(1)} = \begin{pmatrix} 1.096 \\ 1.096 \\ 1.096 \\ 1.048 \end{pmatrix}$$

$$\underline{\Phi}^{(1)} = \begin{pmatrix} 1.096/1.116 \\ 1.096/1.116 \\ 1.096/1.116 \\ 1.048/1.116 \end{pmatrix} = \begin{pmatrix} 9.4483 \\ 9.4483 \\ 9.4483 \\ 9.0345 \end{pmatrix}$$

This method is known
as the Jacobi method

(splitting $\underline{A} = \underline{D} + \underline{B}$)

$$\begin{array}{l} a_{11}\phi_1^{(m)} + a_{12}\phi_2^{(m-1)} + \dots + a_{1N}\phi_N^{(m-1)} = S_1 \\ a_{21}\phi_1^{(m-1)} + a_{22}\phi_2^{(m)} + \dots = S_2 \\ \vdots \\ a_{i1}\phi_1^{(m-1)} + \dots + a_{ii}\phi_i^{(m)} + \dots = S_i \\ \vdots \\ a_{N1}\phi_1^{(m-1)} + \dots + a_{NN}\phi_N^{(m)} = S_N \end{array}$$

Note we have used previous iterates (or guesses) for the off-diagonal terms and put them on the right hand side (RHS) as part of the source term. We then solve the set of trivial algebraic equations by inspection.

Results (FNR) - Jacobi Iteration

X	EXACT $\Phi(X)$	$\Phi^{(0)}$	$\Phi^{(1)}$	$\Phi^{(10)}$	$\Phi^{(30)}$	$\Phi^{(61)}$
0.0	44.28	44.28 1.0	9.448	22.23	35.29	40.78
5.0	42.75	42.75 1.0	9.448	22.16	34.23	39.26
10.0	37.37	37.37 1.0	9.448	20.61	30.08	33.97
15.0	25.27	25.27 1.0	9.034	15.35	20.47	22.56
20.0	0.0	0.0	0.0	0.0	0.0	0.0

MAXIMUM ERROR \rightarrow -
(between succeeding iterations)

26% 5.9% 1%

Note how the Jacobi method has converged within 1% after 61 iterations. Now let us turn to the Gauss-Siedel method, which is a simple modification of the Jacobi method.

Describe by \underline{A} being
split up into a lower TRIANGULAR
MATRIX \underline{L} (with diagonal)

$$\underline{L} = \begin{pmatrix} a_{11} & 0 & 0 & \dots & 0 \\ a_{21} & a_{22} & 0 & \dots & 0 \\ a_{31} & & \dots & \dots & 0 \\ \vdots & & & \dots & \vdots \\ a_{n1} & a_{n2} & \dots & \dots & a_{nn} \end{pmatrix}$$

AND AN UPPER TRIANGULAR
MATRIX \underline{U} (ZERO DIAGONAL)

Gauss-Seidel

Use latest estimate AS
SOON AS it is AVAILABLE :

$$a_{11}\phi_1^{(m)} + a_{12}\phi_2^{(m-1)} + \dots + a_{1N}\phi_N^{(m-1)} = S_1$$

$$a_{21}\phi_1^{(m)} + a_{22}\phi_2^{(m)} + a_{23}\phi_3^{(m-1)} + \dots = S_2$$

$$a_{31}\phi_1^{(m)} + a_{32}\phi_2^{(m)} + a_{33}\phi_3^{(m)} + \dots = S_3$$

$$a_{N1}\phi_1^{(m)} + a_{N2}\phi_2^{(m)} + \dots + a_{NN-1}\phi_{N-1}^{(m)} + a_{NN}\phi_N^{(m)} = S_N$$

With a computer, one would probably solve the set of equations in a systematic order, beginning with the first equation. In that case, one may as well use the latest result as soon as it is available.

$$\underline{U} = \begin{pmatrix} 0 & a_{12} & a_{13} & \dots & a_{1N} \\ 0 & 0 & a_{23} & & a_{2N} \\ \vdots & & 0 & a_{34} & \dots \\ \vdots & 0 & & \ddots & \vdots \\ 0 & & & & 0 \end{pmatrix}$$

iteration: (Guess $\underline{\phi}^{(0)}$)

FOR $m=1, 2, \dots$

solve

$$\underline{\phi}^{(m)} = \underline{S} - \underline{U} \underline{\phi}^{(m-1)}$$

until $\underline{\phi}^{(m)}, \underline{\phi}^{(m-1)}$ agree.

Results (FNR) Gauss-Seidel Iteration

X	exact	$\phi^{(0)}$	$\phi^{(1)}$	$\phi^{(10)}$	$\phi^{(30)}$	$\phi^{(41)}$
	$\phi(x)$					
0.0	44.28	1.0	8.621	32.16	40.99	41.76
5.0	42.75	1.0	9.034	28.44	39.12	40.04
10.0	37.37	1.0	9.034	23.21	33.53	34.46
15.0	25.27	1.0	9.034	15.85	22.08	22.74
MAX ERROR →	—	—	—	32%	3.3%	1%
				26%	5.9%	3.2%

Note we are now within 1% relative error after only 41 iterations, versus 61 iterations for the Jacobi method.

ADVANTAGES

1. NO MORE WORK THAN
JACOBI METHOD

2. FASTER CONVERGENCE
IN GENERAL

(FEWER ITERATIONS TO
OBTAIN CONVERGENCE)

LECTURE 21

DIFFUSION IN MULTIPLYING MEDIA

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 196-198, 202-207.

EXERCISES:

- 21.1. Duderstadt & Hamilton, problem #5-32
- 21.2. Duderstadt & Hamilton, problem #5-36

FISSION SOURCE

$$\nabla \cdot \underline{J}(\underline{r}) + \Sigma_a(\underline{r})\Phi(\underline{r}) = S(\underline{r})$$

\nearrow leakage
 \uparrow absorption
 \uparrow "KNOWN" source

$$\underline{J} = -D(\underline{r})\nabla\Phi(\underline{r}) \leftarrow \text{"diffusion APPROX"}$$

Let us now turn back to the diffusion equation and allow the source to be a fission source. This has a radically different effect on the physical behavior of the system.

The diffusion approximation

$$\underline{J} = -D(\underline{r})\nabla\Phi(\underline{r})$$

combined with the continuity equation yielded the neutron diffusion equation

$$-\nabla \cdot D(\underline{r})\nabla\Phi(\underline{r}) + \Sigma_a(\underline{r})\Phi(\underline{r}) = S(\underline{r}) \quad \text{--- (1)}$$

$\underline{r} \in V$

leakage + absorption = source

Recall our derivation of the diffusion equation and our assumption the source was known. In this case, the source "drives" the system - the system "responds" to the source.

• Given the source $S(\underline{r})$ within V
 and sufficient boundary conditions
 on S (boundary of V), Eq. (1)
 can be solved for $\phi(\underline{r})$.

• Physically - turn on the
 source of neutrons and (after
 the system equilibrates) observe
 the resultant neutron flux $\phi(\underline{r})$

• What if there is no
 given source of neutrons
 except due to fissions
 inside V ?

$$\text{fission source} = \underbrace{\sum_f(\underline{r})\phi(\underline{r})}_{\text{fission rate}} = S_f(\underline{r})$$

(# neutrons/cm³.s) (# fissions/cm³.s)

If there is a fission source, then it will depend
 on the system response. Thus the source and system
 will be coupled in a self-consistent manner.

• Then one might expect
the diffusion equation
to become

$$-\nabla \cdot D(\underline{r}) \nabla \phi(\underline{r}) + \Sigma_a(\underline{r}) \phi(\underline{r}) = \nu \overbrace{\Sigma_f(\underline{r})}^{S_f(\underline{r})} \phi(\underline{r})$$

$\underline{r} \in V$

• Fundamental difference -
 $S_f(\underline{r})$ IS NOT KNOWN

i.e., $S_f(\underline{r})$ depends on $\phi(\underline{r})$

depends on $\phi(\underline{r})$ — UNKNOWN flux
↓
leakage + absorption \neq source

• Possible that the right combination
of $D(\underline{r})$, $\Sigma_a(\underline{r})$, $\nu \Sigma_f(\underline{r})$ (MATERIAL
PROPERTIES) AND the geometry of V
will result in NEUTRON BALANCE

Now it appears we have an indeterminate equation,
hence an unsolvable equation, since the source
is not known. Seems reasonable from a physical
standpoint, though, that there is a source-system
configuration wherein neutron balance is achieved.

- Impractical to shuffle
Through various combinations
of material properties to
attain neutron balance

- Alternative (assume for
convenience constant properties
 $D, \Sigma_a, \nu \Sigma_f$)

Scale the fission source by a
factor λ ,

$$-\nabla \cdot D \nabla \phi + \Sigma_a \phi(\mathbf{r}) = \frac{1}{\lambda} \nu \Sigma_f \phi(\mathbf{r})$$

- For $\lambda = \infty$ $-\nabla \cdot D \nabla \phi + \Sigma_a \phi = \frac{1}{\lambda} \nu \Sigma_f \phi$

$$\frac{1}{\lambda} \times \text{fission source} = \frac{1}{\lambda} \times S_F(\mathbf{r}) = 0$$

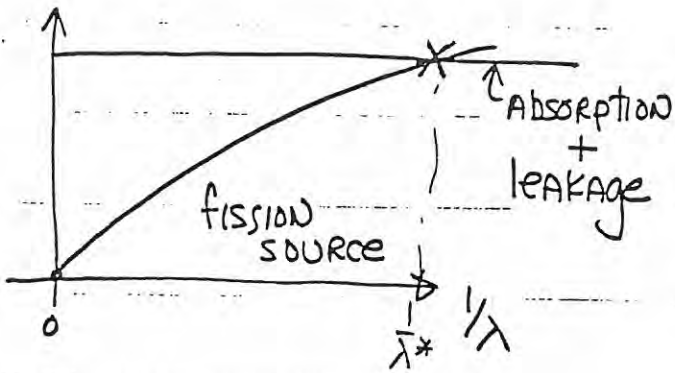
leakage + absorption > source

- Decrease λ , source will increase

- At some λ , we will have

$$\text{leakage} + \text{absorption} = \text{source}$$

The idea that for some value for the source,
neutron balance will be achieved.



$$-\nabla \cdot D \nabla \phi + \Sigma_a \phi = \frac{1}{\lambda} \nu \Sigma_f \phi$$

largest λ such that neutron balance is attained

Statement of problem - find

the maximum λ and associated flux $\phi(\underline{x})$ to solve

$$-\nabla \cdot D \nabla \phi(\underline{x}) + \Sigma_a \phi(\underline{x}) = \frac{1}{\lambda} \nu \Sigma_f \phi(\underline{x})$$

$$\underline{x} \in V$$

mathematics (plus b.c. on S)

↓
 • Well-posed problem with a maximum $\lambda > 0$ and positive flux $\phi(\underline{x})$

Mathematically - known as an eigenvalue problem. The eigenvalue λ and the flux $\phi(\underline{x})$ correspond to one another.

Interpretation of λ

$$-\nabla \cdot D \nabla \phi + \Sigma_a \phi = \frac{1}{\lambda} \nu \Sigma_f \phi \quad \forall \Omega \in V$$

$$\iiint_V [-\nabla \cdot D \nabla \phi + \Sigma_a \phi] d^3r = \frac{1}{\lambda} \iiint_V \nu \Sigma_f \phi d^3r$$

$$\iiint_V -\nabla \cdot D \nabla \phi d^3r = - \oint_S D(\mathbf{r}_s) \nabla \phi(\mathbf{r}_s) \cdot \hat{\mathbf{n}}_s dA = \mathcal{L}$$

$$\iiint_V \Sigma_a \phi d^3r = A \text{ (Abs Rate)} \quad \begin{array}{l} \text{leakage} \\ \text{RATE} \end{array}$$

$$\text{And } \iiint_V \nu \Sigma_f \phi d^3r = S_F V = P$$

where \mathcal{L} = leakage rate ($\frac{\# \text{ neutrons leaking out}}{\text{second}}$)

A = absorption rate ($\frac{\# \text{ neutrons absorbed}}{\text{second}}$)

P = production rate ($\frac{\# \text{ neutrons produced}}{\text{second}}$)

$$\therefore \lambda = \frac{P}{\mathcal{L} + A}$$

Recall from Lecture #10
that the multiplication factor k ,

$$k = \epsilon p \eta f P_{FNL} P_{TNL}$$

could be expressed as

$$k = \frac{P}{\lambda + A} = \lambda$$

$$\therefore \boxed{\lambda = k}$$

Scaling factor is the
multiplication factor k

$$-\nabla \cdot D \nabla \phi(\mathbf{r}) + \sum_a \phi(\mathbf{r}) = \frac{1}{k} \nu \sum_f \phi(\mathbf{r})$$

$$\mathbf{r} \in V$$

$$\text{leakage} + \text{absorption} = \frac{1}{k} \times \text{fission source}$$

(i) fission source too large, $k > 1$ to
force balance

(ii) fission source too small, $k < 1$ to
force balance

$$-\nabla \cdot D(\underline{r}) \nabla \phi(\underline{r}) + \Sigma_a(\underline{r}) \phi(\underline{r}) = \frac{1}{k} \nu \Sigma_f(\underline{r}) \phi(\underline{r}), \quad \underline{r} \in V \quad (*)$$

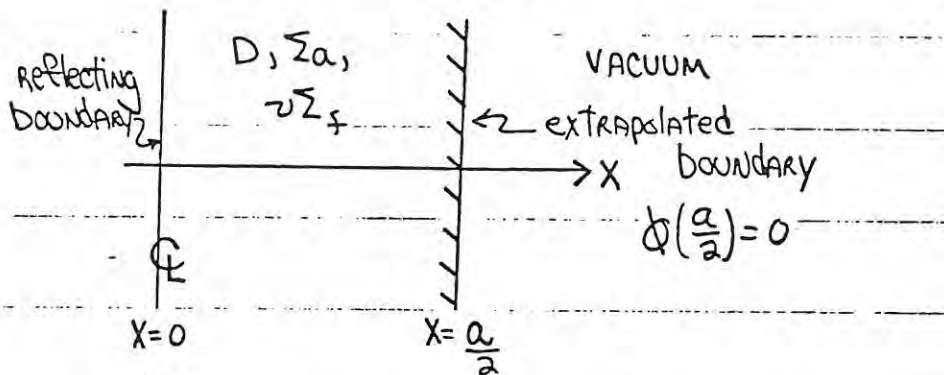
subject to VACUUM

b.c. $\phi(\underline{r}_s) = 0$ on S

(OR possibly reflecting b.c. also)

- Solve (*) for multiplication factor k AND corresponding flux $\phi(\underline{r})$ "eigenfunction"
"eigenvalue" $(\phi_k(\underline{r}))$

The Critical Slab Reactor (BARE)



$$-D \frac{d^2 \phi}{dx^2} + \Sigma_a \phi(x) = \frac{1}{k} \nu \Sigma_f \phi(x), \quad 0 \leq x \leq \frac{a}{2}$$

$$\left. \frac{d\phi}{dx} \right|_{x=0} = 0 \quad \phi\left(\frac{a}{2}\right) = 0$$

$$\frac{d^2\phi}{dx^2} + \frac{1}{D} \left[\frac{1}{k} v \Sigma_f - \Sigma_a \right] \phi(x) = 0$$

(i) k is NOT KNOWN

(ii) Homogeneous equation

$\phi(x)$ is A solution

$d\phi(x)$ " " " where

α is A CONSTANT

Define $B^2 = \frac{1}{D} \left[\frac{1}{k} v \Sigma_f - \Sigma_a \right]$

$$\frac{d^2\phi}{dx^2} + B^2 \phi(x) = 0 \quad (2)$$

↑ still UNKNOWN

• calculate $B^2 \Rightarrow k$ is KNOWN

$$\left. \frac{d\phi}{dx} \right|_{x=0} = 0 \quad (2a)$$

$x=0$

$$\phi\left(\frac{a}{2}\right) = 0 \quad (2b)$$

Equation (2) is simply a convenient manipulation of (1).

Assume solutions $\left(\frac{d^2\phi}{dx^2} + B^2\phi = 0 \right)$

$$\phi(x) = A_1 \cos Bx + A_2 \sin Bx$$

$$(a) \Rightarrow \left. \frac{d\phi}{dx} \right|_{x=0} = 0 \Rightarrow \boxed{A_2 = 0}$$

$$\therefore \phi(x) = A \cos Bx$$

$$(b) \Rightarrow \phi\left(\frac{a}{2}\right) = A \cos B\frac{a}{2} = 0$$

$$\text{OR } \boxed{\cos B\frac{a}{2} = 0} \quad (3)$$

Note the boundary condition led to the condition (3).

$$\cos \theta = 0 \Rightarrow \theta = \frac{\pi}{2}, 3\frac{\pi}{2}, \dots, (2m+1)\frac{\pi}{2}, \dots$$

$$m = 0, 1, 2, \dots$$

$$\therefore \cos\left(\frac{Ba}{2}\right) = 0$$

$$\text{if } B\frac{a}{2} = (2m+1)\frac{\pi}{2} \quad m = 0, 1, 2, \dots$$

$$\text{OR } B_m^2 = (2m+1)^2 \left(\frac{\pi}{a}\right)^2 \quad m = 0, 1, 2, \dots$$

Appears to be an infinite number of eigenvalues, since each B_m^2 gives a different k :

$$k_m = \frac{v \Sigma_f}{\Sigma_a + DB_m^2}$$

$$B_m^2 = \frac{1}{D} \left[\frac{1}{k_m} v \Sigma_f - \Sigma_a \right]$$

Wanted the largest
factor k

$$B_m^2 = (2m+1)^2 \left(\frac{\pi}{a} \right)^2$$

$$B_0^2 < B_1^2 < B_2^2 < \dots$$

$$k_0 > k_1 > k_2 > \dots$$

$$k = k_0 = \frac{v \Sigma_f}{\Sigma_a + DB^2}$$

$$B^2 = \left(\frac{\pi}{a} \right)^2$$

$a = \text{width}$

$$k = \frac{\nu \Sigma_f}{\Sigma_a + DB^2}$$

$$B^2 = \left(\frac{\pi}{a}\right)^2 \quad \text{where } a = \text{width of slab}$$

$$\text{Then } \Phi(x) = A \cos Bx$$

is the neutron flux
corresponding to k

NOTATION: $\Phi(x)$ is the "FUNDAMENTAL Mode"

Normally denote the flux corresponding to the largest eigenvalue as the "Fundamental Mode"

LECTURE 22

CRITICALITY CALCULATIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 207-211

EXERCISES:

22.1 Duderstadt & Hamilton, problem #5-34

22.2 Duderstadt & Hamilton, problem #5-35

Bare Slab Reactor of width a

• Eigenvalue
(multiplication factor) $k = \frac{\nu \Sigma_f}{\Sigma_a + DB^2}$

$$B^2 = \left(\frac{\pi}{a}\right)^2$$

$$\frac{d^2\phi}{dx^2} + B^2\phi(x) = 0$$

$$0 \leq x \leq \frac{a}{2}$$

• Corresponding flux

$$\phi(x) = A \cos Bx$$

$\phi(x) \quad \uparrow ?$

How can we calculate the factor A when any A will suffice to solve the diffusion equation? The answer is we have yet to impose the specified power level.

22-2

$$\text{FISSION RATE} = \underbrace{2}_{\text{AREA}} \underbrace{A}_{\uparrow} \int_0^{a/2} \Sigma_f(x) \phi(x) dx$$

$$\text{POWER} = \underbrace{\mathcal{K}}_{\uparrow} \times 200 \frac{\text{MeV}}{\text{FISSION}} \times \text{FISSION RATE} = Q$$

(CONVERSION FACTOR) MW

$$Q = 2 \cdot A \cdot \mathcal{K} \cdot 200 \int_0^{a/2} \Sigma_f \phi(x) dx$$

$$= 2 \cdot A \cdot \mathcal{K} \cdot 200 \cdot \underbrace{A}_{\text{"A cos Bx"}} \cdot \frac{1}{B} \sin Bx \Big|_0^{a/2} = Q$$

$$A = \frac{\pi Q}{400K \underbrace{Aa}_{V} \Sigma_f} \quad B = \pi/a$$

$$A = \frac{\pi Q}{400K V \Sigma_f}$$

$V = \text{volume of the REACTOR (cm}^3\text{)}$
 $Q = \text{power of the REACTOR (MWth)}$

$$\phi(x) = \frac{\pi Q}{400K V \Sigma_f} \cos Bx \quad \text{1-D bare slab reactor}$$

This is the analytical flux for a 1-D bare slab reactor with a total thermal power Q .

22-4 Criticality Condition

$$k = \frac{\nu \Sigma_f}{\Sigma_a + DB^2} = 1 \quad \text{FOR CRITICAL REACTOR}$$

$$\therefore \nu \Sigma_f = \Sigma_a + DB^2$$

$$\text{OR } B^2 = \frac{\nu \Sigma_f - \Sigma_a}{D}$$

FOR A CRITICAL REACTOR
 where $B^2 = \left(\frac{\pi}{a}\right)^2$
 (s/lb)

note: LHS depends on geometry
 RHS depends on MATERIAL properties

Define $B_m^2 \equiv \frac{\nu \Sigma_f - \Sigma_a}{D}$ "MATERIAL buckling"

What if we wanted to know the conditions for which the reactor were "critical"?

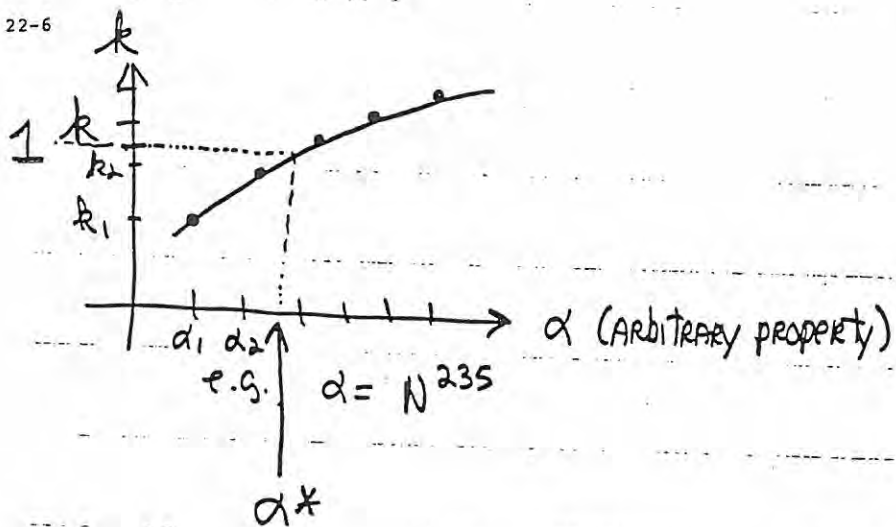
B^2 denoted "geometric buckling"

criticality : $B^2 = B_m^2 \Rightarrow k = 1$

geometric buckling = material buckling

- Yields the proper combination of geometry AND material properties to attain criticality with a bare 1-D slab reactor

22-6



One might expect the multiplication factor to be an increasing function of the ${}^{235}_{92}\text{U}$ loading. At some specific loading we should find $k = 1$.

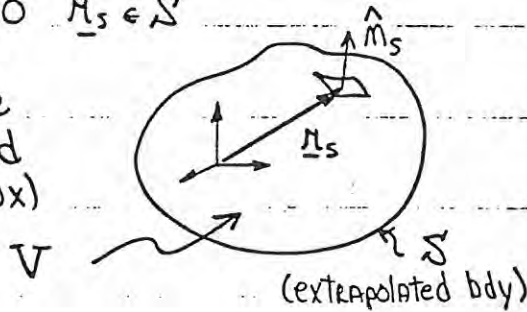
General Geometry

eigenvalue problem

$$-\nabla \cdot D(\underline{x}) \nabla \Phi(\underline{x}) + \Sigma_a(\underline{x}) \Phi(\underline{x}) = \frac{1}{k} \nu \Sigma_f(\underline{x}) \Phi(\underline{x}), \quad \underline{x} \in V$$

$$\Phi(\underline{x}_s) = 0, \quad \underline{x}_s \in \mathcal{S}$$

goal - find eigenvalue k and associated eigenfunction (flux) $\Phi(\underline{x})$



The criticality problem can also be posed in other geometries.

- Assume uniform composition,

$$\nabla^2 \Phi(\underline{x}) + B^2 \Phi(\underline{x}) = 0, \quad \underline{x} \in V \quad (1)$$

$$\Phi(\underline{x}_s) = 0, \quad \underline{x}_s \in \mathcal{S}$$

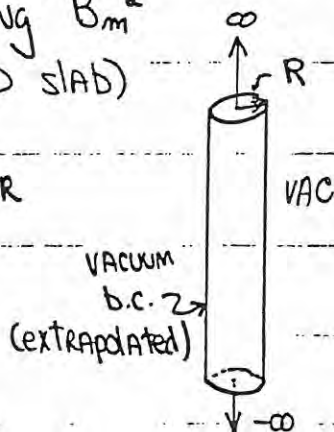
where $B^2 = \frac{1}{D} \left[\frac{1}{k} \nu \Sigma_f - \Sigma_a \right]$

- Eq. (1) is known as the Helmholtz equation and has been solved for many different geometries. The end

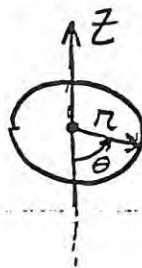
result is a relation between
 the geometric buckling B^2
 (different for slab vs. sphere)
 and the material buckling B_m^2
 (as in the case of the 1-D slab)

$$B^2 = B_m^2$$

EXAMPLE infinite cylinder
 of radius R



Helmholtz Equation
 in Cylindrical Coordinates



$$\Phi(r) = \Phi(r) \quad (\text{NOT ON } z \text{ OR } \theta)$$

$$\frac{1}{r} \frac{d}{dr} r \frac{d\Phi}{dr} + B^2 \Phi(r) = 0, \quad 0 \leq r \leq R$$

$$\Phi(R) = 0 \quad B^2 = \frac{1}{D} \left[\frac{1}{k} \nu_f - \Sigma_a \right]$$

$$\text{Solution: } \left(\Phi_m(r) = A J_0 \left(\frac{\nu_m r}{R} \right) \right)$$

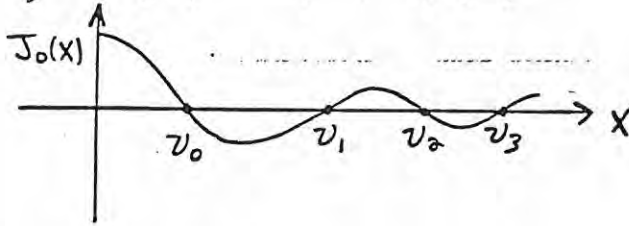
Instead of $\cos Bx$ for slab geometry, one gets $J_0 \left(\frac{\nu_m r}{R} \right)$
 for cylindrical geometry.

where $B_0^2 < B_1^2 < B_2^2 \dots$

$$B_m^2 = \left(\frac{v_m}{R}\right)^2 \quad m=0, 1, 2, \dots$$

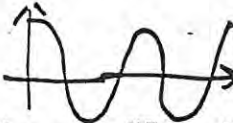
AND v_m is the $(m+1)^{\text{th}}$ zero of the Bessel function $J_0(x)$ Bessel function

i.e., $J_0(v_m) = 0$, $m=0, 1, 2, \dots$



Don't be frightened by Bessel functions!
They are similar to our friends the trigonometric functions $\sin x$ or $\cos x$.

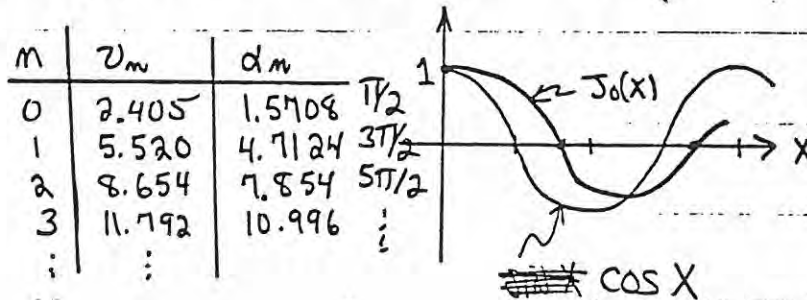
22-12

$J_0(x)$ is similar to $\cos x$: 

• $\cos x = 0$ AT $x = \alpha_m$, $m=0, 1, 2, \dots$

— where $\alpha_m = (m+1)\frac{\pi}{2}$
is the $(m+1)^{\text{th}}$ zero of $\cos x$

• $J_0(x) = 0$ AT $x = v_m$, $m=0, 1, 2, \dots$



Largest $k \Rightarrow$ smallest B_m^2

$$\therefore k = \frac{v \Sigma_f}{\Sigma_a + DB^2}$$

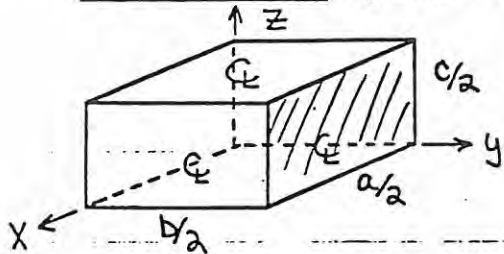
where $B^2 = B_0^2 = \left(\frac{z_0}{R}\right)^2$

(compare with $B^2 = \left(\frac{\pi}{a}\right)^2$ for slab
of width a)

criticality condition ($k=1$): for infinite cyl

$$B_m^2 = B^2 \quad \text{OR} \quad \boxed{\frac{v \Sigma_f - \Sigma_a}{D} = \left(\frac{v_0}{R}\right)^2} \quad k=1$$

3-D Block (sides a, b, c)



SYMMETRY ABOUT
 x, y, z AXES
(Solve for $\frac{1}{8}$ CORE
ONLY)

$$\nabla^2 \phi + B^2 \phi = 0$$

$$B^2 = -\frac{1}{D} \left[\frac{1}{R} v \Sigma_f - \Sigma_a \right]$$

$$\phi(\underline{r}) = \phi(x, y, z)$$

$$\phi\left(\frac{a}{2}, y, z\right) = 0$$

$$\phi\left(x, \frac{b}{2}, z\right) = 0$$

$$\phi\left(x, y, \frac{c}{2}\right) = 0$$

extrapolated
BOUNDARY CONDITIONS

Define the B^2 terms as before

$$\text{Symmetry} \Rightarrow \underline{J} \cdot \hat{n} = 0$$

$$\nabla \Phi \cdot \hat{n} = 0 \text{ AT } x=0 \text{ PLANE}$$

$$\text{IS } \nabla \Phi \cdot \hat{e}_x = \left. \frac{\partial \Phi}{\partial x} \right|_{x=0} = 0 \quad \left(\nabla \Phi = \frac{\partial \Phi}{\partial x} \hat{e}_x + \frac{\partial \Phi}{\partial y} \hat{e}_y + \frac{\partial \Phi}{\partial z} \hat{e}_z \right)$$

$$\text{AT } y=0 \Rightarrow \left. \frac{\partial \Phi}{\partial y} \right|_{y=0} = 0$$

$$\left. \frac{\partial \Phi}{\partial z} \right|_{z=0} = 0$$

$$\nabla^2 \Phi = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} \quad \nabla^2 \Phi + B^2 \Phi = 0$$

\therefore Helmholtz equation becomes

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} + B^2 \Phi(x, y, z) = 0 \quad (1)$$

+ b.c.

Solution - [SEPARATION OF VARIABLES]

$$\text{Assume } \Phi(x, y, z) = X(x) Y(y) Z(z)$$

AND substitute into (1) AND divide by $\Phi(x, y, z)$:

• But now the b.c. become

$$X\left(\frac{a}{2}\right) = 0 \quad Y\left(\frac{b}{2}\right) = 0 \quad Z\left(\frac{c}{2}\right) = 0 \quad \text{- extrapolated b.c.}$$

$$\left. \frac{dX}{dx} \right|_{x=0} = 0 \quad \left. \frac{dY}{dy} \right|_{y=0} = 0 \quad \left. \frac{dZ}{dz} \right|_{z=0} = 0 \quad \text{- symmetry}$$

• Now have 3 eigenvalue problems identical to the 1D slab problem,

$$\left[\frac{d^2\phi}{dx^2} + \beta^2 \phi(x) = 0 \right] \quad \left[\left. \frac{d\phi}{dx} \right|_{x=0} = 0, \phi\left(\frac{a}{2}\right) = 0 \right]$$

$$\underbrace{\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2}}_{\substack{\text{function} \\ \text{of } x \text{ only} \\ -\alpha^2}} + \underbrace{\frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2}}_{\substack{y \text{ only} \\ -\beta^2}} + \underbrace{\frac{1}{Z(z)} \frac{d^2 Z(z)}{dz^2} + B^2}_{\substack{z \text{ only} \\ \text{CONSTANT} \\ -\gamma^2}} = 0$$

Then each term must equal a constant

$$\left. \begin{aligned} \therefore \frac{d^2 X}{dx^2} &= -\alpha^2 X(x) \\ \frac{d^2 Y}{dy^2} &= -\beta^2 Y(y) \\ \frac{d^2 Z}{dz^2} &= -\gamma^2 Z(z) \end{aligned} \right\} \alpha^2 + \beta^2 + \gamma^2 = B^2$$

$$\therefore X_i(x) = A_1 \cos d_i x \quad A \cos Bx$$

$$\text{where } d_i^2 = (2i+1)^2 \left(\frac{\pi}{a}\right)^2, \quad i=0,1,2,\dots$$

$$\cdot Y_j(y) = A_2 \cos \beta_j y$$

$$\text{where } \beta_j^2 = (2j+1)^2 \left(\frac{\pi}{b}\right)^2, \quad j=0,1,2,\dots$$

$$\cdot Z_k(z) = A_3 \cos \gamma_k z$$

$$\text{where } \gamma_k^2 = (2k+1)^2 \left(\frac{\pi}{c}\right)^2, \quad k=0,1,2,\dots$$

$$\text{But } \Phi(x,y,z) = X(x)Y(y)Z(z)$$

\therefore The general homogeneous solution will depend on each of the indices

$i, j,$ and k : $A_1 A_2 A_3$

$$\Phi_{ijk}(x,y,z) = A X_i(x) Y_j(y) Z_k(z)$$

$$\text{or } \Phi_{ijk}(x,y,z) = A \cos d_i x \cos \beta_j y \cos \gamma_k z$$

Φ_{ijk} is a solution to (1) which satisfies the boundary conditions

$$\text{Since } B^2 = \alpha^2 + \beta^2 + \gamma^2$$

Then corresponding to $d_{ijk}(x, y, z)$

$$B_{ijk}^2 = \alpha_i^2 + \beta_j^2 + \gamma_k^2$$

$$k_{ijk} = \frac{v \Sigma_f}{\Sigma a + D B_{ijk}^2}$$

$$k_{ijk}$$



LARGEST

$$\frac{v \Sigma_f}{\Sigma a + D B_{ijk}^2}$$



SMALLEST

$$i=0$$

$$j=0$$

$$k=0$$

The smallest B_{ijk}^2 corresponds
to $i=j=k=0$.

Define $B^2 = \text{MINIMUM } B_{ijk}^2$

then $B^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$ geometric buckling

is Then the largest eigenvalue for a block with sides a, b, c

$$k = \frac{\nu \Sigma_f}{\Sigma_a + DB^2}$$

LECTURE 23

CRITICALITY CALCULATIONS (cont.)

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 211-214.

EXERCISES:

- 23.1. Duderstadt & Hamilton, problem #5-37
- 23.2. Duderstadt & Hamilton, problem #5-38
- 23.3. Use your computer code from the problem set with Lectures #19-20 and repeat the reflected reactor calculations (PWR and FNR) presented in the lecture. Try a few different mesh sizes and reflector thicknesses.

