

# THE USE OF COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

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ABSTRACT

For many years the Chemical Engineering Department of The University of Michigan has been employing electronic computers in its various research and educational programs. During the past three years, in particular, the Department has made a special effort to integrate the use of analog and digital computers throughout the required undergraduate curriculum. This report describes some of the characteristics of these machines which make them useful not only as problem solving tools but also as purely educational devices, and relates the faculty's experiences with computers in both the undergraduate and graduate programs. The Department's curriculum is discussed with special emphasis on courses in which computers have been used extensively.

Twelve computer-oriented example engineering problems with complete analog or digital computer solutions are also included. This set of problems may be considered as a supplement to the 111 example engineering problems, including several of interest to chemical engineers, which have been published previously by the Project on the Use of Computers in Engineering Education at The University of Michigan.

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## USE OF COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

### I. INTRODUCTION

As early as 1948, in what may have been a pioneering venture, graduate students in the Department of Chemical and Metallurgical Engineering at The University of Michigan began to use the digital computer in their doctoral research. During subsequent years, digital computer work was introduced into graduate courses, first at the doctoral level in 1952 and later at the master's level in 1955. Analog computer work in both graduate and undergraduate courses was initiated in 1952. By 1958 the University had acquired a large-scale digital computer with an easy-to-use procedure-oriented language. A pilot program was implemented to experiment with and to study digital computer applications in several undergraduate courses. The success and promise of the early programs, and the results of the Department's pilot program in particular, led to the submission of the original proposal of the Engineering College to The Ford Foundation for support of a demonstration project on the "Use of Computers in Engineering Education."

During the past three years, the Department has intensified its efforts to integrate the use of both analog and digital electronic computers throughout its undergraduate and graduate programs. The current extensive use of these machines, in undergraduate courses in particular, came about as the result of several factors: (1) The University has a large and accessible digital computing facility and a sizable amount of analog computing equipment. (2) There has been extensive support of faculty computer training by the Ford Foundation Project on the Use of Computers in Engineering Education. (3) Every chemical engineering student is now required to take a one-hour sophomore-level computing course which introduces him to digital computing concepts and teaches him the procedure-oriented language (MAD) used on the University's computer. With adequate facilities, and a computer-cognizant faculty and student body, it is possible to use computers extensively in junior and senior level engineering courses. Details of the faculty and student training programs may be found elsewhere.<sup>1,2</sup> MAD (Michigan Algorithm Decoder), whose elements are a mixture of English vocabulary and mathematical notation, is a formal language especially designed to make as simple as presently possible, the communication of scientific computation procedures (sometimes called algorithms) to the digital computer (currently an IBM 7090). The language is similar to the more familiar ALGOL and FORTRAN languages. Students write their programs in this language, but do not operate the machine. Details of language structure and grammar can be found in Reference 3.

This report presents a viewpoint based upon the chemical engineering faculty's experience with computers in the undergraduate curriculum and of the characteristics of computers which make them useful as problem-solving tools and as purely educational devices. This report describes the curriculum and current methods of introducing computers into the chemical engineering program and includes several completely solved chemical engineering problems suitable for educational use.

## II. THE CHEMICAL ENGINEERING DEPARTMENT AND ITS CURRICULUM

Since chemical engineering is offered in a department which also includes three other programs, Metallurgical, Materials, and Science Engineering, the faculty represents a wide variety of research and professional interests. An extensive array of courses is available to implement elective programs.

The chemical engineering student group is well balanced between graduates and undergraduates, with about 60 baccalaureate degrees, 30 master's degrees and 15 doctorates awarded annually. The junior class is larger than the sophomore class because of the relatively high transfer rate from other universities and community colleges after the second year. Undergraduates have the customary diversity of interests while the doctoral students show strong inclinations toward research and teaching. Development of facility in computer application seems to follow the individual student's preference.

There is no sharp demarcation between the metallurgical and the chemical engineering faculty. Those departmental faculty members who have taken part in one or more of the training programs of the Michigan Computer Project are listed in Table II.

As might be expected with the relatively large graduate enrollment, faculty and students are productive in the research area. About seventy-five publications per year have resulted from the research program in recent years. The effect of computer availability is readily apparent in these publications.

Those interested in a more detailed description of staff and student research activities may request a booklet published by the Department of Chemical and Metallurgical Engineering by writing the Departmental office.

TABLE II  
Chemical and Metallurgical Engineering Faculty Members  
Who Have Participated in Programs of the Computer Project

<u>Name</u>	<u>Rank</u>	<u>Name</u>	<u>Rank</u>
R. E. Balzhiser	Assistant Professor	R. D. Pehlke	Assistant Professor
W. C. Bigelow	Professor	D. F. Rudd*	Assistant Professor
L. E. Brownell	Professor	M. R. Tek	Associate Professor
S. W. Churchill	Professor, Dept. Chairman	L. H. Van Vlack	Professor
K. F. Gordon	Associate Professor	Brymer Williams	Professor
L. L. Kempe	Professor	J. L. York	Professor

\* Now at The University of Wisconsin

Figure 1 shows the sequence of courses in the baccalaureate program in chemical engineering at The University of Michigan. The program has an unusually high degree of freedom for a student. Over forty percent of the total credit hours required for graduation are elective; over sixty percent of the courses beyond the "common core" are elective. Each student has the privilege of choosing a program to develop his own interests and abilities. With such individuality possible, a student may concentrate in courses in computer-related fields or he may avoid such courses entirely except for the required minimum. An undergraduate interested in computers would find the courses shown in Table I2 available. (A graduate student has even greater opportunity to concentrate in computer-related areas).

Chemical Engineering BSE Program  
The University of Michigan

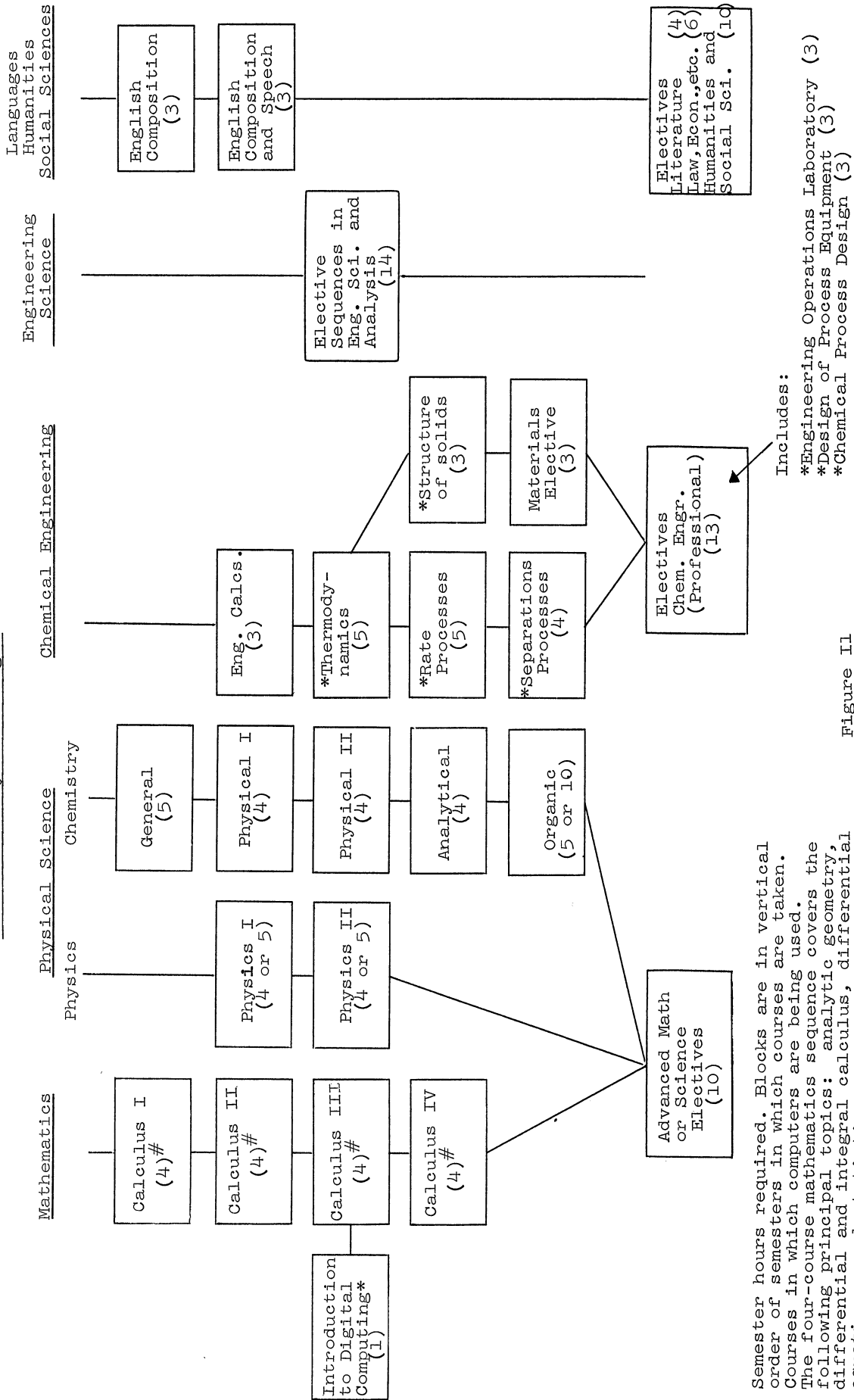


Figure 11

( ) Semester hours required. Blocks are in vertical order of semesters in which courses are taken. Courses in which computers are being used. The four-course mathematics sequence covers the following principal topics: analytic geometry, differential and integral calculus, differential equations, and statistics.

\* #

TABLE I2

Philosophy 414, 415.	Mathematical Logic I and II Introduction and application to computer theory, switches and artificial intelligence.
Philosophy 418.	Philosophy of Mathematics.
Philosophy 428.	Philosophy of Science.
Communication Sciences 400, 401.	Introduction to Communication Sciences I and II. Concepts of communication and processing of information.
Business Administration Statistics 450, 550.	Electronic Data Processing Systems I and II.
Electrical Engr. 465.	Electronic Computers.
Electrical Engr. 467.	Switching Circuits and Logical Design.
Electrical Engr. 565.	Analog and Digital Computer Technology.
Instrumentation Engineering 510.	Application of the Electronic Differential Analyzer.
*Mathematics 373:	Introduction to Digital Computing.
Mathematics 473.	Methods of High Speed Computation.
Industrial Engr. 373.	Data Processing.

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\* The introductory computer course required of all undergraduate chemical engineering students.

### III. COMPUTERS AND THE ENGINEERING SCIENCES

In considering the significant impact which the high-speed electronic computer will have on our future technological development, several questions arise concerning the role of computers in engineering education. There seems little doubt that a good fraction of today's engineering graduates (who may well be working as engineers in the year 2000) will see computers used in their technical work. This probable involvement of computers in engineering work requires that the engineer know more about computers than he can learn from the "giant brain" articles in the Sunday supplements. Two pertinent questions are: "Where should he learn about computers - on the job or in the engineering school?", and "What is the minimum computer experience necessary?" The maximum depth of ability and experience will be limited, of course, only by individual capacity and desire.

In planning a university program in any branch of engineering, the faculty must always consider present engineering technology and the probable course of science and engineering in the future. That is, students must be prepared not only for today's work, but must have the fundamental training to adapt to tomorrow's challenges. What is best learned in school and what should be taught by industry must always be resolved. The responsibility is acute for universities because they must accomplish their work in a brief few years, no more than the first tenth of a man's professional or technical career.



## Use of Computers in Chemical Engineering Education

The development, growth, and acceptance of large electronic computers, particularly the high-speed digital machine, have been so dramatic and rapid that most schools have not been permitted time to study and to experiment with their use. Obviously we cannot ignore these powerful new tools, but as yet are not certain of the best methods of using them in the curriculum. It is certain that we do not always foresee the future correctly and consequently may make errors in curriculum planning.

The Department now believes that the minimum computer experience necessary for graduation should be the successful solution of at least one comprehensive and several simple engineering problems. Since it is most desirable to have the student learn the basic logic and mathematics of computing, all undergraduates are required to take an introductory course in digital computing. In this introductory course the student solves four simple problems, (usually some elementary numerical problems involving interpolation, approximation, root finding, and so forth) which serve to teach the MAD language used extensively throughout the University. The student is taught some useful numerical mathematics as well. Thus the student comes to his engineering problem courses with sufficient background to use computers to solve his engineering problems without the need for time-consuming training. Properly done, computer use should not necessitate removal of any essential material and should enhance the value of material covered in the course. Needless to say, it is essential that an instructor requiring computer use in his course must have a greater depth of programming experience than he expects of his students. Faculty preparation is without question the most important factor in successful computer integration into the engineering classroom. The most successful cases of classroom computer use in the Department have been by instructors willing to spend extra non-class time on computer work. Certainly the instructor should program any proposed problem himself before assigning it to his students. This permits him to gauge the amount of student effort which will be needed and also to foresee any omissions or inconsistencies in the problem statement or in the solution procedure.

The intent of this effort is not to produce computer programmers (although many engineers will certainly be programming their own engineering problems after graduation), but rather to produce engineers with an appreciation for and the ability to use these new engineering tools. If the history of American science and industry is a guide, it is probable that specialization will develop in the use of computers as in most other technical areas. That is, although we are certain that nearly all engineering work forty years hence will in some way involve computers, it is reasonable to assume that not all engineers will actually be involved in programming their computer problems. To forecast otherwise would be to ignore differences in individual preferences and abilities.

However, it is safe to predict continued development in the means of communication with computers. The engineers who wish to do so will find that the writing of programs will be a much simpler task in the future. Arbitrary and meaningless jargon, special and obscure forms will hopefully be eliminated. Programming languages are likely to be improved to the point where the statement of the problem and a simple unambiguous outline of its solution (perhaps in a flow diagram form only) will suffice.

However, regardless of the advances in methods of presenting problems to the computer, engineers will find limitations in their mathematical ability. That is, there are the engineering and scientific aspects of problems and the mathematical aspects. It is clear that many engineers and engineering students will become interested and thoroughly competent in the use of the new mathematical techniques for solving their development and research problems. Others, perhaps a majority, will be primarily interested in work such as development, experimentation, and problem formulation, and will be willing to accept major assistance in mathematics and computer usage as they now accept expert advice in electronics and the sciences.

It is essential that the students' computer experience emphasize pitfalls and possible abuses of computer use as well as the more obvious advantages. Good practices can probably be best instilled by example; the teacher's judgement in selection of problems, the solution approach, explanation of errors, etc., are very important for the student if he is to appreciate fully the value of a computer in his work.

#### IV. EDUCATIONAL ASPECTS OF COMPUTERS

For engineers, the purposes of computing will continue to be the obtaining of usable answers and insight into problems. For engineering teachers the computer can also supply valuable assistance in the learning process. Of the purely educational aspects of a computer (as distinguished from its use as a machine which supplies answers to engineering problems) the following should be considered:

- a. Precise Definition. The computer is a rather rigid taskmaster which requires precision in the statement of the problem and its method of solution. Preparation of procedures for computer solution introduces the student to a precise formal language (usually a mixture of English and algebraic notation). Because of the nature of such languages, the student's communication skill should be enhanced, he should tend to be more accurate, and he should achieve added understanding of mathematical notation and manipulation.
- b. Logical Organization. Complex engineering problems require both an analytical ability (to subdivide the overall problem into simpler ones which can be handled more easily) and an ability to synthesize (bring together solutions of individual parts of the whole). The preparation of algorithms (problem solving procedures, flow diagrams) for a computer requires just such analysis and synthesis abilities.

This training in logical organization should be of value to the student in all of his work. The instructor may also benefit from such computer experiences, resulting in better organization of material and a better presentation of problem solutions, even when the computer is not involved. The engineering teacher must, of course, be aware that logical organization of a problem solution is not equivalent to correct formulation of the problem in the first place. Thus, one can produce a perfectly logical solution to a set of equations which, in fact, do not represent the physical situation under study. Certainly computer training does not lessen the importance of engineering fundamentals.

- c. Minimize Ambiguity. Because a computer solution requires the preparation of an orderly and detailed step-by-step procedure, the approach to the solution must be an unambiguous one (formal languages used by computers allow no ambiguity). No gaps in the logic are permitted.
- d. Recognition of Assumptions. During preparation of organized detailed procedures, assumptions which may be overlooked in a hand computation are frequently brought to the forefront. Of course, a bad assumption in a computer program has just as deleterious an effect as in a hand solution; however, because of the great computational speed, assumptions necessary to permit hand computation may often be removed entirely.
- e. Solution of the General Problem. Because of the nature of the digital computer, i.e., its ability to read parameter values as data, it is usually possible (with little extra effort) to produce a general program which will solve a whole class of problems rather than one specific problem with a single set of parameter values. This necessitates an essentially symbolic approach to problem solving and is rather different from the customary solution technique involving mostly numbers. Such an approach requires a more abstract analysis which focuses on problem structure, rather than on "slide rule" details.
- f. Problem Complexity. Because of high computational speed, the computer permits solution of significantly more complex (and hence, frequently more realistic) problems than can be "hand" solved. The drudgery of tedious repetitive calculations is removed. Unfortunately, it is usually wise, and indeed essential, to work at least one example problem in detail by hand for checkout purposes. However, for iterative procedures it may only be necessary to hand compute through the first two or three iterations to establish correctness of the algorithm.
- g. Numerical Solutions. The high speed computer solution permits numerical approximation of problems which are intractable analytically.
- h. Logical Non-Numeric Problems. Since the digital computer is in fact a symbol manipulator rather than a mere number manipulator, it can solve a large class of essentially non-numeric logical problems.

## V. THE ANALOG COMPUTER

For reasons of speed, economy, capacity and ability to solve an almost unlimited spectrum of problems, the digital computer has in recent years tended to overshadow the analog (differential analyzer) computer. The analog computer is a more specialized machine, particularly well suited for solving differential equations. Because differential equations can be used to describe so many chemical engineering phenomena and processes, its use should be included in any undergraduate chemical engineering program.

Consider the advantage of the differential analyzer for teaching purposes. It is an inexpensive device which may be operated directly by the student; programming of simple problems is very easy to learn, requiring a few hours at most; the output is presented instantly in graphical form. Mistakes may be promptly identified and corrected without the currently unavoidable turn-around delay time for large digital facilities; variations of parameters of the problem may be studied easily with suitable programming.

In addition to teaching advantages there are certain types of problems in which the analog computer may always be superior. Process simulation is the important one for chemical engineers. It is ideal for the illustration and study of control modes and process control, and for the study of process stability and the factors which affect it. In the Michigan curriculum the best course for analog use seems to be the process design course (CME 481). Another successful use has been in the senior laboratory course in which the experimental determination of unsteady-state fixed bed ion-exchange rates were correlated and the ion exchange process simulated by both analog and digital methods.

It is recognized that increasing complexity of problems tends to favor digital computation, and that the complicated and non-linear behavior of most chemical systems may require unrealistic simplifications in order to fit problems to analog equipment which we can afford, whereas the price paid in a digital solution may be primarily in computer time. Nevertheless, any chemical engineering department would do well to have and use at least one of the several small differential analyzers. Under the sponsorship of the National Science Foundation, Bernet Swanson and James Stice of the Illinois Institute of Technology have prepared an excellent report on the use of analog equipment in chemical engineering.<sup>4</sup>

## VI. COMPUTER APPLICATIONS IN THE DEPARTMENT

Chemical engineering is such an all-embracing subject that departments of chemical engineering can develop individual characteristics and personalities. The program at The University of Michigan might be described as a physical-chemical engineering program. Strong faculty interests have developed for research applications and engineering problems in physical chemistry, thermodynamics, and fluid dynamics. The use of computers in course work is largely in the application to solution or evaluation of analytical functions or equations, frequently by numerical

techniques. There has been little work involving either stochastic processes, or processes in which discrete operations or objects as opposed to continua are treated. However, there is growing interest, (and a new graduate course) in such subjects as queueing theory, searching, optimization, scheduling, linear programming, and disjoint processes which are susceptible to the concept of dynamic programming. These subjects, too, are beginning to appear in process design and increased awareness of these fields is expected.

The following is an account to date of the use of computers in the chemical engineering program.

### Required Courses

1. Introduction to Engineering Calculations (CME 200 - 3 credit hours)

This course may be elected as early as the second semester in the freshman year, at a time when students cannot yet be expected to have any computer programming ability. The student learns to analyze engineering problems and to solve them with the application of a few principles - the conservation principles and the first law of thermodynamics, stated formally. The problems are necessarily relatively short and the students learn to solve them under fairly close supervision. The combination of short problems and the need for immediate answers emphasizes the need for hand calculations rather than computer solutions.

In one early attempt to introduce computer work into the course the students were required to write the algorithm for computing the theoretical flame temperature of a combustion process with various fuel to air ratios, after attending four two-hour non-credit lectures on programming in the MAD language. Perhaps one-tenth of the class developed some proficiency in about fifteen hours of study. This experiment showed the desirability of separating the teaching of computer programming from engineering instruction. Since Math. 373, the computer course, is scheduled after this course, the introductory engineering course does not currently include problems for which computer solutions are required.

2. Thermodynamics I (CME 230 - 5 credit hours including a laboratory)

This course is usually elected when the student has had sufficient preparation in mathematics to elect the introductory computer course (Math. 373) at least concurrently.

Thermodynamics is a subject in which machine computation has been used and can be instructive. It seems advisable in some cases to supply workable programs to the students in order to reduce their time to that required for preparation of data and interpretation of results. Experience so far suggests that the best computer problems are those which require tedious, repetitive operations such as the calculation and tabulation of the thermodynamic properties from equations of state or from tabulations of generalized characteristics.

Two of the example problems shown later have been used in this course. No. 117, "Adiabatic Flame Temperature for Carbon Monoxide Oxidation," involves computation of adiabatic flame temperatures for various fuel to air ratios, and determination of the fuel-air mixture which produces the maximum flame temperature. No. 118, "Vapor-Liquid Equilibrium," involves the calculation of the complete vapor-liquid equilibrium composition diagram and of the temperature-composition diagram (at constant pressure) for the acetone-methanol

system based on three experimental vapor-liquid equilibrium concentration measurements taken in the laboratory part of the course. The complete composition diagrams are determined by computing the activity coefficients and using the Gibbs-Duhem and Margules equations. A trial and error (one of the root finding methods) procedure is required.

3. Rate Processes (CME 340 - 5 credit hours including a laboratory)

Much of the Rate Processes course deals with establishing and solving differential equations governing specific problems in the fields of momentum, heat and mass transfer, and reaction kinetics. Also, the associated laboratory is primarily concerned with the taking and correlating of rate data. Consequently, there is a wide variety of choice in the selection of computer problems for this course. One problem is assigned each semester, and the students may work individually or in pairs. Typical problems deal with longitudinal reactor calculations, unsteady and steady state heat conduction, and the processing of experimental data which would otherwise require tedious hand calculation.

The problem being used this semester is shown as example problem No. 116, "Pyrolysis of Ethane in a Tubular Reactor." It is solved by two different methods, one using a straightforward stepping procedure to solve the difference forms of the differential equations; the other uses the Runge-Kutta library subroutine to do the numerical integration. Example problem 120, "Dynamic Heat Exchange," has also been used in this course. It involves the unsteady state behavior of a single-tube, single-shell heat exchanger subjected to a time dependent inlet temperature function.

It is in this course that numerical methods of solution are first introduced into the sequence of courses offered by the Chemical Engineering Department. Whenever possible, numerical solutions are treated alongside the analytical solution to the same problem. The advantage of numerical methods is emphasized for those problems in which analytical solutions are either unknown or very complicated.

4. Separations Processes. (CME 339 - 3 credit hours including a laboratory)

There are numerous and obvious examples of the possibility for use of machine computation in this course. All of the equilibrium stage processes are taught with the awareness of the existence of the many generalized programs for solving problems in this area. However, the digital computer has not yet been used directly in this course. The election of the course by both chemical and metallurgical engineering students requires the inclusion of a wider scope (and hence a briefer treatment) of topics than customarily given to chemical engineers alone; the time available for classroom discussion and problems has been severely reduced by emphasis upon the laboratory.

The course has been in existence for only one year. In each semester, one short analog computer problem related to the separation achieved by the zone melting process has been assigned. The course has recently been changed by the addition of one credit hour and by limiting it to chemical engineering students. Use of the computer can be expected when these changes are effected. Example problem number 119, "Solvent Allocation in Multi-State Cross Current Extraction," is illustrative of the kind of problem which could be considered applicable to this area.

Elective Professional Courses

The elective courses are all in the area of engineering synthesis whereas the required courses are in the category of engineering analysis or science. The work in the professional group of courses includes recognition and formulation of the problem as well as its solution and presentation in a report form. The student, by now in his senior year, is presumed to be competent in the use of the principles of the pure and engineering sciences. He now practices application of the principles in practical engineering problems.

As a consequence, problems tend to be unique and each is attacked by a student in his own fashion. Use of the computer, either digital or analog, is permitted at all times. The extent of use by students varies; in some courses a specific assignment is made to insure that each student will have solved at least one comprehensive problem on the computer before his graduation. Most of the senior level students who have solved several simple and at least one such comprehensive problems feel that they are as competent in computer use as they are in any other specific area of their engineering training. There is little doubt that most students regard their computer work as useful; job interviewers are now familiar with such questions as "What kind of computer do you have?", "Are engineers permitted to do their own programming?", "What kind and how much expert assistance is available for computer work?", and so forth.

There are too many elective courses available to discuss in detail. The following discussion treats those in which machine computation has been successfully used.

1. Engineering Operations Laboratory (CME 460 - 3 credit hours)

The course is developing from the older unit operations laboratory into one with projects which require some originality by the student. Since the emphasis has been upon the value of direct experimental information, the computer has not been used extensively. However, a fixed-bed ion exchange experiment has been used in conjunction with solution of the equations for the unsteady-state process by digital, analog and hand methods.

2. Design of Process Equipment (CME 480 - 3 credit hours)

The problem which is fully described as example problem No. 122, "Economic Design of a Heat Exchanger," is used in this course. To allow students to examine thoroughly the parameters involved in creating an optimum design, the instructor has written several subroutines to do some of the tedious calculations. These routines produce results which are necessary for successful design but which would otherwise require an inordinately large amount of the student's time and divert his attention from the main design problem. The students seem to have a genuine feeling of satisfaction and accomplishment upon completion of the assignment.

3. Chemical Process Design (CME 481 - 3 credit hours)

Since the digital computer is used extensively in the equipment design course, an effort is made to show the utility of the analog computer in process analysis. The most suitable problems are in the field of process dynamics and control. The operation and control of a continuous stirred-tank reactor is a good example. It can be used to show such factors as the difficulties in the formulation of a mathematical model, the evaluation of errors

which arise from the assumptions necessary to fit the process to the available analog equipment, the different modes of control, and so forth. A two-hour lecture-demonstration with the computer and the descriptive pamphlet are usually sufficient to prepare a student for individual work in the formulation and solution of process models which can be expressed by linear differential equations with constant coefficients. Example problem No. 121, "Use of Computers in an Undergraduate Engineering Design Course," describes student solutions to two problems associated with the design of a benzene nitration process. A digital program was written to determine the equipment costs for the plant. A simulation of the nitrator under various control modes was investigated on the analog computer.

The computer can also be helpful in illustrating the use of some of the more powerful mathematical tools such as linear and dynamic programming.

### Graduate Instruction

Many students enter graduate school from other universities with no previous computer experience. They are expected to learn programming either by attending the extra-curricular eight-hour lecture series, by self-teaching, or by taking one of the courses. Since graduate students usually have well-developed interests and abilities focused on purely technical and scientific subjects, they learn computer programming readily and some become extremely proficient.

Only two courses are specifically required of graduate students: Rate Operations and Thermodynamics. In the former, at least two computer problems, one digital and one analog, are required. In the latter, usually one digital problem is assigned. A wide variety of problems is, of course, possible at the graduate level. One problem which has been used, "Adiabatic Reaction to Produce Methanol from Hydrogen and Carbon Monoxide," is shown as Example problem no. 114. It is not uncommon for instructors to be presented with complete computer solutions to problems in which use of the computer was not requested or even suggested.

The Heat Transfer Seminar (CM 840), in which usually only candidates for the doctorate are enrolled, has probably involved the computer solution of a larger number of different problems than any other course in the Department. During the semester, every student is required to present four papers to the class, each of which discusses in some depth a particular topic of interest in the field of heat transfer. Although it has not been the main purpose of the seminar to generate a series of computer problems, these papers have frequently dealt with situations whose governing equations are capable only of numerical solution. Consequently, the computer has made a significant contribution to the success of the seminar. In the last two years, the following topics have been among those leading to problems requiring numerical solution: radiant transfer in gas between parallel plates (integral equation), unsteady state conduction (involving moving freezing fronts), cross-flow heat exchanger, computation of view factors for radiant transfer, and the finite difference computation of natural convection at a vertical heated plate.



## Use of Computers in Chemical Engineering Education

A new graduate-senior level course covering numerical and computer oriented solutions to chemical engineering problems will be given for the first time in the spring semester, 1963. The problems, to be taken from any appropriate chemical engineering area, will illustrate the use of such techniques as numerical interpolation and approximation, numerical integration, elementary operations involving matrices, and numerical solution of linear and non-linear equations, ordinary and partial differential equations. Statistical and optimization procedures will also be discussed. Particular emphasis will be placed on the development and numerical solution of partial differential equations. Announcement of the course produced a substantial student response; twenty-five students have already elected to take the course.

### Research

The effect of large high-speed computers is most noticeable in graduate research. It is a rare doctoral thesis which does not have at least a regression analysis of the data. Any form of assistance has always resulted in the willingness of students to enlarge this scope of research effort, and computers are making as large a contribution to doctoral research as have methods of instrumental analysis.

The experience with the graduate students and the computer is revealing. The essential factor seems to be the presentation of the computer as an opportunity. There follows a development of individual capacities and interests. The individual responses vary from those who become so facile and competent that they are destined for a career as computer specialists to those who, having used machines, prefer to work in fields such as experimental research where the computer may be only a minor adjunct. Several recent experimental theses have involved considerable computer use, not only for data processing, but also to compare experimental results with those computed on the basis of assumed theoretical models.

### VII. EXAMPLE PROBLEMS

Several complete example problems solved on electronic computers have been prepared by departmental faculty and by chemical engineering faculty from other universities who have participated in the faculty training programs of the Project on the Use of Computers in Engineering Education at The University of Michigan. Table I3 lists the problem titles and authors of those problems which are included here. Both digital and analog solutions are presented. Most of the digital programs are written in the MAD (Michigan Algorithm Decoder) language<sup>3</sup>, and have been solved on the IBM 704, 709, or 7090 computers; one is written in the ACT III language for the LGP-30 digital computer.

Problems 114, 116, 117, 118, 120, 121, and 122 have been used for homework assignments in Departmental courses at The University of Michigan. The others have not been used at Michigan, but are thought to be suitable for classroom assignments.

These problems may be considered as a supplement to the 111 example engineering problems previously published by the Project. Others which may be of special interest are problems 1, 6, 7, 12, 18, 19, 20, 41, and 44, in the First Annual Report and numbers 52 and 54 in the Second Annual Report.

TABLE I3  
List of Example Problems

<u>Number</u>	<u>Title</u>	<u>Author</u>	<u>Page</u>
112	Temperatures and Heat Flux in a Radiant Thermal Circuit	W. C. Phelps	I17
113	Minimum Cost of Reactor Operation	A. I. Johnson	I21
114	Adiabatic Reactor	R. E. Balzhiser	I25
115	Successive and Simultaneous First Order Chemical Reactions	R. N. Pease	I32
116	Pyrolysis of Ethane in a Tubular Reactor	J. O. Wilkes	I39
117	Adiabatic Flame Temperature for Carbon Monoxide Oxidation	B. Carnahan and J. J. Martin	I49
118	Vapor-Liquid Equilibrium	R. Bonnacaze	I65
119	Solvent Allocation in Multi-Stage Cross-Current Extraction	A. O. Converse	I75
120	Dynamic Heat Exchange	J. Famularo	I84
121	Use of Computers in an Undergraduate Chemical Engineering Design Course	D. F. Rudd	I96
122	Economic Design of a Condenser	D. E. Briggs	I117

#### VIII. REFERENCES

1. Electronic Computers in Engineering Education, First Annual Report of Project on Use of Computers in Engineering Education, The Univ. of Mich., Ann Arbor, August 26, 1960.
2. Use of Computers in Engineering Education, Second Annual Report of Project on Use of Computers in Engineering Education, The Univ. of Mich., Ann Arbor, December 15, 1961.
3. A Computer Primer for the MAD Language, Organick, E. I., 1962.
4. Theory and Applications of Electronic Analog Computers, Stice, James A., and Bernet F. Swanson, Dept. of Chem. Engr., Illinois Inst. of Technology, 1961.