Reactor Criticality Problem

• Loss rate (absorption + leakage) is a function of $\Phi(\underline{r})$

• Production rate (fissions)

is also a function of $\Phi(\underline{r})$

$$\nu \Sigma_f(\underline{r}) \Phi(\underline{r})$$

do not have $S(\underline{r})$

23-2

• Neutron Balance (steady-state)

$$\text{Loss} = \text{Production}$$

• Mathematically

$$-\nabla \cdot D(\underline{r}) \nabla \Phi(\underline{r}) + \Sigma_a(\underline{r}) \Phi(\underline{r}) = \nu \Sigma_f(\underline{r}) \Phi(\underline{r})$$

$$\underline{r} \in V$$

$$\Phi(\underline{r}_s) = 0, \underline{r} \in S$$

(assume extrapolated b.c.)

CANNOT GUARANTEE
A solution exists
(other than $\Phi(\underline{r}) = 0$)
to this equation

Alternative approach - scale

The fission source by
 a parameter λ and find
 the largest λ (and corresponding
 $\Phi(x)$) such that

$$-\nabla \cdot D(x) \nabla \Phi(x) + \Sigma_a(x) \Phi(x) = \frac{1}{\lambda} \nu \Sigma_f(x) \Phi(x), \quad x \in V$$

$$\Phi(x_s) = 0, \quad x_s \in S$$

Mathematically - an eigenvalue problem

• Have shown that λ is the
 multiplication factor k

• Assume constant material
 properties and divide by $-D$:

$$\boxed{+\nabla^2 \Phi(x) + B^2 \Phi(x) = 0 \quad x \in V} \quad \text{Helmholtz Equation}$$

$$\text{subject to: } \Phi(x_s) = 0 \quad x_s \in S \quad (*)$$

where $B^2 = \frac{1}{D} \left[\frac{1}{k} \nu \Sigma_f - \Sigma_a \right]$

Equation (*) has solutions only for certain values of B^2 . These B^2 yield a value for k ,

$$k = \frac{-\nu \Sigma_f}{\Sigma_a + DB^2}$$

AND SINCE WE WANT THE LARGEST k

THIS MEANS THE SMALLEST B^2 .

definition - $B_g^2 = \text{geometric buckling}$

$B_g^2 \equiv$ MINIMUM B^2 of the Helmholtz equation

$$\nabla^2 \phi + B^2 \phi(\underline{r}) = 0, \underline{r} \in V$$

$$\phi(\underline{r}_s) = 0, \underline{r}_s \in S$$

(Note B_g^2 is a function of geometry only)

MATERIAL Buckling

$$B_m^2 \equiv \frac{1}{D} (\nu \Sigma_f - \Sigma_a) \quad B^2 \text{ with } k=1$$


$$\text{CRITICALITY} \Rightarrow B_g^2 = B_m^2$$

The geometric buckling is the smallest eigenvalue of the Helmholtz equation and is a function of geometry only.

The material buckling is a function of composition only.

SUMMARY of Solutions to the Critical Problem

SLAB

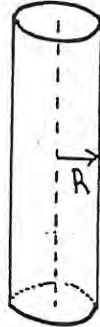


geometric buckling = $(\frac{\pi}{a})^2$

fundamental mode
(the flux profile) = $\cos(\frac{\pi x}{a})$

$\phi(x)$ →

Infinite
Cylinder

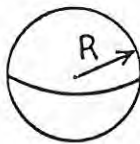


geometric buckling
 $B_g^2 = (\frac{v_0}{R})^2$

fundamental mode
 $\phi(r) = J_0(\frac{v_0 r}{R})$

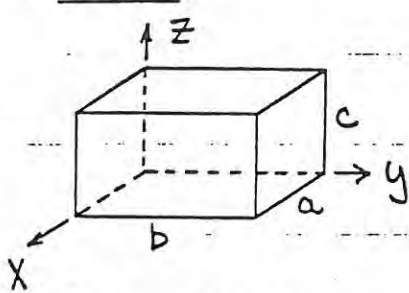
$$\nabla^2 \phi(r) + B^2 \phi(r) = 0$$

Sphere



$B_g^2 = (\frac{\pi}{R})^2$

$\phi(r) = \frac{1}{r} \sin(\frac{\pi r}{R})$

Block

$$B^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$$

$$\Phi(x, y, z) = \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{b}\right) \cos\left(\frac{\pi z}{c}\right)$$

Finite Cylinder

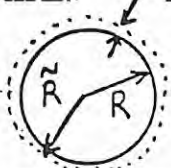
$$B^2 = \left(\frac{\nu_0}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$$

$$\Phi(r, z) = J_0\left(\frac{\nu_0 r}{R}\right) \cos\left(\frac{\pi z}{H}\right)$$

Application - MINIMUM
CRITICAL MASS FOR A
sphere of some
fissile MATERIAL F

$$\tilde{R} = R + 2D$$

$$s = 2D$$



criticality \Rightarrow production = loss

$$k = 1$$

$$B_g^2 = B_m^2$$

For a sphere, the lowest B^2
of the Helmholtz equation = $\left(\frac{\pi}{\tilde{R}}\right)^2 = B_g^2$

- CAUTION - have always assumed that outside dimensions were extrapolated values. But in this case we want the physical MASS \therefore we should differentiate between the two values

$$\tilde{R} = R + 2D$$

• MATERIAL buckling $B_g^2 = \left(\frac{\pi}{R}\right)^2 = B_m^2$

$$B_m^2 = \frac{1}{D} [v\Sigma_f - \Sigma_a] \quad \uparrow \text{calculate (given)}$$

$$\Sigma_a = NF \sigma_a$$

$$v\Sigma_f = NF v\sigma_f$$

$$B_m^2 = \frac{1}{D} [v\Sigma_f - \Sigma_a]$$

$$B_g^2 = B_m^2$$

$$\left(\frac{\pi}{R}\right)^2 = \frac{NF}{D} [v\sigma_f - \sigma_a]$$

$$NF = \left(\frac{D}{v\sigma_f - \sigma_a}\right) \left(\frac{\pi}{R}\right)^2 \quad \begin{array}{l} \# \text{ density} \\ \#/\text{cm}^3 \end{array}$$

$$\boxed{\text{CRITICAL MASS} = NF \times \frac{4}{3}\pi R^3 \times \left(\frac{A_F}{A}\right)}$$

$A_F = \text{ATOMIC MASS}$

$$A = 6.02 \times 10^{23}$$

Reflected Reactors

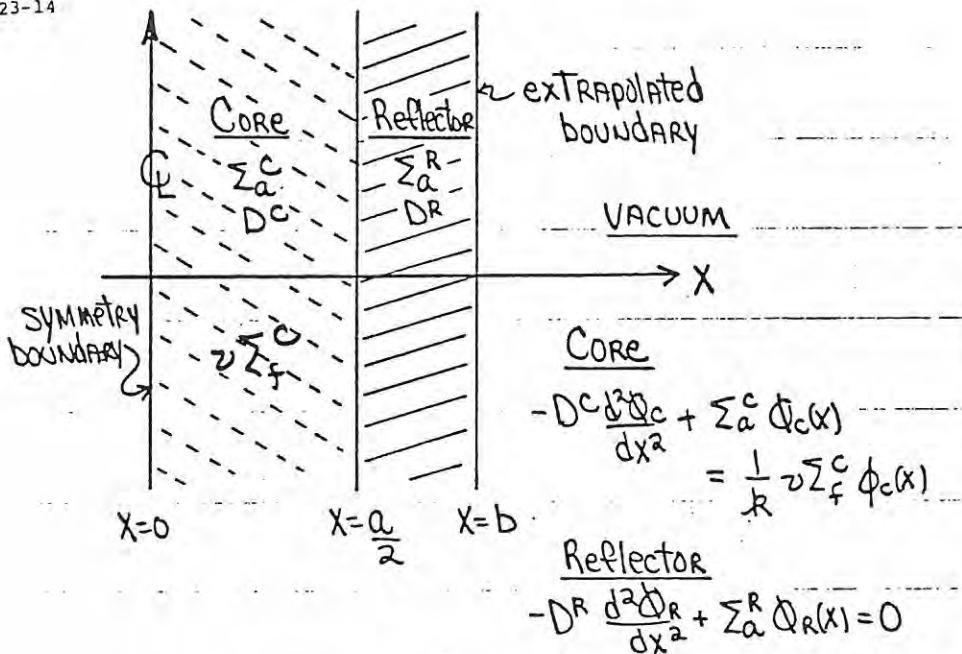
Helmholtz equation

$$\left. \begin{aligned} \nabla^2 \phi(\underline{r}) + B^2 \phi(\underline{r}) &= 0, \quad \underline{r} \in V \\ \phi(\underline{r}_s) &= 0, \quad \underline{r}_s \in S \end{aligned} \right\} \begin{array}{l} \text{have solved} \\ \text{for homogeneous} \\ \text{domains } \cup \\ \text{(slab, sphere, etc.)} \end{array}$$

Consider the solution to the Helmholtz equation for a two-region (reflected reactor) configuration

Now we consider a more realistic problem - a two-region reactor (e.g., core + reflector).

23-14



Boundary Conditions

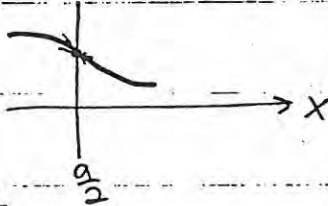
$$X=0: \left. \frac{d\phi_c}{dx} \right|_{X=0} = 0 \text{ (symmetry)}$$

~~$$X=b: \phi_R(b) = 0$$~~
$$X=b: \phi_R(b) = 0 \text{ extrapolated b.c.}$$

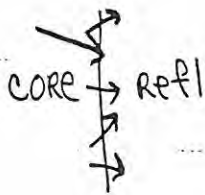
Interface Conditions ($X = \frac{a}{2}$)

$$\phi_c\left(\frac{a}{2}\right) = \phi_R\left(\frac{a}{2}\right)$$

$$-D_c \left. \frac{d\phi_c}{dx} \right|_{X=\frac{a}{2}} = -D_R \left. \frac{d\phi_R}{dx} \right|_{X=\frac{a}{2}}$$



- MANY solutions $\phi_c(x)$ corresponding to the VARIOUS B_c
- $\phi_c(x)$ will depend on the REFLECTOR MATERIAL properties
- $-D_R \frac{d^2\phi_R}{dx^2} + \Sigma_a^R \phi_R(x) = 0, \frac{a}{2} \leq x \leq b$



VIEW THIS AS A SOURCE problem, The source being the IN-leakage from the core

- Rearrange core equation as before,
- $$-D^c \frac{d^2 \phi_c}{dx^2} + \Sigma_a^c \phi_c(x) = \frac{1}{k} \nu \Sigma_f^c(x) \phi_c(x)$$

$$\frac{d^2 \phi_c}{dx^2} + B_c^2 \phi_c(x) = 0, \quad 0 \leq x \leq a/2$$

$$\text{where } B_c^2 = \frac{1}{D^c} \left[\frac{1}{k} \nu \Sigma_f^c - \Sigma_a^c \right]$$

(Material buckling for the core)

- For the reflector,

if $k=1$

$$-\frac{d^2 \phi_R}{dx^2} + \frac{1}{L_R^2} \phi_R(x) = 0, \quad \frac{a}{2} \leq x \leq b$$

$$\text{where } L_R^2 = \left(D^R / \Sigma_a^R \right)$$

Solution

Core $0 \leq x \leq a/2$

$$\phi_c(x) = A_1 \cos B_c x + A_2 \sin B_c x$$

$$\left. \frac{d\phi_c}{dx} \right|_{x=0} = 0 \Rightarrow \boxed{A_2 = 0}$$

$$\therefore \phi_c(x) = A_1 \cos B_c x$$

Reflector $\frac{a}{2} \leq x \leq b$

$$\phi_R(x) = A_3 \cosh\left(\frac{x}{L_R}\right) + A_4 \sinh\left(\frac{x}{L_R}\right)$$

$$\phi_R(x) = A_5 \sinh\left(\frac{b-x}{L_R}\right)$$

$$\phi_R(b) = 0$$

$$\left. \begin{aligned} \phi_C(x) &= A_1 \cos B_C x \\ \phi_R(x) &= A_5 \sinh\left(\frac{b-x}{L_R}\right) \end{aligned} \right\} \begin{array}{l} \text{2 interface} \\ \text{cond at} \\ x = \frac{a}{2} \end{array}$$

INTERFACE CONDITIONS

$$(i) \phi_C\left(\frac{a}{2}\right) = \phi_R\left(\frac{a}{2}\right)$$

$$\Rightarrow A_1 \cos\left(B_C \frac{a}{2}\right) = A_5 \sinh\left(\frac{b - \frac{a}{2}}{L_R}\right) \quad (1)$$

$$(ii) -D_C \frac{d\phi_C}{dx} \Big|_{x=\frac{a}{2}} = -D_R \frac{d\phi_R}{dx} \Big|_{x=\frac{a}{2}}$$

$$\Rightarrow D_C B_C A_1 \sin\left(\frac{B_C a}{2}\right) = D_R \frac{1}{L_R} A_5 \cosh\left(\frac{b - \frac{a}{2}}{L_R}\right) \quad (2)$$

- Divide Eq. (2) by Eq. (1),

$$D^c B_c \tan\left(\frac{B_c a}{2}\right) = \frac{D^R}{L_R} \coth\left(\frac{b - \frac{a}{2}}{L_R}\right) \quad (†)$$

$$w = b - \frac{a}{2} \quad \text{width of reflector}$$

- REARRANGE,

$$\frac{B_c a}{2} \tan\left(\frac{B_c a}{2}\right) = \left(\frac{D^R}{D^c}\right) \left(\frac{a}{2L_R}\right) \coth\left(\frac{w}{L_R}\right) \quad (*)$$

Given the geometry (a and w)
and the MATERIAL properties (D^R, D^c, L_R)
Eq. (*) is AN EQUATION FOR THE ALLOWABLE B_c

Solution of (*)

Observation - for a bare core, the
allowable values for B
satisfied

$$\cos\left(\frac{Ba}{2}\right) = 0$$

This could be solved by
inspection,

$$B_m^2 = (2m+1)^2 \frac{\pi^2}{a^2} \quad m=0,1,2,\dots$$

(*) isn't so easy!

The simple criticality condition for the bare reactor
becomes quite complicated for the reflected reactor.
(Think of the complications for a real commercial reactor).

Define

$$X = \frac{B_c a}{2}$$

$$C = \frac{D^R}{D_c} \left(\frac{a}{2L_R} \right) \coth\left(\frac{\omega}{L_R}\right)$$

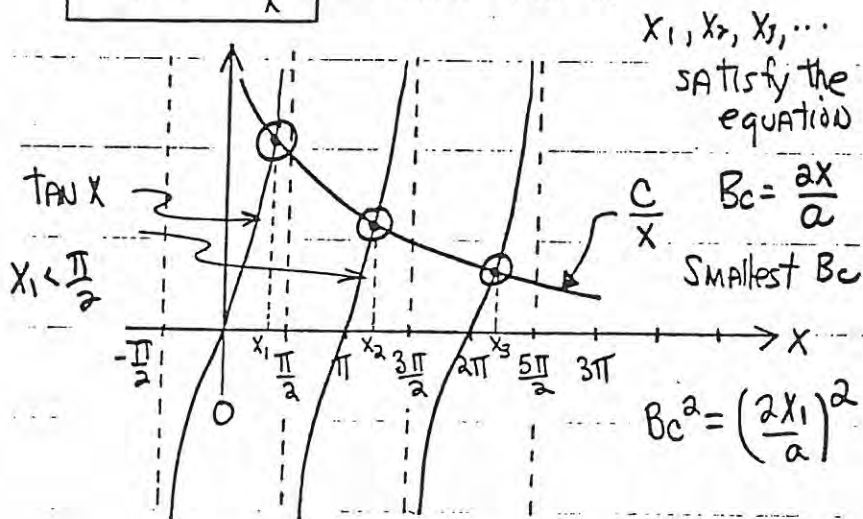
$$(*) \Rightarrow \boxed{X \tan X = C}$$

$$B_c = \frac{2X}{a}$$

23-24

Graphical Solution

$$\boxed{\tan X = \frac{C}{X}} \leftarrow \text{solve for } X$$



• FOR A BARE REACTOR
 of half-width $\frac{a}{2}$
 $B^2 = \left(\frac{\pi}{a}\right)^2$ $\tilde{a} \approx a$
 (LARGE REACTORS)

• FOR THE REFLECTED REACTOR
 with CORE half-width $\frac{a}{2}$,

$$B_c^2 = \left(\frac{\alpha x_1}{a}\right)^2$$

• FROM THE GRAPH, $x_1 < \frac{\pi}{2}$

$$\therefore B_c^2 < B^2$$

$$k = \frac{\nu \Sigma_f}{\Sigma_a + D B_c^2}$$

SINCE $B_c^2 < B^2$ (BARE CORE)

THEN

$$k \text{ (REFLECTED CORE)} > k \text{ (BARE CORE)}$$

REFLECTOR \Rightarrow LESS LEAKAGE FROM CORE
 $\Rightarrow k \uparrow$

LECTURE 24

NUMERICAL SOLUTION OF CRITICALITY PROBLEM

READING ASSIGNMENT:

Duderstadt and Hamilton, pp. 214-218.

EXERCISES:

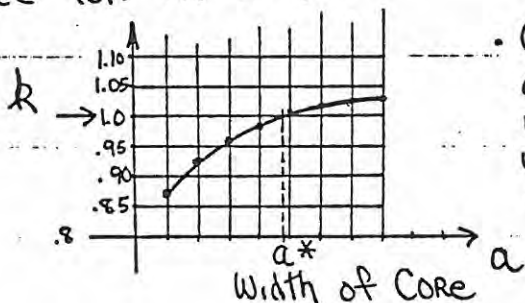
- 24.1. (cont'd) Complete the computer problem assigned in the previous lecture.

Critical Width

- Given the material properties of the core and reflector, what is the width a^* needed for $k=1$?

$$k = \frac{\nu \Sigma_f}{\Sigma_a + D B_c^2}$$

$$B_c^2 = \left(\frac{2.41}{a} \right)^2$$



- Calculated value of k from the above analysis using indicated value for a

24-2

- Recall

$$B_c^2 = \frac{1}{D} \left[\frac{1}{k} \nu \Sigma_f - \Sigma_a \right]$$

- For $k=1$,

$$B_c^2 = \frac{1}{D} (\nu \Sigma_f - \Sigma_a) \equiv B_m^2$$

$$\therefore \boxed{B_c^2 = B_m^2} \text{ for criticality}$$

(AS ALWAYS)

- Our graphical solution for the critical width a^* is equivalent to solving

the equation

$$\frac{B_c a^*}{2} \tanh\left(\frac{B_c a^*}{2}\right) = \frac{D^R}{D_c} \left(\frac{a^*}{2L_R}\right) \coth\left(\frac{b - \frac{a^*}{2}}{L_R}\right) \quad (*)$$

$$\text{where } B_c^2 = \frac{1}{D} (\nu \Sigma_f - \Sigma_a) \equiv B_{m^2}$$

for the quantity a^* .

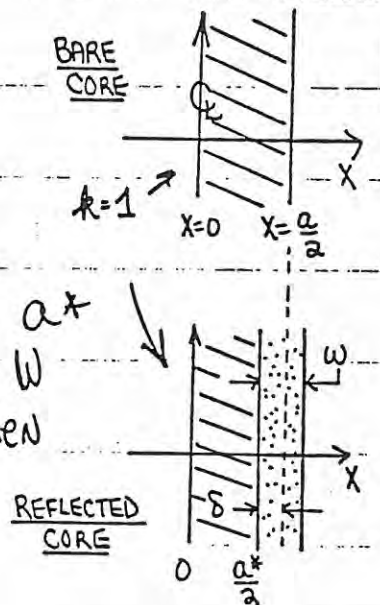
(ACTUAL PROCEDURE - solved (*) for k given values for a , then found the $a = a^*$ that yielded $k = 1$)

Reflector Savings

• Given a bare core of specified composition that has a critical width a , what is the critical width a^* if a reflector of thickness W is added to each side? Then having a^* , we define

$$\delta \equiv \frac{1}{2}(a - a^*)$$

reflector savings



• For the critical core
(bare or reflected), we
have $B_c^2 = B_m^2 = \frac{1}{D} (\nu \Sigma_f - \Sigma_a)$
↑
same

• For the bare core,

$$a = \frac{\pi}{B_c}$$

$$\delta = \frac{1}{2} (a - a^*) = \frac{\pi}{2B_c} - \frac{a^*}{2}$$

OR $\frac{a^*}{2} = \frac{\pi}{2B_c} - \delta$

• Substitute into Eq. (†),

$$D^c B_c \tan\left(\frac{\pi}{2} - B_c \delta\right) = \frac{D^R}{L_R} \coth\left(\frac{W}{L_R}\right)$$

• But $\tan\left(\frac{\pi}{2} - \theta\right) = \cot \theta$

$$\therefore D^c B_c \cot(B_c \delta) = \frac{D^R}{L_R} \coth\left(\frac{W}{L_R}\right)$$

Invert,

$$\frac{1}{D^c B_c} \tan(B_c \delta) = \frac{L_R}{D_R} \tanh\left(\frac{W}{L_R}\right)$$

$$\tan(B_c \delta) = \frac{D^c B_c L_R}{D_R} \tanh\left(\frac{W}{L_R}\right)$$

$$\Rightarrow \delta = \frac{1}{B_c} \tan^{-1} \left[\frac{D^c B_c L_R}{D_R} \tanh\left(\frac{W}{L_R}\right) \right]$$

" Reflector savings "

Amount the half-width of a ^{critical} core can be decreased if a reflector of width W is added

Since a reflector will increase the multiplication factor, then a system that is critical without a reflector can be made smaller if a reflector is added (and still be critical). The amount by which the core can be made smaller is the reflector savings.

Numerical Criticality Calculations

• Analytical solutions to

$$-\nabla \cdot D(\mathbf{r}) \nabla \phi(\mathbf{r}) + \Sigma_a(\mathbf{r}) \phi(\mathbf{r}) = \frac{1}{k} \nu \Sigma_f(\mathbf{r}) \phi(\mathbf{r})$$

(+ b.c.)

are practical only for simple

configurations, i.e.,

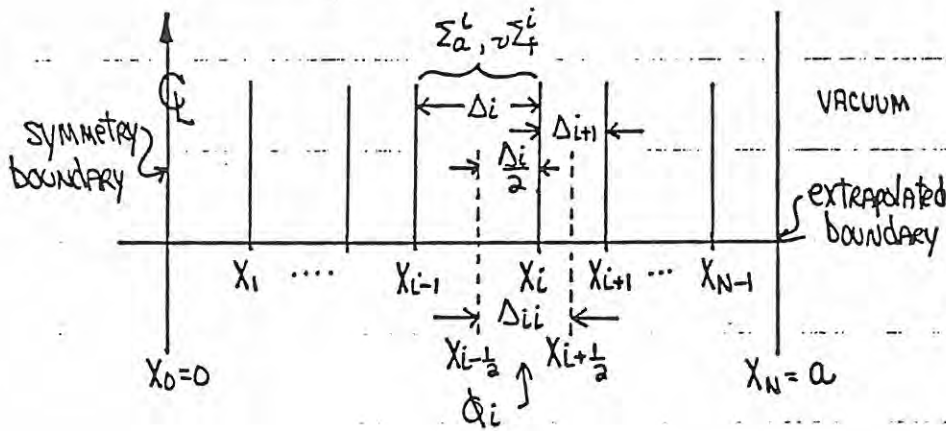
slab, sphere, cylinder, reflected

slab, etc

\Rightarrow COMPUTER!

Again, realistic configurations force one to use computers.

Computer solution of
The 1-D Criticality
Equation in Slab Geometry



Back to the same mesh structure but now we have to add the fission cross section

$$-\frac{d}{dx} D(x) \frac{d\phi}{dx} + \Sigma_a(x)\phi(x) = \frac{1}{k} \nu \Sigma_f(x)\phi(x) \quad (1)$$

$$0 \leq x \leq a$$

$$\text{subject to } \left. \frac{d\phi}{dx} \right|_{x=0} = 0$$

$$\phi(a) = 0$$

only
 difference

Recall (source problem)

$$-\frac{d}{dx} D(x) \frac{d\phi}{dx} + \Sigma_a(x)\phi(x) = S(x)$$

$$0 \leq x \leq a$$

+ SAME b.c.

- Only difference-

The source term is

$$\frac{1}{k} \nu \Sigma_f(x) \Phi(x) \text{ vs. } S(x)$$

- Integrating Eq. (1) from $x_{i-\frac{1}{2}}$ to $x_{i+\frac{1}{2}}$ (As we did for the source problem)

The LHS is the same as before, and

the RHS:

$$\frac{1}{k} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \nu \Sigma_f(x) \Phi(x) dx = \frac{1}{k} \nu \Sigma_{fii} \Phi_i \Delta_{ii}$$

The fission source term is identical to the absorption term (except for the cross section).

where $\nu \Sigma_{fii} \equiv \frac{1}{\Delta_{ii}} \left[\nu \Sigma_{fi} \frac{\Delta_i}{2} + \nu \Sigma_{f(i+1)} \frac{\Delta_{i+1}}{2} \right]$

(similar to the definition for Σ_{aii})

- The treatment of the boundary conditions is identical to the source problem

- The equation for the i^{th} flux is then

$$a_{i(i-1)} \Phi_{i-1} + a_{ii} \Phi_i + a_{i(i+1)} \Phi_{i+1} = \frac{1}{k} \nu \Sigma_{fii} \Phi_i$$

$i=1, 2, \dots, N-1 \quad (\text{vs. } S_i)$

$$\underline{F} = \begin{pmatrix} \nu \Sigma_{f00} & 0 & \dots & 0 \\ 0 & \nu \Sigma_{f10} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \nu \Sigma_{fN-1 N-1} \end{pmatrix}$$

$$\underline{A} \underline{\phi} = \frac{1}{k} \underline{F} \underline{\phi} \quad \underline{\phi} = \begin{pmatrix} \phi_0 \\ \vdots \\ \phi_{N-1} \end{pmatrix}$$

F is a diagonal matrix.

where

$$\underline{A} = \begin{pmatrix} a_{00} & a_{01} & 0 & \dots & 0 \\ a_{10} & a_{11} & a_{12} & \dots & 0 \\ 0 & a_{21} & a_{22} & a_{23} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \end{pmatrix}$$

$$\underline{\phi} = \begin{pmatrix} \phi_0 \\ \phi_1 \\ \vdots \\ \phi_{N-1} \end{pmatrix}$$

A is the same as before.

$$\underline{A} \underline{\phi} = \frac{1}{k} \underline{F} \underline{\phi}$$

How do we solve this
for k and $\underline{\phi}$?

Iterative Method

• Guess $\underline{\phi}^{(0)}$ and $k^{(0)}$

e.g., $\underline{\phi}^{(0)} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}, k^{(0)} = 1$

Now we have to solve for both the eigenvalue k and associated eigenvector $\underline{\phi}$. However, we don't want the trivial solution $\underline{\phi} = 0$, which is clearly a solution to the above equation. To solve, we must use an iterative technique, known as "inverse power iterations".

Define

$$\underline{S}^{(0)} = \frac{1}{k^{(0)}} \underline{F} \underline{\phi}^{(0)}$$

$$\underline{A} \underline{\phi}^{(1)} = \underline{S}^{(0)}$$

solve this
for $\underline{\phi}^{(1)}$

using

Gauss-Seidel, Jacobi

OR Gauss elimination

• New estimate for k

$$k = \frac{\text{Production}}{\text{Absorption} + \text{leakage}} \quad \phi^{(1)} \rightarrow \phi'(x)$$

$$= \frac{\int_0^a v \Sigma_f(x) \phi(x) dx}{\int_0^a \Sigma_a(x) \phi(x) dx + \int_0^a \left[-\frac{d}{dx} D(x) \frac{d\phi}{dx} \right] dx}$$

Then if we have the flux estimate $\phi^{(1)}(x)$, we calculate $k^{(1)}$ from the above.

The idea will be to use the latest estimate of the flux to calculate k . The terms in the expression for k can be calculated using our finite difference definitions.

• Recall $\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} v \Sigma_f(x) \phi(x) dx \approx v \Sigma_{fii} \phi_i \Delta x_i$

• However $\int_0^a v \Sigma_f(x) \phi(x) dx = \sum_{i=0}^{N-1} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} v \Sigma_f(x) \phi(x) dx$
 $(x_{-\frac{1}{2}} = 0)$

• Then $\int_0^a v \Sigma_f(x) \phi^{(1)}(x) dx \approx \sum_{i=0}^{N-1} v \Sigma_{fii} \phi_i^{(1)} \Delta x_i$

• Moreover, solving $\underline{A} \underline{\phi}^{(1)} = \frac{1}{k^{(0)}} \underline{F} \underline{\phi}^{(0)}$ is equivalent to solving the finite difference form of

$$-\frac{d}{dx} D(x) \frac{d\phi^{(1)}}{dx} + \sum_a(x) \phi^{(1)}(x) = \frac{1}{k^{(0)}} \nu \sum_f(x) \phi^{(0)}(x)$$

(verify by integrating this equation over the mesh interval $x_{i-\frac{1}{2}}$ to $x_{i+\frac{1}{2}}$)

$$\begin{aligned} \therefore \int_0^a \left[-\frac{d}{dx} D(x) \frac{d\phi^{(1)}}{dx} + \sum_a(x) \phi^{(1)}(x) \right] dx \\ = \frac{1}{k^{(0)}} \int_0^a \nu \sum_f(x) \phi^{(0)}(x) dx \\ \approx \frac{1}{k^{(0)}} \sum_{i=0}^{N-1} \nu \sum_{fii} \phi_i^{(0)} \Delta_{ii} \end{aligned}$$

Then

$$k^{(1)} = \frac{\sum_{i=0}^N \nu \sum_{fii} \phi_i^{(1)} \Delta_{ii}}{\frac{1}{k^{(0)}} \sum_{i=0}^{N-1} \nu \sum_{fii} \phi_i^{(0)} \Delta_{ii}}$$

$$\therefore k^{(1)} = k^{(0)} \frac{\sum_{i=0}^{N-1} \nu \sum_{fii} \phi_i^{(1)} \Delta_{ii}}{\sum_{i=0}^{N-1} \nu \sum_{fii} \phi_i^{(0)} \Delta_{ii}}$$

updated estimate for k

GENERAL ALGORITHM

FOR $m=1, 2, \dots$

(1) Calculate the fission

SOURCE

$$\underline{S}^{(m-1)} = \frac{1}{k^{(m-1)}} \underline{F} \underline{\Phi}^{(m-1)}$$

(2) Solve for $\underline{\Phi}^{(m)}$:

$$\underline{A} \underline{\Phi}^{(m)} = \underline{S}^{(m-1)} \quad (\text{SIMPLY A SOURCE PROBLEM})$$

Note this is the equation we solved previously (the source problem)

(3) Update k : fission source

$$k^{(m)} = k^{(m-1)} \frac{\sum_{i=0}^{N-1} v \Sigma_{fii} \Phi_i^{(m)} \Delta_{ii}}{\sum_{i=0}^{N-1} v \Sigma_{fii} \Phi_i^{(m-1)} \Delta_{ii}}$$

for the m^{th} iter

for the $(N-1)^{\text{th}}$ iter

Repeated until $\underline{\Phi}^{(m)}$ agrees with $\underline{\Phi}^{(m-1)}$ AND $k^{(m)}$ agrees with $k^{(m-1)}$

The algorithm then consists of a sequence of source calculations separated by auxiliary calculations to update the multiplication factor.

- Inverse power iteration method
- Converge to the largest eigenvalue k AND corresponding flux (eigenfunction) $\underline{\phi}$ to:

$$\underline{A} \underline{\phi} = \frac{1}{k} \underline{F} \underline{\phi}$$

Straightforward to show that the inverse power iteration method converges to the smallest eigenvalue $\frac{1}{k}$; hence, the largest k .

LECTURE 25

NEUTRON ENERGY DEPENDENCE

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 81 - 82
pp. 285 - 288

EXERCISES:

- 25.1. Sketch the derivation of the energy-dependent diffusion equation.
- 25.2. Compare the multigroup method with the "discretization" of the spatial variable used in the numerical solution of the diffusion equation.

25-1

Neutron Energy Dependence

- One-Speed Diffusion Model
- Energy Dependence
- Energy-Dependent Diffusion Theory
- Energy Groups
- Example: Two-Group Model

Will review one-speed model to learn how to generalize it.
 Energy dependence: enormous range; complex dependence
 Energy dependent diffusion equation too complex. Need computer solution. Discretize energy into intervals or "groups".

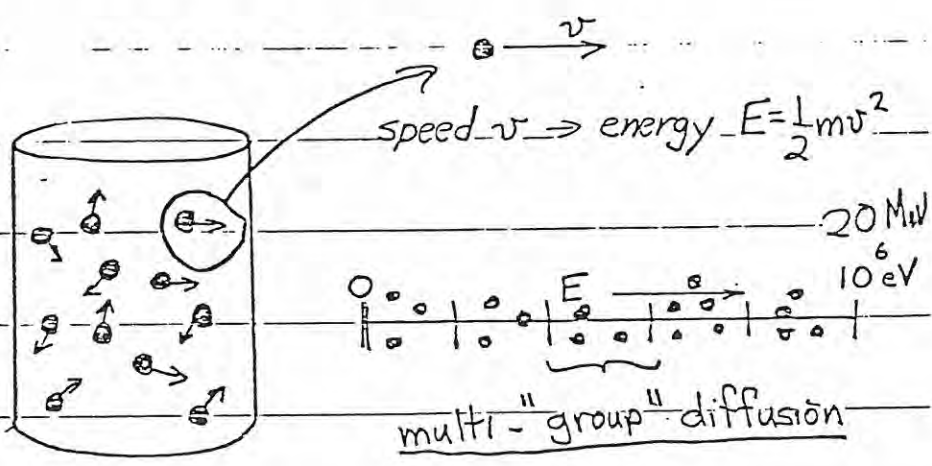
Will develop a specific example: two-group model.

Key questions: How to derive?

How to evaluate parameters (group constants)?

25-2

Multigroup Diffusion Theory



Cornerstone of reactor analysis: multigroup diffusion theory

Theory takes account of the fact that the kinetic energy of neutrons spans an enormous range from 0 to 20 million electron volts.

Simply cannot represent all neutrons by a single energy.

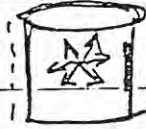
25-3 One-Speed Diffusion Model

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot \underline{D} \nabla \phi + \Sigma_a \phi(r,t) = \nu \Sigma_f \phi + S$$

time rate of change leakage absorption fission external source

Key Assumptions:

i) diffusion approximation
transport effects



ii) one-speed approximation

$$\nabla \cdot \underline{D} \nabla \phi \rightarrow \underline{D} \nabla^2 \phi \rightarrow D \frac{d^2 \phi}{dx^2}$$

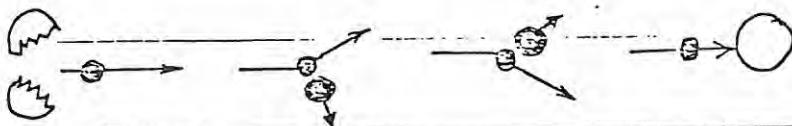
During previous sessions we developed the simplest model of a reactor: one-speed diffusion theory.

Key assumptions: i) neutron distribution only weakly dependent on direction, ii) all neutrons are characterized by a single speed or energy

First approximation is reasonably well satisfied in large power reactors provided we modify analysis a bit in vicinity of boundaries and strong absorbers.

One-speed approximation is usually lousy!

25-4 Neutron Energy Dependence



Fission

Scattering

Absorption

1-20 MeV

1 MeV → 1 eV

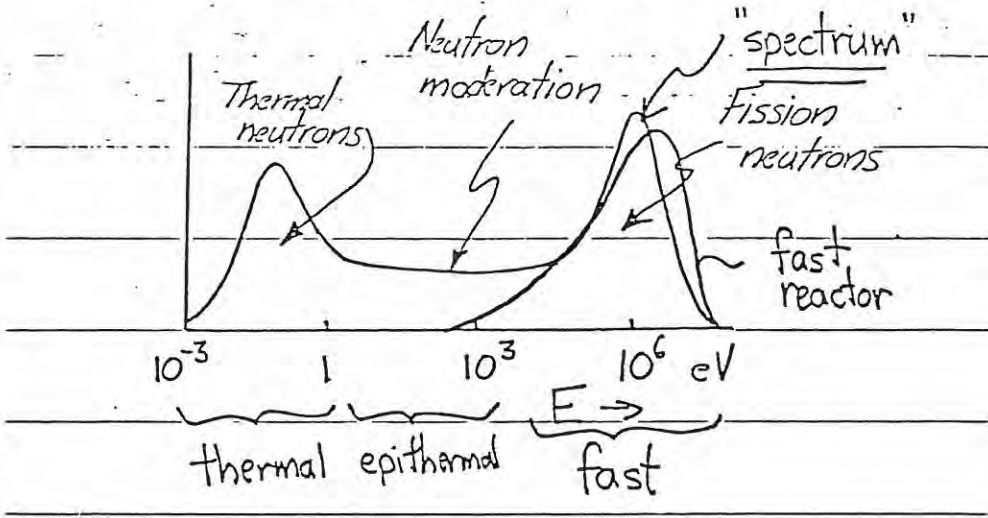
1 eV → 0.01 eV

Consider events in neutron lifetime.

Neutrons in a reactor generally have energies ranging over nine orders of magnitude.

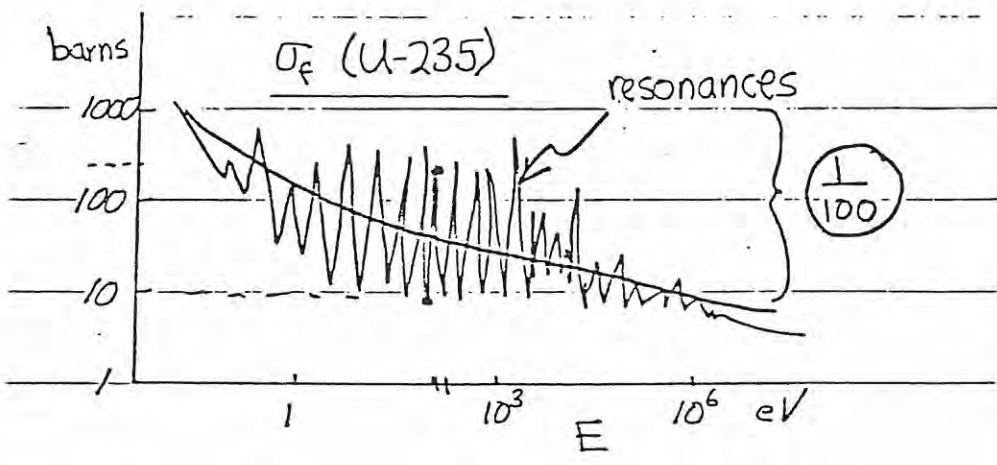
What is significance for calculations? Cross sections (i.e., reactor rates) depend sensitively on energy!!!

25-5 Distribution of neutron energies



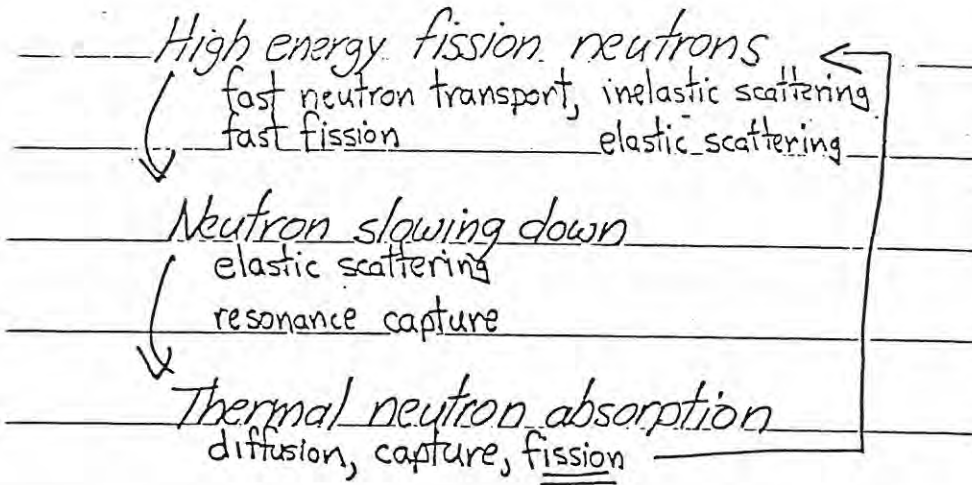
Look at the energy distribution in a typical power reactor.
 Note: Sometimes refer to this energy distribution as the neutron energy "spectrum".
 Contrast LWR vs LMFBR spectra.

25-6 Cross section energy dependence



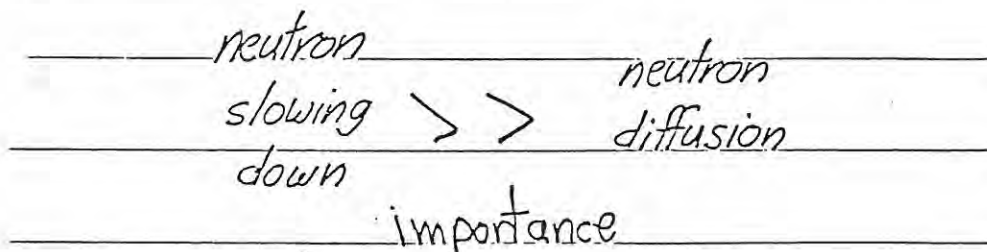
In each energy range, the probability of neutrons inducing a nuclear reaction is different. Neutron-nuclear cross sections depend very sensitively on the incident neutron energy. Not only vary over two orders of magnitude, but exhibit complex resonance behavior.

25-7) Energy changes over neutron lifetime



Examine neutron energy changes during a neutron lifetime.
 Note three different ranges: fast, slowing down, and thermal
 A wonder that treating all neutrons as if they had only one
 speed or energy works at all.
 It is apparent that neutrons "travel further" in energy than
 they do in space.

25-8) An accurate treatment of neutron energy dependence is far more important than that of their spatial dependence!!!



Note most nuclear reactor theory courses spend more time on
 neutron diffusion than slowing down and thermalization.
 Most effort is in development of cross section libraries and
 infinite medium spectrum calculations.
 But difficult to conceptualize "motion" in neutron energy
 "space".
 Diffusion equation is similar to heat conduction equation--
 slowing down is new mathematics.

25-9 Question: How do we generalize

one-speed diffusion theory?

$$-\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D \nabla \phi + \Sigma_a \phi(r, t) = v \Sigma_f \phi + S$$

$$\phi(r, t) \rightarrow \phi(r, E, t) \quad \Sigma_i \rightarrow \Sigma_i(E)$$

$$-\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(E) \nabla \phi + \Sigma_a(E) \phi(r, E, t) = v \Sigma_f(E) \phi(r, E, t) + S(r, E, t)$$

How do we take account of this strong energy dependence?

Try to generalize one-speed diffusion equation.

Perhaps we can simply let the flux and cross sections be energy dependent.

This would suggest a "energy-dependent diffusion equation" as shown. But this would not allow neutrons to change energies. Must be more sophisticated.

25-10 Be careful! Neutrons can change energy by scattering or fission.

Scattering: $\int_0^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi(r, E', t)$

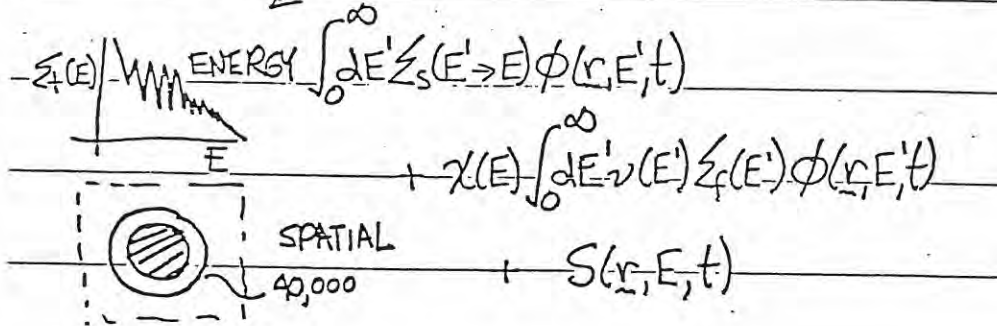
differential scattering cross section

Fission: $\chi(E) \int_0^{\infty} dE' v(E') \Sigma_f(E') \phi(r, E', t)$

This simple minded approach ignores the fact that neutrons can change energy either directly through scattering or indirectly through fission ("born again" neutrons). Use definitions of differential scattering cross section developed earlier in this course. Fission term can be written in a similar sense.

25-11 Energy-dependent diffusion equation:

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(E) \nabla \phi + \Sigma_f(E) \phi(r, E, t) =$$

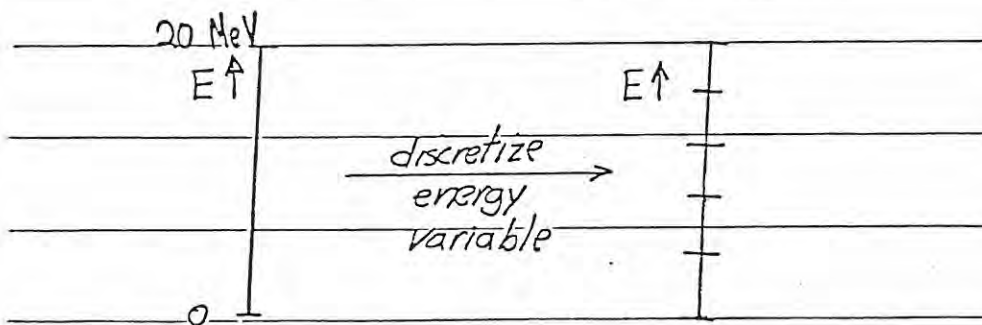
$$\Sigma_f(E) \int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi(r, E', t) + \chi(E) \int_0^\infty dE' v(E') \Sigma_f(E') \phi(r, E', t) + S(r, E, t)$$


Discuss each term in equation in terms of its physical significance.

Note that with the complex spatial and energy dependence, the equation is far too difficult to solve directly.

25-12 Too complex! Can only solve on a computer.

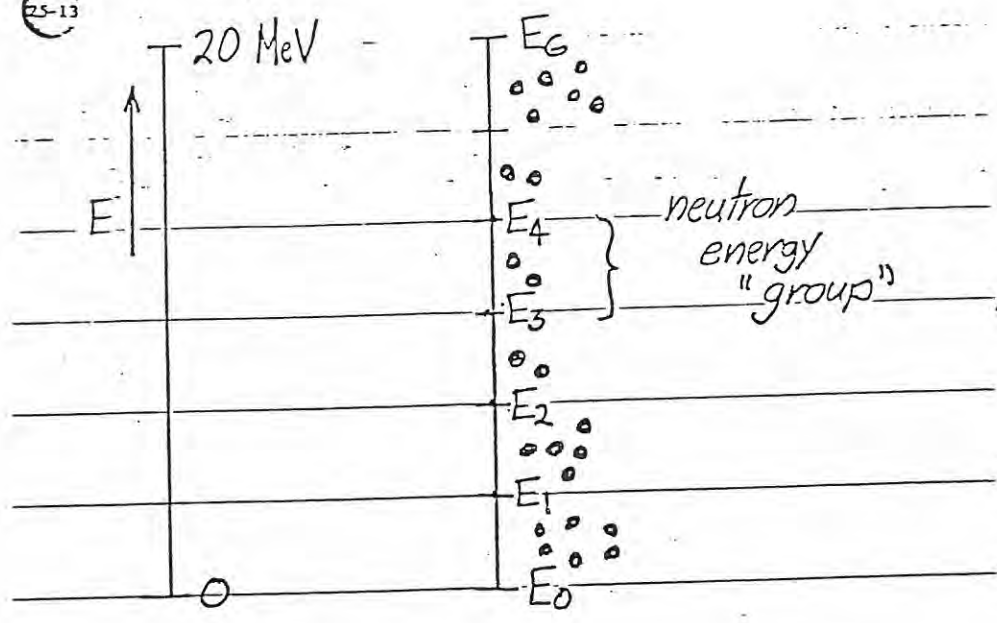
Key Idea: "Discretize" energy E



Computers were originally developed for nuclear calculations! When confronted with such a beast, retreat to the nearest computer (BIG computer!!).

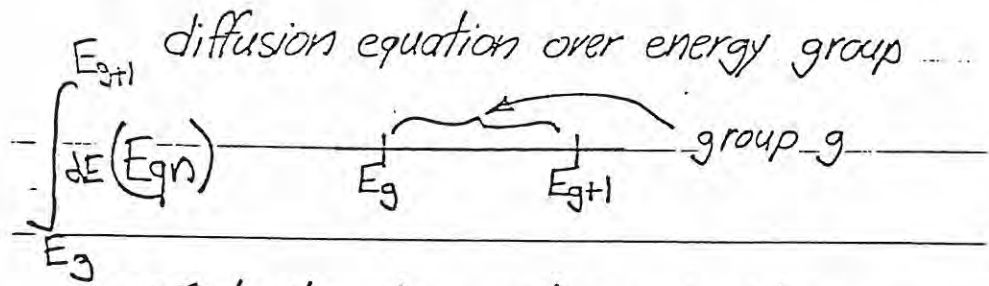
General idea is always to discretize the independent variables-- just as with spatial dependence.

In this case, we wish to discretize the energy variable.



Motive energy range.
 Discretize by chopping up into intervals.
 We call each interval an energy group.
 If we think of each neutron in reactor as having an energy lying in one of the intervals, then we have now broken up the neutrons into a number of groups characterized by their energy.

Procedure: average energy-dependent



Treat all neutrons with energies in group as if they had the same energy:

$$\phi(r, E, t) \xrightarrow{E_g < E < E_{g+1}} \phi_g(r, t) \text{ group flux}$$

We follow a procedure very similar to that used to derive finite-difference equations to solve for spatial dependence.
 Each group will be characterized by a flux -- a "group" flux.

Find a diffusion equation for each group

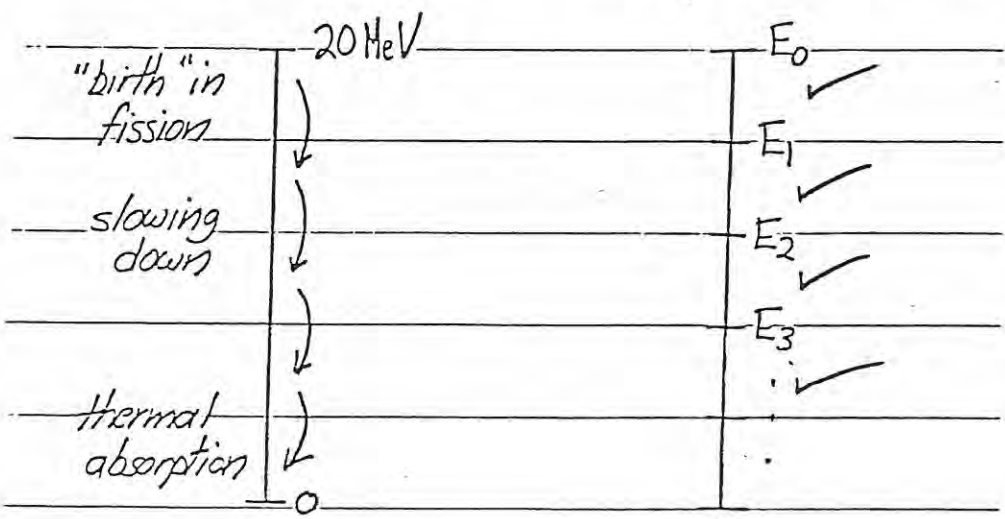
$$\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} - \nabla \cdot D_g \nabla \phi_g + \Sigma_{tg} \phi_g (r, t) = \text{"group } g \text{"}$$

$$\sum_{g'=1}^G \Sigma_{sg'} \phi_{g'} + \lambda_g \sum_{g'=1}^G v_{g'} \Sigma_{fg'} \phi_{g'} + S_g$$

Multigroup diffusion equations

Go over each term in the equation.
 We find one such diffusion equation for each group.
 Multigroup diffusion equations are coupled to each other since neutrons may experience changes in energy and hence pass from group to group.
 Note we have "traded" complex energy dependence for a set of equation.
 These equations, known as the multigroup diffusion equations, form the basis of nuclear reactor analysis.

Technicality: Neutrons generally lose energy during their lifetime:



Example: Fission neutrons will be born in highest energy group and then cascade downward in energy from group to group as they are moderated by scattering collisions.
 Technicality: Note that neutrons usually lose energy during their lifetime, slowing down from high fission energies. It is convenient to index ("label") the groups backwards, from high to low energies.

A cardinal rule of reactor calculations: ---

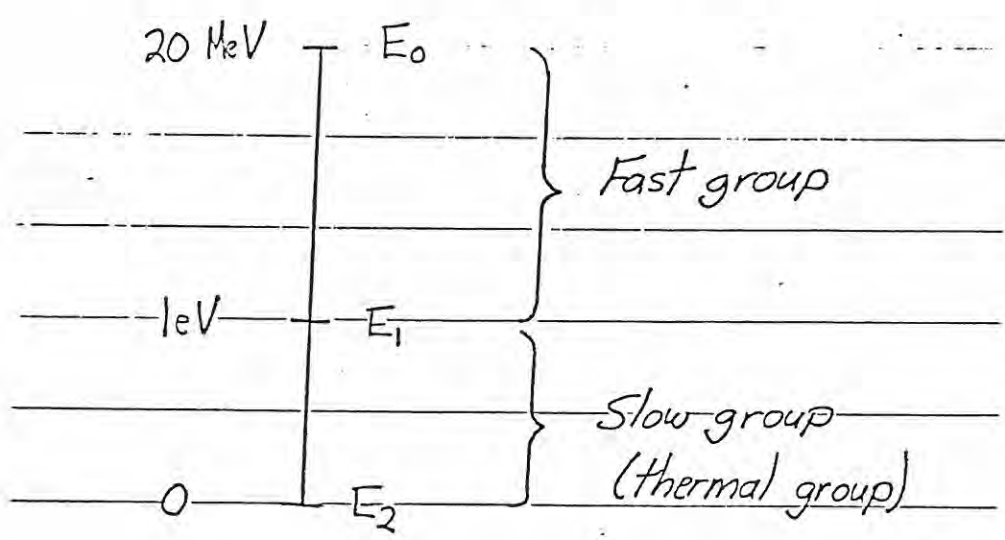
"Follow the neutron!"

Always solve equations in direction
of neutron flow
(high energy to low energy)

Hence we can use the index scheme to solve from low index (high energy) to high index (low energy) in the direction of neutron flow.

This scheme is also used in neutron transport (discrete ordinates of S-N codes).

Example: Two-Group Equations



Usually break up groups into fast and thermal neutrons, Quite popular for "guessestimates". Best for LWRs and we will use these frequently.

$$-\nabla \cdot \underline{D}_1 \nabla \phi_1 + \sum_{R_1} \phi_1 = \nu_1 \sum_{F_1} \phi_1 + \nu_2 \sum_{F_2} \phi_1 + S_2 \text{ fast}$$

↑ coupled

$$-\nabla \cdot \underline{D}_2 \nabla \phi_2 + \sum_{A_2} \phi_2 = \sum_{S_1 \rightarrow 2} \phi_1 + S_1 \text{ thermal}$$

group fluxes: ϕ_1, ϕ_2

group constants: $D_1, \sum_{R_1}, D_2, \sum_{A_2}$

Explain each term in equations. Note coupling.
 Point out group fluxes and group-constants.
 These equations can be simplified considerably.
 We will devote an entire lecture to studying this model
 in detail.

LECTURE 26

DERIVATION OF THE MULTIGROUP DIFFUSION EQUATIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 288 - 295

EXERCISES:

- 26.1. Estimate the fast group constants characterizing water if the fast group is taken from 1 eV to 10 MeV and the neutron energy spectrum over this group is taken to depend on E as $1/E$.
- 26.2. Estimate the minimum group spacing that will yield directly coupled multigroup equations for C-12, D-2, Be-9, and Na-22.
- 26.3. Write out the detailed form of the multigroup diffusion equations for a four-group model in which: a) there is direct coupling, b) the fission source exists only in the upper two groups, and c) only the lowest group contains thermal neutrons.

1) Derivation of Multigroup Diffusion Equations

- Derivation of two-group equations
- Special case: one-group equations
- Generalization to G groups
- Calculation of multigroup constants

Note: The derivation of the multigroup-diffusion equations is not just for culture.

It is an essential task if we are to determine the group constants appearing in the equations.

2) Previous Lecture

- noted complicated neutron energy dependence
- introduced energy-dependent diffusion equation
- discretized energy variable \rightarrow energy groups
- suggested form of multigroup equations

We now must derive the multigroup equations

(only way to determine the "group constants")

In this session we will continue with our study of the multigroup diffusion method, the cornerstone of nuclear reactor analysis.

-3) Energy-dependent diffusion equation:

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(E) \nabla \phi + \Sigma(E) \phi(r, E, t) = \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi(r, E', t) + \chi(E) \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \phi(r, E', t) + S(r, E, t)$$

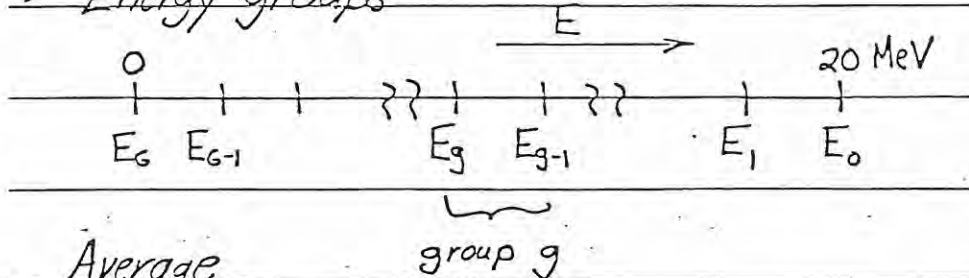
Approach:

i) Break up energy range into groups.

ii) Average (integrate) equation over each group.

We will begin with the energy-dependent diffusion equation. The approach will be quite simple. We first break up the energy range into intervals or groups, and then integrate the equation over each group (in effect, averaging the equation over each group).

-4) Energy groups

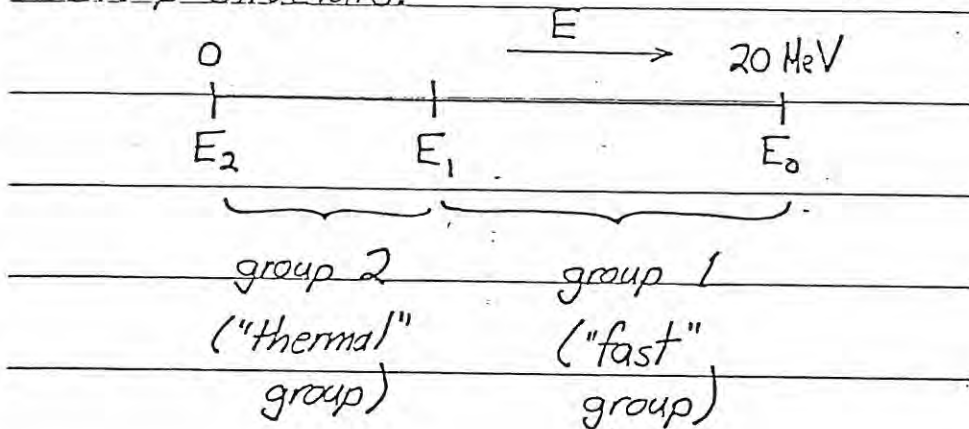


$$\int_{E_g}^{E_{g-1}} dE \text{ (energy-dependent diffusion equation)} \Rightarrow \text{multigroup diffusion equations}$$

Let's begin by determine the group structure. Recall the backwards group indexing scheme demanded by our desire to follow the neutron flow from high energies to low energies as the neutrons slow down. Key will be to introduce key definitions to arrive at the multigroup diffusion equations. Actually, general case is rather messy. Consider a special case first: two groups.

5) Two-group diffusion equations

Group structure:



To make life simple, we will begin with the two-group diffusion equation.

The appropriate group structure is as shown. Note fast and thermal group choices.

We are now ready to proceed to integrate energy-dependent diffusion equation over each of these groups.

6) Recall energy-dependent diffusion equation

$$\begin{aligned} -\nabla \cdot D(E) \nabla \phi + \Sigma_t(E) \phi(r, E) \\ = \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi(r, E') \\ + \chi(E) \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \phi(r, E') \\ + S(r, E) \end{aligned}$$

Recall the form of this equation.

Henceforth we will throw out the time dependence (only important in reactor kinetics -- to be covered in the next course in this series).

Now we will integrate the energy dependent diffusion equation over each of the groups, here noted by the group indices.

To be specific, consider the integration over the fast group in which $g = 1$.

7) Let us examine a typical term

$$\int_{E_1}^{E_0} dE \Sigma_t(\underline{r}, E) \phi(\underline{r}, E)$$

Now define: $\phi_1(\underline{r}) \equiv \int_{E_1}^{E_0} dE \phi(\underline{r}, E)$

$$\Sigma_{t_1} \equiv \frac{1}{\phi_1} \int_{E_1}^{E_0} dE \Sigma_t(\underline{r}, E) \phi(\underline{r}, E)$$

so that

$$\int_{E_1}^{E_0} dE \Sigma_t(\underline{r}, E) \phi(\underline{r}, E) \rightarrow \Sigma_{t_1} \phi_1(\underline{r})$$

The trick is to introduce appropriate definitions. We will rewrite each term in terms of group variables essentially by definition.

That is, we define the group flux and group cross section so that the integrated term can be written in terms of these quantities.

Notice how formal this is.

8) Here

$$\phi_1(\underline{r}) \rightarrow \text{fast flux}$$

$$\Sigma_{t_1} \rightarrow \text{fast group cross section}$$

("group constant")

We can proceed in a similar fashion with

other terms in the equation

$$\int_{E_1}^{E_0} dE S(\underline{r}, E) \equiv S_1(\underline{r})$$

We really have done nothing but introduce convenient definitions.

Here we introduce some terminology.

We can proceed in a similar fashion with each term.

For example, the source term is written as shown.

$$\begin{aligned}
 & \int_{E_1}^{E_0} dE \left[\int_{E_1}^{E_0} dE' \Sigma_s(E' \rightarrow E) \phi(\underline{r}, E') \right] \\
 & \quad + \int_{E_2}^{E_1} dE' \Sigma_s(E' \rightarrow E) \phi(\underline{r}, E') \\
 & \equiv \Sigma_{s1 \rightarrow 1} \phi_1(\underline{r}) + \Sigma_{s2 \rightarrow 1} \phi_2(\underline{r})
 \end{aligned}$$

$$\begin{aligned}
 & \int_{E_1}^{E_0} dE \chi(E) \int_{E_2}^{E_0} dE' \nu(E') \Sigma_f(E') \phi(\underline{r}, E') \\
 & \equiv \chi_1 \nu_1 \Sigma_{f1} \phi_1(\underline{r}) + \chi_2 \nu_2 \Sigma_{f2} \phi_2(\underline{r})
 \end{aligned}$$

The scattering and fission terms are only slightly more complicated. We need only break up the integrals into each group and define the appropriate group fluxes and group constants.

Incidentally, the group constants here are known as "group transfer cross sections" since they correspond to scattering collisions which scatter the neutrons from one group to another.

The fission term can also be handled like this.

-10) Put it all together and what do we find...

$$\begin{aligned}
 -\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{t1} \phi_1 &= \Sigma_{s1 \rightarrow 1} \phi_1 + \Sigma_{s2 \rightarrow 1} \phi_2 \\
 &+ \chi_1 \nu_1 \Sigma_{f1} \phi_1 + \chi_1 \nu_2 \Sigma_{f2} \phi_2 + S_1
 \end{aligned}$$

$$\begin{aligned}
 -\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{t2} \phi_2 &= \Sigma_{s1 \rightarrow 2} \phi_1 + \Sigma_{s2 \rightarrow 2} \phi_2 \\
 &+ \chi_2 \nu_1 \Sigma_{f1} \phi_1 + \chi_2 \nu_2 \Sigma_{f2} \phi_2 + S_2
 \end{aligned}$$

two-group diffusion equations

After making these definitions, we can write the integral of the energy dependent diffusion equation over the fast group as shown.

A similar exercise can be performed for the thermal group. Comments: i) note coupling due to scattering and fission; ii) Note that these two equations can be simplified rather considerably; iii) note that the group constants are still undetermined.

6-1) One-group diffusion theory:

Group structure:
$$\begin{array}{ccc} 0 & \xrightarrow{E} & 20 \text{ MeV} \\ | & & | \\ E_1 & & E_0 \end{array}$$

Group flux:
$$\phi_1(\underline{r}) = \int_{E_1}^{E_0} dE \phi(\underline{r}, E)$$

Group constants:

$$\Sigma_{t_1} \equiv \frac{1}{\phi_1} \int_{E_1}^{E_0} dE \Sigma_t(E) \phi(\underline{r}, E)$$

We can repeat this process to derive the one-group diffusion equation.

Define the group structure as shown.

Just integrate over energy and use definitions as before.

Note:
$$\int_{E_1}^{E_0} dE \chi(E) = \int_0^{20} dE \chi(E) = 1$$

Then

$$\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{t_1} \phi_1 = \Sigma_{s_1} \phi_1 + \nu \Sigma_{f_1} \phi_1 + S_1$$

or

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{a_1} \phi_1 = \nu \Sigma_{f_1} \phi_1 + S_1$$

Consider the fission term.

There is a more direct way to derive this equation. We can always reduce the number of groups.

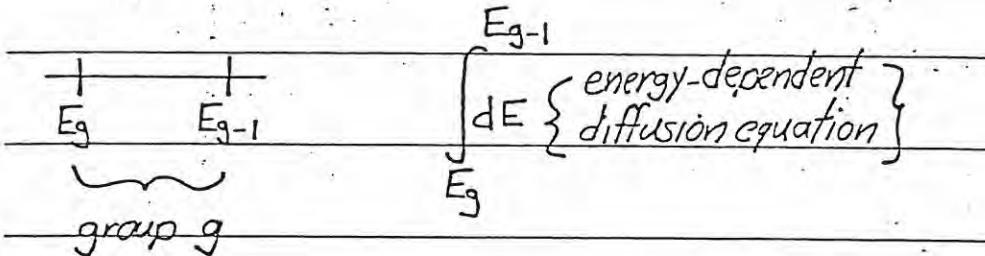
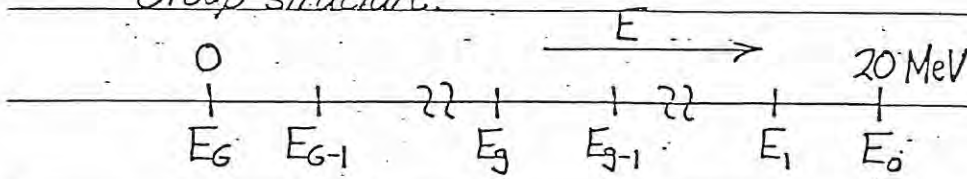
This is known as "group collapsing".

We should note that this equation is still only of formal significance until we define the group constants.

It is comforting to know that one-speed theory does have some justification, however.

13) General Multigroup Equations

Group structure:



We are now ready to tackle the general case.
 Once again we introduce a suitable group structure.
 Then we integrate the energy dependent diffusion equation over an arbitrary group g .
 I will spare you the agony of going through each term and introducing the appropriate definition.

14) Multigroup diffusion equations:

$$-\nabla \cdot D_g \nabla \phi_g + \Sigma_{t_g} \phi_g(\underline{r})$$

$$= \sum_{g'=1}^G \Sigma_{s_{g'g}} \phi_{g'} + \chi_g \sum_{g'=1}^G \nu_{g'} \Sigma_{f_{g'}} \phi_{g'} + S_g$$

$$g = 1, 2, \dots, G$$

where

$$\phi_g(\underline{r}) = \int_{E_g}^{E_{g-1}} dE \phi(\underline{r}, E) \rightarrow \text{group fluxes}$$

Suffice it to say that when the smoke clears away, we find the equations shown.
 Here the group fluxes are defined as shown.

-15) Some comments:

i) MGD equations are still only formal

ii) Define

$$\Sigma_{Rg} \equiv \Sigma_{tg} - \Sigma_{sgg} \quad \begin{array}{l} \text{removal} \\ \text{cross section} \end{array}$$

iii) Usually only downscattering

$$\sum_{g'=1}^G \Sigma_{sg'g} \phi_{g'} = \sum_{g'=1}^{g-1} \Sigma_{sg'g} \phi_{g'} + \Sigma_{sgg}$$

Comments:

- i) The multigroup diffusion equations are still only for formal significance since we don't know how to calculate the group constants yet.
- ii) It is customary to subtract the within-group scattering or transfer cross section from the total cross section to get the "removal" group cross section.
- iii) In most cases the neutrons will only lose energy in a collision--that is, they will only slow down. Hence we can retain only slowing down terms from higher energy groups.

16)

$$-\nabla \cdot \underline{D}_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = S_{f1}$$

$$-\nabla \cdot \underline{D}_2 \nabla \phi_2 + \Sigma_{R2} \phi_2 = \Sigma_{s1 \rightarrow 2} \phi_1 + S_{f2}$$

$$-\nabla \cdot \underline{D}_3 \nabla \phi_3 + \Sigma_{R3} \phi_3 = \Sigma_{s1 \rightarrow 3} \phi_1 + \Sigma_{s2 \rightarrow 3} \phi_2 + S_{f3}$$

$$\vdots$$

$$-\nabla \cdot \underline{D}_g \nabla \phi_g + \Sigma_{Rg} \phi_g = \Sigma_{s1 \rightarrow g} \phi_1 + \dots + \Sigma_{s_{g-1} \rightarrow g} \phi_{g-1} + S_{fg}$$

Note the slowing down structure of the equations. Here the fission and external source terms have been lumped together.

Note lower triangular structure of these scattering terms.

25-1)

How do we calculate the group constants?

$$\Sigma_{tg} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(E) \phi(r, E)}{\int_{E_g}^{E_{g-1}} dE \phi(r, E)}$$

Note Σ_{tg} depends on the intragroup flux $\phi(r, E)$!

How do we calculate the group constants?

Recall the formal definition,

But we don't know the intragroup flux yet.

Note also that the group constant will depend on space even if the cross section is independent of space since the flux is spatially dependent.

5-18)

Idea: approximate

$$\phi(r, E) \approx \phi_{\text{approx}}(r, E)$$

Then

$$\Sigma_{tg} \approx \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(E) \phi_{\text{approx}}(r, E)}{\int_{E_g}^{E_{g-1}} dE \phi_{\text{approx}}(r, E)}$$

Same for

$$D_g, \Sigma_{Rg}, \Sigma_{g \rightarrow g}, \chi_g, \nu_g, \Sigma_{fg}$$

We will approximate the intragroup flux to calculate the multigroup constants.

But what approximations can we use?

-19) What approximations might we use?

i) $\phi_{\text{approx}}(r, E) \sim \text{constant}$

-- too crude

ii) $\phi_{\text{approx}}(r, E) \sim 1/E$ or $M(E)$

-- too crude

iii) CALCULATE ϕ_{approx} using a model

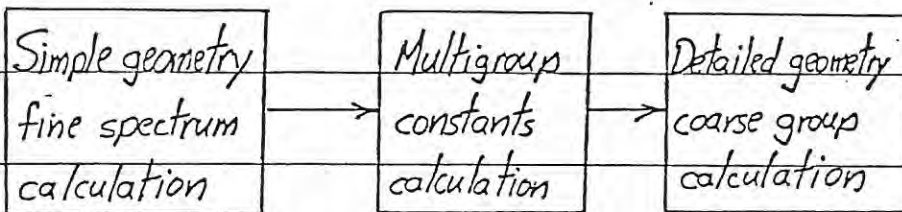
with a very simple space dependence

A constant flux is quite similar to the way one would go about discretizing the spatial dependence. But too crude for the complex cross section energy dependence.

In the fast region, flux behaves as $1/E$. In the thermal region, as a Maxwell-Boltzmann distribution. Still too crude.

Only recourse is to actually calculate the energy dependence. To do so, we sacrifice a detailed spatial treatment.