Example Problem No. 112

TEMPERATURES AND HEAT FLUX IN A RADIANT THERMAL CIRCUIT

by

W. C. Phelps

School of Metallurgical Engineering

Purdue University

Course: Heat Transfer and Fluid Flow

Credit hours: 2

Level: Sophomore

Statement of Problem

Write a MAD program which determines the heat flux and temperatures of radiation shields in a thermal circuit in which heat transfer is by radiation alone. The source of heat is separated from the heat sink by a series of parallel radiation shields which are thin and closely spaced. Data to be used include temperatures of the heat source and heat sink, properties of the materials and surface condition of the thermal elements, i.e., the total thermal emissivity of each.

The program should be written to deal with up to ten radiation shields of not necessarily the same emissivity. The program should be tested using the following data.

Number of Shields: 5

Composition of Source: Graphite (emissivity 0.850)

Composition of Shields 1, 2, and 3: Platinum (emissivity 0.126)

Composition of Shields 4 and 5: Aluminum (emissivity 0.050)

Composition of Sink: Rolled Sheet Steel (emissivity 0.660)

Temperature of Source: 2600° R.

Temperature of Sink: 500° R.

Solution

The radiant heat flux between two adjacent thermal elements (elements k and k-1) is given by

$$\frac{q}{A} = 0.173 F_{k-1,k} \left[ \left( \frac{T_{k-1}}{100} \right)^4 - \left( \frac{T_k}{100} \right)^4 \right], \quad (1)$$

where  $F_{k-1,k}$  is a factor which represents the geometrical relationship between the two surfaces and the effect of their thermal emissivities and absorptivities. In this case,

$$F_{k-1,k} = \frac{1}{\frac{1}{\epsilon_{k-1}} + \frac{1}{\epsilon_k} - 1} \quad (2)$$

Since the heat flux must be the same between each successive pair of elements, it can be shown that

Temperatures and Heat Flux in a Radiant Thermal Circuit

$$\frac{q}{A} = \frac{0.173 \left[ \left( \frac{T_0}{100} \right)^4 - \left( \frac{T_{n+1}}{100} \right)^4 \right]}{\frac{1}{\epsilon_0} + \frac{2}{\epsilon_1} + \frac{2}{\epsilon_2} + \dots + \frac{2}{\epsilon_n} + \frac{1}{\epsilon_{n+1}} - n-1} \quad (3)$$

Once the heat flux is obtained, the temperature of the  $k$  th radiation shield can be calculated by rearranging Equation 1:

$$T_k = 100 \left[ \left( \frac{T_{k-1}}{100} \right)^4 - \frac{q/A}{0.173} \left( \frac{1}{\epsilon_{k-1}} + \frac{1}{\epsilon_k} - 1 \right) \right]^{1/4} \quad (4)$$

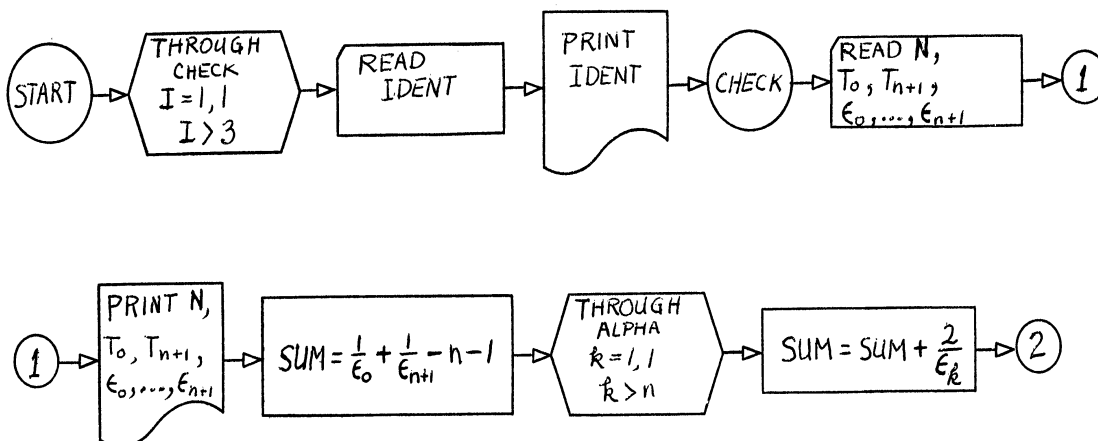
By starting with the known temperature of the heat source (the zeroth thermal element), this equation can be used to determine the temperatures of successive radiation shields. In any procedure of this type it is advisable to compute the temperature of the heat sink (the  $(n+1)$ st element as a check. This check has been included in the program.

A discussion of the theory is given in Reference 1.

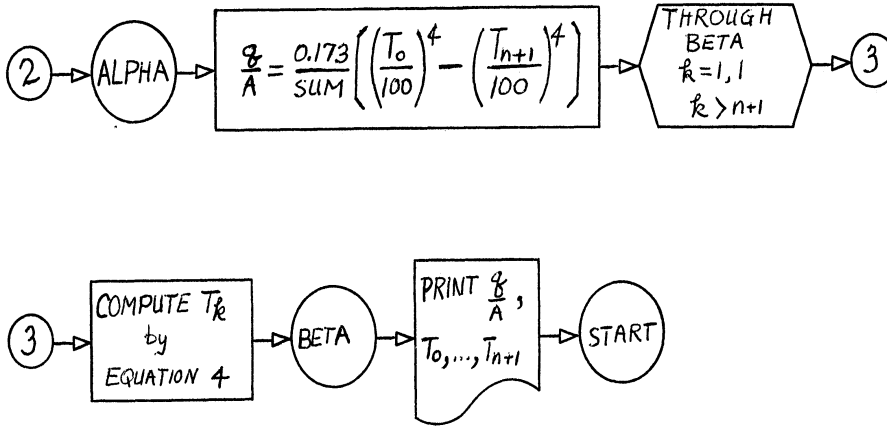
List of Symbols

<u>Problem variable</u>	<u>MAD Program variable</u>	<u>Definition and Units</u>
$n$	$N$	Number of radiation shields, up to ten.
$\frac{q}{A}$	$RADFLX$	Heat flux, BTU per hour per sq. ft.
$T_0$	$T(O)$	Temperature of the heat source, °R.
$T_k$	$T(K)$	Temperature of $k$ th radiation shield, °R.
$T_{n+1}$	$T(N+1)$	Temperature of the heat sink, °R.
$\epsilon_0$	$E(O)$	Total thermal emissivity of the heat source.
$\epsilon_k$	$E(K)$	Total thermal emissivity of the $k$ th radiation shield.
$\epsilon_{n+1}$	$E(N+1)$	Total thermal emissivity of the heat sink.

Flow Diagram



Flow Diagram (continued)



MAD Program and Data

```

WILLIAM PHELPS          D041N          0 2  002  020      RAD 000
WILLIAM PHELPS          D041N          0 2  002  020      RAD 000
$COMPILE MAD, PRINT OBJECT, EXECUTE, DUMP
R
R   THIS PROGRAM COMPUTES THE TEMPERATURES OF INDIVIDUAL
RRADIATION SHIELDS AND THE HEAT FLUX IN A THERMAL CIRCUIT.....
R
R   DIMENSION T(20), E(20)
R   INTEGER I,K,N
START THROUGH CHECK, FOR I=1,1,I.G.3
CHECK READ FORMAT IDENT
PRINT FORMAT IDENT
VECTOR VALUES IDENT =$72H
1
1   READ FORMAT DATA,N,T(0),T(N+1),E(0)...E(N+1)
VECTOR VALUES DATA=$I2,S2,2F6.1,10F5.3/12F5.3*$
PRINT FORMAT ECHO,N,T(0),T(N+1),E(0)...E(N+1)
VECTOR VALUES ECHO=$1H0,I2,S2,F6.1,S2,F6.1,12(S1,F4.3)*$
SUM=1./E(0)+1./E(N+1)-N-1.
THROUGH ALPHA, FOR K=1,1,K.G.N
ALPHA SUM=SUM+2./E(K)
RADFLX=0.173*((T(0)/100.)4-(T(N+1)/100.)4)/SUM
THROUGH BETA, FOR K=1,1,K.G.N+1
BETA T(K)=100.*SQRT.(SQRT.(((T(K-1)/100.)4-RADFLX/0.173*(1./
1E(K-1)+1./E(K)-1.)))
PRINT FORMAT RESULT,RADFLX,T(0)...T(N+1)
VECTOR VALUES RESULT=$1H ,18HRDIANT HEAT FLUX=F10.2,S2,
115HBTU PER HR-SQFT//68H0ABSOLUTE TEMPERATURES OF THE THERMAL
2ELEMENTS, FROM THE HEAT SOURCE,/40H THROUGH THE HEAT SINK, RE
3SPECTIVELY..../1H0,12(F6.1,S2)*$
TRANSFER TO START
END OF PROGRAM

$DATA
1 W C PHELPS AUG 15, 1961 RADIANT HEAT TRANSFER FROM A GRAPHITE HEAT
SOURCE, THROUGH THREE PLATINUM AND TWO ALUMINUM RADIATION SHIELDS, TO A
ROLLED SHEET STEEL HEAT SINK.
5 2600. 500. .850 .126 .126 .126 .050 .050 .660
  
```

Temperatures and Heat Flux in a Radiant Thermal Circuit

Computer Output

W C PHELPS AUG 15, 1961 RADIANT HEAT TRANSFER FROM A GRAPHITE HEAT SOURCE, THROUGH THREE PLATINUM AND TWO ALUMINUM RADIATION SHIELDS, TO A ROLLED SHEET STEEL HEAT SINK.

5 2600.0 500.0 .850 .126 .126 .126 .050 .050 .660

RADIANT HEAT FLUX= 635.09 BTU PER HR-SQFT

ABSOLUTE TEMPERATURES OF THE THERMAL ELEMENTS, FROM THE HEAT SOURCE THROUGH THE HEAT SINK, RESPECTIVELY.....

2600.0 2556.6 2470.6 2374.7 2163.5 1660.0 499.9

Discussion of Results

Note that for the particular set of data chosen the temperature of the hottest aluminum radiation shield is above its melting point.

Critique

This problem is a very simple one and is easily programmed. It should serve as a good introductory problem for students learning to use the computer. Since the problem can be solved by hand, it is not difficult to check the computer program.

Reference

1. Schuhmann, Metallurgical Engineering, Volume I, Principles, Addison-Wesley. (1952)  
Chapter 7.

Example Problem No. 113

MINIMUM COST OF REACTOR OPERATION

by

A. I. Johnson

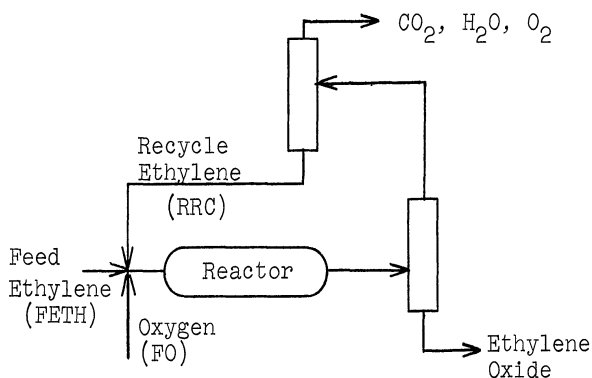
Department of Chemical Engineering

McMaster University

Course: Introductory Chemical Engineering      Credit Hours: 3      Level: Sophomore

Statement of Problem

Ethylene is converted to ethylene oxide using pure oxygen by the scheme shown at the right. The number of moles,  $M$ , of ethylene oxide produced per 100 moles of ethylene fed to the reactor as a function of feed concentration,  $C$  (mole percent ethylene in the feed to the reactor), and temperature,  $T$ , is given by:



$$M(C,T) = (30.4 + 0.2025C - 0.007375C^2)(-3.56 + 0.0357T - 0.00007T^2) \quad (1)$$

In addition, it is found that the activity of the reactor is decreased by the presence of impurity in the recycle and values of  $M$  given by equation (1) should be multiplied by

$$CF = 1 - \frac{RRC}{20,000} \quad (2)$$

where RRC is the moles of recycle per day.

The cost of oxygen is \$1.00 per lb.mole, of feed ethylene is \$2.00 per mole and of recycle ethylene, \$1.00 per mole. You are to determine the most suitable recycle rate, mole percent ethylene in the feed, and reactor temperature for a plant producing 20 tons of ethylene oxide per day.

- Notes: 1. This problem has been adapted from one in Money and the Chemical Engineer, by Osborn and Kammermeyer.
2. This problem would be more realistic and interesting if the information given by equations (1) and (2) were supplied to the students in tabular form.

Solution

The flow diagram below outlines a method for searching for a minimum cost starting from arbitrary values of recycle rate, composition of feed to the reactor, and temperature.

Using a random number generator (the subroutine RAM2B.) to produce three random numbers, the three variables are changed simultaneously ten times, and costs for each set are tabulated;

## Minimum Cost of Reactor Operation

this table also includes the cost at the starting point. The values of the variables at the minimum cost in this table are then used as the starting values for the next set of ten trials. This is repeated until there is essentially no further improvement in minimum cost (determined by tolerance EPSI).

### Table of Symbols

C	Mole percent ethylene in feed (dummy variable for COST. subroutine).
COST.	Subroutine to determine cost, given arguments RRC, C, T.
CCOST	Array for storing the minimum cost for the Kth trial set.
DM*	Maximum possible variation in MPCER during the Kth trial set.
DR*	Maximum possible variation in RETH during the Kth trial set.
DT*	Maximum possible variation in TEMP during the Kth trial set.
EPSI	A tolerance. Used for terminating the optimization procedure. When the improvement in minimum cost between the Kth and the K-1th trial set is less than EPSI.
FETH	New ethylene feed rate.
FO	Oxygen feed rate (moles).
J	Subscript corresponding to the set of parameter values associated with MIN, i.e., RRETH(J), etc.
K	A counter on the number of trial sets.
M.	Internal function to determine the moles of ethylene oxide produced per hundred moles of ethylene feed, given arguments C and T.
MIN	The minimum of the generated set of ten NCOST values.
NCOST	Array for storing cost values for the ten sets of trial parameter values in the arrays RRETH, MMP CER, TTEMP.
MMP CER	Array for ten trial values of MPCER.
MPCER	Best mole percent ethylene in feed (main program), during Kth trial set.
R	A random number. $0.0 \leq R \leq 1.0$
RAM2B.	Subroutine which generates random numbers.
RETH	Best recycle ethylene rate (main program), during Kth trial set.
RRC	Recycle ethylene rate (dummy variable for COST. subroutine).
RRETH	Array for ten trial values of RETH.
T	Reactor temperature (dummy variable for COST. subroutine).
TEMP	Best reactor temperature (main program), during Kth trial set.
TTEMP	Array for ten trial values of TEMP.

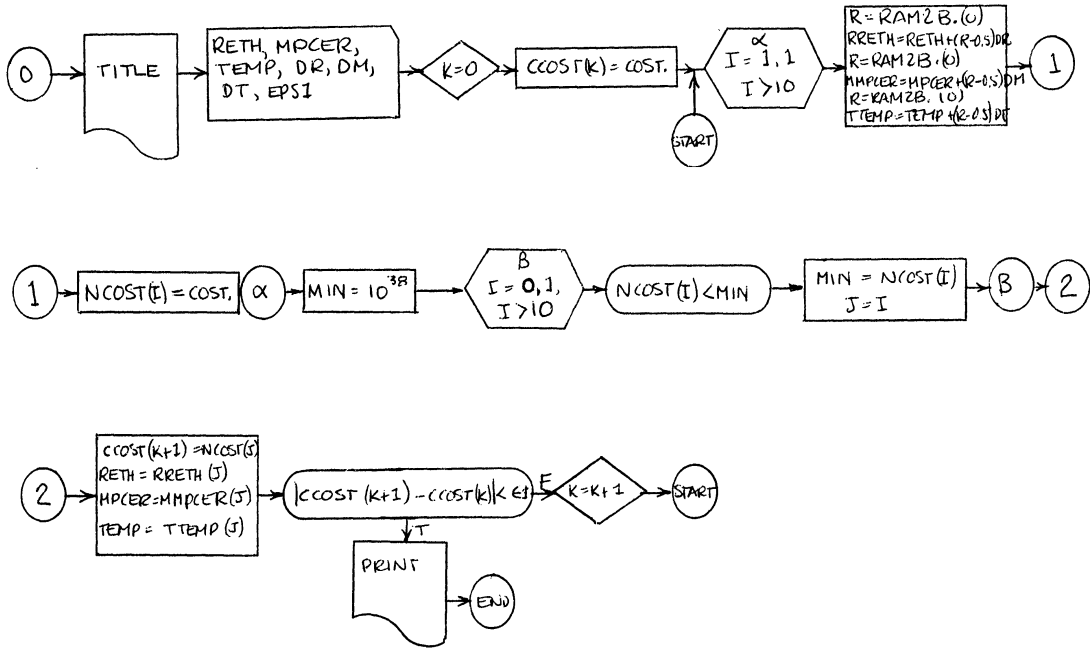
---

\* Actual variation is determined by the random number, R.



Example Problem No. 113

Flow Diagram



MAD Program and Data

```

PRINT FORMAT TITLE
DIMENSION CCOST(500),RRETH(10),MMP CER(10),TTEMP(10),
INCCOST(10)
INTEGER I,J,K, MA
READ DATA
READ FORMAT DATA,RETH,MPCER,TEMP,DR,DM,DT,EPS1
PRINT FORMAT UDATA,RETH,MPCER,TEMP,DR,DM,DT,EPS1
K=0
CCOST(K)=CCOST.(RETH,MPCER,TEMP)
START
RRETH(0) = RETH
MMP CER(0) = MPCER
TTEMP(0) = TEMP
THROUGH ALPHA, FOR I=1,1,I.G.10
R=RAM2B.(0)
RRETH(I)=RETH+(R-0.5)*DR
R=RAM2B.(0)
MMP CER(I)=MPCER+(R-0.5)*DM
R=RAM2B.(0)
TTEMP(I)=TEMP+(R-0.5)*DT
ALPHA
NCCOST(I)=CCSI.(RRETH(I),MMP CER(I),TTEMP(I))
NCCOST(0)=CCOST(K)
MIN=1.E38
THROUGH BETA, FOR I=0,1,I.G.10
WHENEVER NCCOST(I).L.MIN
MIN=NCCOST(I)
J=I
BETA
END OF CONDITIONAL
CCOST(K+1)=NCCOST(J)
RETH=RRETH(J)
MPCER=MMP CER(J)
TEMP=TTEMP(J)
WHENEVER .ABS.(CCOST(K+1)-CCOST(K)).L.EPS1
PRINT FORMAT OUT,CCOST(K+1),RETH,MPCER,TEMP
PRINT FORMAT NUM,K
TRANSFER TO END
OTHERWISE
K=K+1
TRANSFER TO START
END OF CONDITIONAL
    
```

Minimum Cost of Reactor Operation

MAD Program and Data (continued)

```

VECTOR VALUES TITLE=$1H1,24H OPTIMIZATION OF REACTOR*$
VECTOR VALUES DATA=$7F10,2*$
VECTOR VALUES DDATA=$1H0,7F10,2*$
VECTOR VALUES OUT=$1H0,16H MINIMUM COST OF,F10,2,/28H OCCURRE
1D AT RECYCLE RATE OF,F10,2,/22H FEED CONCENTRATION OF,F10,2,/
219H AND TEMPERATURE OF,F10,2*$
VECTOR VALUES NUM=$1H0,21H NUMBER OF TRIALS WAS,12*$
END
END OF PROGRAM

$COMPILE MAD, PRINT OBJECT
EXTERNAL FUNCTION(RRC,C,T)
ENTRY TO COST.
INTERNAL FUNCTION M.(C,T)=(30.4+0.2025*C
1-0.007375*C.P.2)*(-3.56+ .0357*T-0.00007*T.P.2)
CF=1.- RRC/20000.
TETH=91000./(M.(C,T)*CF)
FO=TETH*(100.-C)/C
FETH=TETH-RRC
COSTT=1.0*FO+2.0*FETH+1. *RRC
FUNCTION RETURN COSTT
END OF FUNCTION

$DATA
2000.    40.    240.    50.    5.    20.    50.

```

Computer Output

```

OPTIMIZATION OF REACTOR
2000.00    40.00    240.00    50.00    5.00    20.00    50.00

MINIMUM COST OF 11293.55
OCCURRED AT RECYCLE RATE OF 2059.74
FEED CONCENTRATION OF 42.37
AND TEMPERATURE OF 254.96

NUMBER OF TRIALS WAS 51

```

Critique

The technique suggested in this problem is easily programmed and does not require much machine time. It should be applicable to a large number of independent variables. It is unfortunate that there was not more time available to make a thorough investigation of the method. In particular the value of EPSI = \$50 should be reduced.

Editor's Note: It would probably be wise to decrease the magnitudes of DR, DM, and DT as the procedure continues, i.e., to narrow the band of permitted variations as the estimates of RETH, MPCER and TEMP are improved. The criterion for termination, namely that the lowest cost value found at the randomly selected 10 operating points inside the space DR·DM·DT with geometric center at RETH, MPCER, TEMP show only minimal improvement (EPSI) over the previous best value is probably inadequate, particularly if DR, DM, and DT are still significant fractions of RETH, MPCER, and TEMP. As with most extrema-finding procedures there is no guarantee that the minimum will be found, only that the method will find successive improvements while heading toward a local minimum. (B.C.)

Example Problem No. 114

ADIABATIC REACTOR

by

R. E. Balzhiser

Department of Chemical Engineering

The University of Michigan

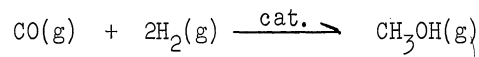
Course: Engineering Thermodynamics

Credit hours: 3

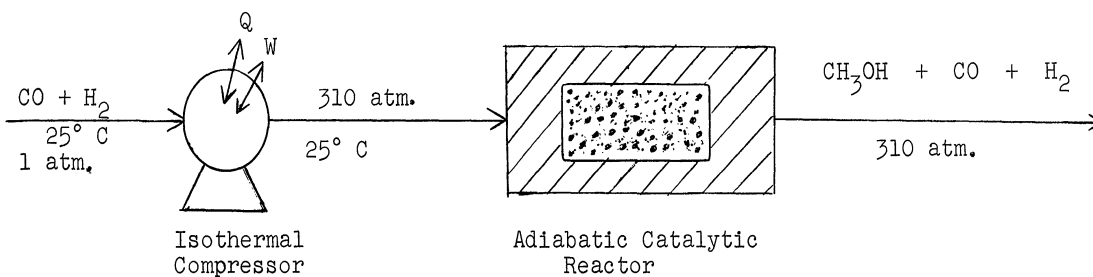
Level: Graduate

Statement of Problem

A plant produces methanol from hydrogen and carbon monoxide. In the process, stoichiometric proportions of CO and H<sub>2</sub> are compressed isothermally and reversibly at 25°C from 1 atmosphere to 310 atmospheres. The compressor discharges the gas continuously to a well-insulated catalytic reactor where the following reaction takes place:



The methanol leaving the reactor is in equilibrium with the CO and H<sub>2</sub> in the stream. There is negligible pressure drop across the reactor. The process is illustrated in the diagram below.



1. Calculate the work done by the compressor in calories per gram-mole of carbon monoxide fed. Also determine on the same basis the amount of heat transferred to the surroundings from the compressor. (Not required as part of computer solution.)
2. What is the per cent conversion of carbon monoxide to methanol?
3. What is the temperature of the exit stream from the reactor?

The following information is to be used.

For methanol at  $P_r = 3.94$  (P = 310 atm.)

Adiabatic Reactor

$$\ln \left( \frac{H^* - H}{T_C} \right) = 3.15 - 0.7 T_r^2$$

$$\ln \left( \frac{f}{P} \right) = -0.43 + \frac{2.46}{T_r} - \frac{3.36}{T_r^2}$$

C<sub>p</sub> at 1 atmosphere      cal/gm-mole-°K

CO(g)                      6.60 + .0012 T

H<sub>2</sub>(g)                      6.62 + .00081 T

CH<sub>3</sub>OH(g)                3.53 + .0256 T

ΔH° (Heat of formation from the elements; standard state of 1 atmosphere and 25°C)

CO(g)                      -26,420 cal/gm-mole

CH<sub>3</sub>OH(g)                -48,080 cal/gm-mole

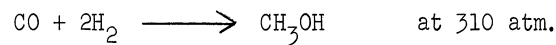
ΔG° (Free energy of formation from the elements; standard state of 1 atmosphere and 25°C)

CO(g)                      -32,808 cal/gm-mole

CH<sub>3</sub>OH(g)                -38,620 cal/gm-mole

<u>Critical Constants</u>	<u>T<sub>c</sub> °K</u>	<u>P<sub>c</sub> atm.</u>
CO	134	35
H <sub>2</sub>	33	12.8
CH <sub>2</sub> OH	513	78.7

Solution



Find conversion and final temperature if reaction proceeds adiabatically.

$$K_a = \frac{a_{\text{CH}_3\text{OH}}}{a_{\text{CO}} a_{\text{H}_2}^2} = \frac{[y(\frac{f}{P})]_{\text{CH}_3\text{OH}}}{[y(\frac{f}{P})]_{\text{CO}} [y(\frac{f}{P})]_{\text{H}_2}^2}$$

where standard states are the pure gases at 1 atmosphere and equilibrium temperature.

At 310 atmospheres ( $\frac{f}{P}$ ) for H<sub>2</sub> and CO ≈ 1.0.

Example Problem No. 114

ADIABATIC REACTOR

by

R. E. Balzhiser

Department of Chemical Engineering

The University of Michigan

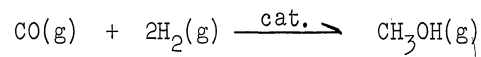
Course: Engineering Thermodynamics

Credit hours: 3

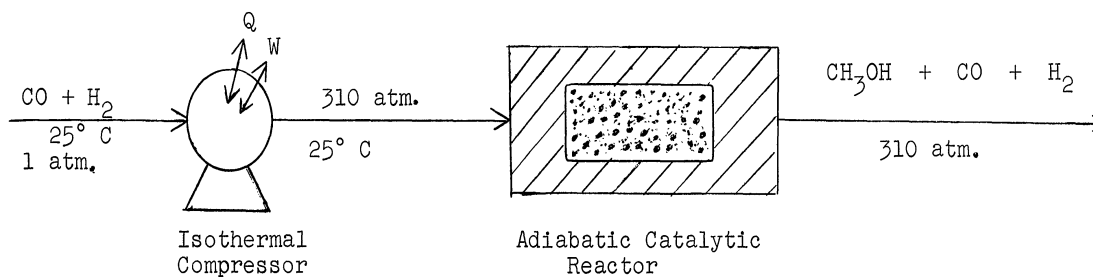
Level: Graduate

Statement of Problem

A plant produces methanol from hydrogen and carbon monoxide. In the process, stoichiometric proportions of CO and H<sub>2</sub> are compressed isothermally and reversibly at 25°C from 1 atmosphere to 310 atmospheres. The compressor discharges the gas continuously to a well-insulated catalytic reactor where the following reaction takes place:



The methanol leaving the reactor is in equilibrium with the CO and H<sub>2</sub> in the stream. There is negligible pressure drop across the reactor. The process is illustrated in the diagram below.



1. Calculate the work done by the compressor in calories per gram-mole of carbon monoxide fed. Also determine on the same basis the amount of heat transferred to the surroundings from the compressor. (Not required as part of computer solution.)
2. What is the per cent conversion of carbon monoxide to methanol?
3. What is the temperature of the exit stream from the reactor?

The following information is to be used.

For methanol at  $P_r = 3.94$  (P = 310 atm.)

Adiabatic Reactor

$$\ln \left( \frac{H^* - H}{T_c} \right) = 3.15 - 0.7 T_r^2$$

$$\ln \left( \frac{f}{P} \right) = -0.43 + \frac{2.46}{T_r} - \frac{3.36}{T_r^2}$$

C<sub>p</sub> at 1 atmosphere      cal/gm-mole-°K

CO(g)                      6.60 + .0012 T

H<sub>2</sub>(g)                      6.62 + .00081 T

CH<sub>3</sub>OH(g)                3.53 + .0256 T

ΔH° (Heat of formation from the elements; standard state of 1 atmosphere and 25°C)

CO(g)                      -26,420 cal/gm-mole

CH<sub>3</sub>OH(g)                -48,080 cal/gm-mole

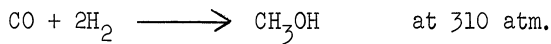
ΔG° (Free energy of formation from the elements; standard state of 1 atmosphere and 25°C)

CO(g)                      -32,808 cal/gm-mole

CH<sub>3</sub>OH(g)                -38,620 cal/gm-mole

<u>Critical Constants</u>	<u>T<sub>c</sub> °K</u>	<u>P<sub>c</sub> atm.</u>
CO	134	35
H <sub>2</sub>	33	12.8
CH <sub>2</sub> OH	513	78.7

Solution



Find conversion and final temperature if reaction proceeds adiabatically.

$$K_a = \frac{a_{\text{CH}_3\text{OH}}}{a_{\text{CO}} a_{\text{H}_2}^2} = \frac{[y(\frac{f}{P})]_{\text{CH}_3\text{OH}}}{[y(\frac{f}{P})]_{\text{CO}} [y(\frac{f}{P})]_{\text{H}_2}^2}$$

where standard states are the pure gases at 1 atmosphere and equilibrium temperature.

At 310 atmospheres ( $\frac{f}{P}$ ) for H<sub>2</sub> and CO  $\cong$  1.0.

Example Problem No. 114

For  $\text{CH}_3\text{OH}$  at 310 atmospheres the following relationship expresses  $\left(\frac{f}{P}\right)$  as a function of  $T_r$ :

$$\ln \left(\frac{f}{P}\right) = -0.43 + \frac{2.46}{T_r} - \frac{3.36}{T_r^2} \quad (1)$$

Incorporating the reaction stoichiometry to eliminate the mole fractions in the above expression for  $K_a$ , yields the following values in terms of the conversion,  $x$ .

Considering 1 mole CO and 2 moles  $\text{H}_2$  entering

	IN	OUT	$y$
CO	1	1-x	$(1-x)/(3-2x)$
$\text{H}_2$	2	2-2x	$(2-2x)/(3-2x)$
$\text{CH}_3\text{OH}$	1	$\frac{x}{3-2x}$	$x/(3-2x)$

where  $x$  = moles  $\text{CH}_3\text{OH}$  produced/mole CO fed.

$$\therefore K_a = \frac{x \left(\frac{f}{P}\right)_{\text{CH}_3\text{OH}} \cdot (3-2x)^2}{(1-x)^3 \cdot 4 \cdot P^2} \quad (2)$$

$$\int_{\ln K_{a,298}}^{\ln K_{a,T}} d[\ln K_a] = \int_{298}^T \frac{\Delta H^\circ}{RT^2} dT$$

$$\Delta H_T^\circ = -21,660 + \int_{298}^T [-16.31 + 0.0226 T] dT$$

$$= 0.0113 T^2 - 16.3 T - 17,805$$

$$\ln K_{a,T} = 0.00568T - 8.2 \ln T + \frac{8,970}{T} + 24.8 \quad (3)$$

For adiabatic reaction,  $Q = 0$ .  $\therefore \Delta H = 0$

or  $H_{\text{products}} = H_{\text{reactants}}$

(a)  $\Delta H_a$  for reactants at 298°K in going from 310 atm. to 1 atm. equals approximately zero.

(b)  $\Delta H_b$  for reaction at 1 atm. and 298°K is equal to -21,660 x per mole of CO fed.

(c)  $\Delta H_c$  for isobaric increase of temperature from 298°K to equilibrium temperature  $T$ :

$$\Delta H_c = x \int_{298}^T (3.53 + 0.0256T) dT + (1-x) \int_{298}^T (6.60 + 0.0012T) dT$$

$$+ (2-2x) \int_{298}^T (6.62 + 0.00081 T) dT$$

Adiabatic Reactor

$$\Delta H_c = (19.84 - 16.31x)T + (0.0113 x + 0.0014)T^2 - 298 (19.84 - 16.31 x) - (0.0113 x + 0.0014)298^2$$

- (d)  $\Delta H_d$  for increasing pressure from 1 atm. to 310 atm. at temperature T: Enthalpy corrections for both CO and H<sub>2</sub> with pressure changes are negligible.

For CH<sub>3</sub>OH at 310 atm.

$$\ln \left( \frac{H^*-H}{T_C} \right) = 3.15 - 0.7 T_r^2 \quad (4)$$

$$\therefore \Delta H_d = -x \left( \frac{H^*-H}{T_C} \right) T_C$$

$$\Delta H = 0 = -21,660 x - 16.31 x T + 0.0113 x T^2 + (298)(16.31)x - (0.0113)(298)^2 x - \left( \frac{H^*-H}{T_C} \right) T_C x + 19.84 T + 0.0014 T^2 - 298(19.84) - (0.0014)(298)^2$$

$$x = \frac{0.0014 T^2 + 19.84T - 6.044}{17,800 + 16.31 T - 0.0113 T^2 + \left( \frac{H^*-H}{T_C} \right) T_C} \quad (5)$$

Table of Symbols

<u>MAD Program</u>	<u>Problem Description</u>	<u>Meaning</u>
	C <sub>p</sub>	Heat capacity at constant pressure.
COMP		<u>±1.0</u> , determines the sign of DELT
DELT	ΔT	Increment in assumed temperature.
ENTH	(H*-H)/T <sub>C</sub>	Enthalpy function.
	f	Fugacity.
FUG	(f/P)	Fugacity coefficient.
	ΔG <sup>o</sup>	Free energy of formation, @ 1 atm., 25°C.
	H	Enthalpy at pressure P and temperature T.
	H*	Enthalpy at pressure P=0 and temperature T.
	ΔH <sup>o</sup>	Heat of formation, @ 1 atm., 25°C.
I		Counter on the number of iterations.
KT	K <sub>a,T</sub>	Equilibrium constant at assumed temperature T.
KX		Equilibrium constant based on conversion, x, computed from heat balance.

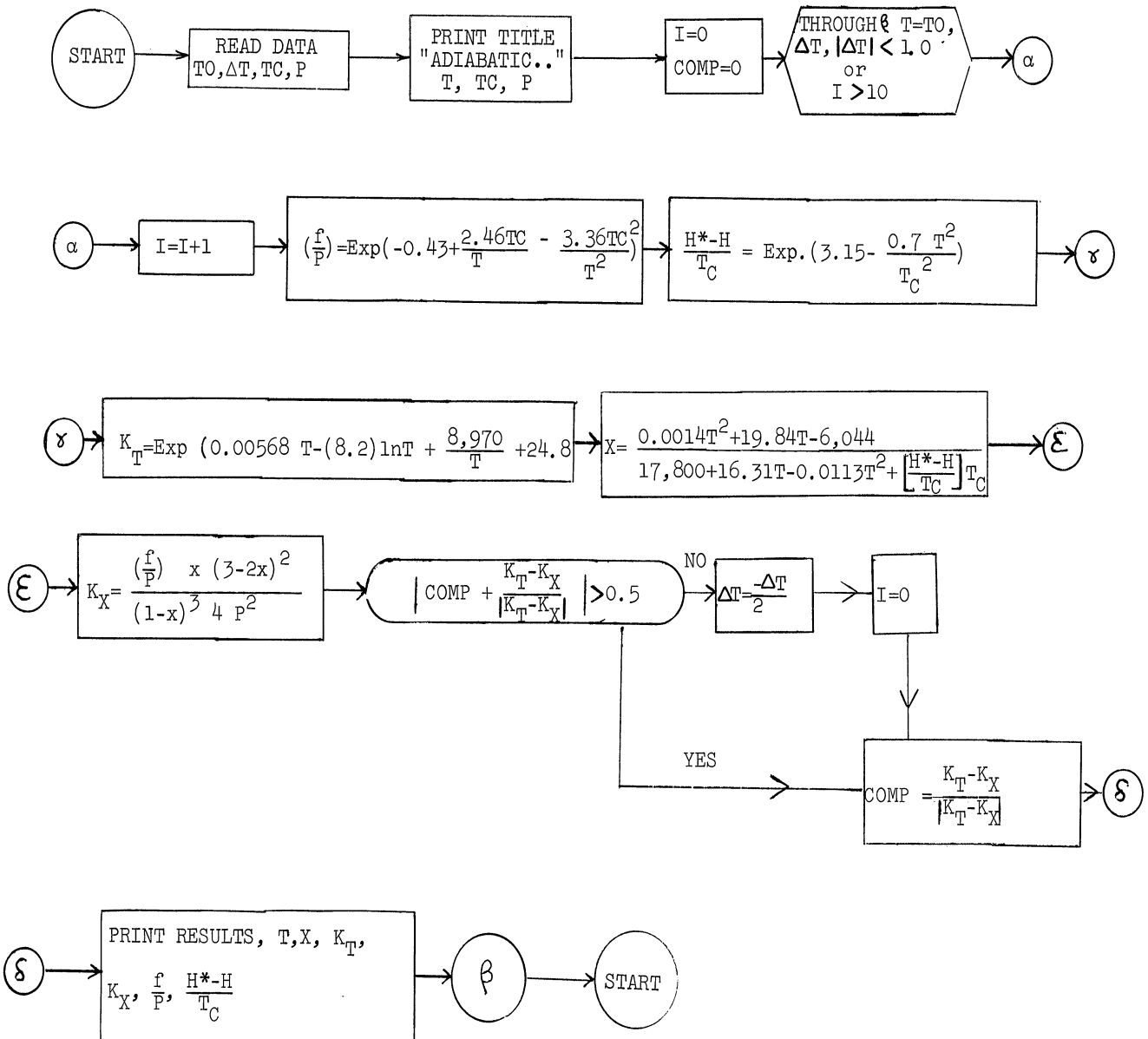


Example Problem No. 114

Table of Symbols, Continued

MAD Program	Problem Description	Meaning
P	P	Pressure.
	$P_r$	Reduced pressure, $P/P_c$ .
T	T	Assumed temperature.
TC	$T_c$	Critical temperature.
TO		Assumed value for T in the first iteration.
X	x	Moles of $CH_3OH$ produced per mole of CO fed.

Flow Diagram



Adiabatic Reactor

MAD Program and Data

```

R. E. BALZHISER          T26-N 2          0 5  010  030
$COMPILE MAD, PRINT OBJECT, EXECUTE, DUMP
START  READ FORMAT DATA,TO,DELT,TC,P
        PRINT FORMAT TITLE,TO,DELT,TC,P
        PRINT COMMENT $ $
        INTEGER I
        I=0
        COMP=0
        THROUGH BETA, FOR T=TO, DELT, .ABS. DELT.L.1 .OR. 1.G.10
        I=I+1
        FUG=EXP.(-0.43+(2.46*TC)/T-(3.36*TC.P.2)/T.P.2)
        ENTH=EXP.(3.15-(0.7*T.P.2.)/TC.P.2.)
        KT=EXP.(0.00568*T-8.2*ELOG.(T)+8970./T+24.8)
        X=(0.0014*T.P.2.+19.84*T-6044.)/(17800.+16.31*T-0.0113*T.P.2.
1+ENTH*TC)
        KX=(FUG*X*(3.0-2.0*X).P.2.)/((1.0-X).P.3*4.0*P.P.2.)
        WHENEVER .ABS.(COMP+((KT-KX)/.ABS.(KT-KX))) .G. 0.5,
1TRANSFER TO ALPHA
        DELT--(DELT/2.)
        I=0
ALPHA  COMP =(KT-KX)/.ABS.(KT-KX)
BETA   PRINT FORMAT RESULT,T,X
        TRANSFER TO START
        VECTOR VALUES DATA=$4F10.4*$
        VECTOR VALUES TITLE=$1H1,S10,17HADIABATIC REACTOR,S6,6HCM 211
1//1H ,4F10.4*$
        VECTOR VALUES RESULT =$S5,6HTEMP =F10.4,S10,12HCONVERSION =F9
1.6*$
        END OF PROGRAM
$DATA
298.0      100.0      513.0      310.0
    
```

Computer Output

```

          ADIABATIC REACTOR          CM 211

298.0000  100.0000  513.0000  310.0000

TEMP = 298.0000      CONVERSION = -0.000236
TEMP = 398.0000      CONVERSION = 0.068324
TEMP = 498.0000      CONVERSION = 0.142736
TEMP = 598.0000      CONVERSION = 0.224651
TEMP = 698.0000      CONVERSION = 0.314837
TEMP = 648.0000      CONVERSION = 0.268686
TEMP = 673.0000      CONVERSION = 0.291495
TEMP = 698.0000      CONVERSION = 0.314837
TEMP = 685.5000      CONVERSION = 0.303099
TEMP = 673.0000      CONVERSION = 0.291495
TEMP = 679.2500      CONVERSION = 0.297280
TEMP = 685.5000      CONVERSION = 0.303099
TEMP = 682.3750      CONVERSION = 0.300185
TEMP = 683.9375      CONVERSION = 0.301641
    
```

Discussion of Results

At the end of each iteration the assumed temperature, in degrees, and the conversion of CO to CH<sub>3</sub>OH were printed. Temperature was the variable incremented in the iterative process. It was initialized to the inlet temperature of the reactants and increased in steps of 100°K until the desired temperature was exceeded as determined by a reversal in the sign of  $K_T - K_X$ . The increment was then halved in magnitude and reversed in sign and the procedure repeated until the absolute temperature increment was less than one degree. The only difficulty anticipated with this program would arise if the temperature assumed initially were too high or if the first increment were too large. Under either of these conditions the sign change in  $K_T - K_X$  would not occur and the assumed temperature would continue to increase by the initialized increment.

Critique

- A) The problem meshed well with the course material. It had been assigned in previous semesters but the exact solution had not been obtained because of the lengthy trial and error procedure involved.
- B) The problem was not extremely difficult to program. It necessitated the use of iterative procedures and demonstrated a practical application for computers in chemical equilibrium problems.
- C) The students reacted very favorably; they were eager to start the problem and most retained their enthusiasm until their program operated satisfactorily.
- D) The last three weeks of the course were devoted to statistical thermodynamics with very little homework assigned. The computer problem was assigned at the end of the classical treatment of thermodynamics and just before the statistical phase began. Additional home assignments during the final three weeks were few and ample time was available in recitation for discussing difficulties. Consequently no interference with the normal course routine was observed.
- E) Both the MAD language and the IBM 704 were quite adequate for the problem.
- F) The problem was extremely worthwhile to both students and instructor.

Example Problem No. 115

SUCCESSIVE AND SIMULTANEOUS FIRST ORDER CHEMICAL REACTIONS

by

Robert N. Pease

Department of Chemical Engineering

The University Michigan

Course: Rate Operations

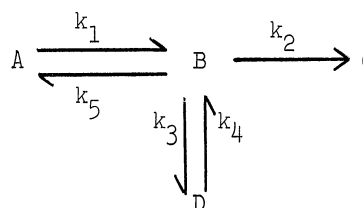
Credit hours: 5

Level: Junior

Statement of Problem

Given the reaction shown at the right for which

$$\begin{aligned} k_1 &= 0.40 \text{ hr}^{-1} \\ k_2 &= 0.16 \text{ hr}^{-1} \\ k_3 &= 0.13 \text{ hr}^{-1} \\ k_4 &= 0.08 \text{ hr}^{-1} \\ k_5 &= 0.10 \text{ hr}^{-1} \end{aligned}$$



Assume that all reactions follow first order kinetics.

$$\begin{aligned} r_1 &= \text{rate of formation of A} \\ r_2 &= \text{rate of formation of B} \\ r_3 &= \text{rate of formation of C} \\ r_4 &= \text{rate of formation of D} \end{aligned}$$

The number of moles of the various components present in the initial reaction mixture are as follows:

- A: 7.00 pound moles per cubic foot
- B: 2.00 pound moles per cubic foot
- C: 0.00 pound moles per cubic foot
- D: 0.50 pound moles per cubic foot

Write a computer program to calculate the number of moles of all the components present as function of time.

Solution

A program was written in the ACT III compiler language and compiled and executed on the LGP-30 digital computer. The problem was solved by step-wise integration. For each time interval, an iteration method was used in which the final concentrations were calculated from rates based on the average concentrations for the interval and then new average concentrations were computed as the arithmetic averages of the initial and final concentrations. The iteration was continued until successive estimates of the final concentrations agreed within a specified convergence limit.

For the first iteration of the first time interval, the starting concentrations were used as the average concentrations.

For the first iteration of each subsequent time interval, the average concentrations were estimated from the concentration changes of the previous interval.

The computation was stopped by the operator when a sufficient number of steps had been computed.

The following symbols were used in the ACT III Program.

ao,bo,co,do	=	concentrations of components A, B, C, D, respectively, at the beginning of the run; pound moles per cubic foot
a,b,c,d	=	average concentrations during an interval
af,bf,cf,df	=	currently computed final concentrations for an interval
paf,pbf,pcf,pdf	=	previously computed final concentrations for the same interval
dela,delb,delc,deld	=	changes in concentrations during an interval.
t	=	time, hours
delt	=	time interval, hours
n	=	number of trials for an interval
conv	=	concentration convergence limit for an interval

The appropriate equations used were

$$\begin{aligned} \text{dela} &= [-k_1 \cdot a + k_5 \cdot b] \cdot \text{delt} \\ \text{delb} &= [k_1 \cdot a - k_6 \cdot b + k_4 \cdot d] \cdot \text{delt} \\ \text{delc} &= k_2 \cdot b \cdot \text{delt} \\ \text{deld} &= [k_3 \cdot b - k_4 \cdot d] \cdot \text{delt} \end{aligned}$$

$$\text{where } k_6 = k_2 + k_3 + k_5$$

$$\begin{aligned} \text{af} &= \text{ai} + \text{dela} \\ \text{bf} &= \text{bi} + \text{delb} \\ \text{cf} &= \text{ci} + \text{delc} \\ \text{df} &= \text{di} + \text{deld} \end{aligned}$$

Successive and Simultaneous First Order Chemical Reactions

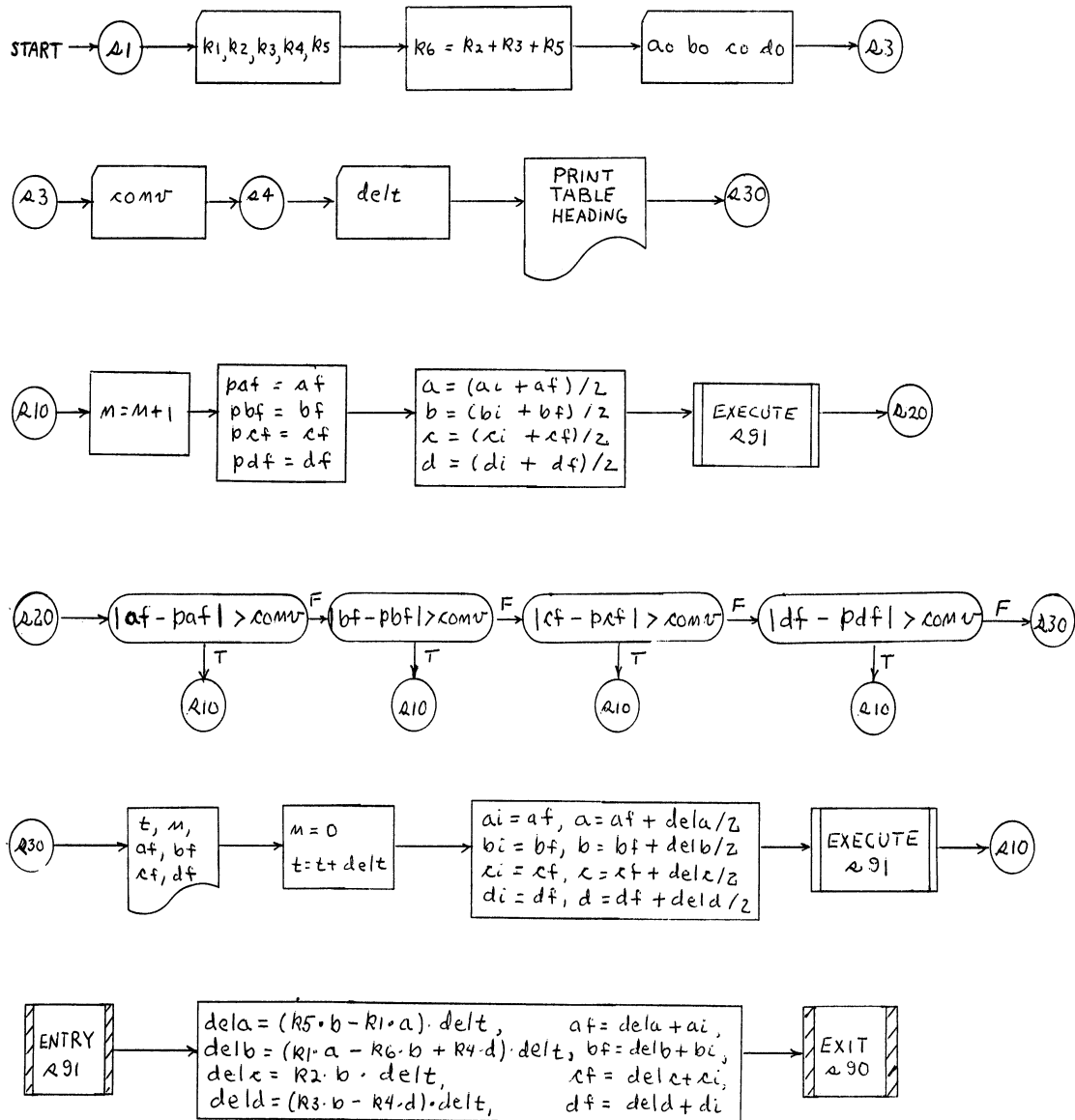
$$a = (a_i + a_f)/2$$

$$b = (b_i + b_f)/2$$

$$c = (c_i + c_f)/2$$

$$d = (d_i + d_f)/2$$

Flow Diagram



ACT III Program and Data

```

s1'cr'read'k1''read'k2''read'k3''read'k4''read'k5''
k2'+k3'+k5';k6''

s2'read'ao''read'bo''read'co''read'do''
s3'read'conv''
s4'read'delt''

s5'cr'cr'daprt' ' 't'tab'daprt' 'n''
tab'daprt' 'a'tab'daprt' 'b''
tab'daprt' 'c'tab'daprt' 'd''

s0'0';'n''prev';'t''prev';'dela''
prev';'delb''prev';'delc''prev';'deld''
s0'ao';'af''bo';'bf''co';'cf''do';'df''
use's30''

s10'n'i+'l';'n''
s12'af';'pa''bf';'pb''cf';'pc''df';'pd''

s14'
, 'ai'+af'. 'x'.5''e'0';'a''
, 'bi'+bf'. 'x'.5''e'0';'b''
, 'ci'+cf'. 'x'.5''e'0';'c''
, 'di'+df'. 'x'.5''e'0';'d''

s16'ret's90'use's91''

s20'
if', 'abs', 'af'-'pa'.'. '-conv'. 'pos's10''
if', 'abs', 'bf'-'pb'.'. '-conv'. 'pos's10''
if', 'abs', 'cf'-'pc'.'. '-conv'. 'pos's10''
if', 'abs', 'df'-'pd'.'. '-conv'. 'pos's10''

s30'cr'703'dprt't'tab'200'iprt'n''
tab'603'dprt'af''tab'603'dprt'bf''
tab'603'dprt'cf''tab'603'dprt'df''

s32'0';'n''t+'delt';'t''
s34'
af';'ai''prev'+dela'x'.5''e'0';'a''
bf';'bi''prev'+delb'x'.5''e'0';'b''
cf';'ci''prev'+delc'x'.5''e'0';'c''
df';'di''prev'+deld'x'.5''e'0';'d''

s40'ret's90'use's91''
use's10''

s91', 'k5'x'b'-'k1'x'a'. 'x'delt';'dela''
prev'+ai';'af''
s92', 'k1'x'a'-'k5'x'b'+k4'x'd'. 'x'delt';'delb''
prev'+bi';'bf''
s93', k2'x'b'x'delt';'delc''
prev'+ci';'cf''
s94', 'k3'x'b'-'k4'x'd'. 'x'delt';'deld''
prev'+di';'df''
s90'go to's0''

```

Data for Run 1

```

+40'+0'+16'+0'
+13'+0'+8'-1'
+10'+0'

+7'+1'+2'+1'
+0'+0'+5'+0'

+2'-2'
+3'+0'

```

Computer Output

Computer Results

Run 1 conv = 0.002 delt = 0.50

.0000502'

+40'+0'+16'+0'

+15'+0'+8'-1'

+10'+0'

+7'+1'+2'+1'

+0'+0'+5'+0'

+2'-2'

+3'+0'

t	n	a	b	c	d
.000	0	7.000	2.000	.000	.500
.300	3	6.272	2.543	.109	.575
.600	2	5.640	2.951	.241	.668
.900	2	5.089	3.250	.390	.772
1.200	2	4.608	3.459	.551	.883
1.500	2	4.186	3.596	.720	.998
1.800	2	3.815	3.676	.895	1.114
2.100	2	3.488	3.710	1.072	1.230
2.400	2	3.198	3.708	1.250	1.344
2.700	2	2.940	3.678	1.427	1.454
3.000	2	2.711	3.626	1.603	1.561
3.300	2	2.506	3.557	1.775	1.662
3.500	2	2.322	3.477	1.944	1.758
3.900	1	2.156	3.387	2.109	1.849
4.200	1	2.006	3.292	2.269	1.933
4.500	1	1.871	3.192	2.424	2.012
4.800	1	1.748	3.091	2.575	2.086
5.100	1	1.636	2.989	2.721	2.153
5.400	1	1.534	2.888	2.862	2.216
5.700	1	1.441	2.789	2.998	2.273
6.000	1	1.355	2.691	3.130	2.324
6.300	1	1.276	2.596	3.257	2.371
6.600	1	1.204	2.504	3.379	2.413
6.900	1	1.137	2.415	3.497	2.451
7.200	1	1.076	2.329	3.611	2.484
7.500	1	1.019	2.247	3.721	2.513
7.800	1	.966	2.169	3.827	2.539
8.100	1	.917	2.094	3.929	2.561
8.400	1	.871	2.022	4.028	2.579
8.700	1	.829	1.953	4.123	2.595
9.000	1	.789	1.888	4.216	2.607
9.300	1	.753	1.825	4.305	2.617
9.500	1	.718	1.767	4.391	2.624
9.900	1	.686	1.711	4.474	2.629
10.200	1	.656	1.657	4.555	2.631
10.500	1	.628	1.607	4.634	2.632
10.800	1	.602	1.558	4.710	2.630
11.100	1	.577	1.513	4.783	2.627
11.400	1	.554	1.469	4.855	2.622
11.700	1	.532	1.428	4.924	2.616
12.000	1	.512	1.388	4.992	2.608
12.300	1	.493	1.351	5.058	2.599
12.600	1	.475	1.315	5.122	2.589
12.900	1	.458	1.281	5.184	2.577
13.200	1	.442	1.249	5.245	2.565
13.500	1	.426	1.218	5.304	2.552
13.800	1	.412	1.189	5.362	2.538
14.100	1	.399	1.161	5.418	2.523
14.400	1	.386	1.134	5.473	2.507
14.700	1	.374	1.108	5.527	2.491
15.000	1	.363	1.084	5.579	2.474



Example Problem No. 115

Computer Output (continued)

Run 2 conv = 0.002 delt = 0.15

.0000302'

+40'+0'+16'+0'  
+13'+0'+8'-1'  
+10'+0'

+7'+1'+2'+1'  
+0'+0'+5'+0'

+2'-2'+15'+0'

t	n	a	b	c	d
.000	0	7.000	2.000	.000	.500
.150	2	6.523	2.289	.051	.535
.300	1	6.273	2.542	.109	.576
.450	1	5.946	2.761	.173	.621
.600	1	5.641	2.949	.242	.668
.750	1	5.357	3.110	.314	.719
.900	1	5.091	3.247	.390	.772
1.050	1	4.842	3.351	.470	.827
1.200	1	4.610	3.455	.552	.883

Run 3 conv = 0.0005 delt = 0.30

.0000302'

+40'+0'+16'+0'  
+13'+0'+8'-1'  
+10'+0'

+7'+1'+2'+1'  
+0'+0'+5'+0'

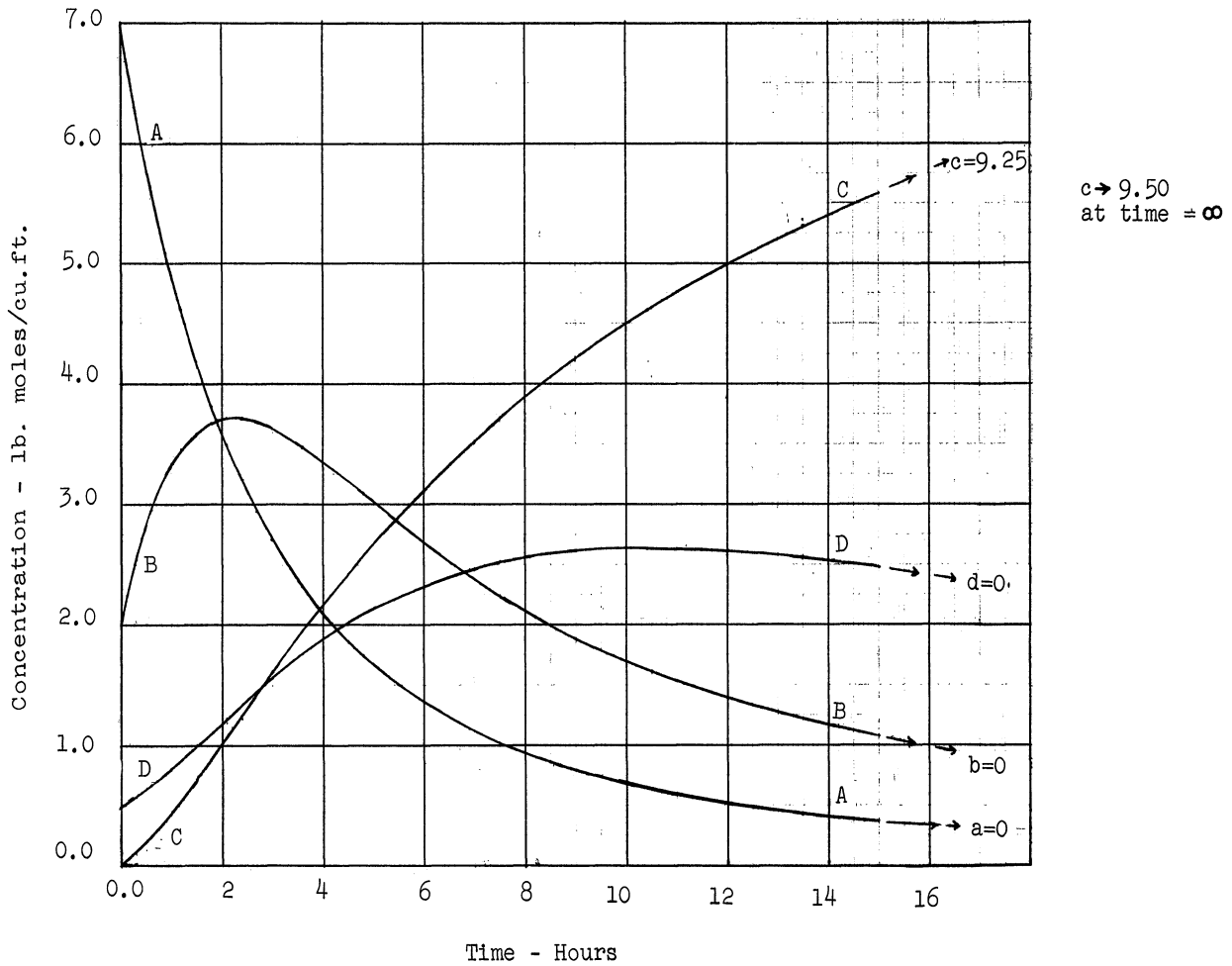
+5'-3'  
+3'+0'

t	n	a	b	c	d
.000	0	7.000	2.000	.000	.500
.300	4	6.272	2.543	.109	.576
.600	3	5.640	2.952	.241	.668
.900	3	5.089	3.250	.390	.772
1.200	3	4.608	3.459	.551	.883
1.500	3	4.186	3.596	.720	.998
1.800	3	3.815	3.676	.895	1.114
2.100	3	3.488	3.711	1.072	1.230

Discussion of Results

The concentrations of each component are plotted as a function of time in the figure on the following page.

Successive and Simultaneous First Order Chemical Reactions



Comparison of Runs 1 and 2 shows that reducing the time interval by half gives a slight improvement in accuracy.

Comparison of Run 1 and 3 shows that reducing the convergence limit increases the number of iterations but does not change the results within the accuracy of printout.

Therefore, one can conclude that the parameters used in Run 1 were reasonable.

Critique

This problem is a good example of one which can be solved on a small computer. The method of solution, however, is applicable for use on a larger computer using any compiler language such as MAD or FORTRAN. While an analytical solution to the problem is possible, it would be very tedious.

Example Problem No. 116

PYROLYSIS OF ETHANE IN A TUBULAR REACTOR

by

J. O. Wilkes

Department of Chemical and Metallurgical Engineering

The University of Michigan

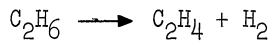
Course: Rate Operations

Credit Hours: 5

Level: Junior

Statement of the Problem

The pyrolysis of ethane in the temperature range 1200-1700 °F is represented essentially by the irreversible first order reaction



1800 lb./hr. of pure ethane are fed at 1200 °F to a 3 in. I.D. tube contained in an ethane pyrolysis furnace. Heat is supplied to the tube at a rate of 5000 B.T.U./hr.ft<sup>2</sup> (of inside tube area). The pressure drop along the tube is small and a mean pressure of 30 psia. may be taken.

Assuming plug flow, calculate the length of tube required to produce 75% decomposition of the ethane. The program should include provision for printing length (ft.), temperature (°R), and conversion after each increment of tube length.

Data (In the following, T is in °K)

	$\Delta H_f$ at 298°K (cal./gm.mole)	$C_p$ (cal./gm.mole.°K)
$\text{C}_2\text{H}_6$ (g)	-20,236	$3.75 + 35.7 \times 10^{-3}T - 10.12 \times 10^{-6}T^2$
$\text{C}_2\text{H}_4$ (g)	12,496	$5.25 + 24.2 \times 10^{-3}T - 6.88 \times 10^{-6}T^2$
$\text{H}_2$ (g)	0	$7.00 - 0.385 \times 10^{-3}T + 0.6 \times 10^{-6}T^2$
Velocity constant:	$k = 5.764 \times 10^{16} e^{-\frac{41,310}{T}} \text{ sec}^{-1}$ .	
Molecular Weights:	C = 12, H = 1	
Gas Constant:	R = 10.73 psia.ft <sup>3</sup> /lb.mole.°R	

Nomenclature

The problem is stated in mixed units. It is here decided to work in B.T.U., lb.mole, °R, ft. and hr. units. Let the following notation be adopted:

- $n_0$  = inlet molal feed rate of ethane, lb.moles/hr.
- $n_{\text{C}_2\text{H}_6}$  = molal flow rate of ethane at any point in the reactor.
- $z$  = fractional conversion.
- $P$  = total pressure, psia.
- $T$  = absolute temperature, °R.