-20) $\phi_{\text{approx}}(r, E) \rightarrow \phi_{\text{approx}}(E)$ "spectrum"



Note: i) cruder $\phi_{\text{approx}}(E)$, more groups required

ii) need accurate $\phi_{\text{approx}}(E)$ for few groups

The cruder the approximation of the spectrum, the more energy groups will be needed.

It takes a pretty good approximate flux or spectrum to allow a few group approximation.

General approach: ignore spatial dependence of problem and perform a detailed multigroup calculation ("fine spectrum").

Then use this to calculate group constants for coarse groups.

Philosophy: We "average" energy dependence

over a calculated spectrum.

KEY: Calculation of spectrum

i) fast spectrum calculations

(neutron slowing down)

ii) thermal spectrum calculations

(neutron thermalization)

Philosophy: In a sense we are "averaging" the energy dependence of the energy dependent diffusion equation over some guessed flux energy dependence or "spectrum". The more accurate the spectrum, the better the calculation. We will devote considerable attention to the spectrum. However first we will study how to solve the equations.

LECTURE 27

TWO-GROUP DIFFUSION THEORY

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 295- 301

EXERCISES:

- 27.1. Calculate the critical size and mass of a bare sphere of pure U-235 metal using the group constants characterizing groups 1 and 2 in Table 1.
- 27.2. Compare the critical radius of a U-235 sphere as given by one-group, two-group, and modified one-group (1.5 group) diffusion models. Again use data from Table 1.
- 27.3. Consider a plane source emitting fast neutrons at the center of a subcritical slab of thickness a . Determine the two-group fluxes established in the assembly.
- 27.4. We have listed in Table 2 typical group constants characterizing a PWR (in both two-group and four-group forms). Calculate the multiplication factor of a PWR core of height 370 cm and diameter 340 cm using two-group diffusion theory.

TABLE 1 ANL Four-Group Microscopic Cross Sections (in barns)[†]

g	Lower Energy E_L	μ [$\ln E_0/E_L$]	Fission Spectrum	H ₂ O		
				σ_{tr}	σ_γ	$\sigma_{g \rightarrow g+1}$
1	1.353 MeV	2	0.575	3.08	0	2.81
2	9.12 keV	7	0.425	10.52	0	4.04
3	0.4 eV	17.03	0	16.55	0.035	4.14
4	0	—	0	68.6	0.57	0

g	U ²³⁵						U ²³⁸					
	σ_{tr}	ν	σ_f	σ_γ	σ_{inR}	σ_{eR}	σ_{tr}	ν	σ_f	σ_γ	σ_{inR}	σ_{eR}
1	4.7	2.65	1.3	0.1	1.4	0	4.7	2.65	0.53	0.04	2.1	0
2	7.0	2.55	1.4	0.3	0	0	7.0	—	0	0.18	0	0
3	51.0	2.5	23.0	18.0	0	0.01	11.0	—	0	0.8	0	0.01
4	597.0	2.5	490	97	0	0	13.0	—	0	2.4	0	0

[†]From *Reactor Physics Constants*, ANL-5800 (1963).

TABLE 2 Few-Group Diffusion Theory Constants for a Typical PWR Reactor Core

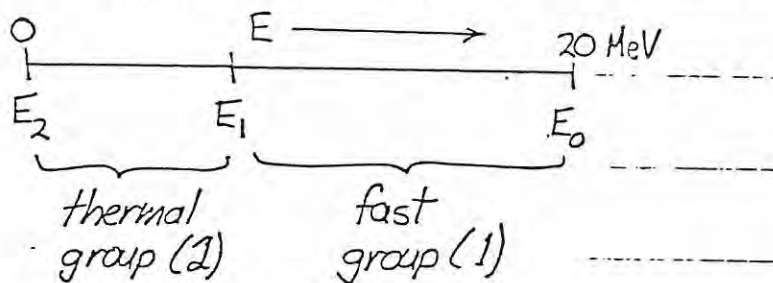
Group Constant	Two-Group		Four-Group			
	1 of 2	2 of 2	1 of 4	3 of 4	3 of 4	4 of 4
$\nu\Sigma_f$.008476	.18514	.009572	.001193	.01768	.18514
Σ_f	.003320	.07537	.003378	.0004850	.006970	.07527
Σ_a	.01207	.1210	.004946	.002840	.03053	.1210
D	1.2627	.3543	2.1623	1.0867	.6318	.3543
Σ_R	.02619	.1210	.08795	.06124	.09506	.1210

27.1) Two-Group Diffusion Theory

- Review of two-group model
- Analysis of reactor criticality
- 6-factor formula
- Collapse to one-group model
- Modified one-group model

To illustrate the multigroup diffusion method more explicitly, in this session we will examine the particular case of two-group diffusion theory.

27.2) Recall two-group structure:



fast group flux: $\phi_1(\underline{r})$

thermal group flux: $\phi_2(\underline{r})$

Recall that this model treats all neutrons as if they had one of two possible energies.

We will follow the usual convention by defining a group structure divided among a fast and thermal group.

The breakpoint energy, E_1 , is generally taken as roughly 1 eV.

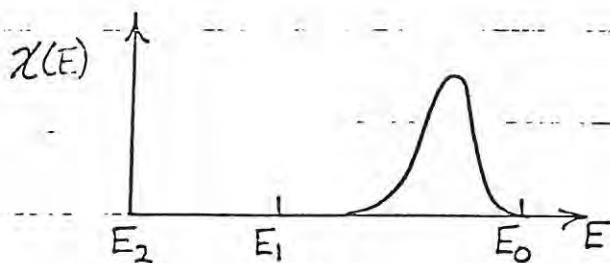
$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{t1} \phi_1 = \Sigma_{S1 \rightarrow 1} \phi_1 + \Sigma_{S2 \rightarrow 1} \phi_2 + \chi_{1\nu_1} \Sigma_{f1} \phi_1 + \chi_{1\nu_2} \Sigma_{f2} \phi_2 + S_1$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{t2} \phi_2 = \Sigma_{S1 \rightarrow 2} \phi_1 + \Sigma_{S2 \rightarrow 2} \phi_2 + \chi_{2\nu_1} \Sigma_{f1} \phi_1 + \chi_{2\nu_2} \Sigma_{f2} \phi_2 + S_2$$

two-group diffusion equations

We can dispense with further details and write down the form of the equations we derived in the last lecture. Note the coupling due to fission and scattering. We can simplify these group constants considerably.

27-4) Simplification of group-constants



$$\chi_1 \equiv \int_{E_1}^{E_0} dE \chi(E) = 1$$

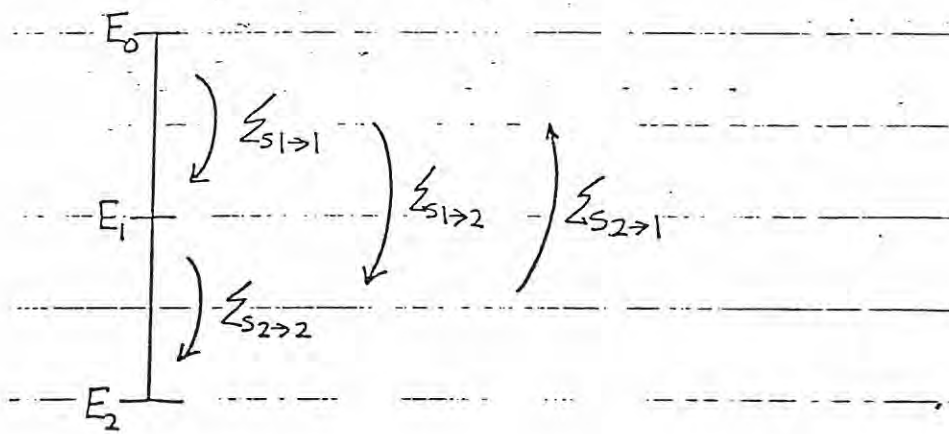
$$\chi_2 \equiv \int_{E_2}^{E_1} dE \chi(E) = 0$$

We will examine several terms in the equations. First look at the fission spectrum.

Essentially all fission neutrons are emitted with energies in the MeV range. Hence all fission neutrons appear in the fast energy group.

We can set the thermal group component equal to zero.

27-5) Neutron slowing down



Next we examine the various components of the scattering or transfer cross sections.

First note that the upscattering term from thermal to fast groups must be zero.

We can identify the within-group scattering cross sections (corresponding to collisions that scatter the neutron to another energy within the group).

27-6) Further simplifications

$$\Sigma_{R1} = \Sigma_{t1} - \Sigma_{S1 \rightarrow 1}$$

$$\Sigma_{S2 \rightarrow 1} = 0$$

$$\Sigma_{S2 \rightarrow 2} = \Sigma_{S2}$$

$$\Sigma_{R2} = \Sigma_{t2} - \Sigma_{S22} = \Sigma_{a2}$$

We can define the removal cross section for the fast group as essentially the sum of the absorption and downscattering cross sections.

The upscattering transfer cross section is set to zero. Note that the only type of scattering that can occur in the thermal group is within-group scattering.

Hence the removal cross section for the thermal group is just the absorption cross section for the group.

27-7)

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = \nu_1 \Sigma_{f1} \phi_1 + \nu_2 \Sigma_{f2} \phi_2 + S_1$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{a2} \phi_2 = \Sigma_{s1 \rightarrow 2} \phi_1 + S_2$$

Note: We still have to face task of calculating
the group constants

If we make these simplifications, we find the forms above. Note that the calculation of the two-group constants would require: i) performing a fine spectrum calculation for each group, ii) averaging appropriate cross section data over this spectrum to obtain the group constants.

7-8) Application: reactor criticality

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = \frac{1}{k} [\nu_1 \Sigma_{f1} \phi_1 + \nu_2 \Sigma_{f2} \phi_2]$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{a2} \phi_2 = \Sigma_{s1 \rightarrow 2} \phi_1$$

$k \equiv$ multiplication factor

Let's turn our attention to an application of the two-group model to a reactor criticality search.

To proceed further we need some information about the reactor geometry and composition.

27-9) Consider a bare, uniform reactor: _____



$$\phi_1(r) = \phi_1 \psi(r)$$

$$\nabla^2 \psi + B_g^2 \psi = 0$$

$$B_g^2 = \left(\frac{2.40}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$$

Hence we can replace _____

$$-\nabla \cdot D_1 \nabla \phi_1 \rightarrow +D_1 B_g^2 \phi_1$$

To simplify the spatial dependence, we will assume a spatial flux shape characteristic of a bare, uniform reactor (a cylindrical shape).

Note how the geometry buckling eliminates the spatial derivatives.

27-10)

$$-D_1 B_g^2 \phi_1 + \Sigma_{R1} \phi_1 = \frac{1}{k} \nu_1 \Sigma_{f1} \phi_1 + \frac{1}{k} \nu_2 \Sigma_{f2} \phi_2$$

$$-D_2 B_g^2 \phi_2 + \Sigma_{a2} \phi_2 = \Sigma_{s1 \rightarrow 2} \phi_1$$

$$(D_1 B_g^2 + \Sigma_{R1} - \frac{1}{k} \nu_1 \Sigma_{f1}) \phi_1 = \frac{1}{k} \nu_2 \Sigma_{f2} \phi_2$$

$$\Sigma_{s1 \rightarrow 2} \phi_1 = (D_2 B_g^2 + \Sigma_{a2}) \phi_2$$

$$(D_1 B_g^2 + \Sigma_{R1} - \frac{1}{k} \nu_1 \Sigma_{f1})(D_2 B_g^2 + \Sigma_{a2}) - \frac{1}{k} \nu_2 \Sigma_{f2} \Sigma_{s1 \rightarrow 2} = 0$$

When we eliminate the derivatives by substituting in the fundamental mode spatial dependence, we find the equations above.

We can rearrange and then solve for k.

27-11) Solve for the multiplication factor

$$k = \frac{\nu_1 \xi_{f1}}{\xi_{R1} + D_1 B_g^2} + \frac{\xi_{S1 \rightarrow 2} \nu_2 \xi_{f2}}{(\xi_{R1} + D_1 B_g^2) (\xi_{a2} + D_2 B_g^2)}$$

due to
fast
fissions

k_1

due to
thermal
fissions

k_2

In this way we can determine the multiplication factor in terms of the two group constants. We have rearranged this into a form more suitable for analysis.

27-12) Examine thermal group contribution:

$$k_2 = \frac{\xi_{S1 \rightarrow 2} \nu_2 \xi_{f2}}{(\xi_{R1} + D_1 B_g^2) (\xi_{a2} + D_2 B_g^2)}$$

$$= \frac{(\xi_{S1 \rightarrow 2} / \xi_{R1}) (\nu_2 \xi_{f2} / \xi_{a2})}{(1 + \frac{D_1}{\xi_{R1}} B_g^2) (1 + \frac{D_2}{\xi_{a2}} B_g^2)}$$

Note we can identify fast and thermal

nonleakage probabilities:

$$P_{NL1} = \frac{1}{(1 + L_1^2 B_g^2)}, \quad P_{NL2} = \frac{1}{(1 + L_2^2 B_g^2)}$$

First examine the thermal contribution (since it is of most importance for LWRs). From our earlier discussion of diffusion theory, it is evident that we can define the nonleakage probabilities. Note the definition of the diffusion lengths for each group.

27-13) Note further

$$\frac{\nu_2 \Sigma_{f2}}{\Sigma_{a2}} \rightarrow \eta_2 f_2$$

$$\frac{\Sigma_{s12}}{\Sigma_{R1}} \rightarrow p \quad (\text{resonance escape probability})$$

Thus

$$k_2 = \eta_2 f_2 P P_{NL1} P_{NL2}$$

We can separate our the fuel and total absorption cross sections to identify the thermal utilization.

Also motivate the resonance escape probability as the ratio between the total downscattering and total being removed.

Hence we can identify the thermal component of the multiplication factor.

7-16) Similarly

$$k_1 = \frac{\nu_1 \Sigma_{f1} / \Sigma_{R1}}{(1 + L_1^2 B_g^2)} = \eta_1 f_1 P_{NL1}$$

Finally, we write

$$k = k_1 + k_2 = \epsilon k_2$$

where

$$\epsilon \equiv \left(1 + \frac{k_1}{k_2}\right) = 1 + \underbrace{\left(\frac{\nu_1 \Sigma_{f1}}{\nu_2 \Sigma_{f2}}\right)}_{\text{fast fission factor}} \left(\frac{\Sigma_{a2} + D_2 B_g^2}{-\Sigma_{s1 \rightarrow 2}}\right)$$

In a similar way we can identify the fast component. Then we can introduce a definition of the fast fission factor to yield the final form of the 6-factor formula.

27-15) Put it all together and we find

$$k = \eta_2 f_2 p \in P_{NL_1} P_{NL_2}$$

$$= \eta_{th} f_{th} p \in P_{FNL} P_{TNL}$$

6-factor formula

Hence we find the usual form of the 6-factor formula.
Note the dependence on 2-group constants.

27-16) Group Collapsing: 2-group \rightarrow 1-group

$$\zeta_a = \frac{\int_{E_2}^{E_0} dE \zeta_a(E) \phi(E)}{\int_{E_2}^{E_0} dE \phi(E)}$$

$$\int_{E_2}^{E_0} dE \phi(E)$$

$$= \frac{\int_{E_1}^{E_0} dE \zeta_a(E) \phi(E) + \int_{E_2}^{E_1} dE \zeta_a(E) \phi(E)}{\int_{E_1}^{E_0} dE \phi(E) + \int_{E_2}^{E_1} dE \phi(E)}$$

$$\int_{E_1}^{E_0} dE \phi(E) + \int_{E_2}^{E_1} dE \phi(E)$$

We have noted that one frequently wishes to generate the group constants for a few-group calculation using the neutron spectrum generated by a many-group calculation.

We can illustrate this "group-collapsing" procedure by calculating the one-group constants in terms of the two-group constants.

27-17) or using our definitions of group

constants

$$\zeta_a = \frac{\zeta_{R_1} \phi_1 + \zeta_{a_2} \phi_2 - \zeta_{S_{12}} \phi_1}{\phi_1 + \phi_2}$$

$$= \frac{(\zeta_{R_1} - \zeta_{S_{1 \rightarrow 2}})(D_2 B_g^2 + \zeta_{a_2}) + \zeta_{S_{1 \rightarrow 2}} \zeta_{a_2}}{D_2 B_g^2 + \zeta_{a_2} + \zeta_{S_{1 \rightarrow 2}}}$$

We have determined 1-group constant ζ_a in terms of 2-group constants.

Here we have used the definition of the geometric buckling.

We can calculate the other one-group constants in terms of the two-group constants in a similar way.

7-18) Similarly

$$D = \frac{D_1 \phi_1 + D_2 \phi_2}{\phi_1 + \phi_2} = \frac{(D_2 B_g^2 + \zeta_{a_2}) D_1 + \zeta_{S_{1 \rightarrow 2}} D_2}{D_2 B_g^2 + \zeta_{a_2} + \zeta_{S_{1 \rightarrow 2}}}$$

$$v \zeta_f = \frac{v_1 \zeta_{f_1} \phi_1 + v_2 \zeta_{f_2} \phi_2}{\phi_1 + \phi_2} = \frac{(D_2 B_g^2 + \zeta_{a_2}) v_1 \zeta_{f_1} + v_2 \zeta_{S_{1 \rightarrow 2}} \zeta_{f_2}}{D_2 B_g^2 + \zeta_{a_2} + \zeta_{S_{1 \rightarrow 2}}}$$

In a similar way we find the other group constants. Again note the importance of this result since it allows us to relate one group constants to two-group constants. This is an example of the group collapsing method.

27-19 Modified One-Group Model

In large power reactors

$$\frac{-D_2 \nabla^2 \phi_2}{\Sigma_{a_2} \phi_2} = \frac{D_2 B_g^2}{\Sigma_{a_2}} \sim \frac{(0.5)(10^{-4})}{(0.1)}$$

$$\sim 5 \times 10^{-4} \ll 1$$

Hence neglect thermal neutron diffusion

$$-\nabla \cdot \cancel{D_2 \nabla} \phi_2 + \Sigma_{a_2} \phi_2 = -\Sigma_{s1 \rightarrow 2} \phi_1$$

In large power reactors we can ignore leakage in the thermal group.

If we neglect this term in the thermal group diffusion equation, we can solve and eliminate the thermal flux appearing in the fast group equation.

27-20 or

$$\phi_2 = \frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{a_2}} \phi_1$$

Thus our fast group equation becomes

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R_1} \phi_1$$

$$= -\nu_1 \Sigma_{f_1} \phi_1 + \nu_2 \Sigma_{f_2} \left(\frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{a_2}} \right) \phi_1$$

That is, we solve for the thermal flux in terms of the fast flux.

This can then be substituted into the fast group equation.

For a uniform reactor, we can rearrange

$$\nabla^2 \phi + \left(\frac{k_{\infty} - 1}{L^2} \right) \phi(r) = 0$$

where

$$k_{\infty} = \frac{\nu_1 \Sigma_{f1}}{\Sigma_{R1}} + \frac{\nu_2 \Sigma_{f2}}{\Sigma_{a2}} \frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{R1}}$$

$$= k_{\infty_1} + k_{\infty_2} p$$

"1/2 group model"

After some rearranging, we find a modified one-group diffusion model.

²⁷⁻²⁸ Aside: Sometimes introduce

$$M^2 = L_1^2 + L_2^2 = \frac{D_1}{\Sigma_{R1}} + \frac{D_2}{\Sigma_{R2}}$$

migration area

Migration area is a measure of mean-square

distance to slow down & be absorbed

$$M^2 = \frac{1}{6} (\text{mean-square distance to slowdown and be absorbed})$$

A useful modification of this scheme which takes some account of both fast and thermal leakage within a one-group treatment is obtained by replacing the diffusion length in the fast group equation by the so-called migration area.

²⁷⁻²² Wrapup Remarks:

• Introduced 1-group and 2-group models

• More common to use 4-group models

• When spatial dependence is more

complex, we must solve multigroup

diffusion equations on a computer.

Our topic for next time...

LECTURE 28

SOLUTION OF THE MULTIGROUP DIFFUSION EQUATIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 301 - 307

EXERCISES:

- 28.1. Derive a general group collapsing expression for N-group constants in terms of N x M group constants (e.g., 2-group in terms of 4-group).
- 28.2. Write out the explicit form of the matrix multigroup equations for a four-group 4 x 4 x 3 three dimensional spatial mesh problem in which the lowest two groups are both taken in the thermal range in which significant upscatter can occur.
- 28.3. Using a source such as ANL-7411, list and contrast various multigroup diffusion codes. In particular, compare their group structure, inner-outer iteration strategy, source-extrapolation methods, criticality search options, and estimated running times.

28-1 Solution of the Multigroup Diffusion Equations

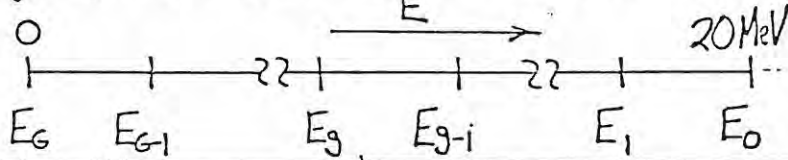
- Review of general form

- Strategy for solution

- Some general comments

In this session we will focus on the computer solution of the multigroup diffusion equations.

28-2 Multigroup structure



E_g E_{g-1}

group g

Let's begin by reminding ourselves of the essential features of the multigroup diffusion equations (MGD). First recall the group structure.

28-3 Multigroup diffusion equations

$$-\nabla \cdot D_g \nabla \phi_g + \Sigma_{t_g} \phi_g(r)$$

$$= \sum_{g'=1}^G \Sigma_{sg'} \phi_{g'} + \chi_g \sum_{g'=1}^G \nu_{g'} \Sigma_{fg'} \phi_{g'} + S_g$$

$$g=1, 2, \dots, G$$

Using this structure, we can proceed to write the MGD as shown.

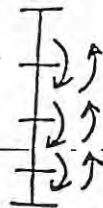
Actually, we will want to simplify this general form a bit.

28-4 Apply to criticality calculations

i) $S_g \rightarrow 0$

ii) no upscattering

iii) fission source



$$\chi_g \sum_{g'=1}^G \nu_{g'} \Sigma_{fg'} \phi_{g'} \rightarrow \chi_g S$$

We will focus our attention on criticality problems (other problems can be solved in a similar way).

We will introduce several assumptions.

With these assumptions, we can rewrite the form of the MGD equations.

$$\textcircled{28-5} \quad -\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = \frac{1}{k} \chi_1 S$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{R2} \phi_2 = \frac{1}{k} \chi_2 S + \Sigma_{S1 \rightarrow 2} \phi_1$$

$$-\nabla \cdot D_3 \nabla \phi_3 + \Sigma_{R3} \phi_3 = \frac{1}{k} \chi_3 S + \Sigma_{S1 \rightarrow 3} \phi_1 + \Sigma_{S2 \rightarrow 3} \phi_2$$

$$-\nabla \cdot D_G \nabla \phi_G + \Sigma_{RG} \phi_G = \frac{1}{k} \chi_G S + \Sigma_{IG} \phi_I$$

$$+ \dots + \Sigma_{SG-1, G} \phi_{G-1}$$

Note the general structure of the MGD equations.

The general strategy is quite similar to that followed in the one-speed method, except we successively solve the diffusion equations characterizing each group.

$\textcircled{28-6}$ Recall strategy for one-speed equation

$$-\nabla \cdot D \nabla \phi + \Sigma_a \phi(r) = \frac{1}{k} \nu \Sigma_f \phi$$

1.) Guess fission source $\frac{1}{k}$

$$S(r) = \nu \Sigma_f \phi \cong S^{(0)}(r), \quad k \cong k^{(0)}$$

2.) Now solve for flux ϕ from this source

$$-\nabla \cdot D \nabla \phi^{(1)} + \Sigma_a \phi^{(1)} = \frac{1}{k^{(0)}} S^{(0)}$$

Lets remind ourselves of the strategy for the one-speed equation.

We begin by guessing values of S and k .

Then we solve for the flux from this source.

Now we can use this to calculate a new source.

28-7 3.) Now calculate new fission source

$$S^{(1)} = \nu \sum_f \phi^{(1)}$$

and value of k

$$k^{(1)} = \frac{\int d^3r S^{(1)}(\underline{r})}{\frac{1}{k^{(0)}} \int d^3r S^{(0)}(\underline{r})}$$

4.) Solve diffusion equation again

$$-\nabla \cdot D \nabla \phi^{(2)} + \sum_a \phi^{(2)} = \frac{1}{k^{(1)}} S^{(1)}$$

We can then calculate a new guess of both S and k .
Then solve the diffusion equation.

We can keep on in this manner, iteratively, to
develop better and better guesses of the value
of k and the flux.

28-8 5.) And so on...

$$-\nabla \cdot D \nabla \phi^{(n+1)} + \sum_a \phi^{(n+1)} = \frac{1}{k^{(n)}} S^{(n)}$$

$$S^{(n+1)} = \nu \sum_f \phi^{(n+1)}$$

$$k^{(n+1)} = \frac{\int d^3r S^{(n+1)}(\underline{r})}{\frac{1}{k^{(n)}} \int d^3r S^{(n)}(\underline{r})}$$

Source iteration method

Eventually, S and k will converge.

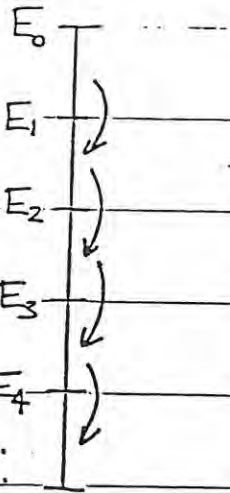
This method is known as the source iteration method. It
is the key technique used in the solution of criticality
problems.

The same idea can be applied to the MGD equations.

²⁸⁻⁹ We can play same game for multigroup

diffusion equations -- provided

there is only upscattering.



Guess fission source \vec{j} k

$$S(\underline{r}) \approx S^{(0)}(\underline{r})$$

$$k \approx k^{(0)}$$

We will assume only downscattering processes (for reasons that will become apparent).

Again we begin by guessing S and k .

Now focus on the highest energy group.

²⁸⁻¹⁰ Now solve for flux ϕ_1 in first (highest)

energy group

$$-\nabla \cdot \underline{D}_1 \nabla \phi_1^{(1)} + \Sigma_{R1} \phi_1^{(1)} = \frac{1}{k^{(0)}} \chi_1 S^{(0)}$$

Consider next group

$$-\nabla \cdot \underline{D}_2 \nabla \phi_2^{(1)} + \Sigma_{R2} \phi_2^{(1)} = \frac{1}{k^{(0)}} \chi_2 S^{(0)} + \Sigma_{S1 \rightarrow 2} \phi_1^{(1)}$$

NOTE: Both terms are known

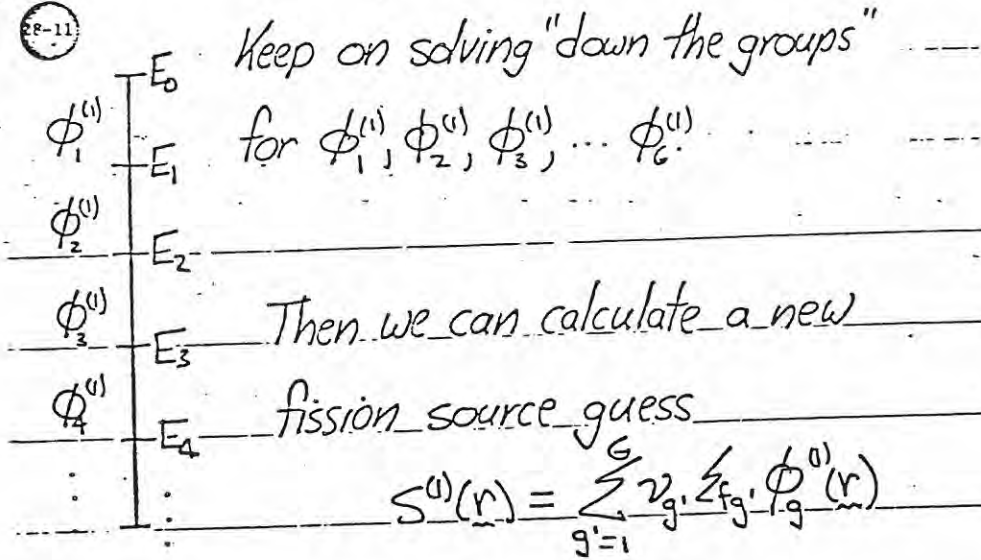
Let's look at the equation for this group.

We can solve for the flux.

Then on to the next group.

The key: each successive group involves only known terms from the higher groups.

28-11



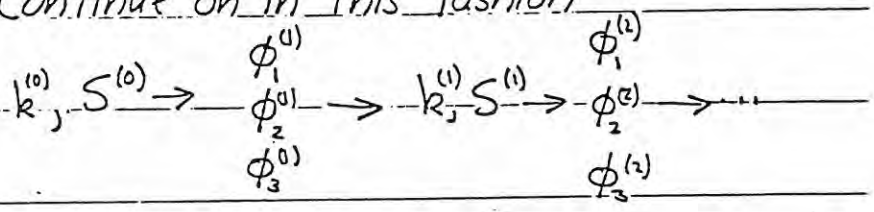
This means we can solve down the groups. Then we calculate a new fission source. With this we can calculate a new value of k.

28-12

and multiplication factor

$$k^{(1)} = \frac{\int d^3r S^{(1)}(r)}{\frac{1}{k^{(0)}} \int d^3r S^{(0)}(r)}$$

Continue on in this fashion



Here we can just use our earlier expression. We keep on iterating in this manner until we have convergence.

$$-\nabla \cdot D_1 \nabla \phi_1^{(n+1)} + \sum_{R_1} \phi_1^{(n+1)} = \frac{1}{k^{(n)}} \chi_1 S^{(n)}$$

$$-\nabla \cdot D_2 \nabla \phi_2^{(n+1)} + \sum_{R_2} \phi_2^{(n+1)} = \frac{1}{k^{(n)}} \chi_2 S^{(n)} + \sum_{S_1 \rightarrow 2} \phi_1^{(n+1)}$$

⋮

$$-\nabla \cdot D_G \nabla \phi_G^{(n+1)} + \sum_{R_G} \phi_G^{(n+1)} = \frac{1}{k^{(n)}} \chi_G S^{(n)} + \sum_{S_1 \rightarrow G} \phi_1^{(n+1)}$$

$$+ \sum_{S_2 \rightarrow G} \phi_2^{(n+1)} + \dots$$

Note importance of downscattering!

The key to this involves the structure of the MGD. Note the importance of downscattering. To handle upscattering, we would have to solve the equations simultaneously. This would require an iterative method. We will leave the topic of the source iteration method applied to the MGD equations and take a somewhat different perspective.

Some reactor analysis philosophy:

separation of variables

or

divide and conquer

PROBLEM:

flux depends on space

energy

direction

time

$$\phi(r, E, \hat{\Omega}, t)$$

We note an important philosophy in reactor analysis. The problem is that the equations generally depend on the complex structure of the cross sections. Even a direct numerical solution is usually impractical without further approximations.

28-15

APPROACH: "decouple" variable dependence

1.) Suppress space, direction, time

$$\phi(\underline{r}, E, \hat{\underline{\Omega}}, t) \rightarrow \phi(E)$$

Calculate energy-dependent spectrum

Average cross sections over spectrum

to get multigroup constants

$$\Sigma_{tg} = \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma_t(E) \phi(E)$$

The key is to decouple or separate the variables.

We will first illustrate this by considering this when solving for the energy dependence.

We will look at this method in detail in the next lecture.

28-16

2.) Suppress energy and time

$$\phi(\underline{r}, E, \hat{\underline{\Omega}}, t) \rightarrow \phi(\underline{r}, \hat{\underline{\Omega}})$$

Calculate flux in fuel cell to

get "homogenized" group constants

$$\langle \Sigma_{tg} \rangle_{\text{cell}} = \frac{\int_{\text{cell}} d^3r \Sigma_{tg}(\underline{r}) \phi(\underline{r})}{\int_{\text{cell}} d^3r \phi(\underline{r})}$$

A variation on this theme involves calculating the detailed spatial dependence of the flux in a fuel pin cell.

28-17

3.) Suppress energy, direction, & time

$$\phi(r, E, \hat{\Omega}, t) \rightarrow \phi(r)$$

Calculate flux & power as functions of space by solving MGD criticality problem

The multigroup diffusion equations themselves are an example of this separation of variables approach.

28-18

4.) Suppress space, energy, direction

$$\phi(r, E, \hat{\Omega}, t) \rightarrow \phi(t)$$

Solve for time dependence reactor kinetics burnup calculations

A final example is the treatment of the time dependence of the flux--reactor kinetics. Hence separation of variables is a very important concept in reactor analysis.

LECTURE 29

GENERATION OF MULTIGROUP CONSTANTS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 290 - 293
pp. 406 - 410

EXERCISES:

- 29.1. Estimate the total number of mesh points needed to adequately describe a nuclear reactor core if brute force discretization were utilized.
- 29.2. Compare the mfp for both thermal and fast neutrons with typical lattice parameters in LWRs and HTGRs.

29-1 Generation of Multigroup Constants

- Overview of MGD calculations
- Multigroup constants
- Energy averaging
- Spatial averaging
- The task ahead

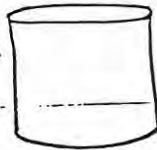
The key to MGD theory involves the determination of the parameters that appear in these equations, the multigroup constants.

This lesson will focus on how these MGC are determined.

3-2 What do we want?

Given:

core geometry & composition



Want:

core multiplication k

flux distribution $\phi(r)$

power distribution $P(r)$

We are usually concerned with calculating the multiplication and power distribution in the reactor.

The key role in this calculation is played by multigroup diffusion theory.

29-3 \odot Where do we start?

Energy-dependent diffusion equation

$$-\nabla \cdot D \nabla \phi + \Sigma_t(\underline{r}, E) \phi(\underline{r}, E)$$

$$= \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi(\underline{r}, E')$$

$$+ \frac{1}{k} \chi(E) \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \phi(\underline{r}, E')$$

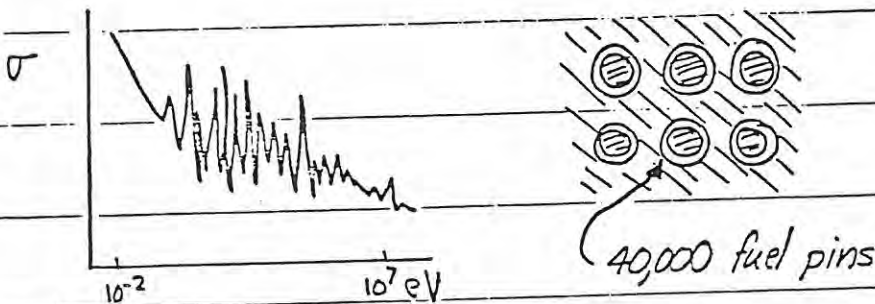
(Note: criticality calculation)

Recall that this method is based upon the energy dependent diffusion equation.

We have assumed: i) no time dependence, ii) a criticality calculation

Why don't we try to solve this equation by simply discretizing it and solving it on a computer?

\odot Problem: A realistic description of core requires realistic treatment of energy; space dependence of cross sections:



The complex energy and spatial dependence prevents this direct approach.

We must find an alternative way to take into account this detailed structure.

29-5

Brute force calculation:

i) thousands of energy points

ii) 40,000 x 25 x 100 space points

forget it!

Instead: Average $\Sigma_t(r, E)$ over space and energy to remove some of this complexity

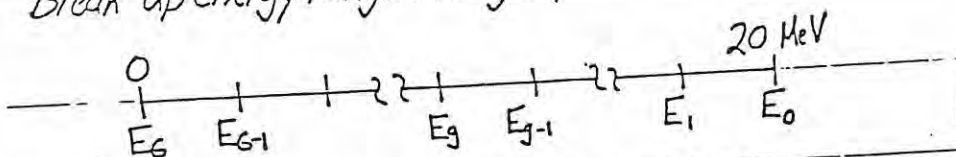
A direct approach would require enormous detail. We need a different approach.

Instead, we will attempt to average the cross sections themselves over the energy and spatial structure characterizing the reactor.