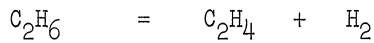
Pyrolysis of Ethane in a Tubular Reactor

Nomenclature, Continued

- k = velocity constant, sec.<sup>-1</sup>
- j = specific reaction rate, (lb.moles ethane/ft<sup>3</sup>hr.)
- c = concentration of ethane, lb.moles/ft<sup>3</sup>.
- A = cross-sectional area of tube, ft<sup>2</sup>.
- q = heat input from furnace, B.T.U./hr.ft (of tube).
- ΔH<sub>R</sub> = heat of reaction, B.T.U./lb.mole.
- C<sub>p</sub> = specific heat, B.T.U./lb.mole.°R.
- x = mole fraction of ethane.
- L = length from reactor inlet, ft.
- V = reactor volume, ft<sup>3</sup>.

Solution

We have, for the reaction.

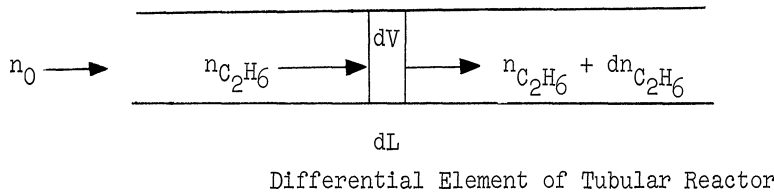


Inlet molal  
flow rate:     $n_0$                       0                      0

Molal flow  
rate when  
conversion  
is z:             $n_0(1-z)$              $n_0z$              $n_0z$

Hence the total moles flowing at any point in the reactor are  $n_0(1+z)$ , and the corresponding mole fraction of ethane is  $x = (1-z)/(1+z)$ .

The problem is now approached by establishing steady state material and thermal balances over a differential element  $dL$  of reactor length, as shown in the figure below:



Material Balance (for moles of ethane)

$$\begin{array}{lclcl} \text{In} & & \text{From Reaction} & = & \text{Out} \\ n_{C_2H_6} & + & j dV & = & n_{C_2H_6} + dn_{C_2H_6} \end{array}$$

whence 
$$j = \frac{dn_{C_2H_6}}{dV} = \frac{d\{n_0(1-z)\}}{AdL} = -\frac{n_0}{A} \frac{dz}{dL} \quad (1)$$

But, for the present irreversible first order reaction, the specific reaction rate is given by

$$j = -kc = -k \frac{xP}{RT} = -k \frac{1-z}{1+z} \frac{P}{RT} \quad (2)$$

Hence, from (1) and (2), the differential increase  $dz$  in conversion over a differential element of length  $dL$  is

$$dz = \frac{AP}{n_0 R} \left(\frac{k}{T}\right) \left(\frac{1-z}{1+z}\right) dL \quad (3)$$

Heat Balance

For a change dz in conversion:

$$\text{Heat liberated due to reaction} = n_0 dz (-\Delta H_R)$$

$$\text{Gain in enthalpy of flowing stream} = (\sum n_i C_{p_i}) dT,$$

where the summation is over the three components ethane, ethylene and hydrogen.

A heat balance on the element of length dL then gives:

$$n_0 dz (-\Delta H_R) + q dL = n_0 \left[ (1-z) C_{p_{C_2H_6}} + z (C_{p_{C_2H_4}} + C_{p_{H_2}}) \right] dT$$

Hence the differential rise in temperature over the element is

$$dT = \frac{Q dL + (-\Delta H_R) dz}{(1-z) C_{p_{C_2H_6}} + z (C_{p_{C_2H_4}} + C_{p_{H_2}})} \quad (4)$$

where  $Q = q/n_0$ .

The problem may now be solved by a stepwise procedure along the length of the reactor, employing the finite difference approximations of equations (3) and (4) (which will then have dT, dL and dz replaced by ΔT, ΔL, and Δz). At the start of any increment ΔL, everything will be known. The increase Δz in conversion may be estimated from equation (3) which then enables the corresponding temperature increase ΔT to be obtained from equation (4). The computation is then repeated for successive elements of length. It is assumed that the elements are sufficiently short so that the values of k, T, z and C<sub>p</sub> at the start of each element may be employed in equations (3) and (4). Strictly speaking, some sort of average values should be taken across each element instead. However, the procedure used here is amply justified by the fact that the computed results are almost invariant over a wide range of values selected for the length increment.

Computation of Various Numerical Constants and Conversion Factors

The computations will be made in B.T.U., lb.mole, °R, ft. and hr. units. The following should be noted:

- a. It is convenient to define a Kelvin temperature  $TK \equiv T/1.8$ .
- b. Cal./gm.mole.°K are numerically the same as B.T.U./lb.mole.°R.
- c. In equation (3), the units of  $AP/n_0 R$  will have to be adjusted to sec.°R/ft., in order to cancel with kdL/T.

i.e., 
$$\frac{AP}{n_0 R} = \frac{(\pi/4) \times (0.25)^2 \times 30.0 \times 3600}{(1800/30) \times 10.73} = \frac{\pi \times 225}{8 \times 10.73} \frac{\text{sec.}^\circ\text{R}}{\text{ft.}}$$

- d. Heat of reaction varies with temperature according to

$$\frac{d(\Delta H_R)}{dT} = \Delta C_p$$

Hence it may be shown that the heat of reaction at any temperature is given by

Pyrolysis of Ethane in a Tubular Reactor

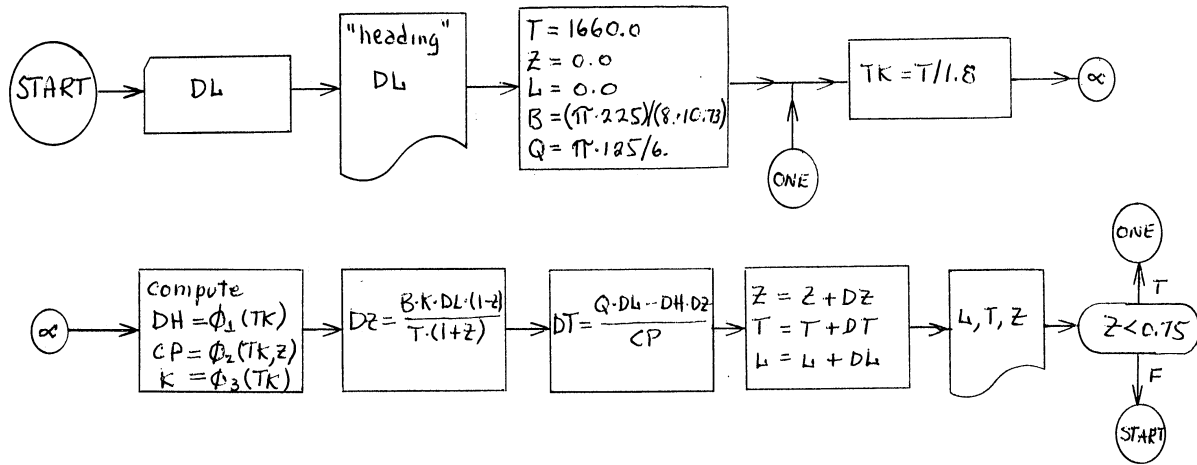
$$(\Delta H_R)_T / 1.8 = 32,732 + 8.50 (TK-298) - 5.942 \times 10^{-3} (TK^2 - 298^2) + 1.28 \times 10^{-6} (TK^3 - 298^3) \text{ B.T.U./lb.mole.}^\circ\text{R.}$$

$$e. \quad Q = \frac{q}{n_0} = \frac{5000 \times \pi / 4}{1800/30} = \frac{125\pi}{6} \frac{\text{B.T.U.hr.}}{\text{ft.lb.mole}}$$

List of Principal Variables

MAD Symbol	Definition
T	Temperature ( $^\circ\text{R}$ )
TK	Temperature ( $^\circ\text{K}$ )
L	Length (ft.)
Z	Conversion
DT, DL, DZ	Increments in temperature, length, and conversion
K	Velocity constant ( $\text{sec.}^{-1}$ )
DH	Heat of reaction
B	$AP/n_0R$
CP	$(1-z) C_{pC_2H_6} + z (C_{pC_2H_4} + C_{pH_2})$
Q	$q/n_0$

Flow Diagram



MAD Program

DECOMPOSITION OF ETHANE IN A TUBULAR REACTOR, WITH A HEAT INPUT AT THE WALL. MATERIAL AND THERMAL BALANCES ON A DIFFERENTIAL ELEMENT OF LENGTH (DL) LEAD TO TWO SIMULTANEOUS ORDINARY DIFFERENTIAL EQUATIONS WHICH GIVE THE INCREASE IN CONVERSION (DZ) AND TEMPERATURE (DT) OVER THE ELEMENT. SOLUTION IS BY STEPWISE COMPUTATION ALONG THE REACTOR LENGTH. TEMPERATURE (T) AND CONVERSION (Z) ARE PRINTED AFTER EACH INCREMENT UNTIL THE CONVERSION REACHES Z = 0.75.

Example Problem No. 116

MAD Program, Continued

```

START   READ DATA DL
        PRINT COMMENT $1      RESULTS FOR ETHANE PYROLYSIS WITH LENGTH
        I INCREMENT$
        PRINT RESULTS DL

        ..... INITIALISE T, Z, L AND COMPUTE CONSTANTS B AND Q .....
        T = 1660.0
        Z = 0.0
        L = 0.0
        B = (3.14159*225.0)/(8.0*10.73)
        Q = 125.0*3.14159/6.0

        ..... PERFORM MATERIAL AND THERMAL BALANCES OVER
        ONE   SUCCESSIVE INCREMENTS OF REACTOR LENGTH .....
        TK = T/1.8
        DH = 1.8*(32732.0 + 8.50*(TK - 298.0) - 5.942E-3*(TK*TK -
        1298.0*298.0) + 1.28E-6*(TK*TK*TK - 298.0*298.0*298.0))
        CP = (1.0 - Z)*(3.75 + 35.7E-3*TK - 10.12E-6*TK*TK) +
        1Z*(12.25 + 23.815E-3*TK - 6.28E-6*TK*TK)
        K = 5.764E16*EXP.(-41310.0/TK)
        DZ = B*K*(1.0 - Z)*DL/(T*(1.0 + Z))
        DT = (Q*DL - DH*DZ)/CP
        Z = Z + DZ
        T = T + DT
        L = L + DL
        PRINT RESULTS L, T, Z
        WHENEVER Z.L.0.75, TRANSFER TO ONE
        TRANSFER TO START
        END OF PROGRAM
    
```

Computer Output

RESULTS FOR ETHANE PYROLYSIS WITH LENGTH INCREMENT

DL =	50.000000		
L =	50.000000,	T = 1775.486313,	Z = 5.028653E-04
L =	100.000000,	T = 1869.406479,	Z = 9.156017E-03
L =	150.000000,	T = 1841.127579,	Z = .075388
L =	200.000000,	T = 1884.386444,	Z = .107355
L =	250.000000,	T = 1840.153625,	Z = .181362
L =	300.000000,	T = 1897.448914,	Z = .206595
L =	350.000000,	T = 1843.791946,	Z = .285262
L =	400.000000,	T = 1907.940247,	Z = .307149
L =	450.000000,	T = 1855.355682,	Z = .385377
L =	500.000000,	T = 1918.359863,	Z = .407688
L =	550.000000,	T = 1869.832809,	Z = .484011
L =	600.000000,	T = 1929.752441,	Z = .507674
L =	650.000000,	T = 1886.067993,	Z = .581698
L =	700.000000,	T = 1942.690582,	Z = .606825
L =	750.000000,	T = 1904.852020,	Z = .678043
L =	800.000000,	T = 1958.121475,	Z = .704669
L =	850.000000,	T = 1927.666519,	Z = .772308

## Pyrolysis of Ethane in a Tubular Reactor

### Discussion of Results

The computed results are shown above for only one value of length increment, viz, DL=50.0 feet. However, runs were also made for several other choices of DL and the results for all runs are summarized in Table 1. which shows the computed reactor lengths in each case corresponding to 75% conversion.

Table 1.  
Computed Reactor Length Corresponding  
to 75% Conversion, for Various Values of DL

Length Increment DL (ft.):	1	5	10	20	50	100
Total Length (ft.):	842.6	842.5	842.3	842.0	833.5	584.5
Exit Temperature (°R):	1949.6	1949.5	1949.5	1949.4	1944.4	1428.7

The results are almost identical for DL = 1, 5 or 10 feet, and the extremely large increment of 100 feet is required before there is serious error introduced. The results for DL = 50 feet are slightly in error but are reproduced above for reasons of economy of space.

Observe that little reaction occurs during the first 100 feet of reactor length. This is a region in which the gas temperature is rising but the velocity constant is still small and only a small amount of ethane decomposes. Thereafter, the longitudinal temperature profile becomes less steep, due to the fact that the reaction is endothermic.

### Solution Using the Runge-Kutta Procedure

The differential equations (3) and (4)

$$\frac{dz}{dL} = \frac{AP}{n_0 R} \left( \frac{k}{T} \right) \left( \frac{1-z}{1+z} \right) \quad (3)$$

$$\frac{dT}{dL} = \frac{Q - \Delta H_R \frac{dz}{dL}}{(1-z)C_{pC_2H_6} + z(C_{pC_2H_4} + C_{pH_2})} \quad (4)$$

can also be solved numerically by using the Runge-Kutta<sup>\*</sup> integration procedure. This procedure, programmed to solve systems of first-order ordinary differential equations, is available as a library subroutine in the Michigan Executive System and can be called upon directly in a MAD program. Briefly, the subroutine has two entries, an initialization entry SETRKD. and an integration entry RKDEQ.

SETRKD. is executed only once and its only function is to supply the names of all pertinent parameters as follows:

---

\* Hildebrand, Introduction to Numerical Analysis, p. 237, McGraw-Hill, 1956.



Example Problem No. 116

EXECUTE SETRKD. (N,Y(1), DERIV(1), DUMMY(1), L, DL)

where N is the number of differential equations, an integer.

Y(1) the first location in an array of length N into which RKDEQ. will put the integrated solution values for the N dependent variables.

DERIV(1) the first location in an array of length N. RKDEQ. expects the main program to evaluate all derivatives of the Y's and put the values into the corresponding elements, e.g.,

$$\text{DERIV}(1) = \frac{dY(1)}{dL}, \quad \text{DERIV}(I) = \frac{dY(I)}{dL}$$

DUMMY(1) the first location in an array of length N which is used by RKDEQ. for working storage.

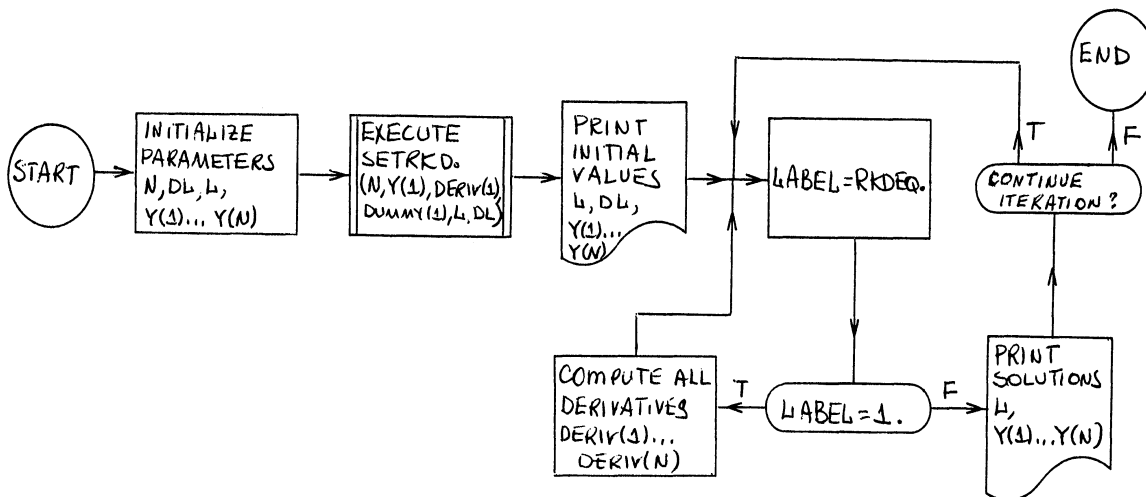
L the independent variable.

DL the step size for the integration procedure.

RKDEQ.(0) is the entry which is called when the subroutine is to integrate numerically to produce solution values Y(1)...Y(N) for the value of the independent variable equal to L + DL, i.e., when the solutions for the equations at the end of the next integration step are wanted.

Since the "fourth-order" Runge-Kutta procedure is used (see Hildebrand), the subroutine needs to have all derivative values computed four times per integration step. The routine indicates that all derivatives are to be evaluated by returning with a value 1.0. After each set of four evaluations, the calling program must return to RKDEQ.(0). After four successive derivative evaluations (all necessary incrementing of L is done automatically by the subroutine) the subroutine returns with a value 2.0 to indicate that the solution values for the N dependent variables at the end of the integration step are available in Y(1) to Y(N). At this point the program can print the results if desired. If integration is to continue across another increment in L, the program calls on RKDEQ.(0) again and the process described above is repeated. The user determines when to stop the integration by testing appropriate dependent or independent variable values.

A rough flow diagram of the Runge-Kutta calling procedure is shown below.



## Pyrolysis of Ethane in a Tubular Reactor

The program which follows is somewhat more general than the earlier one, in that the following parameters are read as data:

TF            Inlet ethane temperature, °F  
P             Pressure in tube, psia.  
MASRAT       Mass rate of ethylene feed, lb./hr.  
ID            Internal diameter of tube, in.  
QPEFSF       Heat input from furnace, B.T.U./hr.ft.<sup>2</sup> of tube (inside tube area)  
CONV         Maximum desired conversion  
DL            Step size for the integration, ft.  
FREQ         Frequency of printout, i.e., results will be printed after every FREQ integration steps.

Most of the MAD symbols with the meanings and units shown on page I42 are used here also.

In addition, the following variables are used.

FACTOR<sup>+</sup>     $\frac{AP}{n_0R}$  × constant part of K.  
LABEL       Value returned by RKDEQ.(0). This is either a 1.0 or 2.0 as indicated above.  
DZDL          $\frac{dz}{dL}$   
DTDL          $\frac{dT}{dL}$

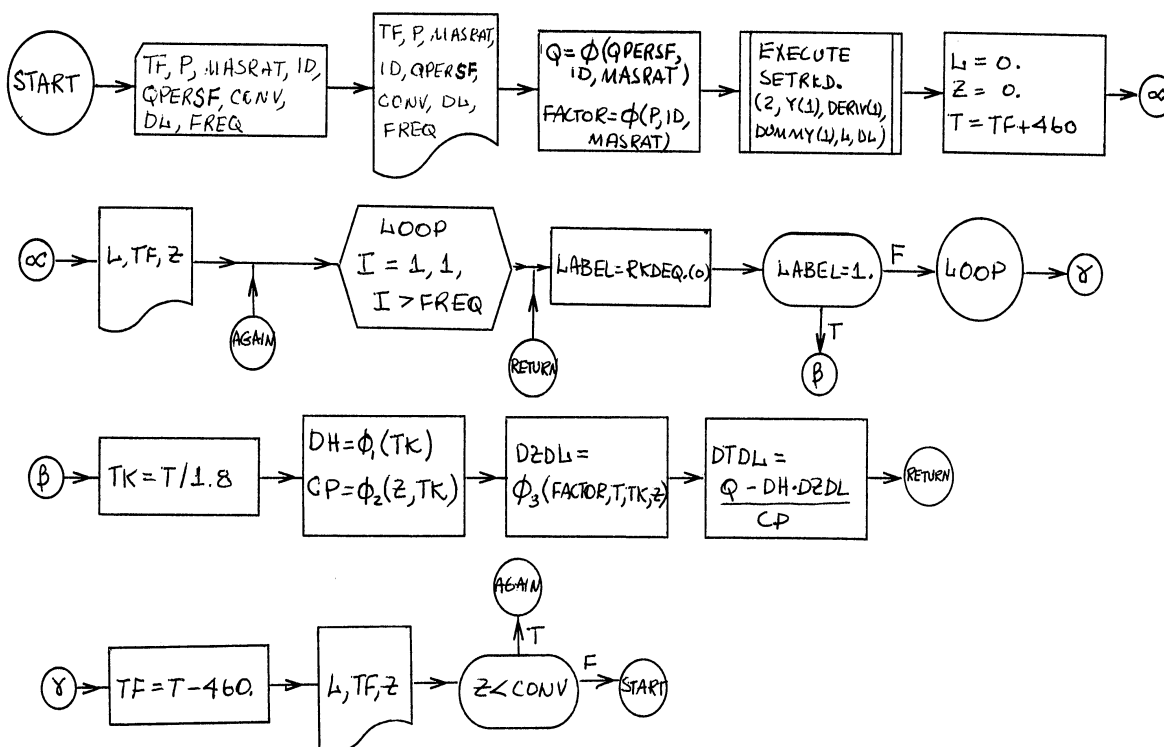
Because of the array nature of some of the subroutine arguments, the following have been made equivalent names for the same values.

Problem Variable	Equivalent MAD Symbols
z	Z, Y(1)
T	T, Y(2)
$\frac{dz}{dL}$	DZDL, DERIV(1)
$\frac{dT}{dL}$	DTDL, DERIV(2)

$$+ \frac{3.14159 \left(\frac{ID}{12}\right)^2}{4} \cdot P \cdot 3600 \cdot 5.764 \times 10^{-16} \cdot \frac{MASRAT}{30} \cdot 10.73$$

Example Problem No. 116

Flow Diagram



MAD Program

```

DIMENSION Y(2), DERIV(2), DUMMY(2)
EQUIVALENCE (Z,Y(1)),(T,Y(2)),(DZDL,DERIV(1)),(DTDL,DERIV(2))
INTEGER I, FREQ

START PRINT COMMENT $1ETHANE PYROLYSIS IN A TUBULAR REACTOR $
READ AND PRINT DATA TF, P, MASRAT, ID, QPERSF, CONV, DL, FREQ
Q = QPERSF*30./MASRAT*3.14159*ID/12.
FACTOR = 2.07504E20*3.14159*ID*ID*P*30./(144.*4.*10.73*MASRAT)

INITIALIZE PARAMETERS FOR RUNGE KUTTA SETUP

EXECUTE SETRKD.(2,Y(1),DERIV(1),DUMMY(1),L,DL)
L = 0.0
Z = 0.0
T = TF + 460.
PRINT RESULTS L, TF, Z

RUNGE KUTTA PROCEDURE CALCULATES T AND Z AT L + DL.
PARAMETER I COUNTS THE NUMBER OF STEPS BETWEEN PRINTOUTS

AGAIN THROUGH LOOP, FOR I=1,1, I.G.FREQ
RETURN LABEL = RKDEQ.(0)
WHENEVER LABEL.E.1.

COMPUTE THE DERIVATIVES DZDL AND DTDL AND RETURN TO RKDEQ.

TK = T/1.8
DH = 1.8*(32732. + 8.50*(TK-298.) - 5.942E-3*(TK*TK-298.*298.
1) + 1.28E-6*(TK*TK*TK-298.*298.*298.))
CP = (1.0-Z)*(3.75+35.7E-3*TK-10.12E-6*TK*TK)+Z*(12.25+23.815
1E-3*TK-6.28E-6*TK*TK)
DZDL = FACTOR*EXP.(-41310./TK)*(1.-Z)/(T*(1.+Z))
DTDL = (Q - DH*DZDL)/CP
TRANSFER TO RETURN

LOOP END OF CONDITIONAL

PRINT THE RESULTS AFTER EVERY FREQ STEPS

TF = T - 460.
PRINT RESULTS L, TF, Z
WHENEVER Z.L.CONV, TRANSFER TO AGAIN
TRANSFER TO START
END OF PROGRAM
    
```

Pyrolysis of Ethane in a Tubular Reactor

Computer Output

ETHANE PYROLYSIS IN A TUBULAR REACTOR

TF = 1200., P = 30., MASRAT = 1800., ID = 3., QPERSF = 5000., CONV = .75,

DL = 50., FREQ = 1 \*

L =	TF =	Z =
.000000,	1200.000000,	.000000
50.000000,	1308.547867,	2.760554E-03
100.000000,	1376.772186,	.023198
150.000000,	1392.900711,	.068156
200.000000,	1402.233643,	.116318
250.000000,	1409.309326,	.165544
300.000000,	1415.354050,	.215257
350.000000,	1420.964020,	.265172
400.000000,	1426.461487,	.315135
450.000000,	1432.027344,	.365059
500.000000,	1437.773926,	.414889
550.000000,	1443.785889,	.464584
600.000000,	1450.143005,	.514104
650.000000,	1456.934540,	.563406
700.000000,	1464.271210,	.612433
750.000000,	1472.298462,	.661114
800.000000,	1481.216476,	.709348
850.000000,	1491.312805,	.756991

Discussion of Results

Computed results for the stepsize DL = 50.0 feet are shown above. The program was also run for values of DL = 1.0, 5.0, 10.0, 25.0, and 100.0. Interpolated results for the tube length necessary for 75% conversion are shown in Table 2.

TABLE 2.  
Computed Reactor Length Corresponding  
to 75% Conversion, for Various Values of DL

Length Increment DL (ft.):	1	5	10	25	50	100
Total Length (ft.):	842.6	842.6	842.6	842.6	842.6	-
Exit Temperature (°F):	1489.6	1489.6	1489.6	1489.6	1489.8	-

Comparison of the results in Table 2 shows that for all stepsizes used, the method produces essentially the same answers. The procedure failed for a DL of 100 ft.; the solution "blew up" after the first integration step, apparently because the temperature computed at the end of the first step was too high. Comparison with the values computed using the simple finite difference stepping procedure (see Table 1.) shows that for this problem the Runge-Kutta procedure produces approximately the same answers for the smaller increments but is more accurate for the larger stepsizes. When comparing the two methods from the standpoint of computing time it should be remembered that the Runge-Kutta method requires at least four (and probably more) times as many machine instructions per integration step as the simple stepping procedure. This difference tends to be offset somewhat, however, by the increased stepsize permitted for the Runge-Kutta method.

Example Problem No. 117

ADIABATIC FLAME TEMPERATURE FOR CARBON MONOXIDE OXIDATION

by

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The University of Michigan

Course: Thermodynamics

Credit Hours: 5

Level: Sophomore-Junior

Statement of the Problem

Carbon monoxide from a water gas plant is burned with air in an adiabatic reactor. Both the carbon monoxide and air are being fed to the reactor at 70°F and atmospheric pressure. Ten percent more air is used than theoretically required by the stoichiometry of the reaction. For the reaction



the following standard free energy change (25°C) has been determined:

$$\Delta G^\circ = -111,600 \text{ B.T.U.}$$

The standard enthalpy change at 25°C has been measured as:

$$\Delta H^\circ = -121,700 \text{ B.T.U.}$$

The standard states for all components are the pure gases at one atmosphere pressure.

The constant pressure heat capacities for the various constituents in calories/(°K.gm.mole) with  $T_K$  in °K are all of the form

$$C_{p_i} = A_i + B_i T_K + C_i T_K^2 \quad (2)$$

For the gases involved here, the constants are as follows:

Gas	A	B	C
CO	6.25	$2.091 \times 10^{-3}$	$-0.459 \times 10^{-6}$
O <sub>2</sub>	6.13	$2.990 \times 10^{-3}$	$-0.806 \times 10^{-6}$
CO <sub>2</sub>	6.85	$8.533 \times 10^{-3}$	$-2.475 \times 10^{-6}$
N <sub>2</sub>	6.30	$1.819 \times 10^{-3}$	$-0.345 \times 10^{-6}$

The ideal gas law may be assumed for this low pressure reaction. If the products from the reactor are at atmospheric pressure:

- What is the maximum temperature which the gases may attain, i.e., the adiabatic flame temperature for the ten percent excess air case described above?
- Show quantitatively what will happen to the flame temperature if the amount of air used is varied from 0.6 to 1.8 times the stoichiometric amount in steps of 0.1.
- How much air should be used to obtain the highest possible flame temperature?

Adiabatic Flame Temperature for Carbon Monoxide Oxidation

Solution Method

1. Nomenclature

- \*  $A_i$  = constant in the heat capacity equation for ith gas.
- \*  $B_i$  = constant in the heat capacity equation for ith gas.
- \*  $C_i$  = constant in the heat capacity equation for ith gas.
- $C_{P_i}$  = heat capacity of ith component gas, cal./(gm.mole<sup>o</sup>K).
- $\Delta C_p$  = heat capacity difference (products minus reactants) for reaction, cal./(gm.mole<sup>o</sup>K).
- $\Delta G_T^o$  = standard free energy change for the reaction at temperature T, cal./gm.mole CO.
- $\Delta H_p$  = enthalpy change for product gases between  $T_r$  and T, cal./gm.mole CO in feed.
- $\Delta H_R$  = enthalpy change of reaction at  $T_r$  for conversion of z gram moles of CO, cal.
- $\Delta H_T^o$  = standard enthalpy change for the reaction at temperature T, cal./gm.mole CO.
- $K_a$  = thermodynamic equilibrium constant.
- $K_p$  = pressure-based equilibrium constant.
- N = total moles of gases in product per mole of CO in feed.
- $n_O$  = moles of oxygen per mole of CO in feed.
- \*  $n_i$  = number of gram moles of ith component gas in product.
- P = total pressure, atm.
- $p_{CO}$  = partial pressure of CO at equilibrium conditions, atm.
- $p_{CO_2}$  = partial pressure of CO<sub>2</sub> at equilibrium conditions, atm.
- $p_{O_2}$  = partial pressure of O<sub>2</sub> at equilibrium conditions, atm.
- T = temperature of product gases, <sup>o</sup>K.
- $T_0$  = reference temperature for which  $\Delta G_T^o$  and  $\Delta H_T^o$  are known, <sup>o</sup>K.
- $T_K$  = temperature in <sup>o</sup>K.
- $T_r$  = temperature of feed gases, <sup>o</sup>K.
- $x_{CO}$  = mole fraction of CO at equilibrium conditions.
- $x_{CO_2}$  = mole fraction of CO<sub>2</sub> at equilibrium conditions.
- $x_{O_2}$  = mole fraction of O<sub>2</sub> at equilibrium conditions.
- z = fractional conversion of CO to CO<sub>2</sub> at equilibrium temperature T.

---

*	<u>i</u>	<u>Component</u>
	1	CO
	2	O <sub>2</sub>
	3	CO <sub>2</sub>
	4	N <sub>2</sub>

2. Material Balance

The problem will be worked where possible in Metric units, basing all calculations on one gram mole of CO in the feed gases. Let  $n_0$  be the number of moles of  $O_2$  per mole of CO in the feed stream and  $z$  be the fractional conversion of CO to  $CO_2$ . Then the moles of the various constituents of the feed and product gases are given by:

	CO	O <sub>2</sub>	CO <sub>2</sub>	N <sub>2</sub>	
Feed (70°F)	1	$n_0$	0.0	$\frac{79}{21} n_0$	(4)
Product (T)	$1-z$	$n_0 - \frac{z}{2}$	$z$	$\frac{79}{21} n_0$	

3. Heat Balance

For an adiabatic reaction, the reacting system exchanges no heat with its surroundings. The enthalpy change for the overall process ( $H_{\text{products}} - H_{\text{reactants}}$ ) must therefore equal zero. The process can be viewed as taking place in two stages: 1) Reaction of the entering gases at the inlet temperature  $T_r$ , and 2) Elevation of the temperature of the products (including any unreacted starting materials) from reaction temperature  $T_r$  to the final adiabatic flame temperature,  $T$ . The enthalpy change of reaction  $\Delta H_R$  at temperature  $T_r$  per mole of CO in the feed at conversion fraction  $z$  is given by

$$\Delta H_R(T_r) = z \cdot \Delta H_{T_r}^{\circ} \quad (5)$$

The enthalpy change for the products  $\Delta H_p$  between temperature  $T_r$  and temperature  $T$  is given by

$$\Delta H_p = \sum_{i=1}^4 \left[ n_i \int_{T_r}^T C_{p_i} dT_K \right] \quad (6)$$

where  $C_{p_i}$  is the heat capacity and  $n_i$  the number of gram moles of the  $i$ th component gas in the product mixture. The subscript  $i$  assumes a different value for each of the component gases, i.e.,  $i=1$  for CO, 2 for  $O_2$ , and so forth. Since the heat capacity equations are in terms of °K,  $T_r$  and  $T$  must be in °K. Both  $\Delta H_R$  and  $\Delta H_p$  are in calories per mole of CO in the inlet gases.