29-6

Energy Averaging

Break up energy range into groups



Integrate energy-dependent diffusion equation

over group g:
$$\int_{E_g}^{E_{g+1}} dE \left\{ \begin{array}{l} \text{energy-dependent} \\ \text{diffusion equation} \end{array} \right\}$$

Averaging over energy corresponds to the multigroup diffusion method.

Recall that our approach began by integrating the energy-dependent diffusion equation over a group g.

29-7 Define

$$\phi_g \equiv \int_{E_g}^{E_{g+1}} dE \phi(\underline{r}, E) \quad \text{group flux}$$

$$\xi_{tg} \equiv \frac{1}{\phi_g} \int_{E_g}^{E_{g+1}} dE \xi(\underline{r}, E) \phi(\underline{r}, E) \quad \text{group constant}$$

to find

$$-\nabla \cdot D_g \nabla \phi_g + \xi_{tg} \phi_g = \sum_{g'=1}^G \xi_{sg'} \phi_{g'} + \frac{1}{k} \chi_g \sum_{g'=1}^G \nu_{g'} \xi_{t_{g'}} \phi_{g'}$$

$g' = 1, \dots, G$

multigroup diffusion equations

We next introduced several key definitions.

This led to the multigroup diffusion equations.

The key ingredient in these equations were the multigroup constants.

29-8

Consider

$$\xi_{tg} \equiv \frac{\int_{E_g}^{E_{g+1}} dE \xi(\underline{r}, E) \phi(\underline{r}, E)}{\int_{E_g}^{E_{g+1}} dE \phi(\underline{r}, E)}$$

Problems:

i) We don't know intragroup flux $\phi(\underline{r}, E)$

ii) $\xi_{tg} = \xi_{tg}(\underline{r})$ since $\phi(\underline{r}, E)$ depends

on space \underline{r}

Let's look at their structure.

Two immediate problems: the fact that this definition depends on the intragroup flux (which is unknown) and indicates a spatial dependence.

We have already hinted as to how we can handle the intragroup flux.

29-9 Idea: Approximate intragroup flux

$$\phi(r, E) \sim \phi_{\text{approx}}(E) \quad \text{spectrum}$$

to find

$$\Sigma_{t9} \approx \frac{\int_{E_9}^{E_{9-1}} dE \Sigma_t(E) \phi_{\text{approx}}(E)}{\int_{E_9}^{E_{9-1}} dE \phi_{\text{approx}}(E)} \quad \text{MGC}$$

Key:

flux spectrum calculation \rightarrow MGC

The idea is to approximate the intragroup flux.
The key here is the calculation of the flux spectrum.
This will be the topic of the next few lectures.

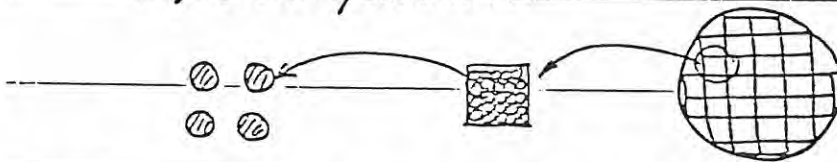
29-10 Spatial Averaging

Fact of life: cores are heterogeneous

i) facilitates thermal design

ii) mechanical design

iii) reactivity control



Let's move on to the spatial dependence.

Reactor cores are highly heterogeneous for a number of reasons,

To realize some of the implications of this structure, it is useful to consider some parameters.

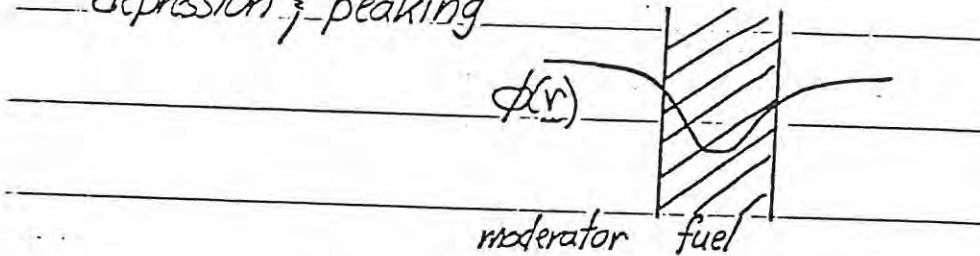
29-11 Some important parameters:

$mfp \sim cm \sim$ fuel element size

$L \sim 5cm \sim$ fuel assembly size

Must account for flux

depression & peaking



Here we note that the neutron mean free path is comparable to a fuel element size, while the neutron diffusion length is comparable to a fuel assembly size.

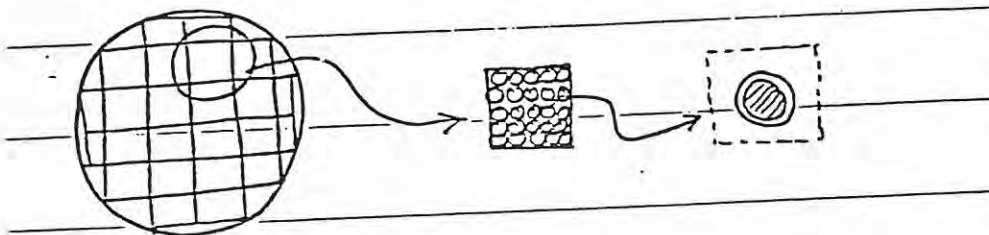
This means that the flux will vary on a scale comparable to the fuel pin structure.

How do we account for this in the multigroup constants?

29-12

Idea: "homogenize" core by spatially averaging

cross sections over spatial dependence



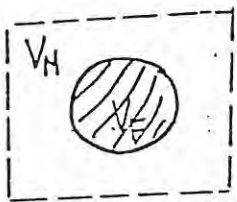
The key idea is to homogenize the core by averaging the cross sections over the spatial dependence of the flux.

This is very similar to the calculation of the multigroup constants themselves.

To make this more concrete, let's look at how we would handle a typical fuel pin cell.

(29-13) Example:

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\int_{V_{\text{cell}}} d^3r \Sigma_g(r) \phi(r)}{\int_{V_{\text{cell}}} d^3r \phi(r)}$$



$$= \frac{\int_{V_H} d^3r \Sigma_g^M \phi(r) + \int_{V_F} d^3r \Sigma_g^F \phi(r)}{\int_{V_H} d^3r \phi(r) + \int_{V_F} d^3r \phi(r)}$$

Define

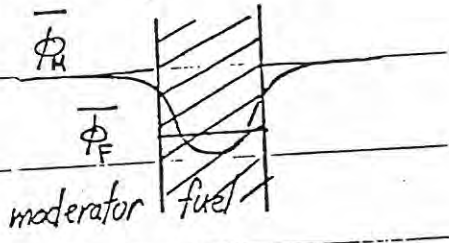
$$\bar{\Phi}_F \equiv \frac{1}{V_F} \int_{V_F} d^3r \phi(r); \quad \bar{\Phi}_M \equiv \frac{1}{V_M} \int_{V_M} d^3r \phi(r)$$

We will consider a two-region fuel cell. Then we can define the cell averaged group constants as shown. It is convenient to introduce the spatially averaged fluxes for each region. Then we can rewrite out cell-averages in a bit simpler form.

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\Sigma_g^M V_M \bar{\Phi}_M + \Sigma_g^F V_F \bar{\Phi}_F}{\Sigma_H \bar{\Phi}_H + V_F \bar{\Phi}_F} \equiv \frac{\Sigma_g^F + \Sigma_g^M \left(\frac{V_M}{V_F}\right) \xi}{1 + \left(\frac{V_M}{V_F}\right) \xi}$$

where

$$\xi \equiv \frac{\bar{\Phi}_H}{\bar{\Phi}_F} = \text{thermal disadvantage factor} > 1$$



We can rearrange this form to identify the thermal disadvantage factor (so called, because it is a measure of the relative disadvantage of fuel nuclei in competing for the absorption of thermal neutrons because of the depressed flux in the fuel relative to the moderator), Thus if we can determine the disadvantage factor, we can calculate the cell-averaged group constants.

We have two major jobs ahead:

i) calculate neutron energy spectrum $\phi(E)$

for energy averaging

$$\xi_g = \frac{\int_{E_g}^{E_{g-1}} dE \cdot \xi(E) \phi(E)}{\int_{E_g}^{E_{g-1}} dE \phi(E)}$$

It is apparent that we have two major jobs ahead of us. First we must calculate the neutron energy spectrum required for the energy averaging to yield the multigroup constants.

ii) calculate spatial dependence of the flux $\phi(r)$ in a fuel pin cell for

spatial averaging

$$\langle \xi_g \rangle_{\text{cell}} = \frac{\int_{V_{\text{cell}}} d^3r \xi_g(r) \phi(r)}{\int_{V_{\text{cell}}} d^3r \phi(r)}$$

Then we must calculate the spatial dependence of the flux in a fuel pin cell to calculate the spatial dependence. These topics will be our primary concern during the remainder of this course.

29-17 Plan of attack:

- 1.) Fast spectrum calculations; fast group constants (neutron slowing down)
- 2.) Thermal spectrum calculations; thermal group constants (neutron thermalization)
- 3.) Lattice cell "homogenization" (for fast and thermal group constants)

Our plan of attack will be as shown above.

LECTURE 30

FAST SPECTRUM CALCULATIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 315 - 321

EXERCISES:

- 30.1. Repeat the solution of the infinite medium slowing down equation in hydrogen for an arbitrary (distributed) source.
- 30.2. Determine the neutron flux resulting from an arbitrary source in an infinite homogeneous medium by: a) solving the infinite medium slowing down equation with a general source term, and then b) using the solution obtained for a monoenergetic source as a Green's function for the more general problem.

30-1 Fast Spectrum Calculations

- Neutron slowing down
- Infinite medium model
- Slowing down in hydrogen

Our task now is to compute the group constants for multi-group diffusion theory. The key will be to average microscopic cross section data over suitable approximations to the energy and spatial dependence of the flux in the fuel pin cell.

We first turn our attention to the study of the neutron spectrum characterizing fast neutrons.

30-2 Recall our goal:

$$\Sigma_{tg} \approx \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(E) \phi(E)}{\int_{E_g}^{E_{g-1}} dE \phi(E)}$$

$\phi(E) \rightarrow$ neutron energy spectrum

Recall our goal: to make an accurate estimate of the neutron energy spectrum (albeit with a crude treatment of the spatial dependence).

The key will be the neutron energy spectrum.

upscattering	elastic scattering (s-wave)	elastic scattering (p-wave)
chemical binding	no upscattering	inelastic scattering
diffraction	resonances (resolved)	resonances (unresolved)
		fission sources
0	1 eV	100 keV
neutron thermalization		fast fission
	neutron slowing down	

The methods used to generate the spectrum vary, depending on the neutron energy range.

It is natural to divide the energy range into regions. Each region is characterized by different physics.

We will focus on fast and neutron slowing down regions.

Key physical phenomena of importance:

i) neutron slowing down

ii) resonance absorption

For the next few lectures we will focus on the fast and slowing down regions.

The key physical theories of importance involve neutron slowing down and resonance absorption.

30-5) General approach:

i) careful treatment of energy dependence

ii) crude approximation of spatial dependence

Assume: neutron slowing down from

sources uniformly distributed throughout

an infinite medium

$$\phi(\underline{r}, E) \rightarrow \phi(E)$$

Our approach will be as shown.

We will assume an infinite medium so that we can ignore the spatial dependence altogether.

30-6) Recall

$$-\nabla \cdot D \nabla \phi + \Sigma(E) \phi(\underline{r}, E)$$

$$- \int_0^{\infty} dE' \Sigma_s(E \rightarrow E) \phi(\underline{r}, E') + \frac{1}{k} \chi(E) \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \phi(\underline{r}, E')$$

Assume:

i) infinite medium: $\nabla \cdot D \nabla \phi \rightarrow 0$

ii) given source term:

$$S(E) = \frac{1}{k} \chi(E) \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \phi(E')$$

\rightarrow known

Recall the form of the energy dependent diffusion equation. We can simplify this by assuming an infinite medium and lumping fission sources into the source term.

30-7) Then find

$$\Sigma_1(E)\phi(E) = \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E)\phi(E') + S(E)$$

infinite medium spectrum equation

(neutron slowing down equation)

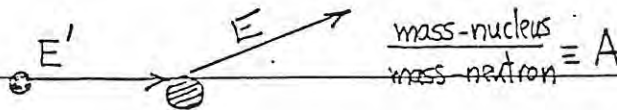
We will apply this to the neutron

slowing down range: $1\text{eV} < E < 20\text{MeV}$

We need information about $\Sigma_1(E)$, $\Sigma_s(E' \rightarrow E)$.

These simplifications lead to the infinite medium spectrum equation. This is an integral equation, in contrast to the differential equations that characterize most of engineering. To proceed further, we need some information about the energy dependence of the cross sections.

30-8) Assume: elastic scattering, isotropic in center of mass frame (s-wave)



Then

$$\frac{\Sigma_s(E')}{(1-\alpha)E'}, \quad E < E' < E/\alpha$$

$$\Sigma_s(E' \rightarrow E) = 0, \quad \text{otherwise}$$

where

$$\alpha \equiv \left(\frac{A-1}{A+1}\right)^2$$

We will consider the form of these cross sections in the most important case: elastic scattering. We can now substitute these into the slowing down equation.

30-9 Neutron slowing down equation becomes

$$[\Sigma_s(E) + \Sigma_a(E)]\phi(E) = \int_E^{E/\alpha} dE' \frac{\Sigma_s(E')\phi(E')}{(1-\alpha)E'} + S(E)$$

We will look at several cases:

i) hydrogen: $A=1$ (with ; without Σ_a)

ii) nonhydrogenous: $A>1$ (with ; without Σ_a)

The slowing down equation then takes the form above. We will break up our study of this equation into several case. We will begin with the simplest, but also the most important case.

30-10 Slowing down in hydrogen, no absorption

Why? i) easiest case

ii) $H_2O \sim H$

iii) $\frac{\sigma_a^H}{\sigma_s^H} \sim 0.01$

Then $A=1$, $\alpha=0$, such that

$$\Sigma_s(E)\phi(E) = \int_E^{\infty} dE' \frac{\Sigma_s(E')\phi(E')}{E'} + S(E)$$

We will consider slowing down in hydrogen with no absorption. This isn't a bad approximation. Then the slowing down equation simplifies as shown.

30-11 Consider neutron slowing down from a

monoenergetic source at energy E_0

$$\Sigma_s(E)\phi(E) = \int_E^{E_0} dE' \frac{\Sigma_s(E')\phi(E')}{E'}$$

$E < E_0$

Introduce

$$F(E) \equiv \Sigma_s(E)\phi(E) \quad \text{collision density}$$

We will solve this for a problem in which a monoenergetic source emits neutrons with energy E_0 .

For energies below the source energy, we can ignore the source term in the equation.

To solve this, we will introduce a new dependent variable. This is just the collision rate density.

30-12 Then slowing down equation becomes

$$F(E) = \int_E^{E_0} dE' \frac{F(E')}{E'}$$

Now differentiate with respect to E .

RECALL:

$$\frac{d}{dx} \left[\int_{b(x)}^{a(x)} dx' F(x, x') \right] = F(x, a) \frac{da}{dx} - F(x, b) \frac{db}{dx} + \int_{b(x)}^{a(x)} dx' \frac{\partial F(x, x')}{\partial x}$$

We can substitute this into the slowing down equation.
 We now differentiate this with respect to energy E .
 We recall the formula from calculus on how to accomplish this.

Hence

$$\frac{d}{dE} \left[\int_E^{E_0} dE' \frac{F(E')}{E'} \right] = - \frac{F(E)}{E} \frac{dE}{dE} = - \frac{F(E)}{E}$$

so that the neutron slowing down equation becomes

$$\frac{dF}{dE} = - \frac{1}{E} F(E)$$

Solution:

$$F(E) = \frac{C}{E}$$

Then differentiating the integral terms gives us the above. We can solve this simple ordinary differential equation. How do we determine C?

Source condition at E_0 determines $C = S_0$

$$F(E) = \frac{S_0}{E} = \Sigma_s(E) \phi(E)$$

Hence

$$\phi(E) = \frac{S_0}{\Sigma_s(E) E}, \quad E > E_0$$

NOTE: $\Sigma_s(E) \sim \text{constant}$

$$\phi(E) \sim \frac{1}{E}$$

for neutron slowing down

We can determine C by simply applying the source condition at energy E

The solution is quite simple. Since the scattering cross section depends only weakly on energy, the flux behaves essentially as $1/E$.

This slowing down behavior of the flux is very simple.

This is a very important result

$$\phi(E) \sim \frac{1}{E}$$

(neutron slowing down)

Thus far: i) hydrogen

ii) no absorption

iii) infinite medium

This is also a very important result.
Let's remember the restrictions, however.

LECTURE 31

NEUTRON SLOWING DOWN (Continued)

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 321 - 325

EXERCISES:

- 31.1. Derive an expression for the neutron balance in a nuclear reactor in terms of the scalar flux and the current density.
- 31.2. Transform the infinite medium slowing down equation (assuming only elastic scattering) from the energy variable to the lethargy variable.
- 31.2. Calculate the mean lethargy loss per collision, the moderating power, and the moderating ratio for light water and heavy water at energies of 1 eV and 100 eV.

31-1 Neutron Slowing Down (continued)

• Neutron slowing down density

• Neutron lethargy

• Moderating parameters

We will continue with our study of neutron slowing down.
In this session we will introduce some important new concepts.

31-2 Neutron slowing down in hydrogen ($\xi_a = 0$)

$$\Sigma_s(E)\phi(E) = \int_E^{\infty} dE' \frac{\Sigma_s(E')\phi(E')}{E'} + S(E)$$

We found

$$\phi(E) = \frac{S_0}{\Sigma_s(E)E}$$

$$\sim \frac{1}{E}$$

We began with the neutron slowing down equation.

We found a simple solution.

We will extend this result to other media, but first we will introduce two important new concepts.

31-3

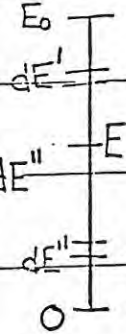
Neutron slowing down density

$q_0(E)$ = number of neutrons slowing down past energy E per second

Note

rate at which neutrons that suffer collisions in dE' slow down past E

$$= \left[\int_0^E dE'' \xi_s(E' \rightarrow E'') \phi(E') \right] dE''$$



We begin by defining the neutron slowing down density. We can calculate this in terms of the scattering cross section.

31-4

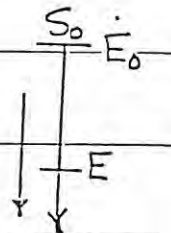
Hence we can integrate over all initial energies

$E' > E$ to find

$$q_0(E) = \int_E^{E_0} dE' \int_0^E dE'' \xi_s(E' \rightarrow E'') \phi(E')$$

For our homogeneous moderator we find

$$q_0(E) = \int_0^E dE'' \int_E^{E_0} dE' \frac{\xi_s(E') \phi(E')}{E'} = EF(E) = S_0$$



(as we might have expected.)

We find the expression above (for slowing down). We can simplify this for the case of hydrogen. In this case, the slowing down density (in the absence of absorption) is equal to the source strength.

31-5: That is, in the absence of absorption

$$q_0(E) = \text{constant} = S_0$$

since all source neutrons must eventually slow-down below energy E .

This result applies for zero absorption.

31-6: Neutron lethargy

Note: $1 \text{ eV} < E < 10^7 \text{ eV}$

Idea: switch to a logarithmic variable

$$u = \ln \frac{E_0}{E} \rightarrow \text{neutron lethargy}$$

(E_0 = source energy or highest energy in problem)

Note: As energy decreases, lethargy u increases.

As neutron slows down, it becomes more "lethargic"

The large energy range suggests the use of a new independent variable related to the logarithm of the energy. This is known as the neutron lethargy. There is another reason for introducing the lethargy variable.

(1-7) It is more convenient to perform fast spectrum calculations in terms of neutron lethargy.

Convert slowing-down equation over to lethargy variable.

$$\text{Note: } du = \frac{d}{dE} \left(\ln \frac{E_0}{E} \right) dE$$
$$= \left(\frac{1}{E} \right) \left(-\frac{E_0}{E^2} \right) dE = -\frac{dE}{E}$$

$$E = E_0 e^{-u}$$

It is more convenient to use in performing slowing down calculations.

We can convert all of the terms in the slowing down equation. First we note.

(1-8) Look at collision density

$$F(u) du = -F(E) dE$$

or $F(u) = E F(E)$

Note that for our infinite, homogeneous medium

$$F(u) = E \left(\frac{S_0}{E} \right) = S_0$$

($F(u)$ is usually more slowly varying than $F(E)$.)

Begin by examining the collision rate density $F(E)$.

Note that in lethargy, $F(u)$ is constant.

This is important for numerical solutions.

31-9

Can also convert:

$$\Sigma_s(E' \rightarrow E) = \frac{\Sigma_s(E')}{(1-\alpha)E'} \quad E < E' < E_0$$

$$0 \quad \text{, otherwise}$$

to

$$\Sigma_s(u' \rightarrow u) = \frac{\Sigma_s(u') e^{u'-u}}{(1-\alpha)} \quad u - \ln \alpha < u' < u$$

$$0 \quad \text{, otherwise}$$

We can also convert the forms of the cross sections.

31-10

For hydrogen, the slowing down equation becomes

$$\Sigma_s(u) \phi(u) = \int_0^u du' e^{u'-u} \Sigma_s(u') \phi(u') + S(u)$$

Aside: for hydrogen

$$q(u) = \int_0^u du' \Sigma_s(u') \phi(u') e^{u'-u}$$

and

$$\frac{dq}{du} = - \underbrace{\int_0^u du' \Sigma_s(u') \phi(u') e^{u'-u}}_{q(u)} + \Sigma_s(u) \phi(u)$$

For hydrogen, the slowing down equation in lethargy becomes as shown.

There is a useful feature of this equation. Note the form of the slowing down density for hydrogen,

By differentiating, we find a simple differential equation for the slowing down density.

31-11

Thus we find

$$\frac{dq}{du} + q(u) = \xi_s(u) \phi(u)$$

We can also rewrite the slowing down equation as

$$\xi_s(u) \phi(u) = \frac{dq}{du} + S(u)$$

(These are more convenient forms to solve on a computer.)

To this differential equation, we can add a second equation by rewriting the slowing down equation in slightly different form. These are far simpler to solve on a computer than the original form of the slowing down equation.

31-12

Parameters characterizing moderators

Let us calculate the average lethargy gain of a neutron in a collision

$$\xi \equiv \langle \Delta u \rangle = \int_{\alpha E_i}^{E_i} \left[\ln\left(\frac{E_0}{E_f}\right) - \ln\left(\frac{E_0}{E_i}\right) \right] \frac{1}{(1-\alpha)E_i} dE_f$$

$$= 1 + \frac{\alpha}{1-\alpha} \ln \alpha = 1 - \frac{(A-1)^2}{2A} \ln \left(\frac{A+1}{A-1} \right)$$

- Example:
- H $\rightarrow \xi = 1$
 - C $\rightarrow \xi = .158$
 - U $\rightarrow \xi = .008$

Suppose we calculate the average lethargy loss in a collision by using the form of the differential scattering cross section. We can use this to calculate the number of scattering collisions required to slow down in a given moderator.

31-13

Application: average number of collisions
necessary to thermalize a fission neutron

$$\langle \# \rangle = \frac{\ln \frac{2 \times 10^6}{1}}{\xi} = \frac{14.5}{\xi}$$



Example: H → 14

C → 91

U → 1730

For example, the average number of collisions necessary to thermalize a fission neutron in various moderators can be estimated as shown. There are a couple of other useful parameters we can use to characterize moderators.

31-14

Other useful parameters:

$$\text{moderating power} \equiv \xi \Sigma_s$$

$$\text{moderating ratio} \equiv \frac{\xi \Sigma_s}{\Sigma_a}$$

We might expect a good moderator would have a large scattering cross section as well as a large value of ξ . But we should also take into account the relative amount of absorption.

A comparison of moderators

Mod	ξ	$\langle \# \rangle$	$\xi \xi_s$	$\xi \xi_s / \xi_a$
H	1	14	—	—
D	.725	20	—	—
H ₂ O	.920	16	1.35	71
D ₂ O	.509	29	0.176	5670
C	.158	91	0.060	192
U	.008	1730	0.003	.0092

We can compare these parameters for various different moderators.

Note in this chart that H and D are gases.

It is apparent that D₂O and C are the best moderators.

Indeed, these two materials can be used to achieve a chain reaction with natural uranium.

However for other reasons, light water (H₂O) is the most popular moderator in power reactors.

LECTURE 32

NEUTRON SLOWING DOWN (One More Time...)

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 325 - 332

EXERCISES:

32.1. Demonstrate that for large mass numbers A ,

$$\xi \sim \frac{2}{A + \frac{2}{3}}$$

32.2. Solve the coupled slowing down equations for an infinite homogeneous medium:

$$\Sigma_a(u)\phi(u) = -\frac{dq}{du} + S(u), \quad \frac{dq}{du} + q(u) = \Sigma_s(u)\phi(u)$$

for a monenergetic source at lethargy $u = 0$.

32.3. Derive an expression for the energy spectrum of the flux in the first collision interval of a moderator of mass A which has an arbitrarily varying scattering cross section and absorption cross section. Assume that the medium is infinite and homogeneous, that neutrons are emitted at a given energy E_0 , and that there is no absorption at this energy.

32-1. Neutron Slowing Down (one more time...)

• Slowing down with absorption

• Nonhydrogenous media ($A > 1$)

• Inelastic scattering

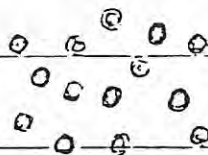
Thus far we have restricted our study with three major assumptions: i) hydrogen, ii) elastic scattering, iii) no absorption.

In this session we will develop the generalizations of the theory.

32-2. Slowing down in hydrogen with absorption

hydrogen (moderator)

absorber



$$[\Sigma_a(E) + \Sigma_s(E)] \phi(E) = \int_E^{E_0} dE' \frac{\Sigma_s(E') \phi(E')}{E} \quad E < E_0$$

Again define

$$F(E) = \Sigma_t(E) \phi(E)$$

We begin by adding a dash of absorption to our hydrogen problem.

We can solve this just as before by introducing the total collision rate density.

32-3

to find

$$F(E) = \int_E^{E_0} \left[\frac{\xi_s(E')}{E' \xi_t(E')} \right] F(E') dE'$$

Again we differentiate to find

$$\frac{dF}{dE} = - \left[\frac{\xi_s(E)}{E \xi_t(E)} \right] F(E)$$

If we plug this in and differentiate as before, we find the indicated differential equation.

We can easily solve this equation.

32-4

Rearrange

$$\int_{F(E)}^{F(E_0)} \frac{dF}{F} = - \int_E^{E_0} \frac{\xi_s(E)}{E \xi_t(E)} dE$$

to arrive at

$$F(E) = \frac{\xi_s(E_0)}{\xi_t(E_0)} \frac{S_0}{E} \exp \left[- \int_E^{E_0} \frac{\xi_s(E')}{E' \xi_t(E')} dE' \right]$$

Note:

$$\xi_s = 0 \Rightarrow F(E) = \frac{S_0}{E}$$

Just rearrange it and then integrate both sides.

Note the special case in which we set the absorption equal to zero.

32-5

We can compute slowing down density as

$$q(E) = EF(E) = S_0 \exp \left[- \int_E^{E_0} dE' \frac{\Sigma_a(E')}{E' \Sigma_t(E')} \right]$$

Note:

$S_0 \equiv$ rate of source neutron emission at E_0

$q(E) =$ rate at which neutrons slow past E

$$\frac{q(E)}{S_0} = \text{probability that source neutron is not absorbed while slowing down from } E_0 \text{ to } E \equiv p(E)$$

We can calculate the slowing down density. But note that the ratio is just the resonance escape probability.

32-6

This is just the resonance escape probability

$$p(E) = \exp \left[- \int_E^{E_0} dE' \frac{\Sigma_a(E')}{E' \Sigma_t(E')} \right]$$

(We'll return later to study this expression in detail.)

Hence we now have an explicit form of the resonance escape probability. We will return later to study this in more detail. For now, however, we will continue with our study of neutron slowing down.

32-7 Neutron moderation for $A > 1$

(no absorption, please...)

$$\Sigma_s(E)\phi(E) = \int_E^{E_0} dE' \frac{\Sigma_s(E')\phi(E')}{(1-\alpha)E'}, \quad E < E_0$$

Again we define

$$F(E) = \Sigma_s(E)\phi(E)$$

Let's look at the case of nonhydrogenous media. Now the slowing down equation is as shown. We can try to repeat our earlier method to solve this. Introduce the collision rate density and then substitute this in.

32-8 to find

$$F(E) = \int_E^{E_0} dE' \frac{F(E')}{(1-\alpha)E'}$$

or differentiating

$$\frac{dF}{dE} = \frac{1}{(1-\alpha)} \left[\frac{F(E_0)}{(E_0)} - \frac{F(E)}{E} \right]$$

(A "differential-difference" equation -- tough to solve!)

But now when we differentiate, we run into problems. The equation we are led to is an example of a differential-difference equation. Such equations are difficult to solve (in fact, the solutions are discontinuous). Instead we will try a different tack.

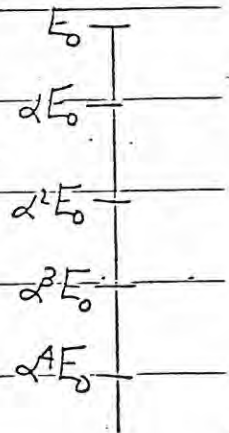
32-9

An important case -- far below source

energy E_0 -- asymptotic solution

Then source term disappears

$$F(E) = \int_E^{E_0} dE' \frac{F(E')}{(1-\alpha)E'}$$



Asymptotic solution:

$$F(E) \sim \frac{S_0}{\sum \xi_s \xi_s(E) E}$$

We will examine the case of energies "far" below the source.
 Note the concept of collision intervals.
 We will seek an asymptotic solution.
 This simple form is very important.

32-10

Hence we arrive at a key result

$$\phi(E) = \frac{S_0}{\sum \xi_s \xi_s(E) E}$$

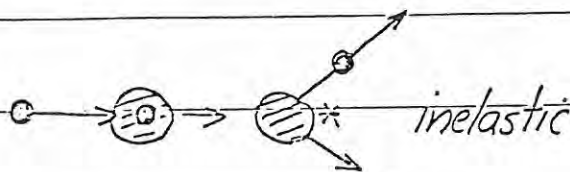
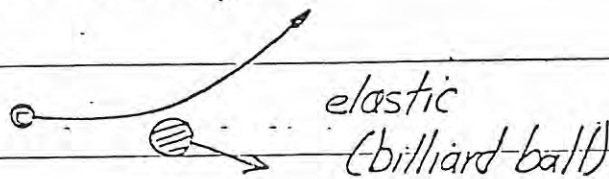
For a mixture of materials

$$\phi(E) \sim \frac{S_0}{\bar{\xi} E \xi_s(E)}$$

$$\bar{\xi} \equiv \frac{\sum_{i=1}^N \xi_i \xi_s^{(i)}(E)}{\sum_{i=1}^N \xi_s^{(i)}(E)}$$

Hence the form of the flux of neutrons slowing down in a moderator is.
 We can generalize this to a mixture of materials.

32-11 Inelastic scattering



Requires $E > 50 \text{ keV}$

Thus far we have considered only elastic scattering. However, for accurate calculations we must also consider inelastic scattering processes.

32-12 Most important for heavy nuclei:

U-238, 1 MeV neutron

$$\Delta E|_{\text{elastic}} = \left(\frac{1-\alpha}{2}\right) E_0 = 0.0085 \text{ MeV}$$

$$\Delta E|_{\text{inelastic}} = 0.6 \text{ MeV}$$

Also an energy threshold:

C-12: 4.4 MeV

O-16: 6.1 MeV

U-238: 45 keV

Inelastic scattering is most important for heavy nuclei. We generally handle inelastic scattering directly on the computer. We will consider this when we look at the detailed methods used to generate fast spectra.

LECTURE 33

RESONANCE ABSORPTION

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 332 - 341

EXERCISES:

- 33.1. Calculate the resonance escape probability in homogeneous media for finite dilution but at zero temperature. Show explicitly that this expression reduces to the infinite dilution result in the limit as

$$\frac{N_A \sigma_0}{N_H \sigma_s} \rightarrow 0$$

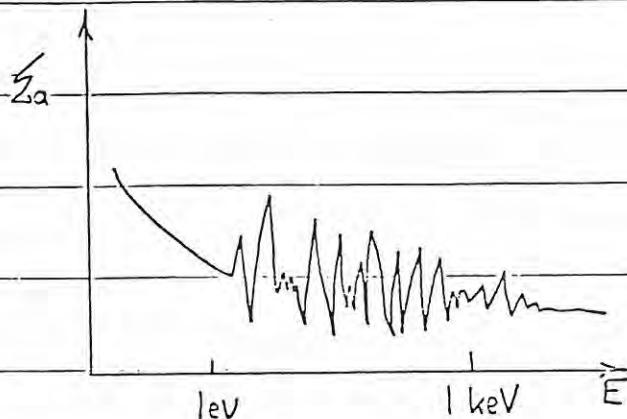
33-1 Resonance Absorption

- Importance of resonance absorption
- Example: hydrogen + absorber
- Doppler effect
- Resonance integrals

In this session we begin the study of the second effect of major importance in fast spectrum calculations: resonance absorption

33-2 Major effect during slowing down:

resonance absorption



Resonance absorption is the primary mechanism of interest during neutron slowing down. Consider the energy dependence of the cross section for a typical material. What aspects of resonance absorption are of most concern?

Major concern: low-lying resonances in heavy isotopes such as U-238, Pu-240

Important for:

i) criticality (reactivity)

ii) conversion, breeding

Premium is on fast & efficient approximate methods

Of major concern are the low lying resonance in heavy isotopes such as U-238 and Pu-240.

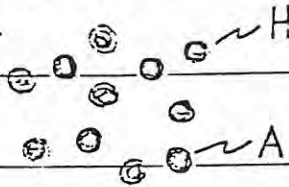
One can always calculate the resonance escape probability using brute force numerical methods.

However the premium is on fast and efficient approximate methods.

To demonstrate this, we will return to consider an old friend.

Example: resonance absorption in hydrogen

plus an infinite mass absorber



hydrogen scatters

absorber absorbs

Recall

$$\phi(E) = \frac{S_0}{E \Sigma_s(E)} P(E)$$

resonance escape prob.

We will begin by considering slowing down in hydrogen plus an infinite mass absorber (so the absorber doesn't also slow down the neutrons).

Recall the form of the solution for this problem.

Here the key quantity of interest is the resonance escape probability.

(33-5) where

$$p(E) = \exp \left[- \int_E^{E_0} \frac{dE'}{E'} \frac{\Sigma_0(E')}{\Sigma_f(E')} \right]$$

$$= \exp \left[- \int_E^{E_0} \frac{dE'}{E'} \frac{N_A \sigma_f^A(E') + N_H \sigma_f^H(E')}{N_A \sigma_s^A + N_H \sigma_s^H + N_A \sigma_f^A + N_H \sigma_f^H} \right]$$

ignore ignore

$$= \exp \left[- \int_E^{E_0} \frac{dE'}{E'} \frac{N_A \sigma_f^A(E')}{N_H \sigma_s^H + N_A \sigma_f^A} \right]$$

Now all we need is $\sigma_f^A(E)$.

In the previous lecture we calculate $p(E)$ as shown. Let's substitute in the forms of the cross sections and simplify.

Now all we need to complete the calculation is the form of the capture cross section for the absorber material. To calculate this, we will use a result from an earlier part of this course.

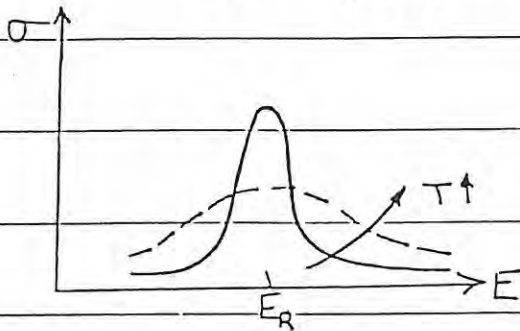
We will use the form of the capture cross section for a Doppler-broadened resonance.