In terms of the heat capacity equations given, the integral of equation 6 is given by:

$$\int_{T_r}^T C_{p_i} dT_K = \int_{T_r}^T \left[ A_i + B_i T_K + C_i T_K^2 \right] dT_K \quad (7)$$

$$= A_i (T - T_r) + \frac{B_i (T^2 - T_r^2)}{2} + \frac{C_i (T^3 - T_r^3)}{3}$$

Combining equations (5) and (7) to produce an enthalpy balance for the overall process,

$$\Delta H_{\text{overall process}} = \Delta H_R(T_r) + \Delta H_p = 0$$

or

$$z \cdot \Delta H_{T_r}^{\circ} = - \sum_{i=1}^4 \left[ n_i \left[ A_i (T - T_r) + \frac{B_i (T^2 - T_r^2)}{2} + \frac{C_i (T^3 - T_r^3)}{3} \right] \right] \quad (8)$$

#### 4. Equilibrium Considerations

Let us define a "pressure-based" equilibrium constant by

$$K_p = \frac{p_{CO_2}}{p_{CO} \cdot p_{O_2}^{1/2}} \quad (9)$$

or, in terms of mole fractions (assuming ideal solution behavior),

$$K_p = \frac{x_{CO_2} P}{x_{CO} \cdot P \cdot (x_{O_2} \cdot P)^{1/2}} \quad (10)$$

Since, at equilibrium, the total number of moles of gas from 4 is given by

$$N = 1 - z + n_0 - \frac{z}{2} + z + \frac{79}{21} n_0 = 1 - \frac{z}{2} + \frac{100}{21} n_0, \quad (11)$$

the appropriate equilibrium mole fractions are given by:

$$\begin{aligned} x_{CO} &= \frac{1 - z}{1 - \frac{z}{2} + \frac{100}{21} n_0} \\ x_{CO_2} &= \frac{z}{1 - \frac{z}{2} + \frac{100}{21} n_0} \\ x_{O_2} &= \frac{n_0 - \frac{z}{2}}{1 - \frac{z}{2} + \frac{100}{21} n_0} \end{aligned} \quad (12)$$

Substitution into equation 10 yields

$$K_p = \frac{z}{1-z} \cdot \left[ \frac{1 - \frac{z}{2} + \frac{100}{21} n_0}{(n_0 - \frac{z}{2}) P} \right]^{1/2} \quad (13)$$

The thermodynamic equilibrium constant  $K_a$  is given by

$$K_a = e^{\frac{-\Delta G_T^{\circ}}{RT}}, \quad (14)$$

where  $\Delta G_T^{\circ}$  is the standard free energy change at temperature T, and R is the gas constant, 1.987 in units of (calories/<sup>o</sup>K.gm.mole). The quantity  $\Delta G_T^{\circ}/T$  can be determined for any temperature T, if its value at one temperature  $T_0$  is known, by integrating the thermodynamic relationship

$$\left[ \frac{\partial \left( \frac{\Delta G_T^{\circ}}{T} \right)}{\partial T} \right]_P = - \frac{\Delta H_T^{\circ}}{T^2} = - \frac{\Delta H_{T_0}^{\circ} + \int_{T_0}^T \Delta C_p dT_K}{T^2} \quad (15)$$



where  $\Delta C_p = C_{pCO_2} - C_{pCO} - 1/2 C_{pO_2}$ . In terms of the constants from (3),

$$\Delta C_p = -2.465 + 4.947 \times 10^{-3} T_K - 1.613 \times 10^{-6} T_K^2 \quad (16)$$

The expression for  $\Delta H_T^0$  as a function of temperature is then given by

$$\Delta H_T^0 = \Delta H_{T_0}^0 + \int_{T_0}^T \Delta C_p \, dT_K$$

or

$$\Delta H_T^0 = \Delta H_{T_0}^0 - 2.465(T-T_0) + 2.473 \times 10^{-3}(T^2-T_0^2) - 0.5376 \times 10^{-6}(T^3-T_0^3). \quad (17)$$

Equation 17 can be rewritten in the form

$$\Delta H_T^0 = -2.465T + 2.473 \times 10^{-3}T^2 - 0.5376 \times 10^{-6}T^3 + INT1, \quad (18)$$

where the integration constant INT1 is given by

$$INT1 = \Delta H_{T_0}^0 + 2.465T_0 - 2.473 \times 10^{-3}T_0^2 + 0.5376 \times 10^{-6}T_0^3 \quad (19)$$

To find  $\Delta G_T^0$ , integrate both sides of equation 15 between temperatures  $T_0$  and  $T$ .

$$\frac{\Delta G_T^0}{T} = - \int_{T_0}^T \frac{\Delta H_T^0}{T^2} \, dT + \frac{\Delta G_{T_0}^0}{T_0} \quad (20)$$

Substitution of  $\Delta H_T^0$  from equation 18 yields, for the value of the integral in 20,

$$- \int_{T_0}^T \frac{\Delta H_T^0}{T^2} \, dT = \frac{INT1}{T} + 2.465 \ln T - 2.473 \times 10^{-3}T + 0.2688 \times 10^{-6}T^2 + INT2 \quad (21)$$

where the integration constant INT2 is given by

$$INT2 = - \frac{INT1}{T_0} - 2.465 \ln T_0 + 2.473 \times 10^{-3}T_0 - 0.2688 \times 10^{-6}T_0^2 \quad (22)$$

Equation 20 can now be evaluated as

$$\frac{\Delta G_T^0}{T} = INT1/T + 2.465 \ln T - 2.473 \times 10^{-3}T + 0.2688 \times 10^{-6}T^2 + INT3 \quad (23)$$

where the integration constant INT3 is given by

$$INT3 = INT2 + \Delta G_{T_0}^0/T_0 \quad (24)$$

Since  $\Delta G^0$  at temperature  $T_0 = 298.15^\circ K$  ( $25^\circ C$ ) is given as -111,600 B.T.U./lb.mole of CO or -62,000 cal./gm.mole of CO) and  $\Delta H^0$  at the same temperature is given as -121,700 B.T.U./lb.mole of CO or -67,611 cal./gm.mole of CO), all the information necessary to compute the equilibrium constant  $K_a$  at any temperature  $T$  is available.

#### 5. The Equations to be Solved:

It can be shown that  $K_a$  of equation 14 is also given by

$$K_a = \frac{a_{CO_2}}{a_{CO} \cdot (a_{O_2})^{1/2}} \quad (25)$$

where the a's are thermodynamic activities. For each constituent,  $a = f/f_0$ , where f is the fugacity of the component and  $f_0$  is the fugacity of the component in the standard state. Since the standard state for each gas is given as one atmosphere, and since the gases are to be assumed ideal,  $f_0=1$ . and  $f=p$  (partial pressure of the component). Therefore,  $K_a$  from equation 14 and  $K_p$  from equation 13 are identical, i.e. the chemical equilibrium relationship is given by:

$$\text{or } \frac{K_p}{(1-z)} \cdot \left[ \frac{1 - \frac{z}{2} + \frac{100 \cdot n_0}{21}}{(n_0 - \frac{z}{2}) \cdot P} \right]^{1/2} - e^{-\frac{[\Delta G_T^0]}{RT}} = 0 \quad (26)$$

The final equation resulting from the enthalpy balance was derived earlier (equation 8) and is reproduced here for convenience.

$$z \cdot \Delta H_{T_r}^0 + \sum_{i=1}^4 \left[ n_i \left[ A_i (T-T_r) + B_i (T^2-T_r^2)/2 + C_i (T^3-T_r^3)/3 \right] \right] = 0 \quad (8)$$

Note that once values for the parameters  $T_0$ ,  $T_r$ ,  $\Delta H_{T_0}^0$ ,  $\Delta H_{T_r}^0$ ,  $\Delta G_{T_0}^0$ , P, and  $n_0$  have been supplied, these two equations (26 and 8) contain only the unknowns z and T. The problem then is to solve this set of two simultaneous equations for z and T, given the following values from the problem statement:

$$\begin{aligned} T_0 &= 298.15^\circ\text{K} \quad (25^\circ\text{C}) \\ T_r &= 294.3^\circ\text{K} \quad (70^\circ\text{F}) \\ \Delta H_{T_r}^0 &= -6761 \text{ cal/gm.mole CO} \\ \Delta G_{T_0}^0 &= -62000 \text{ cal/gm.mole CO} \\ P &= 1 \text{ atm.} \end{aligned}$$

$\Delta H_{T_r}^0$  can be computed from equation 17 with  $T=T_r$ .  $n_0$ , the  $O_2/CO$  ratio, is a variable but assumes a fixed value for any one solution.

#### 6. Mechanism of Solution:

Since the  $n_i$  (see 4) are linear in z, equation 8 is also linear in z. It is therefore possible to solve for z as follows:

$$z = \frac{- \left[ I_{C_{p_1}} + n_0 I_{C_{p_2}} + n_4 I_{C_{p_4}} \right]}{\left[ \Delta H_{T_r}^0 - I_{C_{p_1}} - 1/2 \cdot I_{C_{p_2}} + I_{C_{p_3}} \right]} \quad (27)$$

where

$$I_{C_{p_i}} = A_i (T-T_r) + B_i (T^2-T_r^2)/2 + C_i (T^3-T_r^3)/3 \quad (28)$$

$n_4$  is the number of moles of nitrogen per mole of CO fed. The reason for leaving  $n_4$  in the equation is that it is a simple matter to generalize the computer program to compute the flame temperature for either air or pure oxygen in the feed gases. In the air case,  $n_4 = \frac{79}{21} n_0$ ; for pure oxygen,  $n_4 = 0.0$ .

Substitution of  $z$  from equation 27 into equation 26 results in a single highly non-linear equation in the variable  $T$  of the form

$$g(T) = 0 \quad . \quad (29)$$

The problem is now reduced to finding the value of  $T$ , i.e. the root, which satisfies (29). Since it is not possible to solve for  $T$  analytically, some numerical or trial-and-error solution technique must be employed.

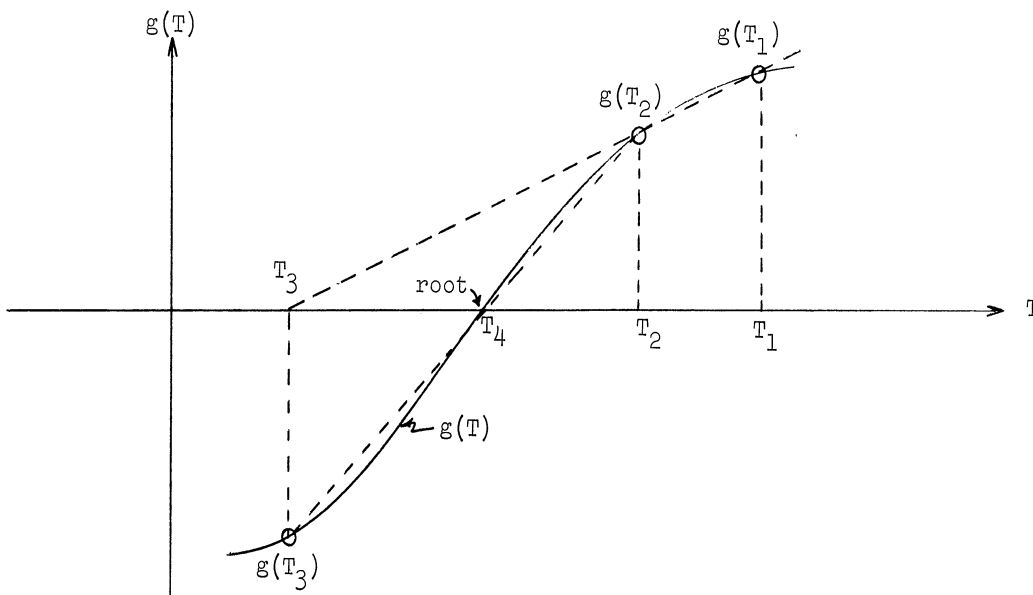
The method used in the computer program which follows is similar to Lin's root-finding procedure. This method involves the evaluation of the function  $g(T)$  for two different values of  $T$ , say  $T_1$  and  $T_2$  (see figure) and then extrapolating (or, as the case may be, interpolating) linearly to find a new, and hopefully better, estimate of the root,  $T_3$ . After evaluation of  $g(T_3)$ , the procedure is repeated, using the straight line determined by the points  $(T_2, g(T_2))$  and  $(T_3, g(T_3))$ . This cycle is continued using the simple algorithm

$$T_{n+1} = \frac{g(T_{n-1}) \times T_n - g(T_n) \times T_{n-1}}{g(T_{n-1}) - g(T_n)} \quad (30)$$

until either

$$\begin{aligned} |g(T_n)| &\ll \epsilon_1 \\ \text{or } |T_{n+1} - T_n| &\ll \epsilon_2 \end{aligned} \quad (31)$$

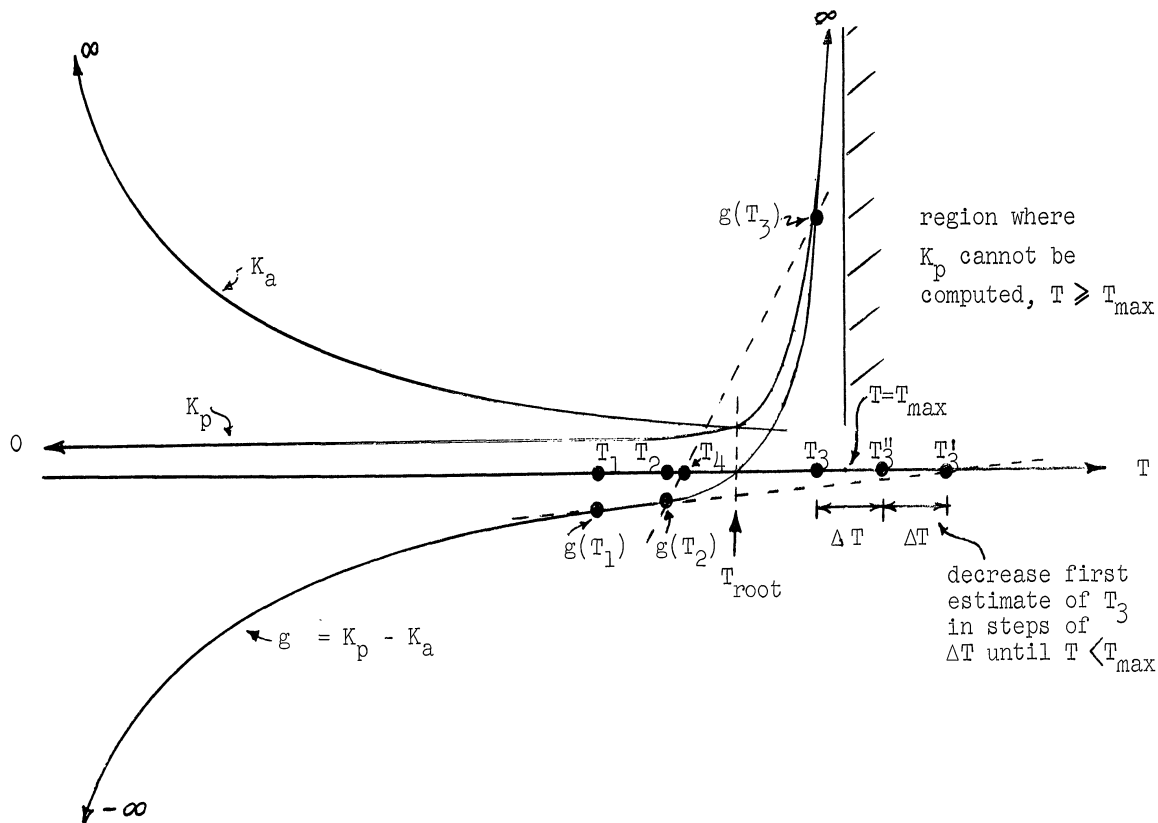
where  $\epsilon_1$  and  $\epsilon_2$  are small positive tolerance values used as criteria for terminating the iteration process. Since the method may not converge, it is also wise to put an upper limit on the number of iterations performed.



Schematic of the Iterative Procedure

The qualitative behavior of  $K_p$ ,  $K_a$ , and  $g$  as functions of temperature  $T$  are shown in the figure below.  $T_{max}$  is the value of  $T$  for which equation (8) yields a value  $z = 2 \cdot n_0$  or  $z = 1$ . Since the factors  $(n_0 - z/2)^{0.5}$  and  $(1 - z)$  appear in the denominator of the expression for  $K_p$  (see equation 13),  $K_p$  becomes infinite when either  $z = 2 \cdot n_0$  or  $z = 1$ . In addition, for  $T > T_{max}$ ,  $K_p$  must not be computed, since this situation corresponds to the physically meaningless cases  $z > 2 \cdot n_0$  (over 100% oxygen consumption) or  $z > 1.0$  (over 100% carbon monoxide consumption). Because of the highly nonlinear character of the function  $g(T)$  for values of  $T$  not near the root  $T_{root}$ , it is possible that a linear extrapolation through two points  $(T_1, g(T_1))$  and  $(T_{i+1}, g(T_{i+1}))$  will produce a new iterate  $T_{i+2} \geq T_{max}$  (or even that the first two values,  $T_1$  and/or  $T_2$ , which are needed to start the iterative procedure, may be in the forbidden region). A special test must be made on the value of  $z$  computed from equation (8) for the new value of  $T$ ,  $T_{i+2}$ . When  $z(T_{i+2}) \geq 2 \cdot n_0$  or  $z(T_{i+2}) \geq 1$ , a new value of  $T_{i+2}$  must be found by some other method before the extrapolation-interpolation algorithm of the previous page can be applied again. In the computer program which follows, the value of  $T_{i+2}$  is simply decremented arbitrarily (and repeatedly) by an amount  $\Delta T$  until  $T_{i+2} < T_{max}$ . The algorithm is then resumed to find  $T_{i+3}$ . Once a computed pair of  $T$  values is sufficiently close to the root  $T_{root}$ , i.e. in the region near  $T_{root}$  where  $g(T)$  is approximately linear, the procedure converges to the answer quite rapidly.

To illustrate the procedure, consider the situation shown in the figure. Two initial assumptions for temperature are  $T_1$  and  $T_2$ . Since both are in the permitted temperature region,  $g(T_1)$  and  $g(T_2)$  can both be computed. Extrapolating linearly produces a new iterate  $T_3' > T_{max}$ . Decrementing  $T_3'$  by an amount  $\Delta T$  produces a new temperature  $T_3''$  which is still larger than  $T_{max}$ . After decrementing by  $\Delta T$  again, a temperature  $T_3$  is found. Since the new value is less than  $T_{max}$ ,  $g(T_3)$  is computed. A linear interpolation produces a new temperature estimate  $T_4$ , etc.



7. The Computer Program

In the computer program which follows, the following symbols are used for the problem variables described in the table of nomenclature, page I50.

<u>MAD Symbol</u>	<u>Problem Variable</u>	<u>MAD Symbol</u>	<u>Problem Variable</u>
A(I)	$A_i$	NITRO	$n_4$
B(I)	$B_i$	NZERO	$n_0$
C(I)	$C_i$	P	P
DGTZ	$\Delta G_{T_0}^0$	T	T
DHTR	$\Delta H_{T_r}$	TR	$T_r$
DHTZ	$\Delta H_{T_0}^0$	TZ	$T_0$
KA	$K_a$	Z	z
KP	$K_p$		

The computer program is written to construct two tables. The first is a table of JMAX+1 line entries. Each line contains four items, RATIO(J), CONV(J), TF(J), and TC(J) where  $0 \leq J \leq JMAX$ . RATIO is a value of NZERO and CONV(J), TF(J) and TC(J) are the corresponding values of conversion z, and flame temperature T in  $^{\circ}F$  and  $^{\circ}C$ . The table is prepared starting with a minimum value of NZERO, MIN, which is placed in RATIO(0). NZERO is incremented by an amount DELTA=BIGD for successive lines; these values of NZERO are stored in successive entries RATIO(1), RATIO(2),... etc., until NZERO > MAX. The value of NZERO=MAX is stored in RATIO(JMAX).

After preparation of this first-pass table which has the flame temperature and conversion information for all values of NZERO=MIN, MIN+BIGD, MIN+2\*BIGD,...,MAX, the table is searched to find the largest value of TF (i.e., the highest computed flame temperature), TBIG. A second table is then prepared using a smaller increment, DELTA=SMALLD, such that RATIO(0)=TBIG-BIGD, RATIO(1)=TBIG-BIGD+SMALLD, RATIO(3)=TBIG-BIGD+2\*SMALLD, etc. This table will then have entries for values of NZERO which differ by no more than an amount BIGD from the value of NZERO at the highest temperature in the first-pass table. The table increment in this case is equal to SMALLD. The completed table is then searched again for the largest value of TF, which is the maximum possible flame temperature ( within a tolerance on NZERO equal to SMALLD).

The same program segment is used to generate both tables. The parameters are adjusted accordingly after preparation of the first-pass table.

This program also allows the option of feeding pure oxygen as well as air by reading as data a value for the variable AIR, AIR=1 for the air case; AIR $\neq$ 1 for the oxygen case. The program is written in a rather general way, and would not require major structural changes to allow the computation of similar tables for any adiabatic-isobaric process.

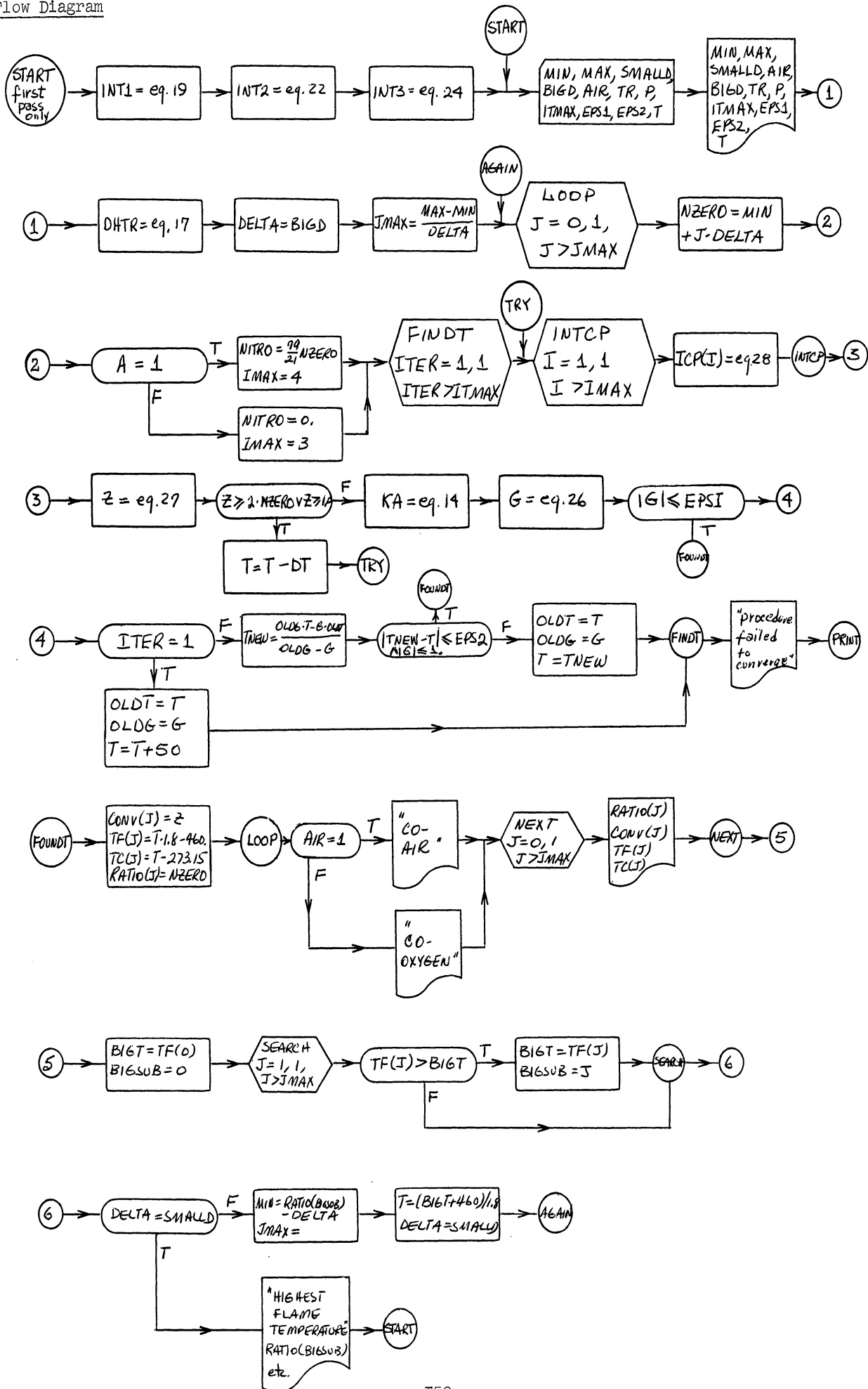
Adiabatic Flame Temperature for Carbon Monoxide Oxidation

Other symbols not previously defined which are used in the program are:

<u>MAD Symbol</u>	<u>Meaning</u>
AIR	AIR=1, feed gas is air; A≠1, feed gas is pure oxygen.
BIGD	Large increment in NZERO for first-pass table.
BIGT	Highest temperature found in first- and second-pass tables.
BIGSUB	Subscript of highest temperature in first- and second-pass tables.
CONV(J)	Conversion (Z) for Jth table entry.
DELTA	Increment in NZERO for tables: =SMALLD on second-pass table, = BIGD on first-pass table.
EPS1	Convergence criterion (See 31).
EPS2	Convergence criterion (See 31).
G	Function of ith value of T whose root is the flame temperature.
I	Counting variable.
IMAX	Maximum number of components in product: 4 when AIR=1; 3 when AIR≠1.
INT1	Integration constant (See 19).
INT2	Integration constant (See 22).
INT3	Integration constant (See 24).
ITER	Counter for the number of iterations to find T.
ITMAX	Maximum number of iterations permitted.
J	Counting variable.
JMAX	Maximum subscript on table entries, $0 \leq J \leq JMAX$ .
MAX	Maximum value of NZERO in table.
MIN	Minimum value of NZERO in table.
NITRO	$n_{N_2}$ , gm.moles of nitrogen: = 0 when AIR=0; = $\frac{79}{21}$ NZERO when AIR=1.
OLDG	i-lth value of function G generated in iterative procedure.
OLDT	i-lth value of temperature T generated in iterative procedure.
RATIO(J)	O <sub>2</sub> /CO ratio (NZERO) for Jth table entry.
SMALLD	Small increment in NZERO for second-pass table.
TC(J)	Flame temperature for Jth table entry, °C.
TF(J)	Flame temperature for Jth table entry, °F.
TNEW	i+1th value of temperature T generated in iteration procedure.
DT	Decrement in temperature $\Delta T$ when $T_{i+1} \geq T_{max}$ (see figure).