(33-6) Use Doppler-broadened resonance

$$\sigma_f^A(E) = \sigma_0 \frac{\Gamma}{v} \psi(\xi, x)$$

$$\psi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dy \frac{e^{-\frac{1}{4}(x-y)^2 \xi^2}}{1+y^2}$$

$$\xi = \Gamma \left(\frac{A}{4E_R kT} \right)^{1/2}, \quad x = 2 \left(\frac{E - E_R}{\Gamma} \right)$$



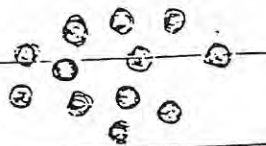
Recall the form taken by the cross section for this case. Note the temperature dependence.

We will now examine the effect of this behavior on the resonance escape probability.

33-7 Simple case: infinite dilution

$$N_A \sigma_s^A(E) < N_A \sigma_s \ll N_H \sigma_s^H$$

$$p \approx \exp \left[- \frac{N_A}{N_H \sigma_s^H} \int_{E_R}^{\infty} dE' \sigma_s^A(E') \right]$$



$$\rightarrow \frac{1}{E_R} \int_{E_R}^{\infty} dE' \sigma_s^A(E') = \frac{1}{E_R} \frac{\sigma_0 \Gamma \pi}{2}$$

or

$$p \rightarrow p^\infty = \exp \left[- \frac{\pi}{2} \frac{N_A \sigma_0 \Gamma}{N_H \sigma_s^H E_R} \right]$$

Let's consider a simple case in which the concentration of the absorber is so small, that is, so dilute, that we can make the following approximation.

Hence our final result for the resonance escape probability is as shown. Here the infinite sign indicates that the infinite dilution limit has been used.

Let's examine this result in more detail.

33-8 Examine:
$$p^\infty = \exp \left[- \frac{\pi}{2} \frac{N_A \sigma_0 \Gamma}{N_H \sigma_s^H E_R} \right]$$

Note:

i) $p^\infty \uparrow$ as $N_H \uparrow$ (Very important in water moderated reactors)

ii) $p^\infty \downarrow$ as $E_R \downarrow$ (most significant absorption occurs in lower resonances -- e.g., 6.67 eV resonance in U-238)

iii) p^∞ does not depend on temperature T (only for infinite dilution)

We will first examine the behavior of the resonance escape probability as we vary different quantities.

First note the dependence on the moderator density.

Then note the dependence on the resonance energy.

Finally, note that this form does not depend on temperature.

This is because of the infinite dilution approximation.

33-9: More complicated case: finite dilution

$$p = \exp \left[- \frac{\int_{E_R}^{\infty} dE' \frac{N_A \sigma_f^A(E')}{N_H \sigma_s^H + N_A \sigma_f^A(E')}}{E_R} \right]$$

$$= \exp \left[- \frac{\Gamma}{E_R} J(\xi, \beta) \right]$$

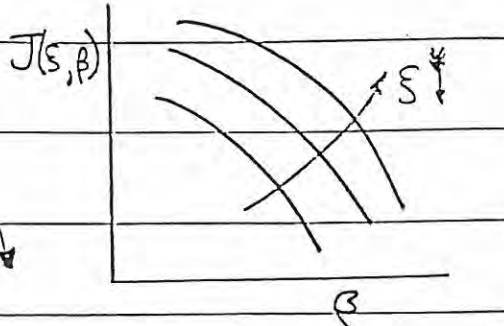
where $J(\xi, \beta) \equiv \int_0^{\infty} dx \frac{\psi(\xi, x)}{\beta + \psi(\xi, x)}$

$$\beta \equiv \frac{N_H \sigma_s^H}{N_A \sigma_0} \frac{\Gamma}{\Gamma_0}, \quad \xi = \Gamma \left(\frac{-A}{4E_R kT} \right)^{1/2}$$

In the more general case of finite dilution, we can write the resonance escape probability as shown. Now there is a temperature dependence, as we can demonstrate.

33-10:

$$p = \exp \left[- \frac{\Gamma}{E_R} J(\xi, \beta) \right]$$



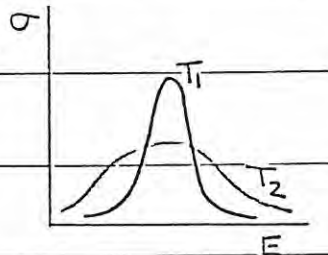
Note:

$$T \uparrow \Rightarrow \xi = \Gamma \left(\frac{-A}{4E_R kT} \right)^{1/2} \downarrow$$

$$\Rightarrow J \uparrow$$

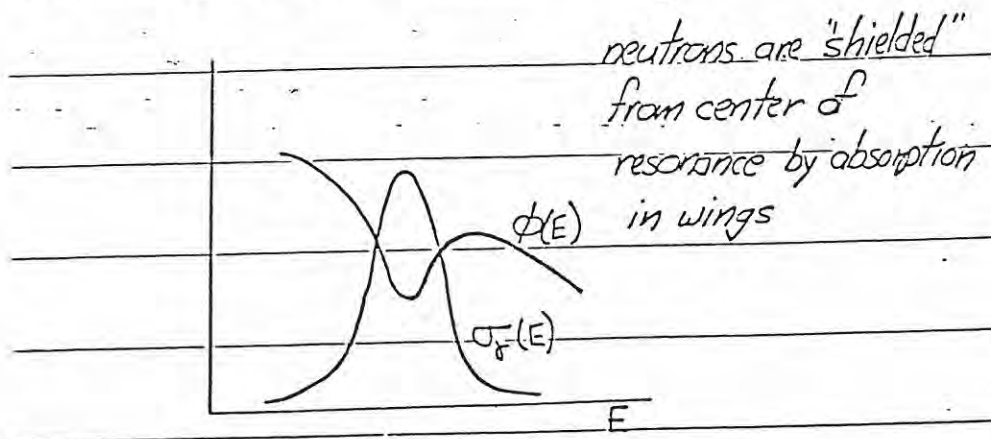
$$\Rightarrow p \downarrow$$

Idea: As $T \uparrow$, resonance broadens and neutrons have a tougher time scattering across it



If we examine the form for the temperature dependence, we note the following. There is an alternative viewpoint that is sometimes useful.

83-11 Alternative view: self-shielding



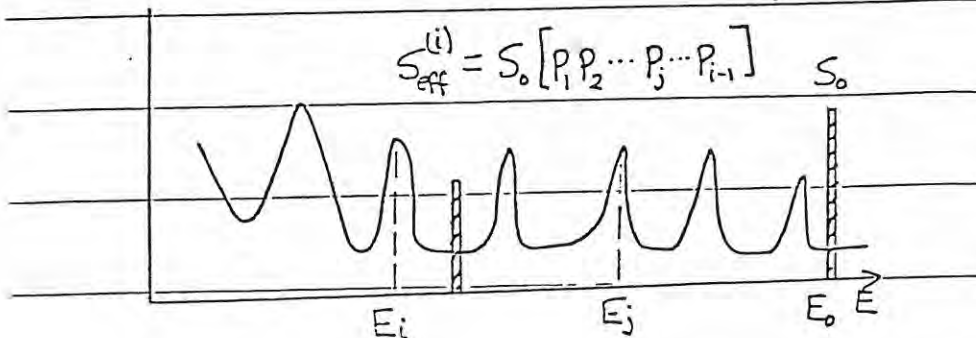
As resonance broadens, self-shielding decreases
and hence resonance absorption increases.

This involves a phenomenon known as self-shielding.
Hence as the resonance broadens, self-shielding decreases
and hence resonance absorption increases.
With this background for hydrogen under our belt, let us
now go on and examine the more general case.

83-12 How do we handle a number of resonances?

Define:

$$p(E) = \frac{S_0 - \text{neutron absorption rate}}{S_0} = 1 - \frac{1}{S_0} \int_E^{E_0} dE' \Sigma_a(E') \phi(E')$$



The first question concerns how we handle a large number of resonances.

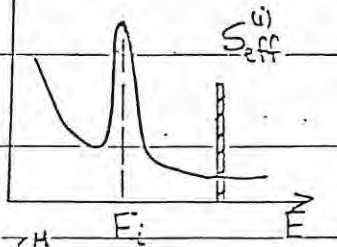
The idea is to break up the resonance absorption for each resonance.

We can now examine the resonance escape probability for any particular resonance.

3-13 The flux above any particular

resonance is given by

$$\phi(E) \sim \phi_{\text{asym}}(E)$$



$$= \frac{S_{\text{eff}}^{(i)}}{\sum \Sigma_s^E}, \quad \frac{1}{\sum \Sigma_s^E} = \frac{\sum \Sigma_s^A + \sum \Sigma_s^H}{\Sigma_s^A + \Sigma_s^H}$$

Hence the resonance escape probability p_i is

$$p_i = 1 - \frac{1}{S_{\text{eff}}^{(i)}} \int_{E_i} dE \Sigma_a^A(E) \phi(E)$$

The flux above any particular resonance is given by our earlier asymptotic solution for slowing down.

We can use this in our expression for the resonance escape probability.

Before continuing, we can introduce some useful notation.

3-14 Some notation: Suppose we normalize the

flux above the resonance to

$$\phi(E) \sim \frac{1}{E}$$

by setting $S_{\text{eff}}^{(i)} = \frac{1}{\sum \Sigma_s}$

Then we can write

$$p_i = 1 - \frac{1}{\sum \Sigma_s} \int_{E_i} dE N_A \sigma_f^A(E) \phi(E)$$

We will normalize the flux above the resonance as shown. This allows us to rewrite the resonance escape probability in a more convenient form.

(33-13) Now the total resonance escape probability is

$$P_{\text{total}} = \prod_i P_i = P_1 P_2 \dots P_i \dots$$

But for any given resonance, $P_i \sim 1$. Hence

$$e^{-(1-P_i)} \sim 1 - (1-P_i) + \dots \sim P_i$$

Why bother? So we can write

$$P_i \cong \exp \left[-\frac{N_A}{\bar{\xi} \bar{\Sigma}_s} \int_{E_i} dE \sigma_f^A(E) \phi(E) \right]$$

Then

$$P_{\text{total}} = \prod_i P_i = \exp \left[-\frac{N_A}{\bar{\xi} \bar{\Sigma}_s} \sum_i \int_{E_i} dE \sigma_f^A(E) \phi(E) \right]$$

Now the total resonance escape probability becomes as shown. But some simplifications are possible. We can replace the product by a sum using the exponential. Let's examine this expression in the argument in more detail.

(33-14) Here we define

$$P_i = \exp \left[-\frac{N_A}{\bar{\xi} \bar{\Sigma}_s} \int_{E_i} dE \sigma_f^A(E) \phi(E) \right]$$

as

$$P_i = \exp \left[-\frac{N_A}{\bar{\xi} \bar{\Sigma}_s} I_i \right]$$

where

$$I_i \equiv \int_{E_i} dE \sigma_f^A(E) \phi(E)$$

effective resonance integral

We can define the resonance escape probability for a single resonance as shown.

It is convenient to introduce the concept of a resonance integral.

33-17: Note \bar{I}_i has dimensions of barns. Thus

$$\bar{I}_i \equiv \int_{E_i} dE \sigma_i^A(E) \phi(E)$$

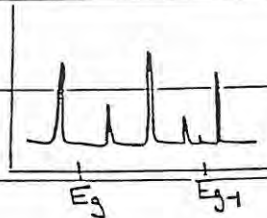
= absorption cross section of resonance
averaged over flux in resonance.

The resonance integral is independent of
properties of moderator.

First note that the resonance integral has dimensions of barns (because of our normalization of the flux). The resonance integral is also independent of the properties of the moderator. There is yet another advantage.

33-18: Another advantage: Suppose we want to
calculate the group constant

$$\bar{\Sigma}_{ag} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_a(E) \phi(E)}{\int_{E_g}^{E_{g-1}} dE \phi(E)}$$



But resonance width is much less than group width

$$\int_{E_g}^{E_{g-1}} dE \phi(E) \sim \int_{E_g}^{E_{g-1}} dE \frac{1}{E} = \ln \frac{E_{g-1}}{E_g} = \Delta U_g$$

$$\int_{E_g}^{E_{g-1}} dE \Sigma_a(E) \phi(E) = N_A \sum_{i \in g} \bar{I}_i$$

Suppose we want to calculate the group constants characterizing absorption from a series of resonances. Since the resonance width is much less than the group width, we can use the asymptotic form of the flux to find the result shown above.

so that we can express absorption group

constants directly in terms of resonance integrals

$$\sum_{ag} = \frac{N_A \sum_{ieg} I_i}{\Delta U_g}$$

Hence key to resonance absorption is the

calculation of the resonance integrals I_i .

Hence we can express the absorption group constants directly in terms of the resonance integrals.

This result will come in handy when we return to consider fast spectrum codes.

LECTURE 34

RESONANCE INTEGRALS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 338 - 347
pp. 427 - 437

EXERCISES:

- 34.1. Consider a medium in which the average lethargy gain and the scattering cross section are independent of energy. A common expression for the resonance escape probability $p(E)$ is

$$p(E) = \exp \left[- \int_E^{E_0} \frac{\Sigma_a(E') dE'}{\xi [\Sigma_s + \Sigma_a(E')] E'} \right]$$

When, if ever, is this expression: a) exact, b) a good approximation, and c) a poor approximation?

- 34.2. Compute the resonance escape probabilities for a $N_H/N_U = 1.0$ mixture of U-238 and hydrogen at temperatures of 0 K and 500 C for the 6.67 eV, 21 eV, and 208 eV resonance of U-238.

54-1 Resonance Integrals

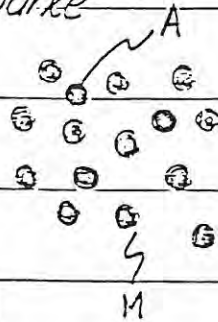
- General problem
- Approximations
- Lattice effects
- Final comments

In this lecture we will focus on how to calculate the resonance integrals. We recall that these are the key to describing resonance absorption.

54-2 Our goal is to calculate the resonance integral for a given material

$$I = \int_{E_0} dE \sigma_r^A(E) \phi(E)$$

$$[\phi(E) \sim \frac{1}{E}]$$



To calculate $\phi(E)$ we need the infinite medium slowing down equation

$$\sum_r^A(E) \phi(E) = \int_E^{E/\alpha_M} \frac{\sum_s^M(E') \phi(E')}{(1-\alpha_M) E'} + \int_E^{E/\alpha_A} \frac{\sum_s^A(E') \phi(E')}{(1-\alpha_A) E'}$$

To calculate the resonance integral, we need information about the neutron flux spectrum.

Hence we will introduce the infinite medium slowing down equation--this type for both species, absorber and moderator. We will introduce some approximations to simplify this equation.

(34-3) Notes: i) Ignore absorption in moderator

$$\Sigma_t^M(E) \sim \Sigma_s^M(E) \equiv \Sigma_p^M$$

ii) Write

$$\Sigma_t^A(E) = \Sigma_0^A(E) + \Sigma_{s, \text{res}}^A(E) + \Sigma_p^A$$

Characterize width of resonance as range over which

$$\Sigma_{\text{res}}^A(E) > \Sigma_p^M + \Sigma_p^A = \Sigma_p$$

Find $\Gamma_p \sim \sqrt{\frac{\Sigma_0}{\Sigma_p}} \Gamma$

Example: U-235

$$\frac{\Sigma_0}{\Sigma_p} \sim 10^3, \quad \Gamma_p \sim 30 \Gamma \sim 0.7 \text{ eV}$$

The first major approximation will be to ignore absorption in the moderator.

Next we introduce the effective resonance width. This provides a basis for comparing the width of the resonance to the neutron energy change in a collision.

To demonstrate how this concept is used, let us consider how it compares to the energy loss of a neutron with a moderator nucleus.

(34-5) But for all resonances

$$\Delta E|_M = \left(\frac{1-\alpha_M}{2}\right) E_0 \gg \Gamma_p$$

Thus for most of range $E < E' < E/\alpha_M$, $\phi(E) \sim Y_E$

$$\int_E^{E/\alpha_M} dE' \frac{\Sigma_s^M \phi(E')}{(1-\alpha_M) E'} \approx \frac{\Sigma_s^M}{(1-\alpha_M)} \int_E^{E/\alpha_M} \frac{dE'}{E'} \left(\frac{1}{E'}\right) = \frac{\Sigma_s^M}{E}$$

so that slowing down equation in the resonance is

$$\left[\Sigma_s^M(E) + \Sigma_0^A(E) + \Sigma_s^A(E) \right] \phi(E) = \int_E^{E/\alpha_A} \frac{dE'}{E'} \frac{\Sigma_s^A(E') \phi(E')}{(1-\alpha_A)} + \frac{\Sigma_s^M}{E}$$

Recall that this energy loss is given by the above.

Hence the form of the slowing down equation we will consider is as shown.

To proceed further, we need a couple of more approximations.

54-5 Narrow Resonance Approximation

$$\overline{\Delta E}|_A = \left(\frac{1-\alpha_A}{2}\right) E_0 \gg \Gamma_p$$

Then

$$\int_E^{E/\alpha_A} \frac{dE' \sum_s^A(E') \phi(E')}{E' (1-\alpha_A)} \approx \frac{\sum_p^A}{(1-\alpha_A)} \int_E^{E/\alpha_A} \frac{dE' (1/E')}{E'} = \frac{\sum_p^A}{E}$$

Thus slowing down equation is

$$\Sigma_t(E) \phi(E) = \frac{\sum_p^A}{E} + \frac{\sum_s^H}{E}$$

so that

$$I^{NR} = \int_{E_0} dE \sigma_f^A(E) \left[\frac{\sum_p^A + \sum_s^H}{\Sigma_t(E) E} \right]$$

The first class of approximations assumes that the average neutron energy loss in a collision with the absorber is large compared to the effective resonance width. This is known as the narrow resonance approximation. It allows us to solve explicitly for the flux and therefore for the resonance integral.

54-6 Narrow Resonance-Infinite Mass Absorber Approximation

$$\overline{\Delta E}|_A = \left(\frac{1-\alpha_A}{2}\right) E_0 \ll \Gamma_p$$

Assume no energy loss in collision with absorber

$$\int_E^{E/\alpha_A} \frac{dE' \sum_s^A(E') \phi(E')}{(1-\alpha_A) E'} \sim \sum_s^A(E) \phi(E) \int_E^{E/\alpha_A} \frac{dE'}{E'} \sim \sum_s^A(E) \phi(E)$$

The slowing down equation becomes

$$\Sigma_t(E) \phi(E) = \sum_s^A(E) \phi(E) + \frac{\sum_s^H}{E}$$

so that

$$I^{NRIM} = \int_{E_0} dE \sigma_f^A(E) \left[\frac{\sum_s^H/E}{\Sigma_t(E) - \sum_s^A(E)} \right]$$

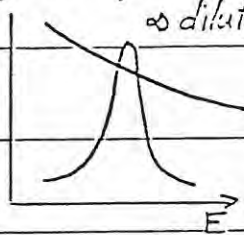
A second class of approximations assumes that the resonance width is wide compared to the average neutron energy loss experienced in a collision with the absorber. This is known as the wide resonance or narrow resonance-infinite mass approximation. It also allows an explicit solution for the resonance integral.

34-7 If absorber concentration is small (infinite

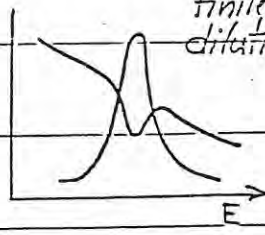
dilution), $\Sigma_s(E) \sim \Sigma_s^M$ and

$$I^{NR} \rightarrow I^{NRIM} \rightarrow I^\infty = \int_{E_0}^{\infty} \frac{dE}{E} \sigma_s^A(E)$$

More generally



∞ dilution



finite dilution

Hence: $I^\infty > I^{NR}$ or I^{NRIM}

If the absorber concentration is small we return to the earlier infinite dilution result.

As we noted earlier, this result does not account for temperature effects.

More generally, we must work with finite absorption concentration. With these approximations, we can now introduce explicit forms for the cross sections themselves.

34-8 Final step: introduce forms of cross sections

$$\sigma_s^A(E) \cong \sigma_0 \frac{\Gamma_n}{\Gamma} \psi(\xi, x) + \sigma_p$$

$$\sigma_p^A(E) \cong \sigma_0 \frac{\Gamma_p}{\Gamma} \psi(\xi, x)$$

to find

$$I^{NR} = \frac{\Sigma_s^M + \Sigma_p^A}{N_A E_0} J(\xi, \beta), \quad \beta \equiv \frac{\Sigma_s^M + \Sigma_p^A}{N_A \sigma_0}$$

$$I^{NRIM} = \frac{\Sigma_s^M \Gamma}{N_A E_0} J(\xi, \beta'), \quad \beta' \equiv \frac{\Sigma_s^M \Gamma}{N_A \sigma_0 \Gamma}$$

\uparrow \uparrow
T dilution

We will introduce the indicated forms for the cross sections. These can be introduced into the NR and NRIM approximations. Generally the functions appearing in these expressions are tabulated in the computer code package. There is a special case of interest.

34-9 Note

$$\text{as } \beta \rightarrow \infty, \quad I \rightarrow I^\infty = \frac{\sigma_0 \Gamma \pi}{2E_0}$$

Which approximation do we use?

$$\Delta E|_A = \left(\frac{1-\alpha_A}{2}\right) E_0 \quad \ll \Gamma_p - \text{NRIM} \\ \gg \Gamma_p - \text{NR}$$

In general

low energy ($E_0 < 100 \text{ eV}$) \Rightarrow NRIM

high energy ($E_0 > 100 \text{ eV}$) \Rightarrow NR

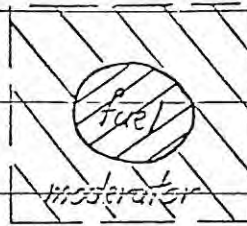
As a reference point, we can calculate the infinite dilution limit.

Note the ranges of validity.

There is one additional effect on resonance absorption that we should consider at this point.

34-10 Lattice effects on resonance absorption:

Important to account
for fuel pin cell transport
effects. Define:



collision probabilities

$$P_{F \rightarrow M}$$



$$P_{M \rightarrow F}$$



(first-flight escape probabilities)

It is very important to account for lattice effects on resonance absorption.

Consider a simple fuel pin cell.

We can introduce the collision probability (first-flight escape probabilities) to rewrite the slowing down equation.

12) We arrive at slowing down equations:

$$V_F \Sigma_F(E) \phi_F(E) = V_F [1 - P_{F \rightarrow H}] \int_E^{E/\alpha_F} dE' \frac{\Sigma_S^F(E') \phi_F(E')}{(1 - \alpha_F) E'} + V_H P_{H \rightarrow F} \int_E^{E/\alpha_H} dE' \frac{\Sigma_S^H(E') \phi_H(E')}{(1 - \alpha_H) E'}$$

$$V_H \Sigma_H(E) \phi_H(E) = V_H [1 - P_{H \rightarrow F}] \int_E^{E/\alpha_H} dE' \frac{\Sigma_S^H(E') \phi_H(E')}{(1 - \alpha_H) E'} + V_F P_{F \rightarrow H} \int_E^{E/\alpha_F} dE' \frac{\Sigma_S^F(E') \phi_F(E')}{(1 - \alpha_F) E'}$$

We now find a slowing down equation for each region of the fuel pin cell.

We could attempt to solve these equations numerically.

However we can also introduce the NR and NRIM approximations we developed earlier.

We will not do so here, but merely note that these are calculated and tabulated in a number of standard books on reactor physics.

13) If we can solve for $\phi_F(E)$ we can solve for

$$I = \int dE \sigma_{\gamma}^F(E) \phi_F(E)$$

This requires approximations:

i) NR, NRIM

ii) $P_{F \rightarrow H}$, $P_{H \rightarrow F}$ (reciprocity relation, rational approximation)

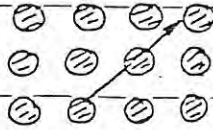
iii) numerical calculation or tabulation

We want to solve for the resonance integrals.

Several additional approximations are generally used to simplify the numerical calculations.

34-13 Further comments:

i) Rod shadowing



(Dancoff correction)

ii) Empirical correlations for resonance integral

$$I^{28} = 11.6 + 22.8 \left(\frac{S_F}{M_F} \right)$$

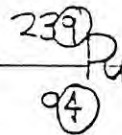
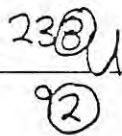
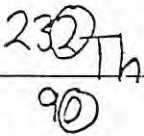
$S_F \rightarrow$ fuel pin surface

$M_F \rightarrow$ fuel pin mass

First, note there will be a rod shadowing effect in the lattice.

Second, one can measure empirical correlations for the resonance integrals.

34-14 Reminder: WW II code



02

28

49

A minor detour to introduce (or remind you) of the simple two number code introduced during World War II.

Example: Strawbridge-Barry correlation

$$I^{28} = 2.16x + 2.56 + [0.279x - 0.0537] \sqrt{x}$$

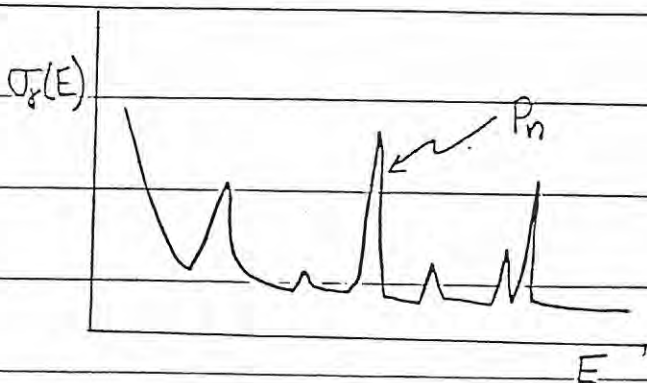
$$x = \left[\frac{\sum P_{F \rightarrow H}}{N_{28}} + \frac{(1-C)}{\langle R \rangle N_{28}} \right]^2$$

(Can use such empirical calculations to
"calibrate" spectrum codes)

One of the most popular correlations is the Strawbridge-Barry correlation.

We can use such correlations to calibrate computer codes.

4-16



Run code -- calculate I^{28} -- compare with correlation -- fudge all P_n 's to agree.

(Note: sometimes only calculate ^{238}U , ^{240}Pu)

The idea is to calculate the total resonance integral for a number of resonances.

Then each resonance escape probability is adjusted "fudged" to yield the empirical result for the total resonance integral.

LECTURE 35

FAST SPECTRUM CODES

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 347 - 363

EXERCISES:

- 35.1. Determine the following quantities in terms of the fine-group MUFT representation: a) source rate, b) slowing down rate to thermal, c) leakage rate, and d) absorption rate. Then calculate the slowing down probability, leakage probability, and absorption probability. Verify that these latter probabilities all add to unity.
- 35.2. Determine the slowing down density established by a monoenergetic plane source at the origin of an infinite moderating medium as given by age-diffusion theory.
- 35.3. Determine the slowing down density resulting from a point source in an infinite moderating medium using age-diffusion theory.

ES-1 Fast Spectrum Codes:

- The task before us
- Spatial effects
- MUFT-type codes
- Group structures

In this lecture we will pull together all of the knowledge we have developed concerning neutron slowing down and resonance absorption in an effort to determine how to calculate the fast neutron spectrum. Let me briefly run through an outline of the lecture.

ES-2 Goal: To determine the energy spectrum $\phi(E)$ characterizing fast neutrons -- to calculate the fast group constants:

$$\Sigma_{t3} \approx \frac{\int_{E_3}^{E_{3-1}} dE \Sigma_t(E) \phi(E)}{\int_{E_3}^{E_{3-1}} dE \phi(E)}$$

REcall that our goal was to calculate the neutron energy spectrum characterizing fast neutrons. This allows us to calculate the fast group constants. Thus far we have examined the spectrum characterizing an infinite medium. Unfortunately, this is a bit too crude for many calculations.

35-3. How do we handle the spatial dependence?

Some simplifications:

i) switch to lethargy variable

$$E \rightarrow u$$

ii) one-dimension $\nabla\phi \rightarrow \frac{\partial\phi}{\partial x}$

iii) only elastic scattering

So how do we handle the spatial dependence of the neutron flux--albeit within a simple approximation. To explain this, let me introduce several assumptions. With these assumptions, I can write the form of the neutron slowing down equations as shown below.

35-4. Begin with

$$\frac{\partial J}{\partial x} + \Sigma_t(u)\phi(x,u) = \int_0^u du' \Sigma_{s_0}(u' \rightarrow u)\phi(x,u') + S(x,u)$$

$$\frac{1}{3} \frac{\partial \phi}{\partial x} + \Sigma_t(u)J(x,u) = \int_0^u du' \Sigma_{s_1}(u' \rightarrow u)J(x,u')$$

Note: $S(x,u) \rightarrow$ external sources
fission sources
inelastic scattering

Actually, these equations are a bit more general and precise than any of our earlier treatment to date. We should note that we have written separate equations for both the flux and the current.

In reactor analysis, these equations are sometimes referred to as the P-1 equations.

We will not dwell on their solution, but rather utilize them to develop several useful approximations to the neutron spatial dependence.

ES-5: Approximation 1: infinite medium

$$\frac{\partial J}{\partial x} = 0, \quad \frac{\partial \phi}{\partial x} = 0$$

$$\xi_s(u) \phi(u) = \int_0^u du' \xi_s(u' \rightarrow u) \phi(u') + S(u)$$

infinite medium slowing down equation

(This is just the equation we have been studying for the past several lectures!!!)

The simplest approximation would be to simply ignore the spatial dependence altogether by applying them to an infinite medium.

This has been our approach for the past few lectures. However, for many problems this is too crude. Some acknowledgement of the effects of leakage during slowing down must be made.

ES-6: Approximation 2: age-diffusion theory

Recall the definition of the slowing

down density:

$$q(x, u) = \int_0^u du' \int_u^\infty du'' \xi_s(u' \rightarrow u'') \phi(x, u'')$$

Now note:

$$\frac{\partial q}{\partial u} = \int_u^\infty du'' \xi_s(u' \rightarrow u'') \phi(x, u'') - \int_0^u du' \xi_s(u' \rightarrow u) \phi(x, u')$$

Historically the first attempt to do this involved a theory known as age-diffusion theory.

This is also known as Fermi age theory.

We begin by introducing the neutron slowing down density.

Now note what happens when we differentiate.

We can use this to simplify the slowing down equations.

35-7 Hence we can write

$$-\frac{\partial J}{\partial x} + \Sigma_a(u)\phi(x,u) = -\frac{\partial q}{\partial x} + S(x,u)$$

Introduce two approximations:

i) diffusion approximation

$$J \cong -D \frac{\partial \phi}{\partial x}$$

ii) age approximation

$$q \cong \xi \Sigma_s \phi$$

We introduce approximations to calculate the two unknown functions appearing in the equation.

The first approximation is an old friend--diffusion theory.

The second approximation is new--age approximation.

It turns out that this is not a bad approximation for neutrons slowing down in materials other than hydrogen (unfortunately however, LWRs have lots of hydrogen--rather, water--in them, so this isn't too good an approximation for these reactors).

35-8 Hence we find

$$-D(u) \frac{\partial^2 \phi}{\partial x^2} + \Sigma_a(u)\phi(x,u) = -\frac{\partial}{\partial u} \left[\xi \Sigma_s \phi(x,u) \right] + S(x,u)$$

age-diffusion equation

Let's rearrange a bit: $S=0$, $q = \xi \Sigma_s \phi$

$$\frac{D(u)}{\xi \Sigma_s(u)} \frac{\partial^2 q}{\partial x^2} - \frac{\Sigma_a(u)}{\xi \Sigma_s(u)} q(x,u) = \frac{\partial q}{\partial u}$$

Introduce

$$\hat{q}(x,u) = q(x,u) \exp \left[\int_0^u \frac{\Sigma_a(u')}{\xi \Sigma_s(u')} du' \right]$$

We can now substitute these in to arrive at a diffusion equation.

We can rearrange this equation a bit.

Now introduce a new dependent variable to get rid of the second term on the left hand side.

Note the exponential term is just the resonance escape probability.

5-9 to find

$$\frac{D(u)}{\xi \xi_s(u)} \frac{\partial^2 \hat{\phi}}{\partial x^2} = \frac{\partial \hat{\phi}}{\partial u}$$

Now make a change of independent variable

$$\tau(u) \equiv \int_0^u \frac{D(u')}{\xi \xi_s(u')} du'$$

$$\frac{\partial}{\partial u} = \frac{\partial \tau}{\partial u} \frac{\partial}{\partial \tau} = \frac{D(u)}{\xi \xi_s(u)} \frac{\partial}{\partial \tau}$$

to find

$$\frac{\partial^2 \hat{\phi}}{\partial x^2} = \frac{\partial \hat{\phi}}{\partial \tau}$$

One last change of variable--this time, the independent variable. Hence we arrive at an equation of the form shown.

5-10 Note

$$\frac{\partial^2 \hat{\phi}}{\partial x^2} = \frac{\partial \hat{\phi}}{\partial \tau}$$

looks like time-dependent diffusion equation.

$$\tau \equiv \int_0^u \frac{D(u')}{\xi \xi_s(u')} du' \equiv \text{Fermi age}$$

Example: Age to thermal $\tau_{th} \equiv \tau(u_{th})$

material	τ (cm ²)
H ₂ O	26
D ₂ O	131
Be	102
C	368

NOTE:

$$\tau = \frac{1}{6} \langle r^2 \rangle$$

↑
slowing down
distance

This looks just like a time-dependent diffusion equation.

Hence we can pull out all of the solutions familiar from heat conduction or neutron diffusion literature

For that reason, the new variable was referred to by

Fermi as the age.

Most useful for graphite moderated reactors.

Nevertheless, the "age to thermal" is a common quantity.

35-11. Approximation 3: P₁ (MUFT) approximation

$$\frac{\partial J}{\partial x} + \Sigma_a(u) \phi(x, u) = -\frac{\partial \rho_0}{\partial u} + S_0(x, u)$$

$$\frac{1}{3} \frac{\partial \phi}{\partial x} + \Sigma_{tr}(u) J(x, u) = -\frac{\partial \rho_1}{\partial u}$$

Approximate: $\phi(x, u) = \phi(u) e^{iBx}$

$$iBJ + \Sigma_a \phi = -\frac{d\rho_0}{du} + \int_0^u du' \Sigma_{in}(u' > u) \phi(u') + S(u)$$

$$\frac{1}{3} iB\phi + \Sigma_{tr} J = -\frac{d\rho_1}{du}$$

The most popular approach was developed at the Naval Reactors Laboratories and first implemented in a code known as MUFT. It begins with the P-1 equations written in terms of the slowing down density.

Now one treats the spatial dependence by assuming it has a simple cosine shape--or more generally, an exponential shape of the form shown.

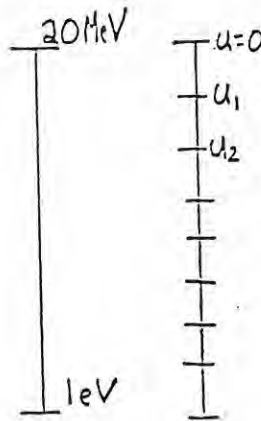
We can substitute this in to eliminate the spatial derivatives. Note leakage is determined by our choice of the buckling B.

35-12 To solve, we break up mesh and derive a "fine" multigroup description:

$$\phi_n = \int_{u_{n-1}}^{u_n} du \phi(u)$$

$$\Sigma_{sn} = \frac{1}{\Delta u_n} \int_{u_{n-1}}^{u_n} du \Sigma_s(u)$$

$$\Sigma_{an}^R = \frac{N_A}{\Delta u_n} \sum_{i \in n} \Gamma_i$$



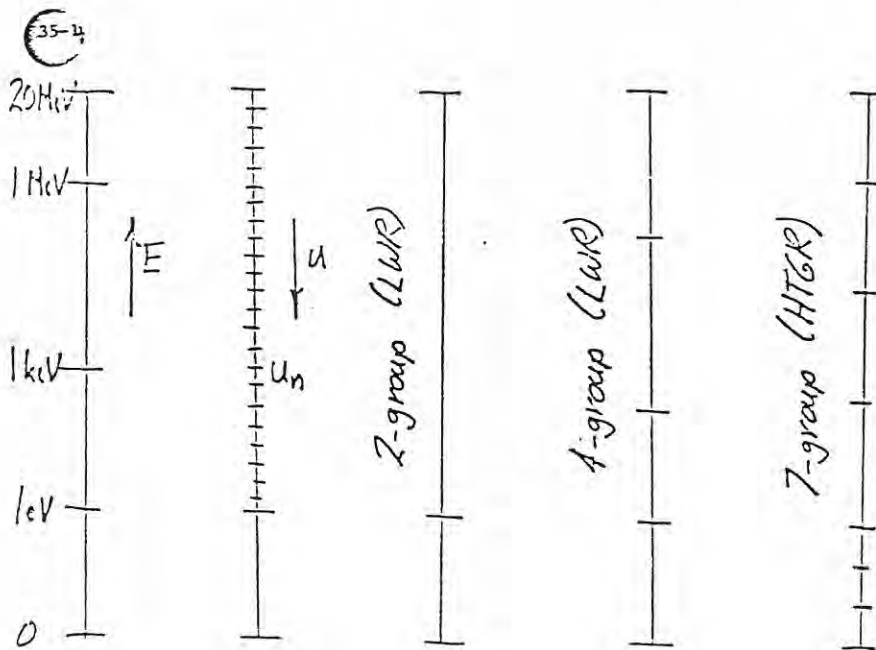
Rather than attempt an analytical solution, we break up these equations over a very fine group structure and solve them numerically as differential equations. This gives us a simple set of algebraic equations over the multigroup structure.

³⁵⁻¹² We can solve the fine spectrum multigroup equations for the ϕ_n and then calculate the fast group constants.

$$\Sigma_{a1} = \frac{\int_0^{u_{1n}} du \Sigma_a(u) \phi(u)}{\int_0^{u_{1n}} du \phi(u)} = \frac{\sum_n \Sigma_{an} \phi_n}{\sum_n \phi_n}$$

Example: fine groups coarse groups
 50-100 1-10

We can then solve the fine spectrum multigroup equations for the fast spectrum. This can be used to calculate the group constants. An example for LWR calculations.



I have sketched the fine and coarse group structures most commonly used in thermal reactors. We will return later to re-examine fast spectrum calculations within the general context of reactor design and analysis.

LECTURE 36

THERMAL SPECTRUM CALCULATIONS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 375 - 394

EXERCISES:

- 36.1. Give three reasons why the neutron energy distribution in a thermal homogeneous reactor is not Maxwellian. What specific physical effects cause deviations at high energies and what physical effects give rise to deviations at low energies?
- 36.2. Calculate the average energy and speed of neutrons in a Maxwellian distribution at a temperature T .

Thermal Spectrum Calculations

- Neutron thermalization
- General features of thermal spectra
- Computational models

We will now turn our attention to the study of the neutron energy dependence when the neutrons have slowed down to thermal energies.

That is, energies comparable to the energy of the thermal motion of the atoms comprising the reactor core.

³⁶⁻² Now turn our attention to generating group constants for low energy neutrons. Here

$$\text{"thermal"} \Rightarrow E \sim kT$$

Special features:

- $E \sim kT \Rightarrow$ upscattering
- $E \sim BE \Rightarrow$ chemical binding
- $\lambda \sim d \Rightarrow$ diffraction

Recall that our mission is to calculate the spectrum characterizing thermal neutrons so that we can generate the thermal group constants.

To be more precise, we will define the term "thermal" as shown above.

Discuss special features of interest.

36-3 Complications:

- i) upscattering
- ii) $mfp \sim 1 \text{ cm} \Rightarrow$ lattice effects

Simplifications:

- i) leakage effects are of minor importance
 $P_{NFL} \sim 97\%$, $P_{NTL} \sim 99\%$
- ii) isotropic scattering
- iii) few thermal resonances

Upscattering complicates the solution of the equations characterizing thermal neutrons (we can no longer simply solve down the groups in energy as we did in the slowing down problem).

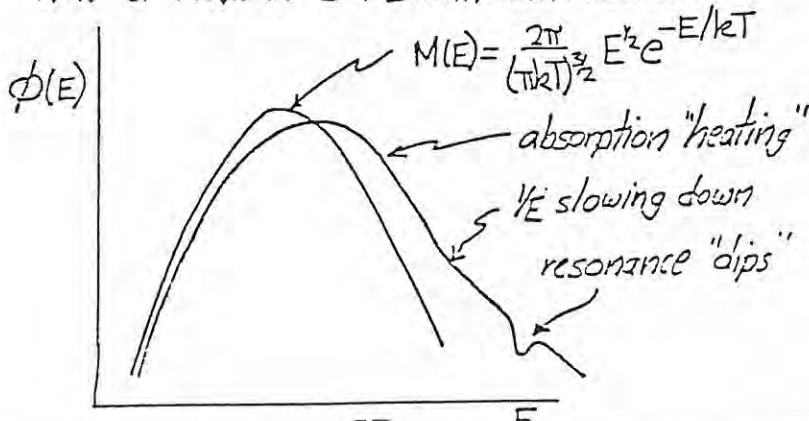
Also must worry about lattice effects--a very important topic that we will return to later.

These complications are offset by a couple of simplifications.

36-4 Some general features:

All thermal spectra look roughly

like a Maxwell-Boltzmann distribution



Since the thermal spectrum characterizes neutrons coming into thermal equilibrium with the material in the reactor, the spectrum usually approximates a Maxwell-Boltzmann distribution. There are some differences caused by absorption, slowing down, and resonances, however.

36-5

This fact, coupled with short mfp, implies

$$\left(\begin{array}{c} \text{spatial} \\ \text{effects} \end{array} \right) \underset{\text{importance}}{> \geq} \left(\begin{array}{c} \text{energy} \\ \text{effects} \end{array} \right)$$

in thermal energy range.

(Not leakage, but rather lattice effects)

This fact, coupled with the short mfp characterizing thermal neutrons, implies that spatial effects are more important than energy effects.

Here we mean lattice effects, not leakage (thermal leakage in a large power reactor is quite small--typically about 1%).

Let us focus first on the energy dependence.

36-6

We will focus here on the energy dependence.

Begin with

$$[\Sigma_a(E) + \Sigma_s(E)]\phi(E) = \int_0^\infty dE' \Sigma_s(E' \rightarrow E)\phi(E') + S(E)$$

infinite medium spectrum equation

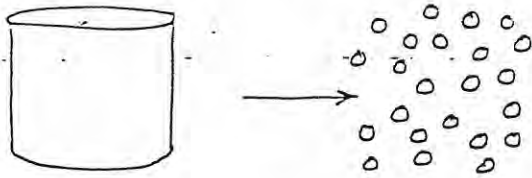
NOTE: If $\Sigma_a = 0, S = 0$ (equilibrium)

$$\phi(E) \rightarrow \phi_{MB}(E) \text{ (Maxwell-Boltzmann)}$$

Once again we begin with an old friend, the infinite medium spectrum equation.

We consider the special case of zero absorption and sources. The steady state solution is the Maxwell-Boltzmann distribution. How do we model the cross sections? They are very complex in general. Fortunately, this doesn't make much difference.

35-7: COMMON MODEL: free proton gas



Accounts for upscattering, but not chemical binding. (Also not a bad model for LWR.)

In light water reactors, one usually models the moderator as a free gas--ignoring binding and diffraction effects, but accounting for upscattering.

To implement this, we can use the particular form of the cross sections for a free proton gas.

36-8 Using two-body kinematics, one can derive form of $\Sigma_s(E' \rightarrow E)$ for proton gas

$$\Sigma_s(E' \rightarrow E) = \begin{cases} \frac{\Sigma_s}{E} \operatorname{erf} \sqrt{E/kT}, & E' > E \\ \frac{\Sigma_s}{E} e^{\frac{E'-E}{kT}} \operatorname{erf} \sqrt{E'/kT}, & E' < E \end{cases}$$

This is great! It transforms integral equation into differential equation

$$\begin{array}{ccc} \text{infinite medium} & & \text{Wigner-Wilkins} \\ \text{spectrum equation} & \rightarrow & \text{equation} \\ \text{(integral)} & & \text{(differential)} \end{array}$$

The form of the cross sections are as shown above. An interesting feature: the spectrum equation is transformed into a differential equation, making it much easier to solve.

This is known as the Wigner-Wilkins equation. How do we solve this?

⑤ We can solve this very cheaply!

(SOFOCATE-type codes)



Break up energy range into
fine groups and solve Wigner-
Wilkins equation on this mesh.

We just break up the energy range into groups and solve the Wigner-Wilkins equation numerically—like any other differential equation.

This method was developed at the Naval Reactors Laboratories and first implemented in the SOFOCATE (or TEMPEST) computer code.

It has become the most popular model for LWR analysis.

⑥ Alternative: Can always solve infinite medium spectrum equation directly

$$\Sigma_t(E) \phi(E) = \int_0^{\infty} \Sigma_s(E' \rightarrow E) \phi(E') + S(E)$$

Just "discretize" on a fine group structure

$$\Sigma_{t_n} \phi_n = \sum_{n'=1}^N \Sigma_{s_{n'n}} \phi_{n'} + S_n$$

We can always get a little bit fancier and just solve the thermalization equation directly.

Just discretize on a fine group structure and solve.

This will yield the thermal spectrum for each fine thermal group.

36-11 We can then calculate the thermal group constants in the usual way:

$$\Sigma_{th} = \frac{\int_0^{1eV} dE \Sigma(E) \phi(E)}{\int_0^1 dE \phi(E)} \rightarrow \frac{\sum_{n=1}^N \Sigma_n \phi_n}{\sum_{n=1}^N \phi_n}$$

Unfortunately, something very important has been left out -- lattice effects. These are very important in thermal group.

We can then calculate the thermal group constants in the usual way.

Hence we can now handle the energy dependence in both neutron slowing down and thermalization.

We must now turn to the spatial dependence caused by the lattice structure.

LECTURE 37

LATTICE EFFECTS

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 398 -409

EXERCISES:

- 37.1. Determine the ratio of neutron mfp to lattice dimension (e.g., fuel-pin diameter or lattice pitch) in LWR, HTGR, and LMFBR cores for both fast and thermal neutrons. Also compare the ratio of core size to migration length in these reactors.
- 37.2. Derive an expression for the thermal utilization of a three region lattice cell (including fuel, clad, and moderator) in terms of thermal disadvantage factors. Also derive an expression for the cell averaged group constants characterizing this cell in terms of the appropriate disadvantage factors.

37-1

Lattice Effects

• Cell averaging

• Qualitative effects

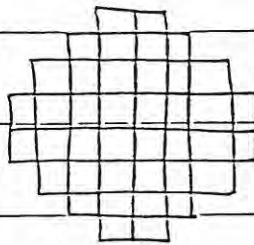
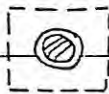
• Effects on k

We have handled the complex energy dependence of the neutron cross sections by averaging them over an approximate energy spectrum. We now turn our attention to the equally important task of averaging the group constants over the complex spatial structure of the reactor. That is, we will examine the effects of the fuel lattice in a reactor core. We will begin by attempting to put this spatial dependence in perspective.

37-2

Thus far we have assumed fuel + moderator + coolant + structure homogeneously mixed.

But

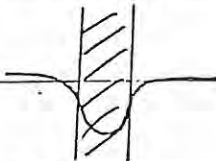


Moreover, $mfp \sim 1\text{ cm}$

\sim size of lattice cell

Flux varies appreciably

over cell.



Thus far most of our analysis has focussed on a uniform reactor composition. That is, we have assumed fuel and moderator and coolant and structure are homogeneously mixed. But we know there is a complex structure. Furthermore, the neutron mfp is comparable to the size of a lattice cell. This implies that the flux varies appreciably over the cell.

57-3

How do we account for this?

Cell-averaging or
homogenization of
group constants

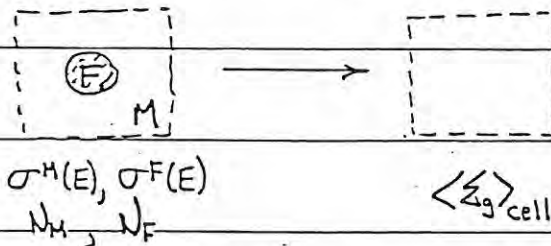
$$\langle \Sigma_g \rangle_{\text{cell}} \equiv \frac{\int_{\text{cell}} d^3r \Sigma_g(\underline{r}) \phi(\underline{r})}{\int_{\text{cell}} d^3r \phi(\underline{r})}$$

But how do we account for this effect of the lattice structure? We attempt to cell-average or "homogenize" the group constants by averaging them over some assumed or approximate flux shape in the cell.

Let me be a bit more precise about this process.

57-4

Note: We really have a double-averaging process:



$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\int_{E_g}^{E_{g-1}} dE \int_{V_{\text{cell}}} d^3r \Sigma(\underline{r}, E) \phi(\underline{r}, E)}{\int_{E_g}^{E_{g-1}} dE \int_{V_{\text{cell}}} d^3r \phi(\underline{r}, E)}$$

In effect we have a double averaging process.

Consider a simple two-region fuel pin cell.

Note that the group constants involve averages over both energy and space.

We will develop this procedure in this and the next session.

First, however, it is useful to describe qualitatively the effects of the fuel lattice on the core behavior.

37-5

Qualitative effects:

homogeneous \rightarrow heterogeneous

$$k = \eta f \epsilon p P_{FNL} P_{TNL}$$

Example: Fermi's "pile" (graphite-natural U)

$$k_{\infty}^{hom} = (1.33)(1.05)(0.59) = 0.85$$

$$k_{\infty}^{het} \longrightarrow = 1.08$$

In particular, let's examine the effect of lumping the fuel in a lattice on the multiplication factor.

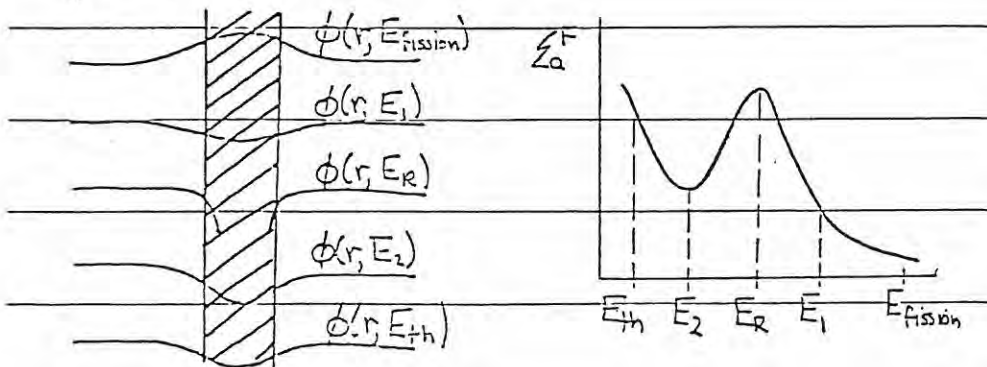
Here we can use the 6-factor formula.

Recall Fermi's pile (Stagg Field).

What effects cause this increase in the multiplication?

37-6

Consider a fuel pin cell



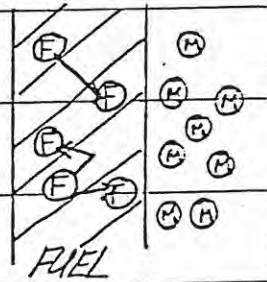
We can consider a two-region fuel cell to make this more precise. If we plot the flux across the fuel cell for various energies, we find the following structure (note we have included a resonance). Hence there will be a mild peaking at fission energies, with a pronounced depression in the flux in the resonance energy region.

57-7) Lattice effects on $k = \eta f \epsilon p P_{FNL} P_{TNL}$

$\eta = \frac{\nu \sigma_f^F}{\sigma_a^F}$: only spectrum effects

ϵ (fast fission factor):

fuel lumping increases probability that neutron will run into fuel (F) before $E < E_{threshold}$



We can now examine the effects on each term in the 6-factor formula. First, there is only a modest effect on eta due to a spectrum shift.

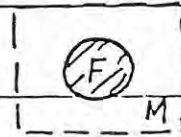
We can ignore this effect to first order.

There is a mild increase in the fast fission factor. (Explain)

Not too much of an impact on leakage (very small in a large power reactor).

57-8) f (thermal utilization):

$$f = \frac{\int_{V_F} \Sigma_a^F(\underline{r}) \phi(\underline{r}) dV}{\int_{V_F} \Sigma_a^F(\underline{r}) \phi(\underline{r}) dV + \int_{V_M} \Sigma_a^M(\underline{r}) \phi(\underline{r}) dV}$$



$$= \frac{\Sigma_a^F \int_{V_F} \phi(\underline{r}) dV}{\Sigma_a^F \int_{V_F} \phi(\underline{r}) dV + \Sigma_a^M \int_{V_M} \phi(\underline{r}) dV} = \frac{\Sigma_a^F V_F \bar{\phi}_F}{\Sigma_a^F V_F \bar{\phi}_F + \Sigma_a^M V_M \bar{\phi}_M}$$

$$= \frac{\Sigma_a^F}{\Sigma_a^F + \Sigma_a^M (V_M/V_F)} \left(\frac{\bar{\phi}_M}{\bar{\phi}_F} \right) \quad \xi = \frac{\bar{\phi}_M}{\bar{\phi}_F}$$

The thermal utilization is strongly sensitive to the fuel lumping. Recall the definition of f .

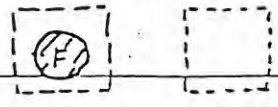
Here we have identified the disadvantage factor.

To see how this affects f , we can compare this with the homogeneous case.

37-9

Compare to homogeneous case

$$f^{hom} = \frac{\sum_a^F hom}{\sum_a^F hom + \sum_a^{H-hom}}$$



$$N_F^{hom} = N_F \left(\frac{V_F}{V_{cell}} \right); \quad N_H^{hom} = N_H \left(\frac{V_H}{V_{cell}} \right)$$

$$f^{hom} = \frac{\sum_a^F}{\sum_a^F + \sum_a^H \left(\frac{V_H}{V_F} \right)}$$

We first have to decide just what we mean by the "homogeneous" case. We will assume that we can simply volume-average the cross sections in the cell to arrive at their homogeneous form. We can now compare this with our heretogeneous result.

37-10

Compare these:

$$f^{hom} = \frac{\sum_a^F}{\sum_a^F + \sum_a^H \left(\frac{V_H}{V_F} \right)}$$

$$f^{het} = \frac{\sum_a^F}{\sum_a^F + \sum_a^H \left(\frac{V_H}{V_F} \right) \xi}$$

$$\xi = \frac{\bar{\Phi}_H}{\bar{\Phi}_F} > 1 \Rightarrow f^{hom} > f^{het}$$

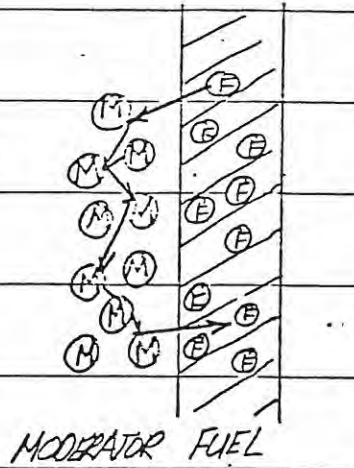
In comparing both forms, we can see the dependence on the disadvantage factor. Since zeta is greater than one, we find that f decreases for a heterogeneous lattice. (Because the fuel is at a "disadvantage"-- it doesn't see as large a flux as the moderator.) We still haven't answered the question as to just what causes the increase in k.

37-11

p (resonance escape probability)

Two effects:

i) geometric separation of slowing down from fuel



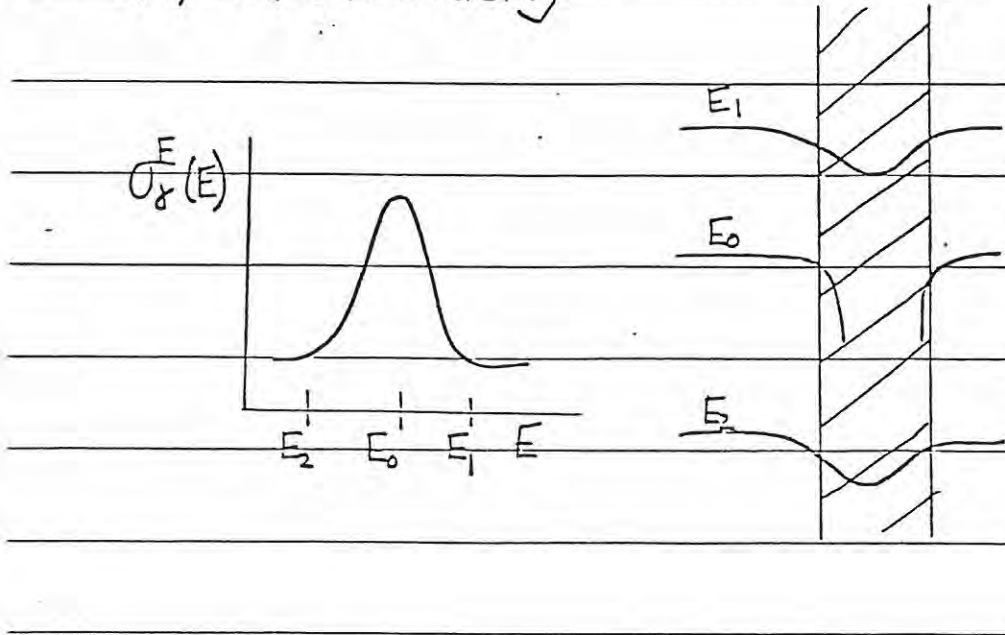
Well, the only remaining possibility is the resonance escape probability.

There are actually two important effects.

First there is the geometrical separation of slowing down from the fuel region.

37-12

ii) spatial self shielding



But of even more importance is a self-shielding effect.

This is similar to the self-shielding in energy we noted in our study of resonance absorption.

We can demonstrate this effect with a simple example.

37-13 Example:

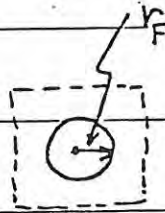
$$I_{\text{hom}}^u = 280 b$$

$$I_{\text{het}}^u = 9 b$$

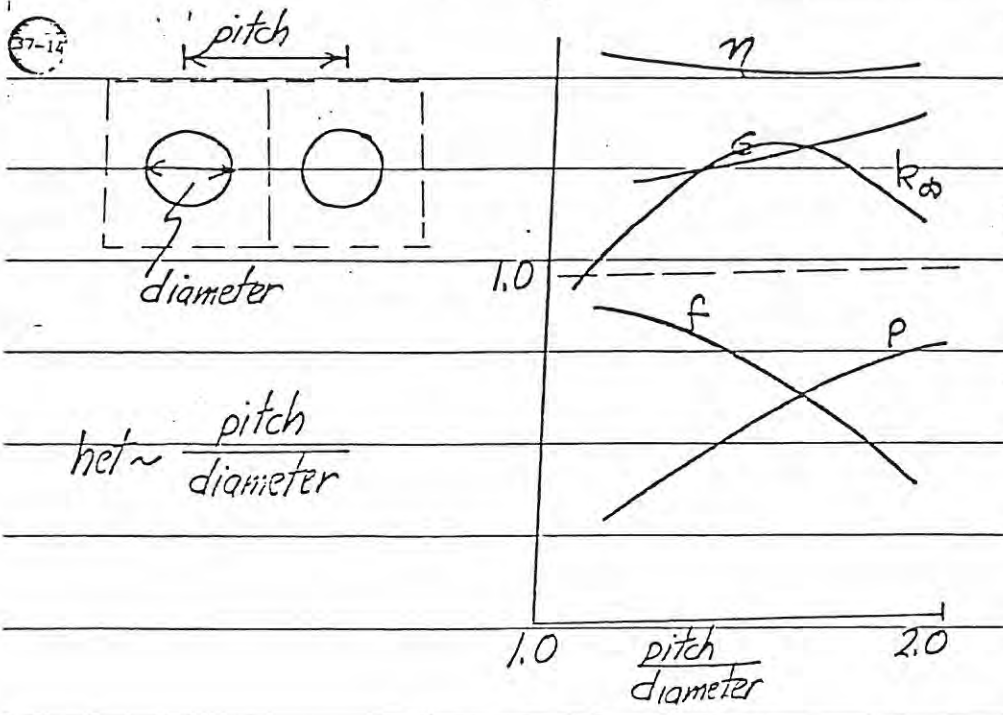
(30-fold reduction)

$$I \sim C_1 + C_2 \left(\frac{A_F}{M_F} \right)$$

$$\frac{A_F}{M_F} \sim \frac{A_F}{V_F} = \frac{2\pi r_F}{\pi r_F^2} = \frac{2}{r_F}$$



Consider the resonance integral for U-238.
 Note the difference due to fuel lumping.
 Can also see this from empirical correlations for the resonance integral.



We can conveniently quantify the degree of heterogeneity of the lattice by its pitch-to-diameter ratio.
 Here we have determined the physical effects which cause the multiplication to increase as the fuel is lumped.
 We must learn how to account for this in analyzing the reactor core.

LECTURE 38

CELL HOMOGENIZATION

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 406 - 427

EXERCISES:

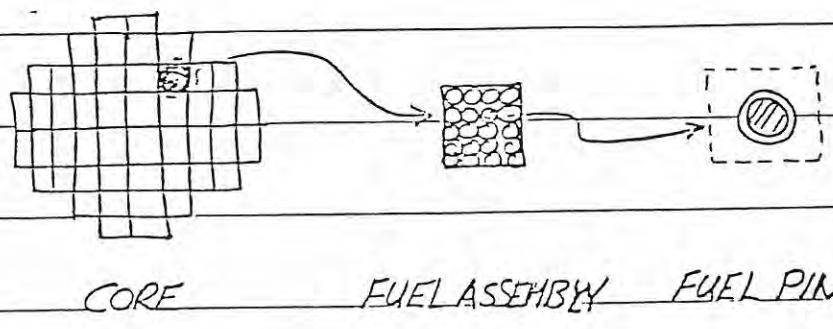
- 38.1. Calculate the disadvantage factor characterizing a two-region slab geometry consisting of a fuel region of width $2a$ surrounded by moderating regions of width b . Use one-speed diffusion theory.
- 38.2. Calculate the self-shielding factor for the lattice cell described in Problem 38.1.

Cell Homogenization

- Basic ideas
- Cell-averaged group constants
- Detailed procedure
- More general approaches

How do we account for the spatial variation of the flux within a fuel pin cell--or on a more global level, across the core of the reactor? We know that the actual structure of the reactor is quite complex. Since the neutron mfp and diffusion length are comparable to this structure, we must account for it. Indeed, we have already seen it makes a strong difference in the core multiplication. In this lecture, we will examine the topic of cell homogenization.

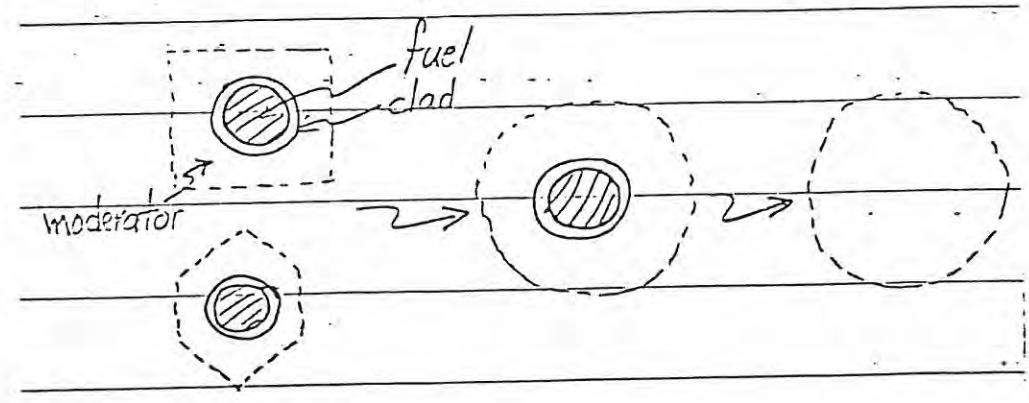
Idea: Generate effective group constants
(spatially averaged)



The general idea is to account for the spatial structure by averaging our group constants over an approximation to the flux in the core. That is, we spatially average. On a gross level, we might visualize the various scales of heterogeneity or structure as shown above. Let's now consider how we might account for this structure in a multigroup diffusion calculation.

38-3

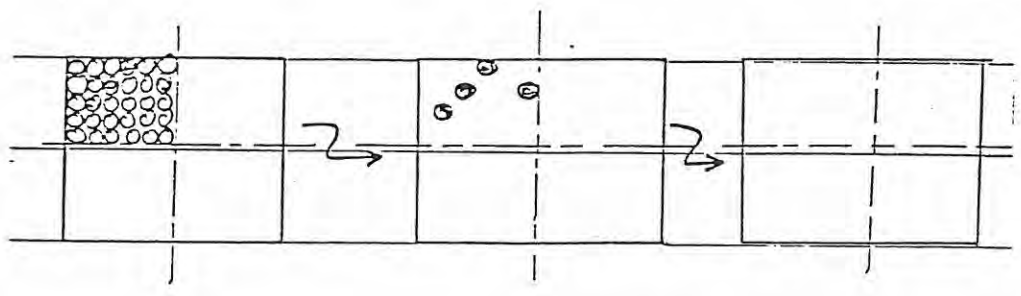
Step 1: "Homogenize" fuel pin cell



One begins by homogenizing a fuel pin cell. That is, we average group constants (cross sections) over the flux typical of a fuel pin cell. This allows us in effect to replace the pin cell by a homogeneous cell. We can then use this homogenized cell to analyze a fuel assembly.

38-4

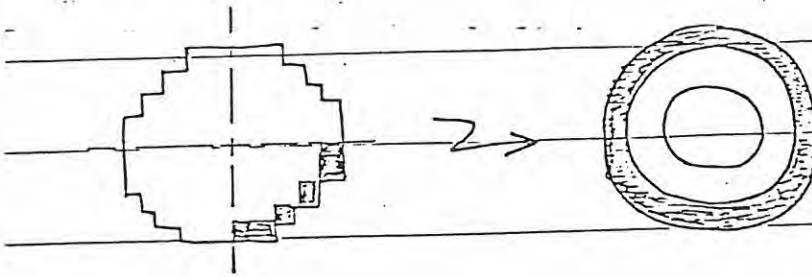
Step 2: "Homogenize" fuel assembly



The same idea holds on the level of the fuel assembly. Note that burnable poisons and control elements may lead to additional heterogeneity. Can carry this finally to the level of a reactor core.

38-5

Step 3: "Homogenize" reactor core



That is, one can represent the reactor core as rings of homogenized fuel assemblies.

Note the zone fuel loading.

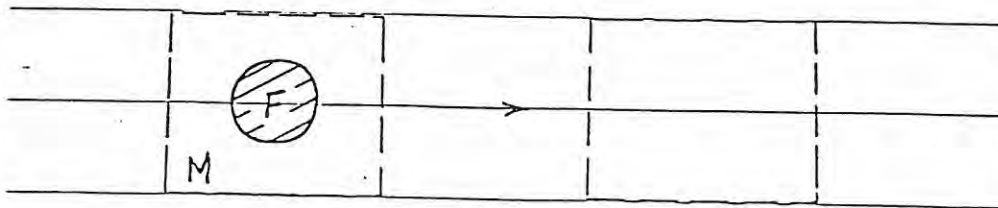
This representation would be used only in gross calculations.

It is more customary to work at the fuel assembly level.

How do we accomplish this "homogenization"?

38-6

Consider a two-region cell:



$$\sigma^M(E), \sigma^F(E)$$

$$N_M, N_F \longrightarrow \langle \Sigma \rangle_{\text{cell}}$$

$$V_M, V_F$$

To be definite, consider a two region fuel pin cell.

Note the quantities we are given.

Our goal is to use this data to calculate a cell-averaged group constant.

38-7

Suppose we can calculate $\phi(\underline{r}, E)$ in cell
 Then define "cell-averaged" or "self-shielded"
 group constant

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\int_{E_g}^{E_{g-1}} dE \int_{V_{\text{cell}}} d^3r \Sigma(\underline{r}, E) \phi(\underline{r}, E)}{\int_{E_g}^{E_{g-1}} dE \int_{V_{\text{cell}}} d^3r \phi(\underline{r}, E)}$$

Suppose we can calculate the flux in the cell. If we knew this in detail, we could easily define the cell-averaged group constant as shown.

Actually, this expression simplifies a bit because of the spatial dependence of the cross section data, as we will indicate.

38-8

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\int_{E_g}^{E_{g-1}} dE \left[\Sigma^H(E) \int_{V_H} d^3r \phi(\underline{r}, E) + \Sigma^F(E) \int_{V_F} d^3r \phi(\underline{r}, E) \right]}{\int_{E_g}^{E_{g-1}} dE \left[\int_{V_H} d^3r \phi(\underline{r}, E) + \int_{V_F} d^3r \phi(\underline{r}, E) \right]}$$

Define: $\bar{\phi}_H(E) = \frac{1}{V_H} \int_{V_H} d^3r \phi(\underline{r}, E)$, $\bar{\phi}_F(E) = \frac{1}{V_F} \int_{V_F} d^3r \phi(\underline{r}, E)$

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{V_H \int_{E_g}^{E_{g-1}} dE \Sigma^H(E) \bar{\phi}_H(E) + V_F \int_{E_g}^{E_{g-1}} dE \Sigma^F(E) \bar{\phi}_F(E)}{V_H \int_{E_g}^{E_{g-1}} dE \bar{\phi}_H(E) + V_F \int_{E_g}^{E_{g-1}} dE \bar{\phi}_F(E)}$$

Go through the analysis showing how the flux averages are defined. This allows us to write the cell-averaged group constants as shown. To proceed further, we need an approximation.

38-9) Suppose: $\phi(r, E) = \phi(r) \psi(E)$

Then

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{V_H \Sigma_g^H \bar{\phi}_H + V_F \Sigma_g^F \bar{\phi}_F}{V_H \bar{\phi}_H + V_F \bar{\phi}_F}$$

where

$$\Sigma_g^F \equiv \frac{\int_{E_g}^{E_{g-1}} dE \Sigma^F(E) \psi(E)}{\int_{E_g}^{E_{g-1}} dE \psi(E)}$$

It is customary to assume that the flux is separable in space and energy.

This allows us to simplify the cell-averaged group constant as shown. Note that the group constants for the fuel and moderator region separately can be calculated using the infinite medium spectrum. We can simplify this expression even further.

38-10) Define:

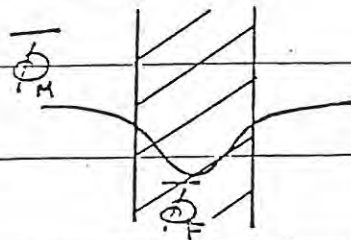
$$\xi \equiv \frac{\phi_H}{\phi_F} \equiv \text{disadvantage factor}$$

so that

$$\langle \Sigma_g \rangle_{\text{cell}} = \frac{\Sigma_g^F + \Sigma_g^H \left(\frac{V_H}{V_F} \right) \xi}{1 + \left(\frac{V_H}{V_F} \right) \xi}$$

Note:

$$\xi > 1$$



Here we can define the ratio of fluxes, the so-called disadvantage factor, to rewrite the cell-average as shown above.

Note that since the flux is depressed in the fuel, the fuel is at a relative disadvantage in competing for neutrons with the moderator.

The key to this analysis is the assumption of space-energy separability.

SE-11 Note: In survey calculations, separability

$$\phi(r, E) = \phi(r) \psi(E)$$

is a common assumption. This separates infinite medium spectrum calculation: $\psi(E)$ from calculation of spatial flux: $\phi(r)$

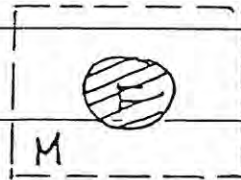
This is usually not a bad assumption for survey calculations. In more detailed calculations, we must use a more complex approach. But for now, let us run through the detailed procedure for calculating the cell averaged group constants.