Example Problem No. 117

Flow Diagram



Adiabatic Flame Temperature for Carbon Monoxide Oxidation

MAD Program and Data

```

$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT, PUNCH OBJECT      FLAME000
R
  DIMENSION CONV(500), TF(500), TC(500), RATIO(500), ICP(4)
  INTEGER I, J, ITER, ITMAX, IMAX, JMAX, AIR, BIGSUB
R
R PRESET HEAT CAPACITY CONSTANTS A(I), B(I), AND C(I), THE
R REFERENCE TEMPERATURE TZ, THE STANDARD FREE ENERGY CHANGE
R AT TEMPERATURE TZ, AND THE STANDARD ENTHALPY CHANGE AT
R TEMPERATURE TZ. COMPUTE THE INTEGRATION CONSTANTS INT1,
R INT2, AND INT3.
R
  VECTOR VALUES A(1) = 6.25, 6.13, 6.85, 6.30
  VECTOR VALUES B(1) = 2.091E-3, 2.990E-3, 8.533E-3, 1.819E-3
  VECTOR VALUES C(1) = -0.459E-6, -0.806E-6, -2.475E-6, -0.345E-6
  VECTOR VALUES TZ = 298.15
  VECTOR VALUES DHTZ = -67611.
  VECTOR VALUES DGTZ = -62000.
  INT1 = DHTZ + 2.465*TZ-2.4735E-3*TZ*TZ+ 0.5376E-6*TZ*TZ*TZ
  INT2 = -INT1/TZ - 2.465*ELOG.(TZ)+2.4735E-3*TZ - 0.2688E-6
  1*TZ*TZ
  INT3 = INT2 + DGTZ/TZ
R
START READ AND PRINT DATA MIN, MAX, SMALLD, BIGD, AIR, TR, P,
  1 ITMAX, EPS1, EPS2, DELTAT, DT, T
  DHTR = -2.465*TR+2.4735E-3*TR*TR - 0.5376E-6*TR*TR*TR + INT1
  DELTA = BIGD
  JMAX = (MAX - MIN + DELTA/2.)/DELTA
AGAIN  R..... STATEMENTS FROM AGAIN THROUGH LOOP PREPARE TABLE .....
  THROUGH LOOP, FOR J=0,1,J.G.JMAX
  NZERO = MIN + J*DELTA
  R..... IS THIS THE AIR OR OXYGEN CASE .....
  WHENEVER AIR.E.1
    NITRO = 79./21.*NZERO
    IMAX = 4
  OTHERWISE
    NITRO = 0.0
    IMAX = 3
  END OF CONDITIONAL
  R..... ITERATE TO FIND T AT EQUILIBRIUM .....
  THROUGH FINDT, FOR ITER=1,1, ITER.G.ITMAX
  R ..... FOR ASSUMED T, COMPUTE ICP(I) VALUES AND Z .....
TRY   THROUGH INTC, FOR I=1,1, I.G. IMAX
INTCP ICP(I) = A(I)*(T-TR) + B(I)*(T*T-TR*TR)/2. + C(I)*(T*T*T-TR*
  1 TR*TR)/3.
  Z = (-ICP(1) - NZERO*ICP(2) - NITRO*ICP(4))/(DHTR - ICP(1) -
  1 ICP(2)/2. + ICP(3))
  R..... IS Z PHYSICALLY MEANINGFUL .....
  WHENEVER Z.GE.2.*NZERO .OR. Z.GE.1.0
    T = T - DT
    TRANSFER TO TRY
  END OF CONDITIONAL
  R..... T ESTIMATE IS LEGITIMATE, COMPUTE KA, KP, AND G .....
  KA = EXP.(-(INT1/T + 2.465*ELOG.(T)-2.4735E-3*T + 0.2688E-6
  1 *T*T + INT3)/1.987)
  KP= Z/(1.-Z)*((1.-Z/2.+NITRO+NZERO)/((NZERO-Z/2.)*P)).P.G.5
  G = KP - KA
  R ..... CONVERGENCE TEST ON SIZE OF FUNCTION G .....
  WHENEVER .ABS.G.LE.EPS1, TRANSFER TO FOUNDT
  R..... USE LINEAR EXTRAPOLATION ALGORITHM TO GET NEW T .....
  WHENEVER ITER.E.1
    OLD T = T
    OLD G = G
    T = T + DELTAT
  OTHERWISE
    TNEW = (OLDG*T - G*OLDT)/(OLDG - G)
  R ..... CONVERGENCE TEST ON SIZE OF TEMPERATURE CHANGE .....
  WHENEVER .ABS.(TNEW-T).LE.EPS2.AND..ABS.G.LE.1., TRANSFER
NEXT1 1 TO FOUNDT
  OLD T = T
  T = TNEW
  OLD G = G
FINCT  END OF CONDIIONAL

```



MAD Program and Data (continued)

```

        PRINT COMMENT $ PROCEDURE FAILED TO CONVERGE ON T $
        PRINT RESULTS J, NZERO, IMAX, NITRO, ITER, ICP(1)...ICP(4),
1 Z, KA, G, TNEW, OLDG, OLDT
        TRANSFER TO PRINT
FOUNDT  CONV(J) = Z
        TF(J) = T*1.8 - 460.
        TC(J) = T - 273.15
LOOP    RATIO(J) = NZERO
PRINT  WHENEVER AIR.E.1
        PRINT COMMENT $ADIABATIC FLAME TEMPERATURE FOR CO-AIR $
        OTHERWISE
        PRINT COMMENT $ADIABATIC FLAME TEMPERATURE FOR CO-OXYGEN$
        END OF CONDITIONAL
        THROUGH NEXT, FOR J=0,1,J.G.JMAX
NEXT    PRINT RESULTS RATIO(J), CONV(J), TF(J), TC(J)
        R..... FIND HIGHEST TEMPERATURE IN TABLE .....
        BIGT = TF(0)
        BIGSUB = 0
        THROUGH SEARCH, FOR J=1,1, J.G.JMAX
        WHENEVER TF(J).G.BIGT
            BIGT = TF(J)
            BIGSUB = J
SEARCH  END OF CONDITIONAL
        WHENEVER DELTA.E.SMALLD
        PRINT COMMENT $THE HIGHEST FLAME TEMPERATURE CONDITIONS W
        ITHIN AN OXYGEN/CARBON MONOXIDE RATIO TOLERANCE SMALLD IS $
        PRINT RESULTS RATIO(BIGSUB), CONV(BIGSUB), TF(BIGSUB),
1 TC(BIGSUB)
        TRANSFER TO START
        END OF CONDITIONAL
        R..... MODIFY PARAMETERS FOR SECOND-PASS TABLE .....
        MIN = RATIO(BIGSUB) - DELTA
        JMAX = (2.*DELTA+SMALLD/2.)/SMALLD
        T = (BIGT + 460.)/1.8
        DELTA = SMALLD
        PRINT COMMENT $1$
        TRANSFER TO AGAIN
        END OF PROGRAM

```

```

$ DATA
MIN = 0.30, MAX = 1.00, SMALLD = 0.005, BIGD = 0.05, AIR = 1, TR = 294.3
P = 1.0, ITMAX = 200, EPS1 = 1.E-4, EPS2 = 0.1, DT = 1.0, DELTAT = 10.5
T = 2400 *
MIN = 0.30, MAX = 1.00, SMALLD = 0.005, BIGD = 0.05, AIR = 0, TR = 294.3
P = 1.0, ITMAX = 200, EPS1 = 1.E-4, EPS2 = 0.1, DT = 1.0, DELTAT = 10.5
T = 3000. *
MIN = 0.30, MAX = 1.00, SMALLD = 0.005, BIGD = 0.05, AIR = 1, TR = 294.3
P = 2.0, ITMAX = 200, EPS1 = 1.E-4, EPS2 = 0.1, DT = 1.0, DELTAT = 10.5
T = 2400 *
MIN = 0.30, MAX = 1.00, SMALLD = 0.005, BIGD = 0.05, AIR = 0, TR = 294.3
P = 2.0, ITMAX = 200, EPS1 = 1.E-4, EPS2 = 0.1, DT = 1.0, DELTAT = 10.5
T = 3000. *

```

Adiabatic Flame Temperature for Carbon Monoxide Oxidation

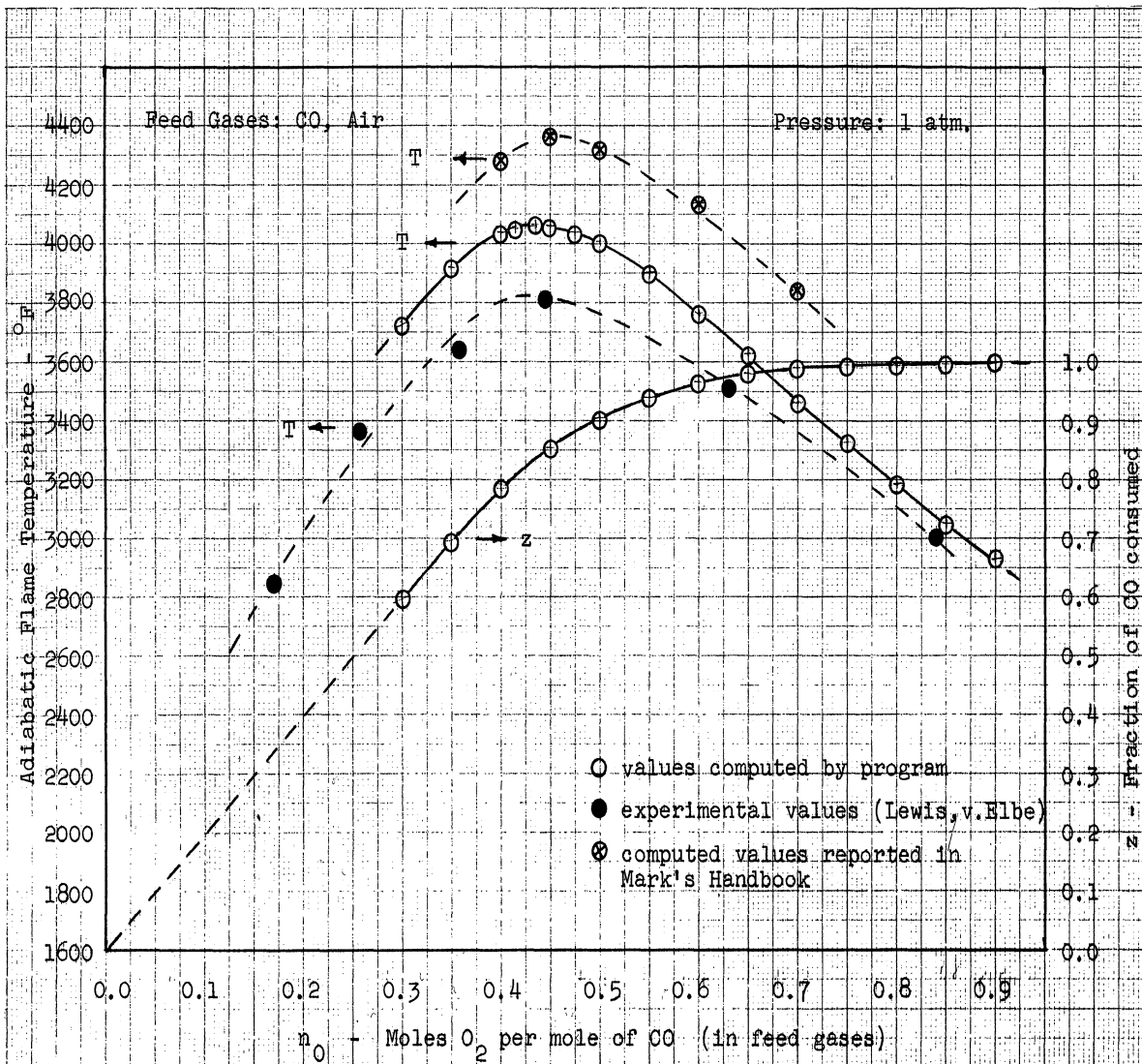
Computer Results

The following are the computed results for CO-air feed for the first and third data sets. These two cases are identical except for the pressure P. The results have been reorganized to conserve space. The flame temperature is given in degrees Fahrenheit and the first and second pass tables have been merged to produce one overall table with smaller increments in  $n_0$  near the maximum flame temperature.

$n_0$ moles $O_2$ /mole CO in feed	P = 1 atm.		P = 2 atm.	
	z fraction of CO converted	T Flame Temp. $^{\circ}F$	z fraction of CO converted	T Flame Temp. $^{\circ}F$
.300000	.599712	3723.942322	.599854	3724.742310
.350000	.697258	3922.688904	.698554	3929.376892
.400000	.784699	4042.157410	.790389	4069.327881
.405000	.792418	4048.224243	.798688	4077.940430
.410000	.799959	4053.363220	.806808	4085.570068
.415000	.807296	4057.464722	.814708	4092.055969
.420000	.814392	4060.392944	.822382	4097.397705
.425000	.821336	4062.574280	.829829	4101.604553
.430000	.828083	4063.825134	.837045	4104.695862
.435000	.834635	4064.177917	.844004	4106.577576
.440000	.840998	4063.675354	.850777	4107.588867
.445000	.847176	4062.360046	.857325	4107.583984
.450000	.853175	4060.273499	.863652	4106.596375
.455000	.859000	4057.455627	.869761	4104.670898
.460000	.864656	4053.944458	.875660	4101.853943
.465000	.870147	4049.775940	.881353	4098.190918
.470000	.875477	4044.983276	.886803	4093.535950
.475000	.880651	4039.598328	.892095	4088.282593
.480000	.885673	4033.650269	.897200	4082.310181
.485000	.890498	4026.968445	.902120	4075.655640
.490000	.895218	4019.951233	.906862	4068.354431
.495000	.899795	4012.444397	.911429	4060.439941
.500000	.904230	4004.469299	.915826	4051.943665
.550000	.941312	3903.070129	.951281	3940.947144
.600000	.966407	3772.191833	.973551	3797.491699
.650000	.981872	3625.161652	.986310	3639.885559
.700000	.990531	3473.495911	.993064	3481.415344
.750000	.995132	3325.872559	.996491	3329.895905
.800000	.997495	3186.568024	.998210	3188.582825
.850000	.998699	3057.110291	.999075	3058.122101
.900000	.999316	2937.504120	.999515	2938.016418

Discussion of Results

1. CO-Air: Tabulated results for the flame temperature and fraction of CO converted at pressures of 1. and 2. atmospheres are shown on the previous page for  $0.3 \leq n_0 \leq 0.9$ , i.e. for  $O_2$  to CO ratios varying from 0.6 to 1.8 times the stoichiometric amount. The flame temperature,  $T$ , and fraction of CO converted,  $z$ , as functions of  $n_0$  are shown in the figure below for a pressure of 1. atmosphere. Computed flame temperature values reported in Mark's Mechanical Engineers Handbook (source unspecified) and the experimental data of Lewis and von Elbe tabulated in Lange's Handbook of Chemistry are shown along with the values computed by the program. Reaction is nearly complete for  $0.4 < n_0$  and  $n_0 > 0.75$ , i.e. the limiting component ( oxygen for  $n_0 < 0.5$  and carbon monoxide for  $n_0 > 0.5$  ) is essentially consumed for these conditions. For  $0.4 \leq n_0 \leq 0.75$  the extent of reaction is smaller than theoretically possible ( from the viewpoint of stoichiometry only), being only 0.916 at the stoichiometric ratio  $n_0 = 0.5$ . As would be expected from the chemical equation, increased pressure (see the tabulated results) raises both the fraction of CO converted and the flame temperature for the same value of  $n_0$ . Maximum flame temperatures occur at  $n_0 = 0.435$  at 1 atm. pressure ( $T=4064.2^\circ F$ ) and at  $n_0 = 0.440$  at 2 atm. pressure ( $T=4107.6^\circ F$ ). In both cases therefore, maximum temperature occurs in a stoichiometrically "fuel rich" (oxygen deficient) reaction mixture.



## Adiabatic Flame Temperature for Carbon Monoxide Oxidation

2. CO-O<sub>2</sub>: Computed results for the combustion of carbon monoxide with pure oxygen are shown in the figure below, along with experimental values of Lewis and von Elbe reported in Lange's Handbook of Chemistry. In this case the fraction of CO reacted is considerably smaller than stoichiometrically possible. At the high temperatures generated, the equilibrium constant is fairly small (of order 1.) and so reaction is not nearly complete in most cases. The highest flame temperature found by the program for 1. atm. pressure was 5436.9°F and occurred at  $n_0 = 0.5$ , i.e. at the stoichiometric ratio, and varies only slightly over the range  $0.45 < n_0 < 0.55$ .

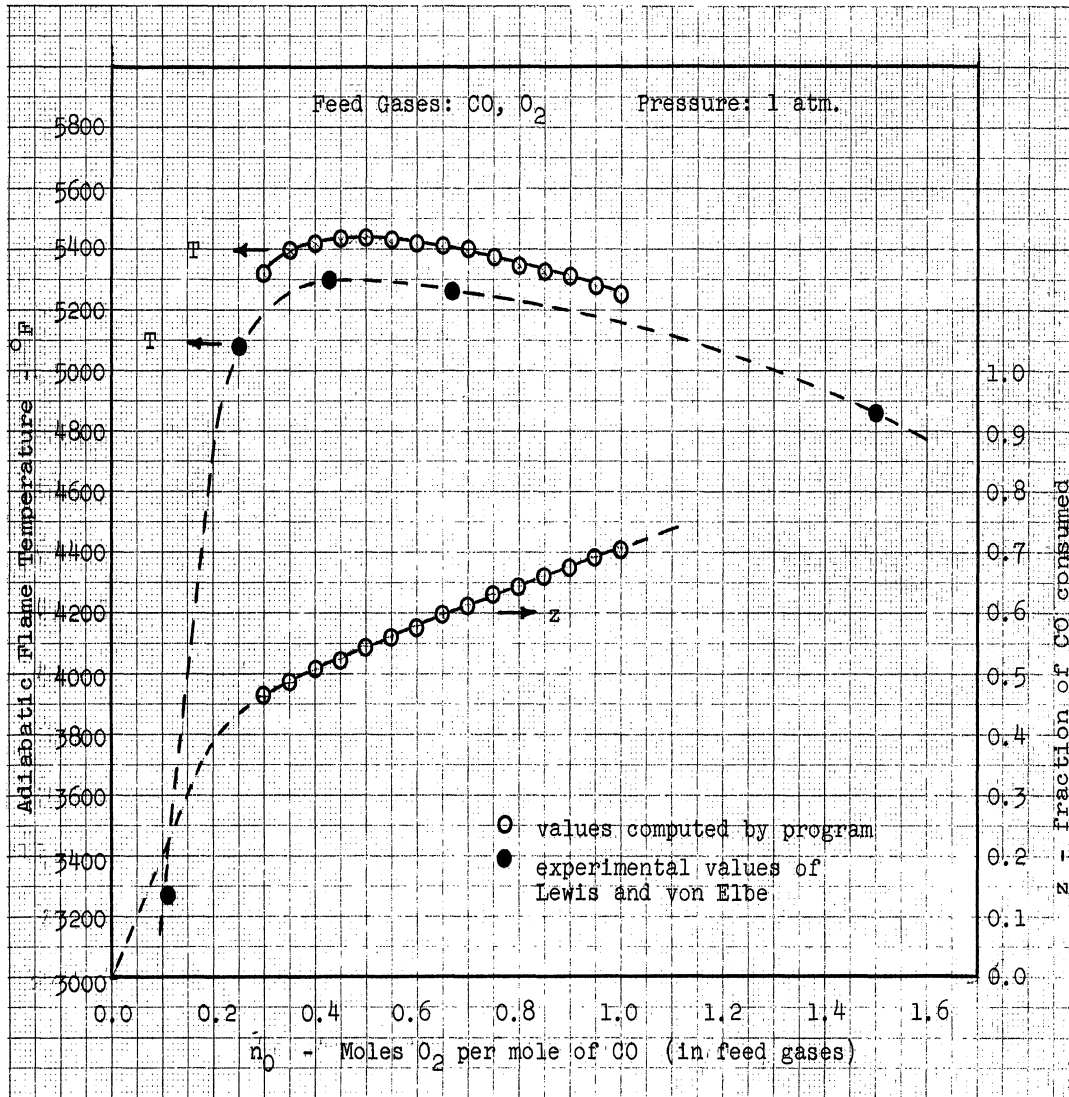


Table of Maximum Adiabatic Flame Temperatures

Components	Pressure	$n_0$	$z$	Flame Temperature
CO - Air	1.0 atm.	0.435	0.8346	4064.2°F
CO - Air	2.0 atm.	0.440	0.8508	4107.6°F
CO - O <sub>2</sub>	1.0 atm.	0.500	0.5446	5436.9°F
CO - O <sub>2</sub>	2.0 atm.	0.500	0.5576	5601.4°F

Example Problem No. 118

VAPOR-LIQUID EQUILIBRIUM

by

Roger Bonnecaze

Department of Chemical and Metallurgical Engineering

The University of Michigan

Course: Thermodynamics I

Credit Hours: 5

Level: Sophomore or Junior

Introduction

The first course in Thermodynamics for chemical engineering undergraduates consists of two hours of lecture, two hours of recitation, and an associated four-hour laboratory session. This problem is a two-fold one involving experimental work in the laboratory and subsequent preparation of a computer program which uses the data.

Statement of the Problem Given to Student

The two parts of the problem are: 1) The determination of the vapor-liquid equilibrium in the acetone-methanol system, and 2) the writing of a MAD program to calculate Y-X and T-X diagrams at constant pressure for the above system. You are expected to understand the significance of equilibrium, activity coefficient, and the Gibbs-Duhem equation.

In this experiment you are to determine the equilibrium relationship for the vapor-liquid system acetone-methanol. For ideal solutions the partial pressure ( $P_i$ ) of the  $i$ th component in the vapor is equal to the product of the mole fraction ( $X_i$ ) of the component in the liquid and its vapor pressure ( $P_i^0$ ) at the boiling temperature of the solution, i.e.,

$$P_i = X_i P_i^0 \quad (\text{Raoult's Law}). \quad (1)$$

For non-ideal solutions, a factor,  $\gamma_i$ , called the activity coefficient, must be included in the above expression, i.e.,

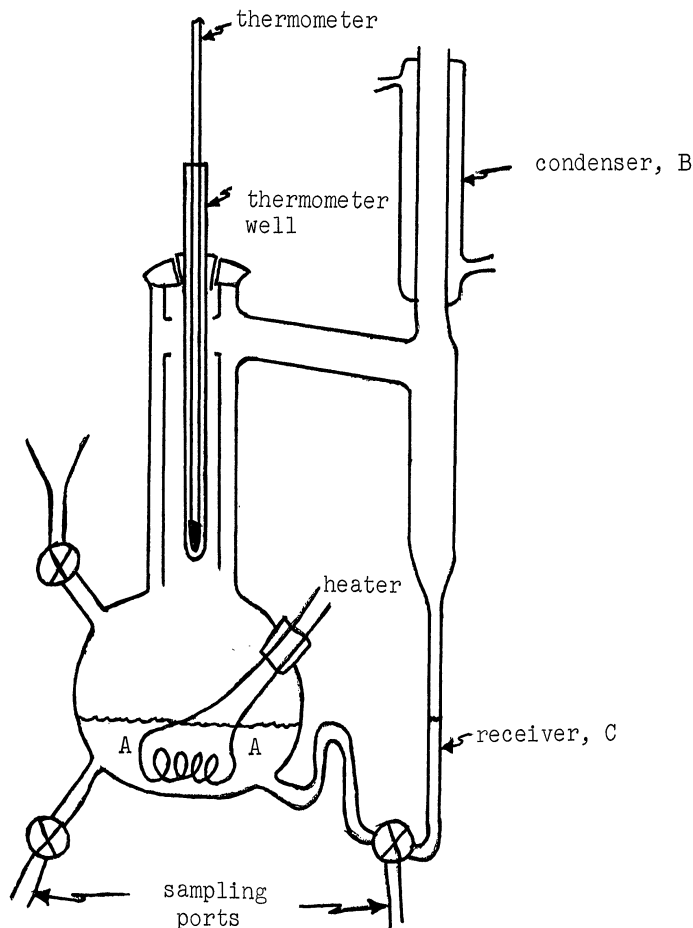
$$P_i = \gamma_i X_i P_i^0 \quad (2)$$

The activity coefficient is a measure of the departure from ideality and it is a function of temperature, pressure and composition. In most cases the temperature and pressure dependency may be assumed negligible. Thus the activity coefficient is primarily a function of composition in the liquid and the problem is to determine this functional dependency.

An Othmer equilibrium still is available for this purpose in the laboratory. This is a circulation still (see schematic below) in which the vapors evolved from the boiling mixture in the distilling flask, A, pass to a total condenser, B, where they are condensed and collected in a receiver, C. After filling the receiver, the condensate returns to the distilling flask A.

## Vapor-Liquid Equilibrium

At steady state the liquid in the distilling flask and the condensate in the receiver are in equilibrium. Since the condensate in the receiver has the same composition as the vapor rising from the boiling liquid, the partial pressure of component  $i$  in the vapor can be calculated from its composition in the condensate and the known pressure exerted on the system.



Othmer Equilibrium Still

### I. Experimental

#### Procedure

- A. Analysis of liquid samples. The composition of the binary mixture will be determined by measuring the refractive index of the unknown sample and comparing this value with a known sample. A refractometer is available in the laboratory. A standard curve may be prepared as follows:
1. Prepare three known samples containing 25, 50, and 75 wt.% acetone. Use the weighing bottles and the analytical balance available in the laboratory.
  2. Measure the refractive indices of these three samples and the two pure components. Note the temperature. Make a plot of refractive index vs. composition. From this plot and the refractive index of any sample of acetone and methanol the approximate composition of the sample may be obtained.

B. Operation of the Othmer Still.

1. Close all ports on the still except the feed port.
2. Fill the distilling flask according to the following table:
 

<u>Run</u>	<u>ml. Acetone</u>	<u>ml. Methanol</u>
1	64	136
2	110	90
3	148	52
3. Turn on the water to the condenser.
4. Adjust the variac so that the current to the heater is 6-7 amp.
5. Note the temperature at 30 sec. intervals.
6. When the receiver is filled with liquid, turn the stopcock connecting the receiver and the distilling flask so that condensate will flow to the boiling liquid.
7. When the temperature becomes steady, start withdrawing samples of liquid and condensate every ten minutes.
8. After about 30 minutes the refractive indices of these samples should remain constant. This indicates that steady state has been obtained. Run the still for 10 more minutes and then withdraw a sample of liquid and condensate. These samples will give the equilibrium compositions of the liquid and vapor for use in later calculations.
9. Record the boiling temperature and the atmospheric pressure.

II. Vapor-Liquid Equilibrium

Having found the equilibrium relationships for acetone-methanol, process the data and determine whether or not it is thermodynamically consistent.

Solution

Adopt the following nomenclature:

- $X_1$  = mole fraction of acetone in liquid.  
 $X_2$  = mole fraction of methanol in liquid.  
 $Y_1$  = mole fraction of acetone in vapor.  
 $P_1$  = partial pressure of acetone in vapor, mm. Hg.  
 $P_1^0$  = vapor pressure of pure acetone at boiling temperature, mm. Hg.  
 $P_2^0$  = vapor pressure of pure methanol at boiling temperature, mm. Hg.  
 $P$  = total pressure, mm. Hg.  
 $T$  = boiling temperature, °K.  
 $A_1$  = constant in vapor pressure equation for pure acetone (see equation 7).  
 $A_2$  = constant in vapor pressure equation for pure methanol (see equation 8).  
 $B_1$  = constant in vapor pressure equation for pure acetone (see equation 7).  
 $B_2$  = constant in vapor pressure equation for pure methanol (see equation 8).  
 $A$  = constant in Margules Equation (see equation 5).  
 $B$  = constant in Margules Equation (see equation 5).  
 $\gamma_1$  = activity coefficient of acetone.  
 $\gamma_2$  = activity coefficient of methanol.

## Vapor-Liquid Equilibrium

### Hand Calculation

The student is expected to use his experimental data in the following calculations, to be done by hand.

Calculate the activity coefficients and their logarithms from the expressions:

$$\gamma_1 = \frac{Y_1 P}{X_1 P_1^0} \qquad \gamma_2 = \frac{Y_2 P}{X_2 P_2^0} \qquad (3)$$

Plot  $\ln \gamma_1$  vs.  $X_1$  and  $\ln \gamma_2$  vs.  $X_2$ . From the Gibbs-Duhem equation we have:

$$\frac{d \ln \gamma_1}{dx_1} = - \frac{X_2}{X_1} \cdot \frac{d \ln \gamma_2}{dX_1} \qquad (4)$$

Measure the appropriate slopes and calculate the values of the left and right side of the above equation for the compositions which have been obtained. Any discrepancies should be explained.

Calculate the constants A and B in the Margules equation:

$$\begin{aligned} \ln \gamma_1 &= X_2^2 [A + 2X_1 (B-A)] \\ \ln \gamma_2 &= X_1^2 [B + 2X_2 (A-B)] \end{aligned} \qquad (5)$$

This may be done by solving for A and B in terms of the activity coefficients and mole fractions. The values obtained in the experiment can be used to calculate A and B. If the three values of A and the three values of B computed from the three experimental measurements do not differ greatly, compute average values for A and B and use these constants in the computer program described below.

### Machine Calculation

The calculation of predicted behavior for the Y-X and T-X diagrams is done as follows. The Margules equation permits calculation of activity coefficients in regions which have not been investigated experimentally. The complete Y-X or T-X diagram at constant pressure can be determined. For this purpose it is first necessary to know the boiling temperature of a given binary liquid from the equation

$$P = X_1 \gamma_1 P_1^0 + X_2 \gamma_2 P_2^0 \qquad , \qquad (6)$$

where

$$\ln P_1^0 = \frac{A_1}{T} + B_1 \qquad (7)$$

$$\ln P_2^0 = \frac{A_2}{T} + B_2 \qquad . \qquad (8)$$

Substituting the values of  $P_1^0$  and  $P_2^0$  from the equations 7 and 8 into equation 6 yields

$$P = X_1 \gamma_1 e^{\left[\frac{A_1}{T} + B_1\right]} + X_2 \gamma_2 e^{\left[\frac{A_2}{T} + B_2\right]} \qquad (9)$$

or

$$P = X_1 \gamma_1 e^{B_1} e^{\frac{A_1}{T}} + X_2 \gamma_2 e^{B_2} e^{\frac{A_2}{T}} \qquad (10)$$



Since  $X_1 + X_2 = 1,$  (11)

equation (10) can be written

$$P = \phi (X_1, T) . \quad (12)$$

For a fixed value of  $X_1$  and a known pressure, equation (10) is then an implicit function of  $T$  only.

$$P = C_1 e^{\frac{A_1}{T}} + C_2 e^{\frac{A_2}{T}} \quad (13)$$

where

$$C_1 = X_1 Y_1 e^{B_1}, \quad C_2 = X_2 Y_2 e^{B_2} . \quad (14)$$

One method of finding the value of  $T$  corresponding to a given value of  $X_1$  is to apply Newton's Method. Briefly, given a function  $f(z) = 0,$  and an initial estimate  $z_0$  of the root  $\alpha,$  Newton's Method is a procedure which iteratively finds a new (and if the method converges, a better) estimate of the root  $\alpha.$  The algorithm is given by

$$z_{i+1} = z_i - \frac{f(z_i)}{f'(z_i)} . \quad (15)$$

where the prime denotes the derivative with respect to  $z$  and the subscripts  $i$  and  $i+1$  are for two successive estimates in the sequence  $z_0, z_1, z_2, \dots, z_i, z_{i+1}, \dots, z_n.$  If the sequence converges, i.e., if  $z_n \rightarrow \alpha,$  then this represents a simple and effective procedure for solving an implicit function of one variable.

Applying Newton's Method to 13 yields:

$$f(T) = C_1 e^{\frac{A_1}{T}} + C_2 e^{\frac{A_2}{T}} - P = 0 \quad (16)$$

$$f'(T) = -C_1 \frac{A_1}{T^2} e^{\frac{A_1}{T}} - C_2 \frac{A_2}{T^2} e^{\frac{A_2}{T}} \quad (17)$$

$$T_{i+1} = T_i - \frac{f(T_i)}{f'(T_i)} \quad (18)$$

or

$$T_{i+1} = T_i + \frac{C_1 e^{\frac{A_1}{T}} + C_2 e^{\frac{A_2}{T}} - P}{C_1 \frac{A_1}{T^2} e^{\frac{A_1}{T}} + C_2 \frac{A_2}{T^2} e^{\frac{A_2}{T}}} . \quad (19)$$

$A_1, A_2, B_1,$  and  $B_2$  are known constants. After hand calculating  $A$  and  $B$  for a given  $P,$  the entire  $X$ - $T$  diagram can now be generated by the following procedure:

1. Select a value of  $X_1.$
2. Compute  $Y_1$  and  $Y_2$  from equations (5).
3. Compute  $C_1$  and  $C_2$  from equations (14)
4. Make an initial estimate of the root,  $T_0.$  On the first pass (small  $X_1$ ) assume that  $T$  is the boiling temperature for  $X_1=0,$  i.e., for pure methanol. On subsequent passes, simply use the temperature found on the previous pass as the first guess for the next pass.

## Vapor-Liquid Equilibrium

5. Use equation 19 to iteratively determine  $T_{i+1}$  from  $T_i$ .
6. If the magnitude of  $f(T)$  for some  $T_i$  has value less than some small number  $\epsilon_1$  or if  $|T_{i+1} - T_i|^*$  is less than some other small number  $\epsilon_2$ , then  $T_i$  or  $T_{i+1}$  represents a good approximation to  $T$ . Provision should also be made for the possibility that the method does not converge by limiting the number of iterations to some maximum value ITMAX.
7. Tabulate the data pair  $X_1 - T$ .
8. Pick a new value of  $X_1$  and return to step 2. Repeat this process until an adequate number of  $X_1$  values have been selected.

To determine values for the X-Y diagram it is necessary to compute the value of  $Y_1$  from

$$Y_1 = \frac{X_1 \gamma_1 P_1^0}{P} \quad (20)$$

When the appropriate value of boiling temperature  $T$  has been found using the procedure above,  $X_1$ ,  $\gamma_1$ ,  $P_1^0$  and  $P$  are all known. The value of  $Y_2$  corresponding to the chosen value of  $X_1$  can then be computed directly.

Since the computer program is the primary concern here, the values of  $A$ ,  $A_1$ ,  $A_2$ ,  $B$ ,  $B_1$ , and  $B_2$  will simply be given. The student would have to hand calculate  $A$  and  $B$ .

$$\begin{aligned} A &= 0.905 \\ B &= 0.570 \\ A_1 &= -3747.37 \\ B_1 &= 18.0131 \\ A_2 &= -4793.23 \\ B_2 &= 20.8237 \\ P &= 747.0 \end{aligned}$$

\* This second test is valid because in general  $|T_{i+1} - T_i|$  becomes small as  $f(T)$  becomes small. In the case of a function with a very steep (essentially infinite) slope far removed from the zero of the function, this criterion may fail. However, for the function involved in this problem, this situation does not arise for the range of temperatures involved.

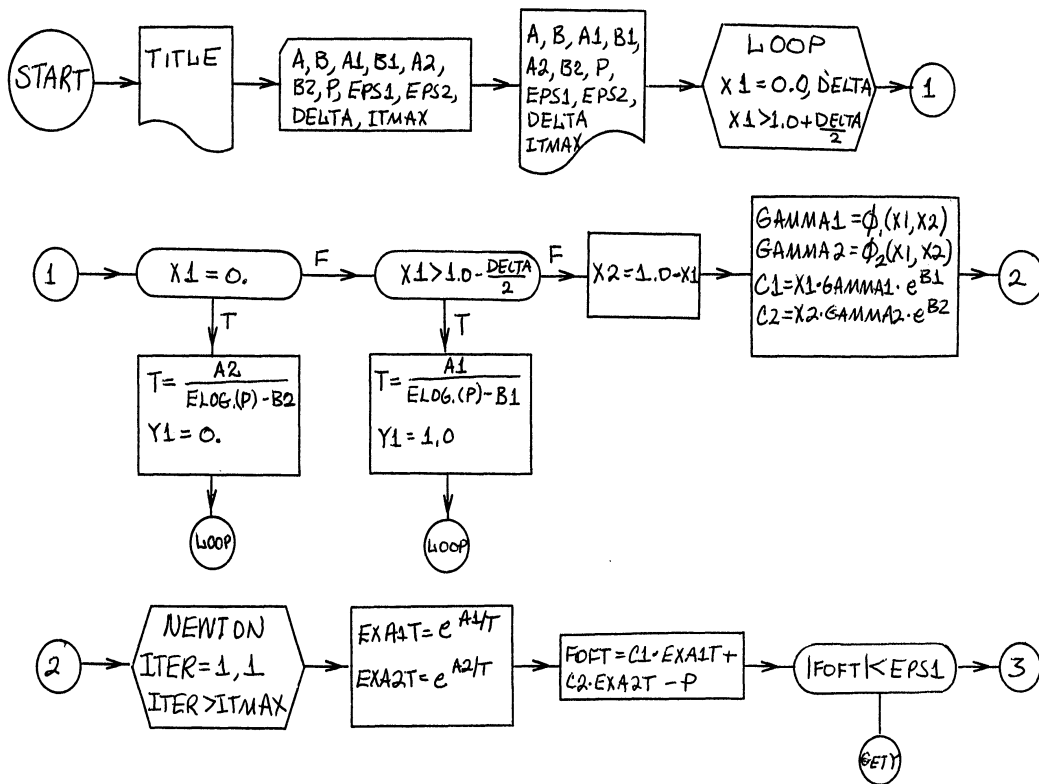
### Table of Symbols

<u>Problem Symbol</u>	<u>MAD Variable</u>	<u>Meaning</u>
A	A	} See Nomenclature, page I65.
B	B	
$A_1$	$A_1$	
$B_1$	$B_1$	
$A_2$	$A_2$	
$B_2$	$B_2$	
$\gamma_1$	GAMMA1	
$\gamma_2$	GAMMA2	

Table of Symbols, Continued

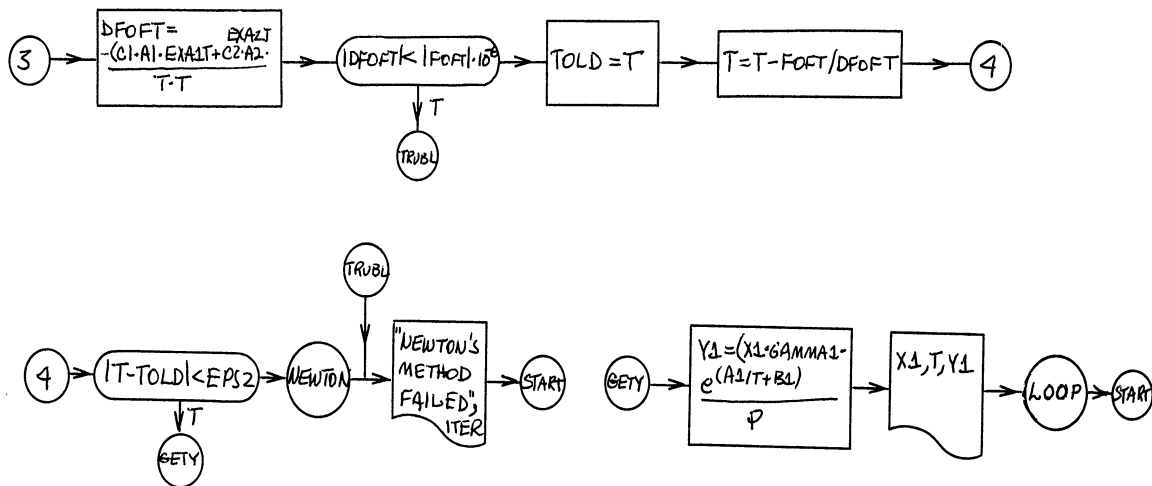
<u>Problem Symbol</u>	<u>MAD Variable</u>	<u>Meaning</u>
$P_1$	P1	} See Nomenclature, Page I65.
$P_1^0$	P1ZERO	
$P_2^0$	P2ZERO	
P	P	
T	T	
$X_1$	X1	
$X_2$	X2	
$Y_1$	Y1	} See Equation 14.
$C_1$	C1	
$C_2$	C2	See Equation 14.
	DELTA	Increment in $X_1$ for tabular calculations.
$f'(T)$	DFOFT	See Equation 17.
$\epsilon_1$	EPS1	Convergence tolerance.
$\epsilon_2$	EPS2	Convergence tolerance.
$f(T)$	FOFT	See Equation 16.
	ITER	A counter for the number of Newton's Method iterations.
	ITMAX	Maximum number of iterations permitted.

Flow Diagram



Vapor-Liquid Equilibrium

Flow Diagram, Continued



MAD Program

PROGRAM TO COMPUTE A TABLE OF X1 VS Y1 AND T FOR THE SYSTEM ACETONE - METHANGL IN VAPOR-LIQUID EQUILIBRIUM AT PRESSURE P

```

START
  INTEGER ITER, ITMAX
  PRINT COMMENT $1VAPOR-LIQUID EQUILIBRIUM FOR THE ACETONE - ME
  1THANGL SYSTEM $
  READ AND PRINT DATA A,B,A1,B1,A2,B2,P,EPS1,EPS2,DELTA,ITMAX
  THROUGH LCOP, FOR X1=C.0, DELTA, X1.G.1.0 + DELTA/2.0
  WHENEVER X1.E.C.C
    Y1 = 0.C
    T = A2/(ELCG.(P) - B2)
    TRANSFER TO LOOP
  OR WHENEVER X1.G.1.0-DELTA/2.0
    Y1 = 1.C
    T = A1/(ELCG.(P) - B1)
    TRANSFER TO LOOP
  END OF CONDITIONAL
  X2 = 1.0 - X1
  GAMMA1 = EXP.(X2*X2*(A+2.*X1*(B-A)))
  GAMMA2 = EXP.(X1*X1*(B+2.*X2*(A-B)))
  C1 = X1*GAMMA1*EXP.(B1)
  C2 = X2*GAMMA2*EXP.(B2)

  BEGIN NEWTONS METHOD ITERATION TO FIND T FOR GIVEN X1

  THROUGH NEWTON, FOR ITER=1,1, ITER.G.ITMAX
  EXA1T = EXP.(A1/T)
  EXA2T = EXP.(A2/T)
  FGFT = C1*EXA1T + C2*EXA2T - P
  WHENEVER .ABS.FOFT .L. EPS1, TRANSFER TO GETY1
  DFOFT = -(C1*A1*EXA1T + C2*A2*EXA2T)/(T*T)
  WHENEVER .ABS.DFOFT.L.1.E-10*.ABS.FOFT, TRANSFER TO TRUFL
  TOLD = T
  T = T - FOFT/DFOFT
  NEWTON
  WHENEVER .ABS.(T-TOLD).L.EPS2, TRANSFER TO GETY1
  TRUFL
  PRINT COMMENT $ NEWTONS METHOD FAILED TO WORK $
  PRINT RESULTS ITER
  TRANSFER TO START
  GETY1
  Y1 = X1*GAMMA1*EXP.(A1/T + B1)/P
  LCOP
  PRINT RESULTS X1, T, Y1
  TRANSFER TO START
  END OF PROGRAM
  
```

Computer Output

The program was run with the indicated data for a stepsize DELTA = 0.05 and 0.1. The results for the DELTA = 0.1 case are shown below.

VAPOR-LIQUID EQUILIBRIUM FOR THE ACETONE - METHANOL SYSTEM

A1 = -3747.37, B1 = 18.0131, A2 = -4793.23, B2 = 20.8237, DELTA = 0.10,

A = 0.905, B = 0.573, P = 747., EPS1 = 1.E-6, EPS2 = 0.01, ITMAX = 20\*

X1 =	.000000,	T =	337.370014,	Y1 =	.000000
X1 =	.100000,	T =	333.407753,	Y1 =	.230874
X1 =	.200000,	T =	331.256516,	Y1 =	.356726
X1 =	.300000,	T =	329.963955,	Y1 =	.441312
X1 =	.400000,	T =	329.120228,	Y1 =	.509109
X1 =	.500000,	T =	328.546825,	Y1 =	.571920
X1 =	.600000,	T =	328.176064,	Y1 =	.636663
X1 =	.700000,	T =	327.996449,	Y1 =	.708182
X1 =	.800000,	T =	328.024136,	Y1 =	.790393
X1 =	.900000,	T =	328.285271,	Y1 =	.886714
X1 =	1.000000,	T =	328.802189,	Y1 =	1.000000

In order to get an indication of the accuracy of the data taken in the laboratory, three experimental points were taken from the acetone-methanol data given by Hala et.al.\* The computed results for the hand calculated values A = 0.659, B = 0.606 and pressure P=760 mm Hg are:

VAPOR-LIQUID EQUILIBRIUM FOR THE ACETONE - METHANOL SYSTEM

A1 = -3747.37, B1 = 18.0131, A2 = -4793.23, B2 = 20.8237, DELTA = 0.10,

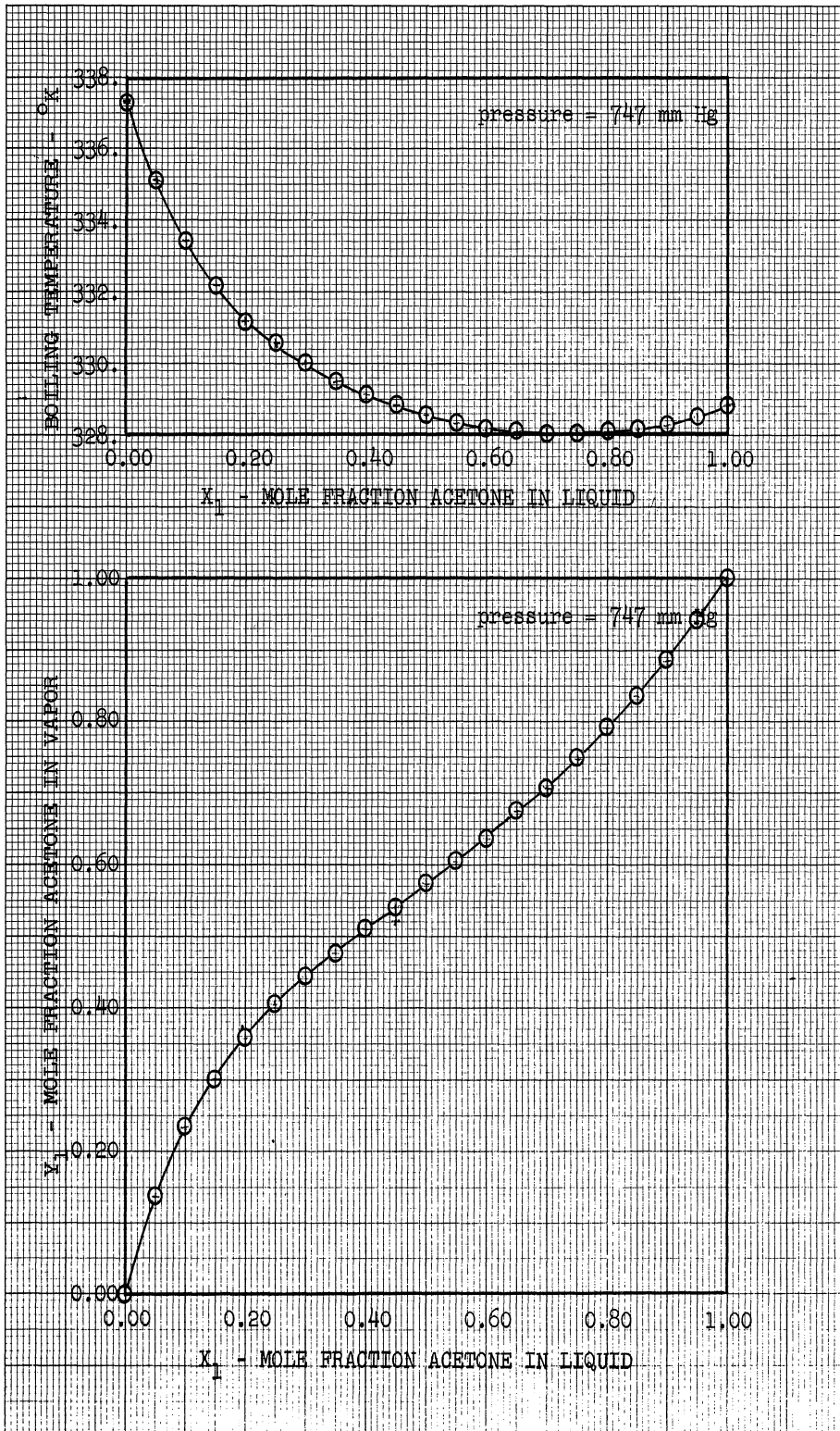
A = 0.659, B = 0.606, P = 760., EPS1 = 1.E-6, EPS2 = 0.01, ITMAX = 20\*

X1 =	.000000,	T =	337.780201,	Y1 =	.000000
X1 =	.100000,	T =	334.736027,	Y1 =	.203396
X1 =	.200000,	T =	332.697346,	Y1 =	.337880
X1 =	.300000,	T =	331.280895,	Y1 =	.436650
X1 =	.400000,	T =	330.269028,	Y1 =	.516361
X1 =	.500000,	T =	329.538387,	Y1 =	.586584
X1 =	.600000,	T =	329.024982,	Y1 =	.653706
X1 =	.700000,	T =	328.707443,	Y1 =	.722830
X1 =	.800000,	T =	328.601143,	Y1 =	.798994
X1 =	.900000,	T =	328.761559,	Y1 =	.888353
X1 =	1.000000,	T =	329.300694,	Y1 =	1.000000

\* Vapour-Liquid Equilibrium by E. Hala, J. Pick, V. Fried, and O. Vilim, Pergamon Press, 1958.

Vapor-Liquid Equilibrium

The X-T and X-Y diagrams for results from the first set of input parameters are shown below.



Example Problem No. 119

SOLVENT ALLOCATION IN MULTI-STAGE CROSS-CURRENT EXTRACTION

by

Alvin O. Converse

Department of Chemical Engineering

Carnegie Institute of Technology

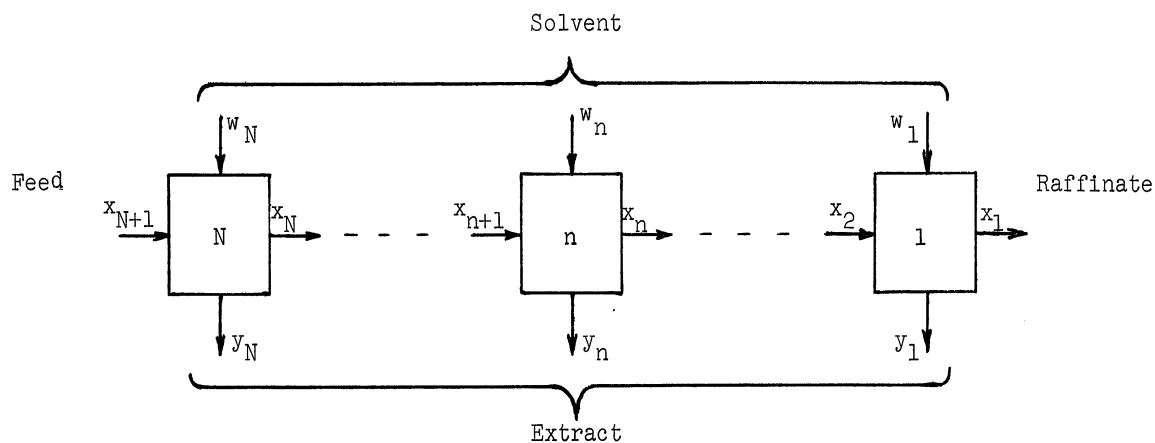
Course: Process Design

Credit hours: 3

Level: Senior or Graduate

Statement of Problem<sup>1</sup>

A schematic of the process under consideration is presented in the figure below.



Assume that the profit from each stage is proportional to

$$p_n = \alpha w_n y_n - \beta w_n \quad (1)$$

For a three-stage process determine the optimum solvent allocation such that the overall profit is maximized. Also determine the maximum overall profit.

In working the problem, assume that the flow rates (pounds/hr.) of feed or raffinate in and out of a stage are equal. Also assume individual stage efficiencies to be 100%.

<sup>1</sup> The general solution to this problem was first reported by R. Aris, D. Rudd, and N. Amundson, Ch. E. Sci., 12, (1960)

A recent paper by the author, "Computer Optimization of a Multi-Stage Allocation Problem by Means of a Non-Embedding Technique" presented at the Dec. 2-6, 1962, meeting of the AIChE (preprint 116) describes a continuation of the material presented here.

## Solvent Allocation in Multi-Stage Cross-Current Extraction

Use the following equilibrium data.

<u>y, wt. fraction</u>	<u>x, wt. fraction</u>
0.000	0.000
0.027	0.010
0.050	0.020
0.073	0.030
0.094	0.040
0.119	0.050
0.138	0.060
0.153	0.070
0.163	0.080
0.170	0.090
0.173	0.100
0.176	0.110
0.178	0.120
0.179	0.130
0.179	0.140
0.180	0.150
0.180	0.160
0.182	0.170
0.186	0.180
0.192	0.190
0.200	0.200

Other necessary data are:

$$\beta/\alpha = 0.05, \quad x_4 = 0.15, \quad \text{and } \alpha = \$1.00/\text{lb.}$$

The following notation is suggested:

p	proportional to the profit from a single stage
q	feed and raffinate flow rate, lbs./hr.
w	solvent flow rate, lbs./hr.
x	wt. fraction of solute in the raffinate
y	wt. fraction of solute in the extract
α	value of the solute extracted, \$/lb.
β	value of the solvent, \$/lb.

Subscripts

n	refers to a stream leaving the n <sup>th</sup> stage (also solvent stream entering n <sup>th</sup> stage)
N	total number of stages

### Solution<sup>1</sup>

This follows the solution given by Aris, Rudd, and Amundson (loc. cit.).

Consider the n<sup>th</sup> stage. A material balance yields

$$q [x_{n+1} - x_n] = w_n y_n \quad (2)$$

The extract and raffinate are assumed to be in equilibrium, hence:

$$y_n = f(x_n) \quad (3)$$

From the problem statement, the profit from the n<sup>th</sup> stage is proportional to:

$$p_n = \alpha w_n y_n - \beta w_n \quad (4)$$

Combination of Equations (2), (3), and (4) yields

---

<sup>1</sup> Much of this would be discussed with the students during class prior to the assignment.



$$\bar{p}_n = [x_{n+1} - x_n] [1 - \lambda f(x_n)] \quad (5)$$

where

$$\begin{aligned} \bar{p}_n &= p_n / (\alpha q) \\ \lambda &= \beta / \alpha \end{aligned}$$

The total profit on all N stages is therefore proportional to

$$P_N = \sum_{n=1}^N p_n = \sum_{n=1}^N [x_{n+1} - x_n] [1 - \lambda f(x_n)] \quad (6)$$

This is to be maximized by the proper choice of  $w_1, \dots, w_n$ , which is reflected in Equation (6) by  $x_1, \dots, x_N$ . Note that as stated in Equation (6)  $P_N$  is to be optimized by the proper, simultaneous choice of N variables. This is spoken of as an N dimensional problem since  $P_N$  is a function of N variables. The concept of dynamic programming is now used to remove the simultaneous aspect of the optimization, and reduce this N dimensional problem to N one-dimensional problems.

Consider now a three stage process

$$\begin{aligned} P_3 &= [x_4 - x_3] [1 - \lambda f(x_3)] + [x_3 - x_2] [1 - \lambda f(x_2)] + [x_2 - x_1] [1 - \lambda f(x_1)] \\ &= \bar{p}_3 + \bar{p}_2 + \bar{p}_1 \end{aligned} \quad (7)$$

Let  $g_1(x_2) = \max_{x_1} \bar{p}_1$ , which is to say, once the proper choice of  $x_1$  has been made so that the profit from the 1<sup>st</sup> stage is maximum, this maximum profit is a function of  $x_2$  only. This can be seen from inspection of the term,  $[x_2 - x_1] [1 - \lambda f(x_1)]$ .

Hence, as a first step in the computation procedure, the function  $g_1(x_2)$  is constructed by choosing various values for  $x_2$  and searching on  $x_1$  to find the maximum value of  $\bar{p}_1$ , for each value of  $x_2$ . This function,  $g_1(x_2)$ , is then used in the next step.

Similarly the function

$$g_2(x_3) = \max_{x_2} [\bar{p}_2 + g_1(x_2)]$$

and

$$g_3(x_4) = \max_{x_3} [\bar{p}_3 + g_2(x_3)]$$

can be constructed. In this problem  $g_3$  is the desired maximum profit and the corresponding values of  $x_1, x_2$ , and  $x_3$  contain the information necessary to compute the optimum solvent distribution,  $w_1, w_2$ , and  $w_3$ , from Equations (2) and (3).

The theoretical aspects of the solution have been described above. The following section describes the implementation of this method of solution on the digital computer.

Input Data:

NOINCG: The maximum profit from a section of stages is to be calculated and tabulated as a function of input concentration. NOINCG is the number of increments in the tabulation. (17 in this example)

NOINCS: For each value of the input concentration, the value of the output concentration from the first stage in the section that yields the maximum profit from the entire section

## Solvent Allocation in Multi-Stage Cross-Current Extraction

is determined by calculating the profit,  $FUNCX$ , for  $NOINCS$  values of the output concentration,  $X$ , which ranges between 0 and the input concentration,  $GX$ .

$NOINCS$ , therefore, is the number of increments in this search. (40 in this example)

$E$  = a small number (0.00005) used as a criterion in the refined search for maximum profit.

$A$  = lowest value of the input concentration which is considered.

$DELTA$  = size of the increment of inlet concentrations,  $GX$ . (0.01 in this example)

$CASES$  = number of different economics cases to be considered. (1 in this example)

$LAMDA$  = the values of the economic parameter,  $\lambda$ , which are to be considered.

One value is needed for each case. (0.05 used)

$IDEN$  = first six letters of the name of person submitting problem.

$NOINCF$  = number of increments in the tabulation  $y$  vs.  $x$  ( $EQY$  vs.  $EQX$ ).

$STAGES$  = number of equilibrium stages in the extraction process

$EQY$ ,  $EQX$  = equilibrium data

$GY$  = maximum profit for stages 1 to  $n+1$

### Procedure

The computation begins with stage number 1 (see the figure). Since there are no stages to the right of this one, the maximum profit on these nonexistent stages is zero; hence  $GY=0$ .

To begin the computation on stage number 1, a series of values of the inlet concentration,  $GX$ , is generated. For each element of  $GX$  a series of values of the outlet concentration,  $X$ , is generated and the profit,  $FUNCX$ , calculated. This last computation requires the values of the solute concentration in the extract which is in equilibrium with the raffinate,  $F$ , and the maximum profit on the stages to the right,  $G$ . Both of these are obtained from a table interpolation subroutine,  $TAB.*$ , since they are both functions of  $X$ . The maximum value of  $FUNCX$  is then selected and refined by a half-interval search. On the flow diagram, this half-interval search extends from the statement labeled  $START$  through the second  $TRANSFER TO START$  statement.

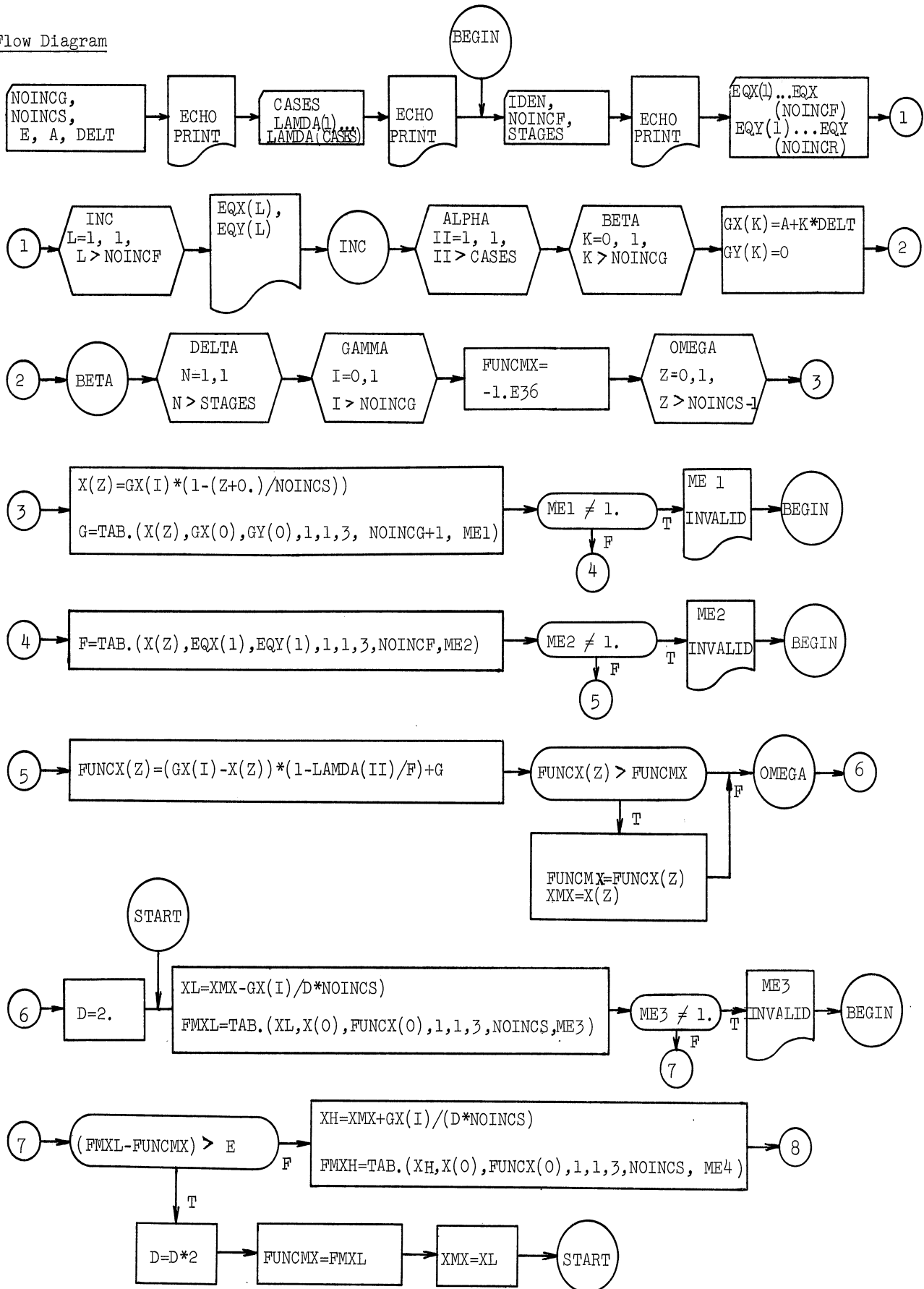
The resulting maximum value of  $FUNCMX$  and the corresponding value of  $X$  are stored in the vectors  $GY$  and  $XX$  respectively. The corresponding values of the solvent to the first stage of the section being considered,  $V$ , are then computed. Elements of  $GY$ ,  $XX$ , and  $V$  are generated and printed out for each element of  $GX$  in the  $THROUGH$  loop which is terminated at the statement labeled  $DELTA$ . The computation is then repeated for stages number 1 and 2, etc., until the final section of stages includes all stages, the maximum profit from the previous section being used in the next. Note that when the computations on a section are finished,  $GY$  is transferred to  $GY$  for use in the next section.

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\* After each execution of this subroutine, the success of the execution is tested, transferring to  $BEGIN$  if unsuccessful.

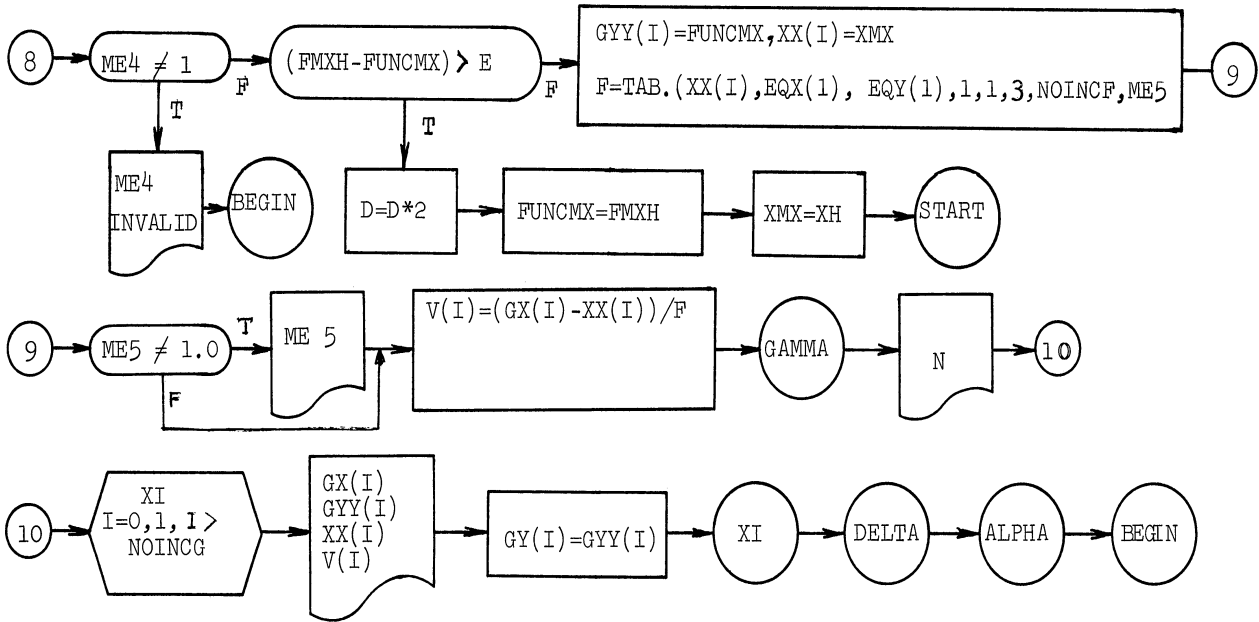
Example Problem No. 119

Flow Diagram



Solvent Allocation in Multi-Stage Cross-Current Extraction

Flow Diagram (continued)



MAD Program and Data

```

A O CONVERSE          D029N          0 3 005 050
$COMPILE MAD, PRINT OBJECT, EXECUTE, DUMP
ROPTIMIZATION OF CROSS-CURRENT EXTRACTION--DYNAMIC PROGRAMMING
R
  READ FORMAT PARAM, NOINCG, NOINCS, E, A, DELT
  VECTOR VALUES PARAM = $ 2I5, 3F10.5*$
  PRINT FORMAT PARAMO, NOINCG, NOINCS, E, A, DELT
  VECTOR VALUES PARAMO = $44H1NO. OF INCREMENTS IN THE PROFIT FU
  INCTION = I3/35H NO. OF INCREMENTS IN THE SEARCH = I3/5H E = F
  I10.5,S10,4HA = F10.5,S10,7HDELT = F10.5*$
  READ FORMAT ECO, CASES, LAMDA(1)...LAMDA(CASES)
  VECTOR VALUES ECO = $ I3, 10F6.4*$
  PRINT FORMAT ECOO, CASES, LAMDA(1)...LAMDA(CASES)
  VECTOR VALUES ECOO = $16H NO. OF CASES = I3/7H LAMDAS10F6.4*$
BEGIN
  READ FORMAT IDENT, IDEN, NOINCF, STAGES
  VECTOR VALUES IDENT = $ C6, 2I3*$
  PRINT FORMAT IDENTO, NOINCF, STAGES
  VECTOR VALUES IDENTO = $27H0NO. OF EQUILIBRIUM DATA = I3,S10,1
  16HNO. OF STAGES = I3*$
  READ FORMAT EQDATA, EQX(1)...EQX(NOINCF)
  READ FORMAT EQDATA, EQY(1)...EQY(NOINCF)
  VECTOR VALUES EQDATA = $(16F5.3)*$
  PRINT FORMAT ECHO1, IDEN
  VECTOR VALUES ECHO1 = $21HQEQUILIBRIUM DATA OF C6/1H0S5,1HYS9,
  11HX*$
  THROUGH INC, FOR L = 1,1,L.G. NOINCF
  PRINT FORMAT ECHO2, EQY(L), EQX(L)
  VECTOR VALUES ECHO2 = $1H S3, F5.3,S5, F5.3*$
  INTEGER L, NOINCF, NOINCG, K, STAGES, N, I, Z, NOINCS, II, CA
  1SES, IDEN
  DIMENSION EQY(50), EQX(50), GX(40), GY(40), X(60), LA
  1MDA(10),FUNCX(60),V(60),GYY(40),XX(40)
  THROUGH ALPHA, FOR II = 1,1, II.G. CASES
  THROUGH BETA, FOR K = 0,1, K.G.NOINCG
  GX(K) = A + K*DELT
  GY(K) = 0
  THROUGH DELTA, FOR N = 1,1, N.G. STAGES
  THROUGH GAMMA, FOR I = 0,1, I.G. NOINCG
  FUNCMX = -1.E36
  