SE-11 Approach:

1) Given:

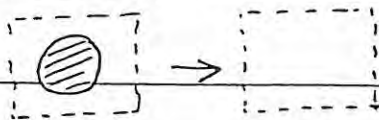
$$\sigma_a^M, \sigma_{tr}^M, \sigma_s^M, N_M, V_M$$

$$\sigma_a^F, \sigma_{tr}^F, \sigma_s^F, \sigma_f^F, V_F, N_F, V_F$$



2) Homogenize cell using volume fractions for

weighting:



$$\Sigma_a^{hom} = \frac{V_M}{V_{cell}} N_M \sigma_a^M + \frac{V_F}{V_{cell}} N_F \sigma_a^F$$

Let us run through all of the steps in this approach.

First note the information we are given.

We next homogenize the cell using simple volume fraction weighting to get cross sections for calculating the infinite medium spectrum.

E8-13

3) Use Σ_a^{hom} , Σ_s^{hom} , Σ_f^{hom} to calculateinfinite medium spectrum $\Psi(E)$

4) Calculate infinite medium group constants

$$\Sigma_{ag}^M = \frac{\int_{E_g}^{E_{g-1}} dE N_M \Sigma_a^M(E) \Psi(E)}{\int_{E_g}^{E_{g-1}} dE \Psi(E)}$$

Same for

$$\Sigma_{sg}^M, \Sigma_{fg}^F, \Sigma_{ag}^F, \Sigma_{gg}^F, \nu_g, \dots$$

Next we use these homogenized cross sections in a fast spectrum code or a thermal spectrum code to calculate the infinite medium spectrum. These can then be used to calculate the infinite medium group constants for both the fuel and the moderator.

To proceed further, we need some information about the spatial dependence of the flux in the cell.

E8-14

5) Calculate disadvantage factor ξ 6) Then use ξ to calculate cell averaged group constants:

$$\langle \Sigma_{ag} \rangle_{\text{cell}} = \frac{\Sigma_{ag}^F + \Sigma_{ag}^M \left(\frac{V_M}{V_F} \right) \xi}{1 + \left(\frac{V_M}{V_F} \right) \xi}$$

Actually, we don't need the detailed flux spatial dependence--only the ratio of the average flux in the moderator to that in the fuel. That is, we need the disadvantage factor. Then we can calculate the cell-averaged group constants.

Big question: Where does ξ come from?

$$\xi = \frac{\bar{\Phi}_M}{\bar{\Phi}_F} = \frac{\text{ave. flux in mod.}}{\text{ave. flux in fuel}}$$



Perform a one-speed calculation.

Still very difficult! Why?

Fuel pin is so highly absorbing that diffusion theory doesn't work!

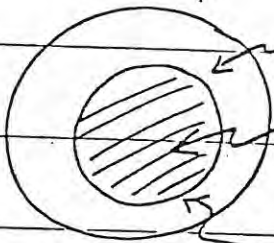
Must use transport theory!

Of course we still have to come to grips with how we calculate the disadvantage factor.

We can usually get by with a one-speed calculation.

But this is still difficult since we must use transport theory.

Common scheme: Amoyal, Benoist, Horowitz (ABH)



diffusion theory

free streaming transport theory (escape probabilities)

match using an "extrapolated boundary"

$$\frac{1}{\bar{\Phi}_M} \left. \frac{d\bar{\Phi}_M}{dr} \right|_{r=a} = \frac{1}{d}$$

The most common approach is called the ABH method. It is a mixture of diffusion theory and free-streaming theory.

One couples these with an extrapolated boundary condition.

Although this is messy, you can work it out in a straightforward fashion.

This gives

$$\xi = \xi(\text{geometry, cross sections})$$

One can then use these in codes.

Problem: Frequently flux in cell is not separable! Then what? Must solve directly for $\phi(r, E)$.

Problem: Highly absorbing nature of fuel requires a transport calculation.

This gives the disadvantage factor as a function of geometry and the cross sections.

One can then use this in computer codes to calculate the cell-averaged group constants.

A problem: In many cases the cell flux is not separable. This is further complicated by the strongly absorbing nature of the fuel.

We will return in the next session to learn how this situation is treated.

LECTURE 39

AN OVERVIEW OF MULTIGROUP DIFFUSION CODES

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 368 - 369
pp. 450 - 452

EXERCISES:

- 39.1. Catalog the various multigroup constant generation codes utilized in your nuclear organization and determine the degree to which these are derived from the MUFT-SOFOCATE-THERMOS schemes.
- 39.2. Sketch a rough diagram of the codes utilized in the nuclear analysis code packages used by your organization.

An Overview of Multigroup Diffusion Codes

- More general cell calculations
- Reactor analysis code packages
- Cross section libraries
- Flux-power-reactivity module

In this lecture we will fill in a few of the gaps in our development of the multigroup diffusion method. We begin with an extension of our cell-homogenization work.

Recall: $\phi(r, E) = \phi(r) \psi(E)$

implied:

$$\langle \xi_g \rangle_{\text{cell}} = \frac{\Sigma_g^F + \Sigma_g^M \left(\frac{V_M}{V_F} \right) \xi}{1 + \left(\frac{V_M}{V_F} \right) \xi}$$

where

$$\xi = \frac{\overline{\phi}_M}{\overline{\phi}_F} = \text{disadvantage factor}$$

Recall that our earlier analysis had been based on the assumption of space-energy separability.

This allowed us to perform the cell-average using only the knowledge of the disadvantage factor.

Problem: frequently flux in cell is not separable! Then what? Must solve directly for $\phi(r, E)$.

Another problem: Highly absorbing nature of fuel requires a transport theory calculation.

However in many situations the flux is not separable in space and energy. Then we must perform a transport calculation to solve directly for the flux in the cell.

How? Monte Carlo or collision probabilities

$$\phi(r, E) = \int d^3r' T(r, r', E) \left[\int_0^{E_{th}} dE' \xi(r', E' \rightarrow E) \phi(r', E') + S(r', E) \right]$$

Break into groups and spatial mesh:

$$\phi_{mg} = \sum_{m=1}^N T_{mn}^g \left[\sum_{g'=1}^G \xi_{sg'g}^m \phi_{mg'} + S_{mg} \right]$$

Solve directly.

This requires a transport calculation. The most common methods involve "collision probabilities". One usually proceeds by directly discretizing the transport equation for the cell (beyond the scope of this course).

~~typical spectrum - multigroup constant codes:~~

~~fast thermal~~

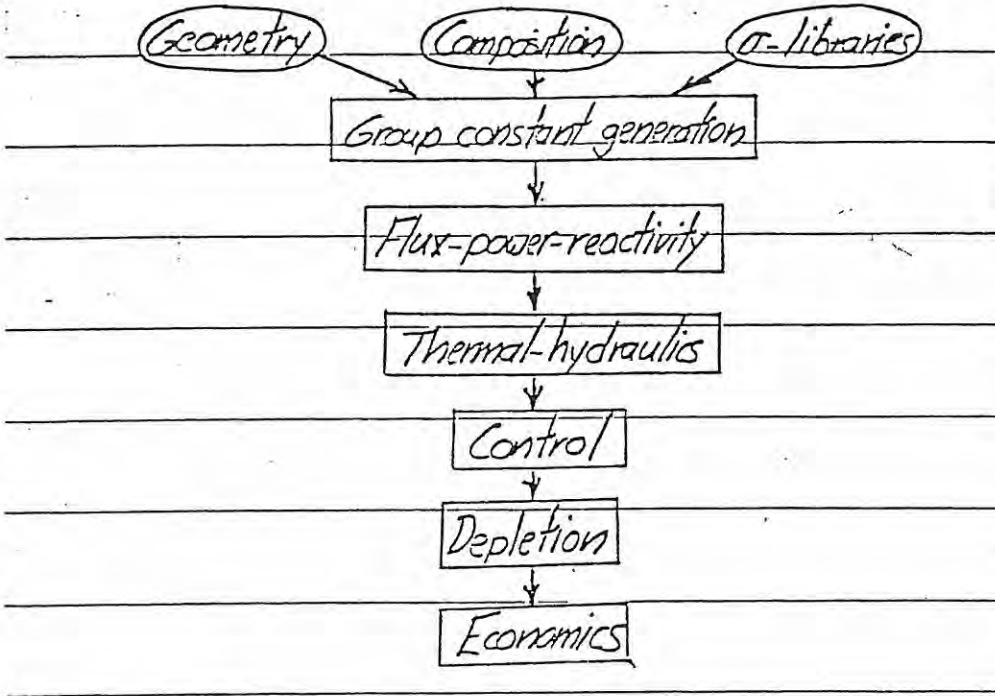
~~LEOPARD: MUFT + SOFOCATE~~

~~LASER: MUFT + THERMOS~~

~~MICROX: GAM + THERMOS~~

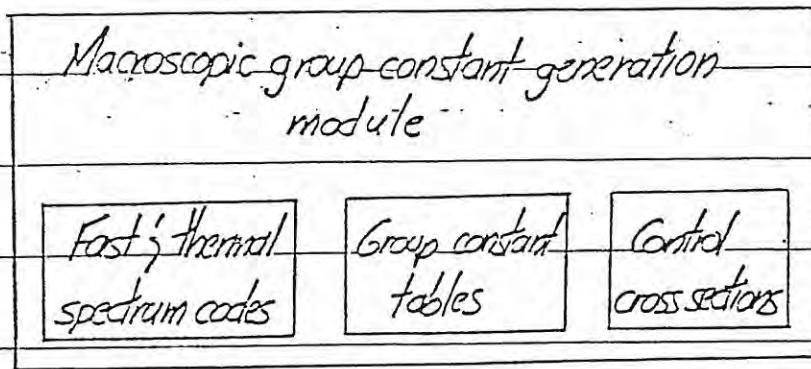
We can classify the various codes used to produce group constants for light water reactors.

The THERMOS code includes a transport calculation of the flux in the cell, while the SOFOCATE code assumes space-energy separability and uses an ABH calculation of the disadvantage factor.



In reactor analysis, one generally relies on a collection or package of computer codes. Let us examine a prototype reactor code package for nuclear reactor analysis.

We have been focussing on the group constant generation module.



Let us look at this module in more detail.

We have focussed our attention on fast and thermal spectrum codes (e.g., MUFT and SOFOCATE).

There are other ways to generate group constants, including tables and special methods to calculate cross sections to account for control elements.

We will consider these in more detail in subsequent courses.

But first we should consider where the cross section data itself comes from.

Microscopic cross section data:

i) Primary source: nuclear data files

ENDF/B (Evaluated Nuclear Data File)

Form: pointwise data (σ)

interpolation parameters

ii) Process into library of microscopic data

suitable for spectrum codes (collapse

over $1/E$ or $\chi(E)$ weighting function)

Nuclear cross section data have been measured and calculate for many decades. These data play the same role as other engineering parameters in other engineering fields.

Explain the ENDF data file.

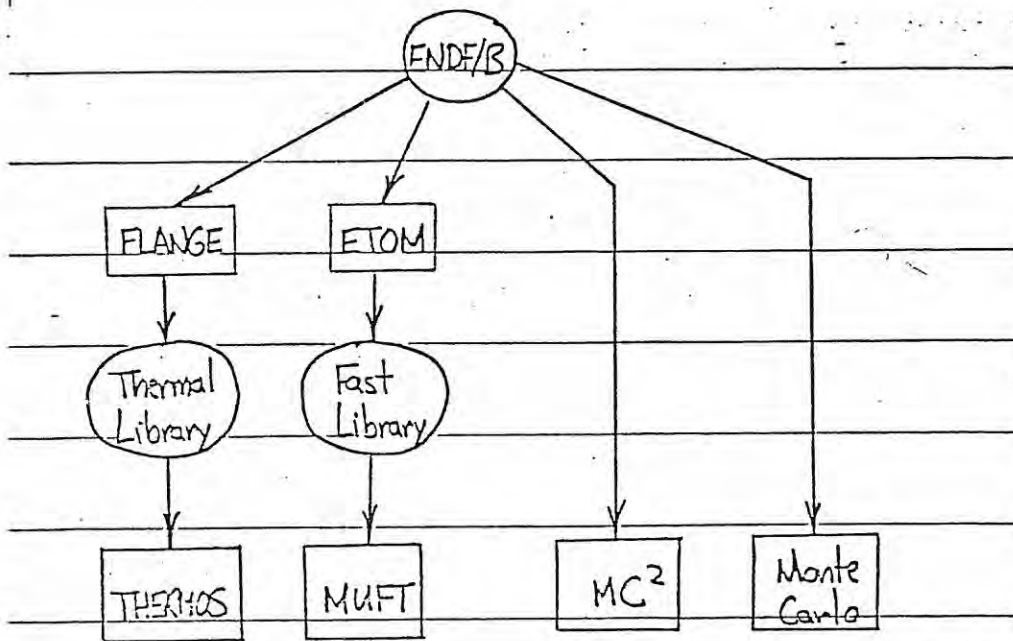
Explain the need for processing codes (and note the expense of processing).

(Note: Frequently fast & thermal libraries are supplied as part of spectrum codes)

iii) Library data is used in calculating spectrum $\phi(E)$

iv) Library data is averaged over spectrum to calculate multigroup constants

Fortunately, most spectrum codes come with fast and thermal libraries already prepared. This library data is also used in calculating the spectrum and in performing the calculating of the multigroup constants.



Shown above is a diagram indicated several routes to preparing cross section data for a spectrum code.

Before leaving this subject of the nitty-gritty of multigroup diffusion calculations, perhaps we should focus for a moment on the flux-power-reactivity module where these calculations are actually performed,

Flux-power-reactivity
module

(static multigroup diffusion
codes)

This module is typically referred to as the flux-power-reactivity module since it is concerned with calculating these quantities. This module consists of the static multigroup diffusion equations we studied several lectures earlier

Flux-power-reactivity module

Goal: Analyze static neutronic behavior in core using multigroup diffusion theory.

Determine:

i) k

ii) $\phi_g(r)$

iii) $P(r) = w_f \sum_{g=1}^{G_f} \epsilon_{fg}(r) \phi_g(r)$

Analyze the module in terms of the general goal of reactor analysis. Go over aspects of the calculation. Why?

Why?

k determines fuel loading

control system adjustment for criticality

also control element worth

reactivity feedback coefficients

reactivity for various fuel

loading patterns

The multiplication factor determines a number of important quantities for reactor analysis.

Moreover, the flux generated by the MGD calculations is also of considerable interest.

$\phi(r)$ determines fuel depletion

isotope buildup (conversion)

$P(r)$ determines thermal-hydraulic performance

hot channel factors

LECTURE 40

A SUMMARY OF THE COURSE

READING ASSIGNMENT:

Duderstadt & Hamilton, pp. 447 - 466

EXERCISES:

None specified

☺ A Summary of the Course

- Nuclear reactor theory
- Neutron-nuclear interactions
- Neutron diffusion
- Multigroup diffusion theory
- Neutron slowing down ; thermalization
- Lattice effects

Hold on to your chairs, sports fans. In this lecture we are going to put it all together by reviewing the topics of this course.

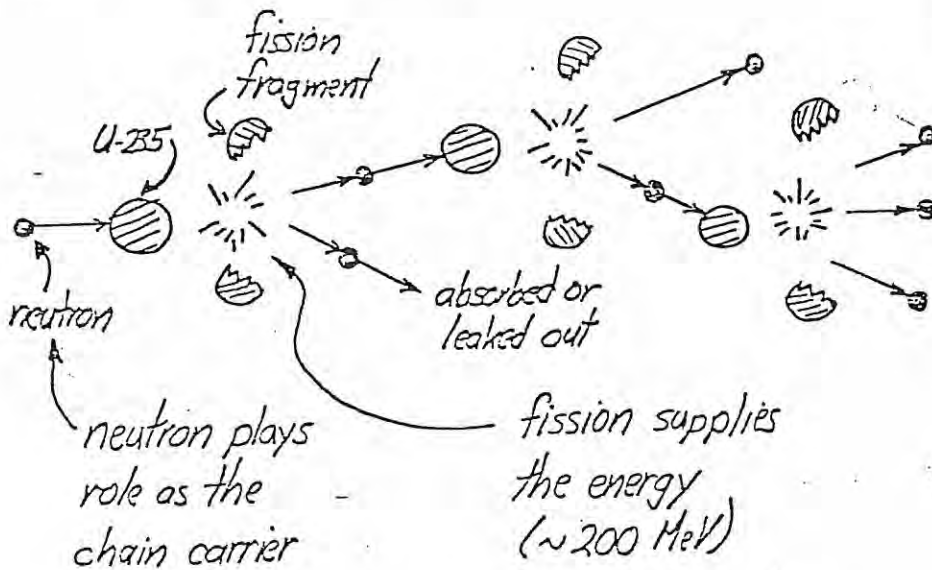
I will fly over this material rather rapidly. However it does seem important to show you once again how all of the pieces fit together.

Otherwise you might lose the forest for the trees.

We can begin with a discussion of just what nuclear reactor theory is all about.

D-2

Fission Chain Reaction



Recall the general features of the fission chain reaction:

Note: neutron -- chain carrier

fission -- energy

From this perspective, we can easily identify the primary jobs of the nuclear engineer.

②-3) Two jobs of the nuclear engineer

- 1.) Follow the neutron "economy" to achieve a stable fission chain reaction
nuclear reactor theory
- 2.) Extract and use fission energy
heat transfer, fluid flow, stress analysis,
power plant analysis

The first job is to follow the neutron "economy"...

The second job is...

In this course we have focussed on the first of these jobs.

②-4) Key problem: Determine the distribution of neutrons in a reactor. Why?

i) Allows one to study neutron economy
(and hence chain reaction)

ii) neutron density & fission rate

& power

The key here is the determination of the distribution of neutrons in a reactor.

Why? ...

There are two aspects of this endeavor.

20-5 Two aspects of this problem:

- i) Study the interaction of neutrons with matter (nuclei).
- ii) Study the motion ("transport") of neutrons within a nuclear reactor and hence their leakage rate out of the core.

Let me review these, since they represent quite different disciplines.


Interaction of neutrons with matter.

Neutron transport (in space and energy).

We can quickly review the key topics in the first of these.

20-6 Interaction of neutrons with matter

Types of neutron-nuclear reactions:

radiative capture 

fission 

scattering: elastic 

inelastic 

other: $(n, 2n)$ - (γ, n)

Recall the principal interactions of interest;

Go over list.

We need to develop a quantitative basis for analyzing these interactions.

to describe interactions quantitatively:

$\sigma \equiv$ microscopic cross section

Note:

$$\sigma_T = \sigma_S + \sigma_f + \sigma_c + \dots$$

$\Sigma \equiv N\sigma \equiv$ macroscopic cross section

$\lambda = 1/\Sigma \equiv$ mean free path

$v\Sigma \equiv$ frequency of interactions

$1/v\Sigma \equiv$ mean time between collisions

To this end, we introduced the concept of a microscopic cross section.

Go over list.

We also developed several generalizations.

40-B Generalizations:

$\sigma(E), \Sigma(r, E)$

$\sigma_s(E' \rightarrow E), \Sigma_s(E' \rightarrow E)$ differential scattering cross section

Calculation of cross sections:

i) Two body kinematics

ii) Nuclear physics

We included the dependence of the cross sections on neutron position and energy.

Also scattering cross sections.

The calculation of cross sections has been developed in this and earlier courses.

We can use these cross sections to make a simple analysis of a fission chain reaction.

Simple theory of fission chain reactions

Define:

$$k \equiv \frac{\text{number of neutrons in one generation}}{\text{number of neutrons in preceding generation}}$$

\equiv multiplication factor

Note: $k > 1$ - supercritical

$k = 1$ - critical

$k < 1$ - subcritical

The key here is the multiplication factor.

Define.

Go over implications.

How do we calculate k ?

By following processes during neutron lifetime
we find

$$k = \eta f p \epsilon P_{FNL} P_{TNL}$$

6-factor formula

Here $\eta = \frac{\nu \sigma_f^F}{\sigma_a^F}$

$$f = \frac{\Sigma_a^F}{\Sigma_a} = \frac{N_F \sigma_a^F}{N_F \sigma_a^F + N_H \sigma_a^H}$$

$p, \epsilon, P_{FNL}, P_{TNL} \Rightarrow$ neutron transport & slowing down

We play a game of follow the neutron. Let me be more precise.

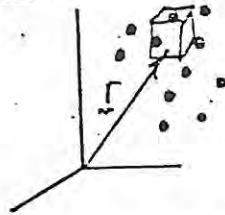
Go over terms in 6-factor formula.

Most of these terms depend on neutron transport in space and energy.

We began by studying neutron motion in space.

Neutron diffusion ("transport")

$n(\underline{r}, t)$ neutron density



$\phi(\underline{r}, t) = \bar{v} n(\underline{r}, t)$ neutron flux

$\underline{J}(\underline{r}, t)$ neutron current density

$\Sigma\phi(\underline{r}, t)$ reaction rate density

Introduced subject of neutron diffusion.

Introduced various definitions.

To calculate these quantities, we developed a simple model: one-speed diffusion theory.



Use

$$\frac{1}{\bar{v}} \frac{\partial \phi}{\partial t} + \nabla \cdot \underline{J} + \Sigma_a \phi(\underline{r}, t) = S(\underline{r}, t)$$

neutron continuity equation

Then approximate

$$\underline{J} \cong -D \nabla \phi$$

to find

$$\frac{1}{\bar{v}} \frac{\partial \phi}{\partial t} - D \nabla^2 \phi + \Sigma_a \phi(\underline{r}, t) = S$$

neutron diffusion equation

We began with the neutron continuity equation.

Go over derivation.

This simple equation formed the basis for our further analysis of the reactor.

Steady-state, non-multiplying media

$$-D\nabla^2\phi + \xi_a\phi = S$$

or dividing by D

$$\nabla^2\phi - \frac{1}{L^2}\phi = -\frac{S}{D}$$

where

$$L \equiv \sqrt{\frac{D}{\xi_a}} \text{ diffusion length}$$

We began by examining the case of a steady-state, nonmultiplying medium.

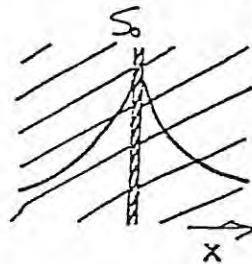
Go over analysis.

We looked at several typical solutions.

Typical solutions

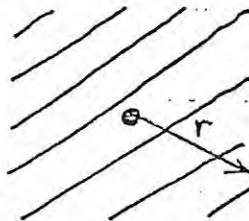
Plane source:

$$\phi(x) = \frac{S_0 L}{2\xi_a} e^{-x/L}$$



Point source:

$$\phi(r) = \frac{S_0}{D} \frac{e^{-r/L}}{4\pi r}$$



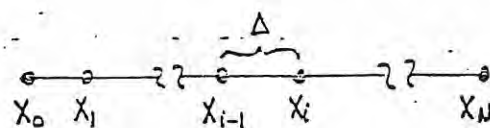
Go over solutions.

Actually, most problems cannot be solved in such simple forms.

Instead we are forced to use a digital computer.

9-15

Numerical solutions:

$$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(x) = -\frac{S(x)}{D}$$


Use

$$\left. \frac{d^2\phi}{dx^2} \right|_{x_i} \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta^2}, \quad \phi_i \equiv \phi(x_i)$$

to find

$$-\frac{1}{\Delta^2}\phi_{i+1} + \left[\frac{2}{\Delta^2} + \frac{1}{L^2}\right]\phi_i - \frac{1}{\Delta^2}\phi_{i-1} = \frac{S_i}{D}$$

$$i = 1, \dots, N-1$$

This led us to the subject of the numerical solution of the diffusion equation.

Go over structure.

Next we considered the extension to multiplying media.

10-16

Multiplying media:

$$S \rightarrow S_f(\underline{r}) = \nu \Sigma_f \phi(\underline{r})$$

Then diffusion equation becomes

$$-D\nabla^2\phi + \Sigma_a\phi(\underline{r}) = \nu \Sigma_f\phi(\underline{r})$$

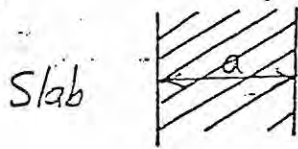
Criticality condition:

$$\text{material buckling } B_m^2 = \frac{\nu \Sigma_f - \Sigma_a}{-D} = B_g^2 \text{ geometric buckling}$$

In multiplying media, the source is provided by fission.

Go over criticality calculation.

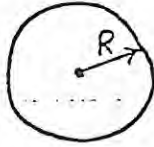
Let me give you some examples.



$$\left(\frac{\pi}{a}\right)^2$$

$$\cos \frac{\pi x}{a}$$

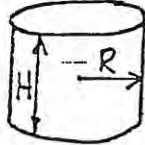
Sphere



$$\left(\frac{\pi}{R}\right)^2$$

$$\frac{\sin \frac{\pi r}{R}}{r}$$

Cylinder



$$\left(\frac{\pi}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$$

$$J_0\left(\frac{\pi r}{R}\right) \cos\left(\frac{\pi z}{H}\right)$$

Go over table of geometric bucklings and shapes.

What happens for more general problems? Again the computer.

More generally:

$$-D\nabla^2\phi + \epsilon_a\phi(r) = \frac{1}{k} v\epsilon_f\phi$$

Guess:

$$S(r) \equiv S^{(0)}(r), \quad k \sim k^{(0)}$$

Solve:

$$-D\nabla^2\phi^{(1)} + \epsilon_a\phi^{(1)} = \frac{1}{k^{(0)}} S^{(0)}$$

Calculate:

$$S^{(1)} \equiv v\epsilon_f\phi^{(1)}, \quad k^{(1)} = \frac{\int d^3r S^{(1)}}{\frac{1}{k^{(0)}} \int d^3r S^{(0)}}$$

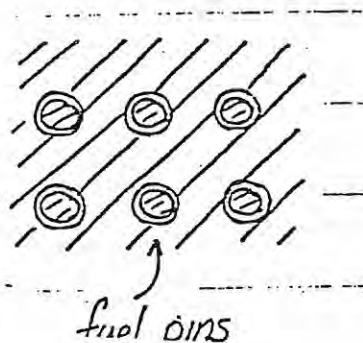
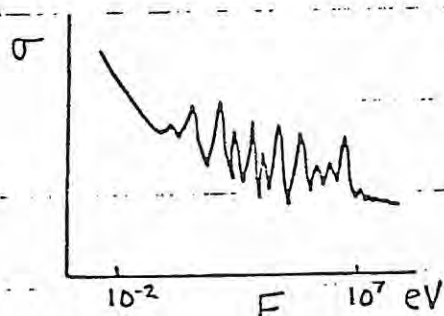
The key here was an iterative solution.

Go over strategy.

We can continue on in this fashion.

40-21

Note: A realistic description of core requires realistic treatment of energy & space dependence of cross sections:



A realistic description of the core requires a realistic treatment of the space and energy dependence of the cross sections. This would overload any computer. What are we to do?

40-22

Key Idea: average $\Sigma(r, E)$ over space and energy to remove complexity

- multigroup diffusion method
- slowing down & resonance absorption
- thermalization
- lattice cell homogenization

The key idea...

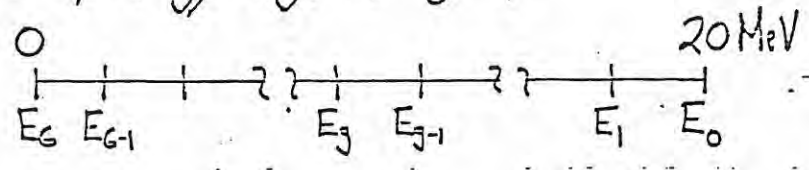
We implemented this through the study of several topics.

Let's briefly review the route we took.

40-23

Energy Averaging:

Break up energy range into groups



Integrate energy-dependent diffusion equation

ORR each group:

$$\int_{E_g}^{E_{g-1}} \{ \text{energy-dependent diffusion equation} \} dE$$

To arrive at the multigroup diffusion equations, we essentially energy averaged...
 Then by introducing some convenient definitions...

40-24

Define

$$\phi_g \equiv \int_{E_g}^{E_{g-1}} dE \phi(r, E) \quad \text{group flux}$$

$$\Sigma_g \equiv \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma(r, E) \phi(r, E) \quad \text{group constant}$$

to find

$$-\nabla \cdot D_g \nabla \phi_g + \Sigma_{g} \phi_g = \sum_{g'=1}^{G'} \Sigma_{s, g'} \phi_{g'} + \frac{1}{k} \sum_{g'=1}^{G'} \chi_{g'} \Sigma_{f, g'} \phi_{g'}$$

$g = 1, \dots, G$

Namely, ...
 we arrived at the multigroup diffusion equations.
 We studied one important example in detail.

40-25 Example: Two group diffusion theory

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = \frac{1}{k} [\nu_1 \Sigma_{f1} \phi_1 + \nu_2 \Sigma_{f2} \phi_2]$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{R2} \phi_2 = \Sigma_{S1 \rightarrow 2} \phi_1$$

Describe the structure of these equations.
More generally, we examined methods for solving the MGD.

40-26 Solution:

$$-\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{R1} \phi_1 = \frac{1}{k} \chi_1 S$$

$$-\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{R2} \phi_2 = \frac{1}{k} \chi_2 S + \Sigma_{S1 \rightarrow 2} \phi_1$$

$$-\nabla \cdot D_3 \nabla \phi_3 + \Sigma_{R3} \phi_3 = \frac{1}{k} \chi_3 S + \Sigma_{S1 \rightarrow 3} \phi_1 + \Sigma_{S2 \rightarrow 3} \phi_2$$

$$-\nabla \cdot D_G \nabla \phi_G + \Sigma_{R_G} \phi_G = \frac{1}{k} \chi_G S + \Sigma_{S1 \rightarrow G} \phi_1 + \dots + \Sigma_{S_{G-1} \rightarrow G} \phi_{G-1}$$

Go over solution strategy.

This behind us, we next turned to a determination of the multigroup constants themselves.

4.0-27

Calculation of multigroup constants

$$\Sigma_{tg} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(\Omega, E) \phi(\Omega, E)}{\int_{E_g}^{E_{g-1}} dE \phi(\Omega, E)}$$

Key idea: Approximate

$$\phi(\Omega, E) \sim \phi(E) \quad \text{spectrum}$$

Recall the definition of the multigroup constants.
We introduced an approximation to the intragroup flux.

4.0-28

Fast spectrum calculations:

neutron slowing down

resonance absorption

We found

$$\phi(E) \sim \frac{S_0}{\xi E \Sigma_s(E)} \sim \frac{1}{E}$$

$$P_i = \exp\left[-\frac{N_A}{\xi \Sigma_s} I_i\right]$$

$$I_i \equiv \int_{E_i} dE \sigma_a(E) \phi(E)$$

To calculate the spectrum, we looked first at the fast energy range.

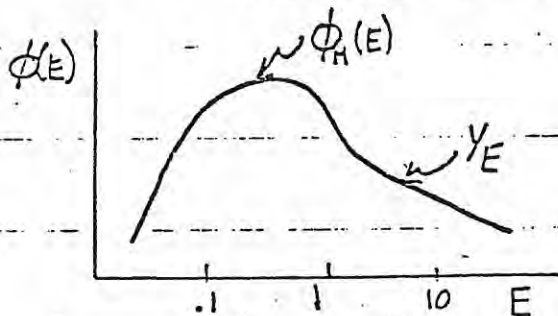
Two topics...

Our key results were...

40-29 Thermal spectrum calculations

$$\phi(E) \sim \Phi_M(E) \sim \frac{2\pi n_0}{(\pi kT)^{3/2}} \left(\frac{2}{m}\right)^{1/2} E e^{-E/kT}$$

Maxwell-Boltzmann distribution



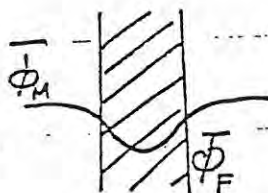
The thermal range was somewhat simpler.
Review essential aspects.
But there was one final task that remained.

40-30 Spatial averaging

$$\begin{aligned} \langle \Sigma_g \rangle_{\text{cell}} &= \frac{\int_{V_{\text{cell}}} d^3r \Sigma_g(\mathbf{r}) \phi(\mathbf{r})}{\int_{V_{\text{cell}}} d^3r \phi(\mathbf{r})} \\ &= \frac{\Sigma_g^F + \Sigma_g^M \left(\frac{V_M}{V_F}\right) \xi}{1 + \left(\frac{V_M}{V_F}\right) \xi} \end{aligned}$$



$$\xi \equiv \frac{\bar{\Phi}_M}{\bar{\Phi}_F} = \text{thermal disadvantage factor}$$



We had to account for the spatial dependence caused by the lattice structure.
The key here was spatial averaging--somewhat akin to energy averaging.
Go over details.
Thus we completed our development of the multigroup diffusion method.

i) Develop the basic theory of fission chain reactions

ii) Develop the principal tool of nuclear reactor analysis: multigroup diffusion theory

The goals of this course were as follows...

It has provided us with the basis both for understanding and analyzing nuclear reactor behavior and design.

ABOUT THE NUCLEAR ENGINEERING DEPARTMENT

The first course in nuclear energy applications at The University of Michigan was taught in the late 1940s, and the Department of Nuclear Engineering was formally established in 1958 on the graduate level. Seven years later it inaugurated an undergraduate program, based on the principle that a sound education in mathematics and the basic sciences should precede specialized training. Since then, the Department has gained increasing recognition for the quality of both its undergraduate and graduate programs, as well as for its ongoing research in such areas as the dynamic behavior of nuclear reactors, computer methods in reactor analysis, nuclear fuel management, the effects of nuclear radiation on materials, the use of liquid metals in cooling nuclear reactors, and both magnetic fusion and inertial confinement (laser and particle-beam) fusion. Among the departmental faculty members participating in this series are:

JAMES J. DUDERSTADT / BE(EE) Yale University / MS (Eng Sci), PhD (Eng Sci/Physics), Caltech
KINETIC THEORY & STATISTICAL PHYSICS / NUCLEAR FISSION & FUSION REACTORS / ENERGY SYSTEMS ANALYSIS



WILLIAM KERR / BS(EE), MS(EE) University of Tennessee / PhD(EE) University of Michigan
REACTOR SAFETY / REACTOR KINETIC BEHAVIOR / SHIELDING / CONTROLLED FUSION TECHNOLOGY / HYDROGEN PRODUCTION & USE



GLENN F. KNOLL / BS(ChE) Case / MS(ChE) Stanford / PhD(Nuc) University of Michigan
NUCLEAR MEASUREMENTS / NEUTRON CROSS SECTIONS / ENGINEERING ASPECTS OF NUCLEAR MEDICINE & RADIOLOGY



JOHN C. LEE / BS(Nuc) Seoul National University / PhD(Nuc) University of California, Berkeley
REACTOR CORE ANALYSIS / REACTOR KINETICS / FUEL CYCLE ANALYSIS / POWER PLANT MODELING



WILLIAM R. MARTIN / BSE(Eng Phys) University of Michigan / MS(Phys) University of Wisconsin / MSE(Nuc), PhD(Nuc) Michigan
NEUTRON TRANSPORT THEORY / REACTOR ANALYSIS METHODS / FUEL MANAGEMENT SCHEMES



RICHARD K. OSBORN / BS(Phys), MS(Phys) Michigan State University / PhD(Phys) Case Institute of Technology
NUCLEAR REACTIONS & KINETIC THEORY / PLASMA PHYSICS / NONLINEAR OPTICS



GEORGE C. SUMMERFIELD / BS(Phys), PhD(Phys) Michigan State University
NEUTRON TRANSPORT THEORY / NEUTRON INTERACTIONS WITH MATTER / GEOPHYSICAL STUDIES USING NUCLEAR TECHNIQUES



DIETRICH H. VINCENT / Diplomphysiker, Dr.Rer.Nat., University of Goettingen
RADIATION EFFECTS ON MATERIALS / GASES IN METALS / ION BEAM ANALYSIS / MÖSSBAUER SPECTROSCOPY



GARY S. WAS / BS(Nuc) University of Michigan / SM(Nuc), PhD(Nuc) MIT
RADIATION DAMAGE IN METALS & ALLOYS / DEGRADATION OF MATERIALS IN ENERGY SYSTEMS / MATERIALS SELECTION FOR ENERGY-SYSTEM COMPONENTS / FUEL BEHAVIOR PERFORMANCE