```

## MAD Program and Data (continued)

```

      THROUGH OMEGA, FOR Z = 0,1, Z.G. NOINCS-1
      X(Z) = GX(I)*(1-((Z+0.)/NOINCS))
      G = TAB.(X(Z), GX(0), GY(0), 1,1,3,NOINCG+1,ME1)
      WHENEVER ME1 .NE. 1.
      PRINT FORMAT MER1
      VECTOR VALUES MER1 =$ 4H ME1*$
      TRANSFER TO BEGIN
      END OF CONDITIONAL
      F = TAB.(X(Z), EQX(1), EQY(1), 1,1,3, NOINCF,ME2)
      WHENEVER ME2 .NE. 1.
      PRINT FORMAT MER2
      VECTOR VALUES MER2 =$ 4H ME2*$
      TRANSFER TO BEGIN
      END OF CONDITIONAL
      FUNCX(Z) = (GX(I) - X(Z))*(1 - LAMDA(I)/F) + G
      WHENEVER FUNCX(Z) .G. FUNCMX
      FUNCMX = FUNCX(Z)
      XMX = X(Z)
      END OF CONDITIONAL
      OMEGA RREFINED SEARCH FOR THE MAXIMUM PROFIT
      D = 2.
      START XL = XMX - GX(I)/(D*NOINCS)
      FMXL = TAB.(XL, X(0), FUNCX(0), 1,1,3,NOINCS ,ME3)
      WHENEVER ME3 .NE. 1.
      PRINT FORMAT MER3
      VECTOR VALUES MER3 =$ 4H ME3*$
      TRANSFER TO BEGIN
      END OF CONDITIONAL
      WHENEVER (FMXL - FUNCMX) .G. E
      D = D*2
      FUNCMX = FMXL
      XMX = XL
      TRANSFER TO START
      OTHERWISE
      XH = XMX + GX(I)/(D*NOINCS)
      FMXH = TAB.(XH,X(0),FUNCX(0),1,1,3,NOINCS ,ME4)
      WHENEVER ME4 .NE. 1.
      PRINT FORMAT MER4
      VECTOR VALUES MER4 =$4H ME4*$
      TRANSFER TO BEGIN
      END OF CONDITIONAL
      END OF CONDITIONAL
      WHENEVER (FMXH - FUNCMX) .G. E
      D = D*2
      FUNCMX = FMXH
      XMX = XH
      TRANSFER TO START
      END OF CONDITIONAL
      GYY(I) = FUNCMX
      XX(I) = XMX
      F = TAB.(XX(I),EQX(1),EQY(1),1,1,3,NOINCF,ME5)
      WHENEVER ME5 .NE. 1.,PRINT FORMAT MER5
      VECTOR VALUES MER5 =$4H ME5*$
      GAMMA V(I) = (GX(I)-XX(I))/F
      PRINT FORMAT HEAD, N
      VECTOR VALUES HEAD =$1H0S20,4HN = I3/S3,6H X(IN)S5,1HGS10,1HX
      1S10,1HV*$
      THROUGH XI, FOR I = 0,1, I.G. NOINCG
      PRINT FORMAT RESULT, GX(I), GYY(I), XX(I), V(I)
      VECTOR VALUES RESULT =$S2,F7.5,3F11.5*$
      XI GY(I) = GYY(I)
      DELTA CONTINUE
      ALPHA CONTINUE
      TRANSFER TO BEGIN
      END OF PROGRAM

      $DATA
      17 40 0.00005 0.03 0.01
      1 0.05
      CONVER 21 3
      0 0.01 0.020 .0300.0400.0500.060 .0700.0800.0900.1000.1100.1200.1300.1400.150
      0.1600.1700.180 .1900.200
      0 0.0270.050 .0730.0940.1190.138 .1530.1630.1700.1730.1760.1780.1790.1790.180
      0.1800.1820.186 .1920.200

```

Solvent Allocation in Multi-Stage Cross-Current Extraction

Computer Output

NO. OF INCREMENTS IN THE PROFIT FUNCTION = 17  
 NO. OF INCREMENTS IN THE SEARCH = 40  
 E = 0.00005      A = 0.03000      DELT = 0.01000

NO. OF CASES = 1  
 LAMDAS0.0500

NO. OF EQUILIBRIUM DATA = 21      NO. OF STAGES = 3

EQUILIBRIUM DATA OF CONVER

Y	X
0.000	0.000
0.027	0.010
0.050	0.020
0.073	0.030
0.094	0.040
0.119	0.050
0.138	0.060
0.153	0.070
0.163	0.080
0.170	0.090
0.173	0.100
0.176	0.110
0.178	0.120
0.179	0.130
0.179	0.140
0.180	0.150
0.180	0.160
0.182	0.170
0.186	0.180
0.192	0.190
0.200	0.200

N = 1

X(IN)	G	X	V
0.03000	0.00095	0.02475	.08600
0.04000	0.00324	0.02800	.17519
0.05000	0.00635	0.03125	.24798
0.06000	0.01002	0.03450	.30970
0.07000	0.01415	0.03675	.38207
0.08000	0.01881	0.04200	.38384
0.09000	0.02390	0.04500	.42204
0.10000	0.02925	0.04750	.46492
0.11000	0.03482	0.04950	.51354
0.12000	0.04052	0.05100	.56960
0.13000	0.04635	0.05200	.63303
0.14000	0.05228	0.05250	.70431
0.15000	0.05826	0.05250	.78481
0.16000	0.06430	0.05600	.79394
0.17000	0.07048	0.05525	.88544
0.18000	0.07665	0.05850	.89698
0.19000	0.08293	0.05700	1.00142
0.20000	0.08928	0.06000	1.01449

N = 2

X(IN)	G	X	V
0.03000	0.00120	0.02625	.05814
0.04000	0.00415	0.03200	.10367
0.05000	0.00803	0.03750	.14107
0.06000	0.01272	0.04350	.16050
0.07000	0.01805	0.04725	.20258
0.08000	0.02375	0.05000	.25210
0.09000	0.02962	0.05175	.31173
0.10000	0.03569	0.05500	.34850
0.11000	0.04192	0.05775	.38950
0.12000	0.04828	0.06000	.43478
0.13000	0.05477	0.06500	.44501
0.14000	0.06136	0.06650	.49573
0.15000	0.06801	0.06750	.55118
0.16000	0.07471	0.07200	.56651
0.17000	0.08150	0.07225	.62815
0.18000	0.08828	0.07200	.69527
0.19000	0.09514	0.07600	.71486
0.20000	0.10200	0.08000	.73620

Computer Output (continued)

N = 3			
X(IN)	G	X	V
0.03000	0.00127	0.02775	0.03312
0.04000	0.00457	0.03400	0.07380
0.05000	0.00883	0.04125	0.09010
0.06000	0.01396	0.04650	0.12226
0.07000	0.01962	0.05075	0.15961
0.08000	0.02560	0.05400	0.20439
0.09000	0.03185	0.06075	0.21001
0.10000	0.03834	0.06500	0.23962
0.11000	0.04498	0.06875	0.27250
0.12000	0.05172	0.07200	0.30901
0.13000	0.05851	0.07475	0.34913
0.14000	0.06537	0.07700	0.39275
0.15000	0.07227	0.07875	0.43994
0.16000	0.07921	0.08400	0.45724
0.17000	0.08620	0.08500	0.50917
0.18000	0.09321	0.08550	0.56490
0.19000	0.10022	0.08550	0.62468
0.20000	0.10727	0.09000	0.64706

Discussion of Results

The feed concentration was given as 0.15. Entering the table of results under the heading of N=3, at the value of X(IN) = 0.15, one finds the maximum profit function G=0.07227. Hence the maximum profit =  $\alpha G = \$0.072/\text{lb. of feed}$ . From the same table the concentration of the solute in the extract from stage no. 3 is X=0.07875; the amount of solvent, V=0.43994 lbs. of solvent/lb. of feed.

Entering the next table (N=2) at X(IN)=0.07875, one finds the solvent allocated to that stage to be V $\approx$ 0.246, by linear interpolation. Similarly X<sub>2</sub>  $\approx$  0.0497.

Entering the last table (N=3) at X(IN)=0.0497 one finds V $\approx$ 0.248 and X<sub>1</sub>  $\approx$  0.031. Hence the total amount of solvent used = 0.934 and is greatly different from an equal distribution.

The program required 1.0 minute for compilation and 1.7 minutes for execution on the IBM 704.

Example Problem No. 120

DYNAMIC HEAT EXCHANGE

by

Jack Famularo

Department of Chemical Engineering

New York University

Course: Rate Operations

Credit hours: 3

Level: Junior-Senior

Statement of Problem

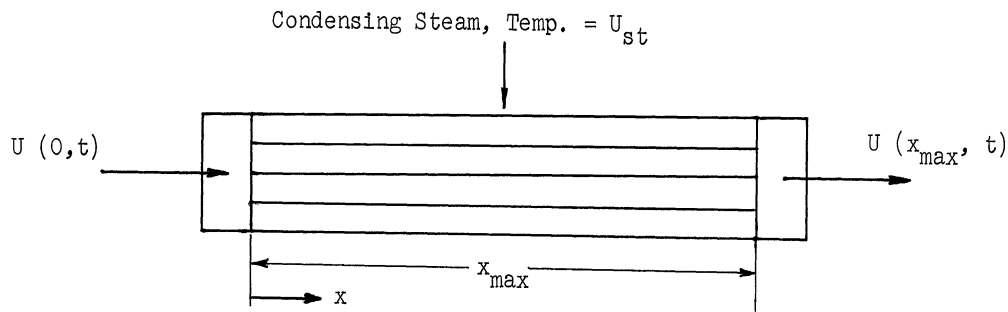
It is desired to study the unsteady state behavior of a shell and tube heat exchanger (1 tube pass, 1 shell pass) which is subjected to a variable inlet fluid temperature on the tube side. To simplify the analysis consider the problem of condensing steam on the shell side with an organic liquid such as toluene on the tube side, and limit the problem to small enough inlet temperature fluctuations so that a constant overall heat transfer coefficient can be assumed.

For the sake of uniformity the following nomenclature will be used:

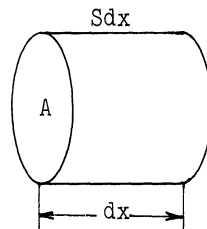
<u>Problem variable</u>	<u>MAD variable</u>	<u>Definition</u>
$U(x,t)$	$U(I,J)$	Fluid temperature at mesh nodes, °F
$U_{st}$	UST	Steam-condensate temperature, °F
$x$	X	Distance into tube bundle, ft.
$t$	T	Time, sec.
$A$	A	Cross-sectional area, ft. <sup>2</sup>
$S$	S	Lateral area, ft. <sup>2</sup> /ft. length
$m$	M	Mass flow rate, lb <sub>m</sub> /sec.
$c$	C	Specific heat of fluid, BTU/lb <sub>m</sub> °F
$D$	D	Density of fluid, lb <sub>m</sub> /ft <sup>3</sup>
$x_{max}$	XMAX	Length of tube bundle, ft.
$v$	V	Fluid velocity, ft./sec.
$Z$	Z	Overall heat transfer coefficient, BTU/sec. ft <sup>2</sup> °F.
$h$	H	Mesh size in $x$ , ft.
$\ell$	L	Mesh size in $t$ , sec.
$i$	I	Position subscript in $x$ .
$j$	J	Position subscript in $t$ .



A schematic diagram of the heat exchanger is shown below.



Rather than consider the flow through individual tubes, the total flow is to be treated as if it were through a single tube with cross-sectional area and lateral area equal to the sum of these terms over all of the tubes.



If the element of fluid shown above is followed as it moves a distance  $dx$  it is observed that the temperature changes. This change in temperature is the result of two contributing effects:

1. Movement of fluid to a region of different temperature, characterized by  $\left. \frac{\partial U}{\partial x} \right|_t$ . This factor is also of importance in the steady state problem, if the inlet temperature is some constant less than  $U_{st}$ .
2. The change in temperature at any given position with time, characterized by  $\left. \frac{\partial U}{\partial t} \right|_x$ . This factor would contribute even if the element of fluid were stationary and originally at some temperature less than  $U_{st}$ .

The total change in temperature as the element moves  $dx$  is constructed as follows:

$$dU = \left. \frac{\partial U}{\partial x} \right|_t dx + \left. \frac{\partial U}{\partial t} \right|_x dt$$

If the element of fluid experiences a change in temperature its energy content is increased by  $m \cdot c \cdot dU$ . However, this energy must be transferred to the fluid from the condensing steam through the resistance  $\frac{1}{Z \cdot S dx}$ .

Dynamic Heat Exchange

Thus:

$$dQ = ZSdx (U_{st} - U)$$

$$dQ = mcdU = mc \frac{\partial U}{\partial x} dx + mc \frac{\partial U}{\partial t} dt$$

Equate:

$$mc \frac{\partial U}{\partial x} dx + mc \frac{\partial U}{\partial t} dt = ZSdx (U_{st} - U)$$

Divide by  $mc dx$ , yielding:

$$\frac{\partial U}{\partial x} + \frac{1}{v} \frac{\partial U}{\partial t} + \frac{ZS}{mc} (U - U_{st}) = 0$$

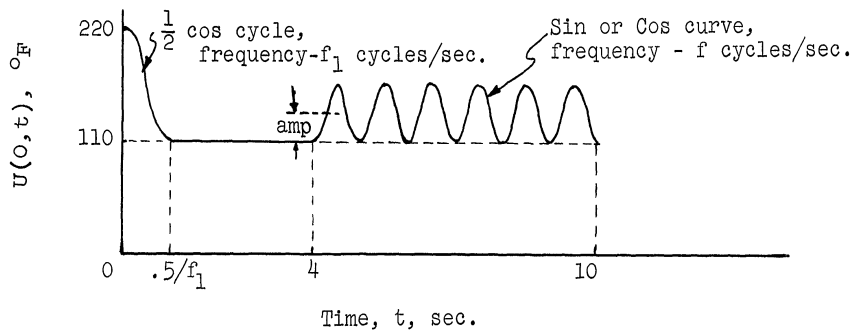
and substitute  $m = DAv$ . This results in:

$$\frac{\partial U}{\partial x} + \frac{1}{v} \frac{\partial U}{\partial t} + \frac{ZS}{cDAv} (U - U_{st}) = 0$$

A more formal statement of the problem is as follows. Transform the differential equation to an appropriate difference equation and write a MAD computer program to simulate the heat exchanger for the following boundary and initial conditions.

$$\text{Initial Condition: } U(x,0) = U_{st}$$

Boundary Condition:  $U(0,t)$  is given by the figure below.

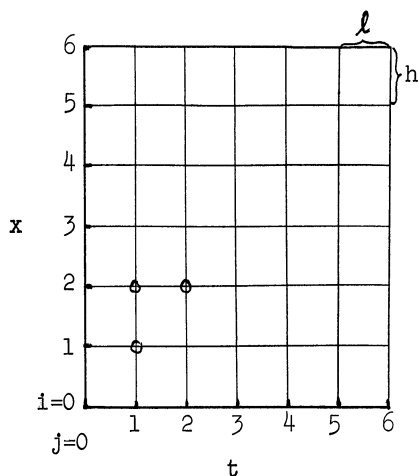


It is suggested that the following data be used in the computation, and that this data be read into storage from data cards.

A	=	0.4 ft. <sup>2</sup>
S	=	30 ft. <sup>2</sup> /ft. length
c	=	0.5 BTU/lb <sub>m</sub> °F.
D	=	54 lb <sub>m</sub> /ft. <sup>3</sup>
v	=	4 ft./sec.
Z	=	0.1 BTU/sec. ft. <sup>2</sup> °F.
U <sub>st</sub>	=	220 °F.
x <sub>max</sub>	=	10 ft.
f <sub>1</sub>	=	1 cycle/sec.
f	=	.5 cycle/sec.
h/l	=	4 ft./sec.
h	=	.4 ft.
amp	=	22 °F.

Solution

The space defined by the coordinates  $x$  in distance and  $t$  in time is partitioned into small rectangular sections of dimensions  $h$  ft. and  $\ell$  sec. as shown in the diagram below.



The partitioning defines a mesh whose pivotal points are defined by the equations:

$$\begin{aligned} x_i &= x_0 + ih \\ t_j &= t_0 + j\ell \end{aligned}$$

Thus the temperature at any of the pivotal points or nodes of the mesh may be represented as follows:

$$U(x_i, t_j) = U_{i,j}$$

The differential equation can now be reduced to a difference equation by substituting for the partial derivatives in the following manner:

$$\left. \frac{\partial U}{\partial x} \right|_{i,j} = \frac{U_{i,j} - U_{i-1,j}}{h} \quad \text{Backward difference quotient}$$

$$\left. \frac{\partial U}{\partial t} \right|_{i,j} = \frac{U_{i,j+1} - U_{i,j}}{\ell} \quad \text{Forward difference quotient}$$

The selection of the above difference quotients is necessary to insure convergence of the solution of the finite-difference equation to the solution of the differential equation. For example, the use of a forward difference for  $\partial U / \partial x$  results in an unstable solution.\* It can also be shown\* that the ratio  $v\ell/h$  must be equal to or less than unity.

Proceeding to the conversion of the differential equation to difference form, the following is obtained.

$$v \frac{\partial U}{\partial x} + \frac{\partial U}{\partial t} + \frac{ZS}{cDA} (U - U_{st}) = 0$$

\* Courant, Isaacson, Rees. "On the Solution of Non-Linear Hyperbolic Differential Equations by Finite Differences," Comm. Pure Appl. Math., 5, 243-255 (1952).

Dynamic Heat Exchange

which becomes in difference form,

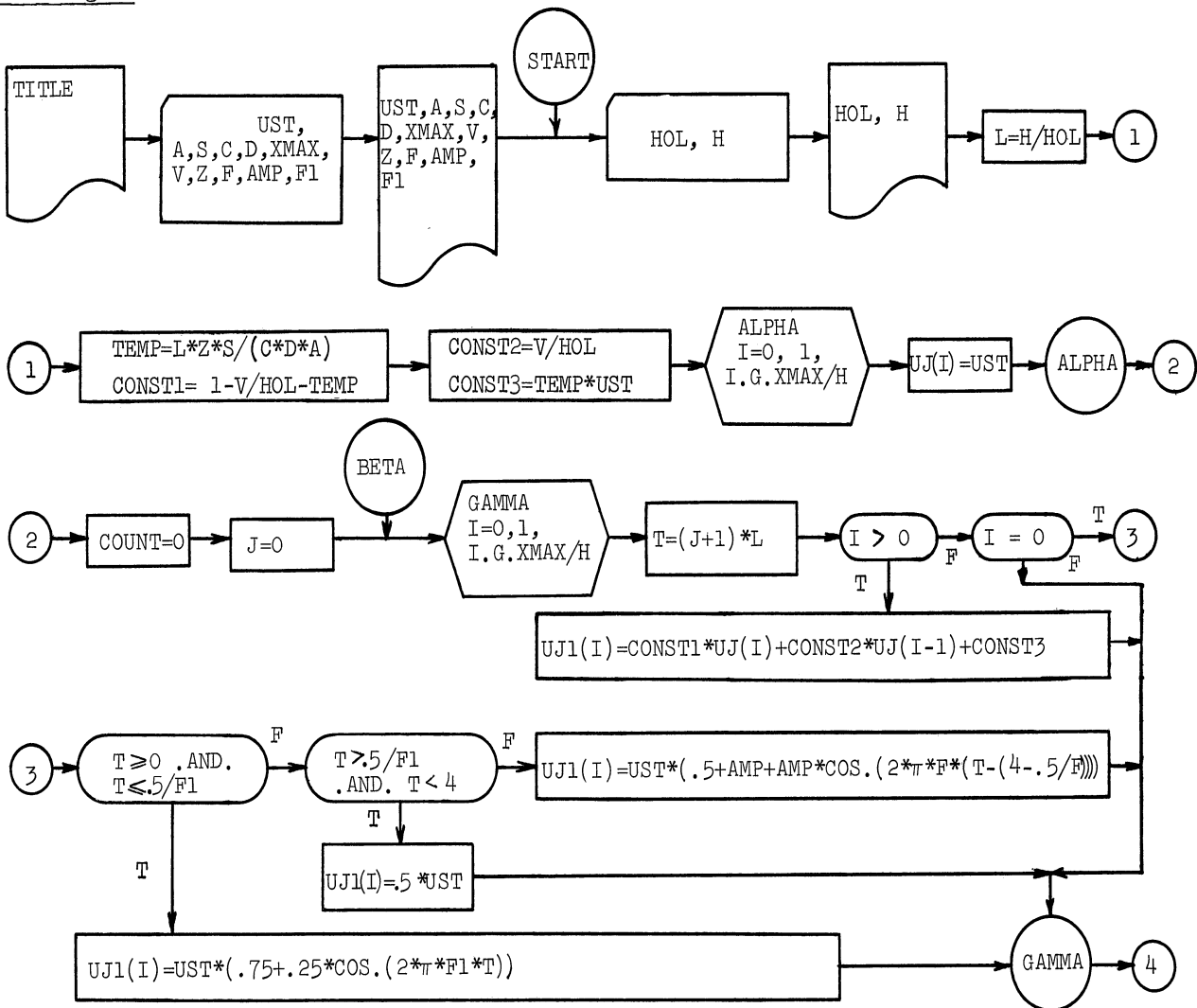
$$v \left[ \frac{U_{i,j} - U_{i-1,j}}{h} \right] + \left[ \frac{U_{i,j+1} - U_{i,j}}{l} \right] + \frac{ZS}{cDA} \left[ U_{i,j} - U_{st} \right] = 0$$

This can be rearranged to yield,

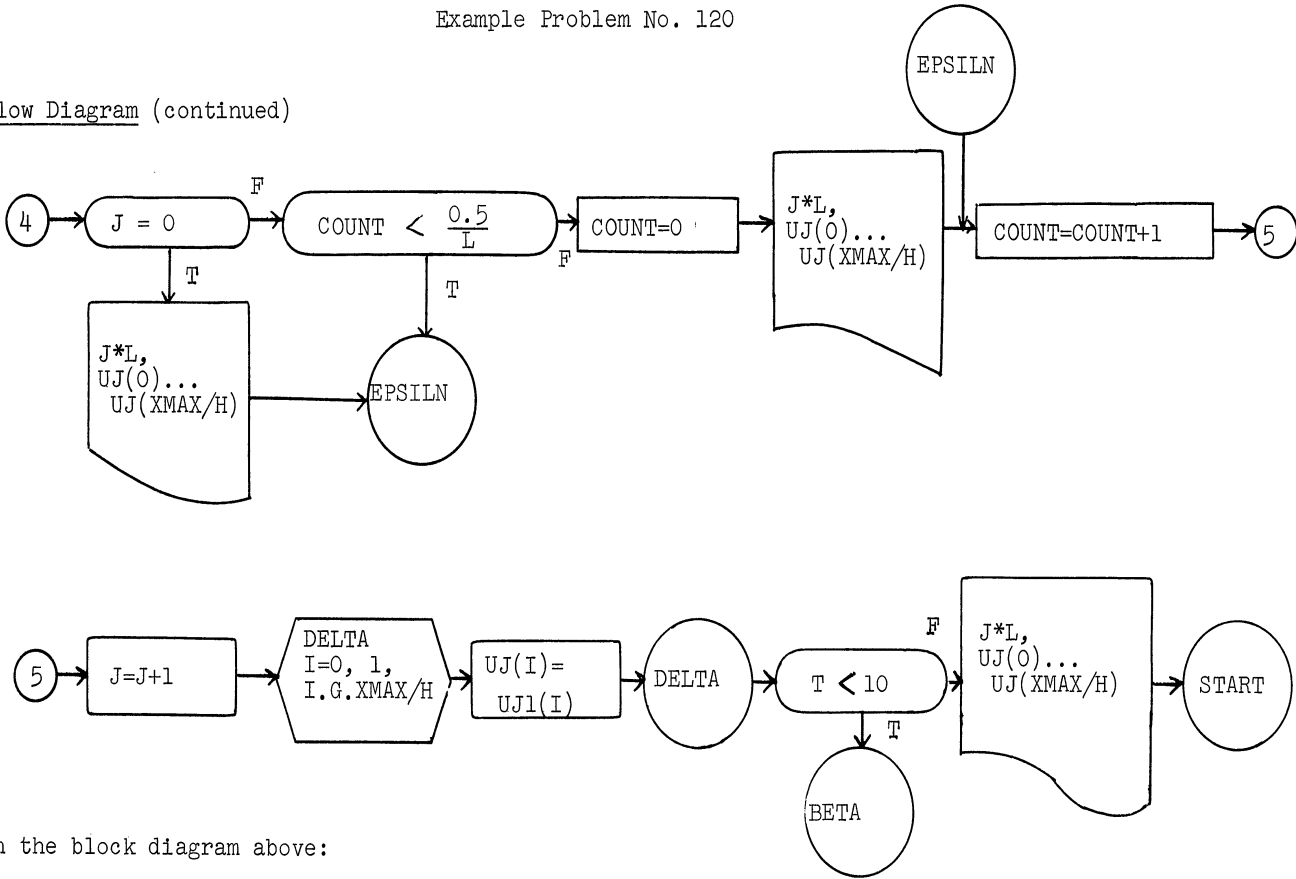
$$U_{i,j+1} = \left( 1 - \frac{v l}{h} - \frac{ZS}{cDA} \right) U_{i,j} + \frac{v l}{h} U_{i-1,j} + \frac{l ZS}{cDA} U_{st}$$

The difference equation is employed to calculate an approximate temperature at every mesh node preceeding from  $i = 0$  to  $i = x_{max}/h$  for every column  $j$ , starting at  $j=0$ . The solution is started by substituting the initial condition for the axis  $j=0$ , and the temperatures along the axis  $i=0$  are obtained from the boundary condition.

Flow Diagram



Flow Diagram (continued)



In the block diagram above:

HOL = H/L

UJ(I) = TEMPERATURE AT TIME = J\*L, I=0,1,2,...,n

UJ1(I) = TEMPERATURE AT TIME = (J+1)\*L, I=0,1,2,...,n

MAD Program and Data

```

J. FAMULARO          T29=N          0 5 400 400  HEATEXCH
J. FAMULARO          T29=N          0 5 400 400  HEATEXCH
$COMPILE MAD, PRINT OBJECT, EXECUTE, DUMP
PRINT FORMAT TITLE
READ FORMAT CONST,UST,A,S,C,D,XMAX,V,Z,F,AMP,F1
PRINT FORMAT CONSTH,UST,A,S,C,D,XMAX,V,Z,F,AMP,F1
START
READ FORMAT RATIO,HOL,H
PRINT FORMAT MESH,HOL,H
L=H/HOL
TEMP=L*Z*S/(C*D*A)
CONST1=1.-V/HOL-TEMP
CONST2=V/HOL
CONST3=TEMP*UST
THROUGH ALPHA, FOR I=0,1,I.G.XMAX/H
ALPHA
UJ(I)=UST
COUNT=0
J=0
BETA
THROUGH GAMMA, FOR I=0,1,I.G.XMAX/H
T=(J+1)*L
WHENEVER I.G.0
UJ1(I)=CONST1*UJ(I)+CONST2*UJ(I-1)+CONST3
OR WHENEVER I.E.0
WHENEVER T.GE.0..AND.T.LE..5/F1
UJ1(I)=UST*(.75+.25*COS.(2*3.1415927*F1*T))
OR WHENEVER T.G..5/F1.AND.T.L.4.
UJ1(I)=.5*UST
OTHERWISE
UJ1(I)=UST*(.5+AMP+AMP*COS.(2*3.1415927*F*(T-(4.-.5/F))))
END OF CONDITIONAL
GAMMA
END OF CONDITIONAL
    
```

MAD Program and Data (continued)

```

WHENEVER J.E.0
PRINT FORMAT RESULT,J*L,UJ(0)...UJ(XMAX/H)
TRANSFER TO EPSILN
OTHERWISE
WHENEVER COUNT.L..5/L,TRANSFER TO EPSILN
END OF CONDITIONAL
COUNT=0
PRINT FORMAT RESULT,J*L,UJ(0)...UJ(XMAX/H)
EPSILN COUNT=COUNT+1
J=J+1
THROUGH DELTA,FOR I=0,1,I.G.XMAX/H
DELTA UJ(I)=UJ1(I)
WHENEVER T.L.10.,TRANSFER TO BETA
PRINT FORMAT RESULT,J*L,UJ(0)...UJ(XMAX/H)
TRANSFER TO START
INTEGER I,J,COUNT
DIMENSION UJ(500)
DIMENSION UJ1(500)
VECTOR VALUES TITLE=$69H1 STUDY OF DYNAMIC HEAT EXCHANGE FOR
1VARIABLE INLET FLUID TEMPERATURE*$
VECTOR VALUES CONST=$11F7.2*$
VECTOR VALUES CONSTH=$1H ,S4,3HUST,S6,1HA,S6,1HS,S6,1HC,S6,1H
1D,S3,4HXMAX,S6,1HV,S6,1HZ,S6,1HF,S4,3HAMP,S5,2HF1/1H ,11F7.2*
2$
VECTOR VALUES RATIO=$1F23.4,1F21.4*$
VECTOR VALUES MESHR=$17H1 MESH RATIO H/L=,F7.4,S3,12HMESH SIZ
1E H=,F7.4*$
VECTOR VALUES RESULT=$40H0 TEMPERATURE PROFILE IN EXCHANGER A
1T T=,F5.2,27H SECS. AT X=0,H,2H,....,XMAX/(1H ,7F10.3)*$
END OF PROGRAM

$DATA
220.00 0.40 30.00 0.50 54.00 10.00 4.00 .10 0.50 0.10 1.00
4.0000 .2000
    
```

Computer Output

The following is an abbreviated form of the computer output obtained using the input data listed with the MAD program above.

STUDY OF DYNAMIC HEAT EXCHANGE FOR VARIABLE INLET FLUID TEMPERATURE

UST	A	S	C	D	XMAX	V	Z	F	AMP	F1
220.00	0.40	30.00	0.50	54.0	10.00	4.00	.10	0.50	0.10	0.00

MESH RATIO H/L= 4.0000 MESH SIZE H= 0.2000

TEMPERATURE PROFILE IN EXCHANGER AT T= 0.00 SECS. AT X=0,H,2H,....,XMAX

220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000
220.000	220.000	220.000	220.000	220.000	220.000	220.000	220.000

TEMPERATURE PROFILE IN EXCHANGER AT T= 1.00 SECS. AT X=0,H,2H,....,XMAX

110.000	111.507	112.993	114.459	115.905	117.331	118.737	
120.124	121.492	122.842	124.173	125.485	126.780	128.057	
129.317	130.558	131.799	132.726	137.500	110.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	
220.000	220.000	220.000	220.000	220.000	220.000	220.000	

TEMPERATURE PROFILE IN EXCHANGER AT T= 4.00 SECS. AT X=0,H,2H,....,XMAX

110.000	111.507	112.993	114.459	115.905	117.331	118.737	
120.124	121.492	122.842	124.173	125.485	126.780	128.057	
129.317	130.559	131.784	132.993	134.184	135.360	136.519	
137.663	138.791	139.903	141.001	142.083	143.150	144.203	
145.241	146.265	147.275	148.272	149.254	150.223	151.179	
152.122	153.052	153.969	154.873	155.765	156.645	157.513	
158.369	159.214	160.046	160.868	161.678	162.476	163.264	
164.042	164.808						

Computer Output (continued)

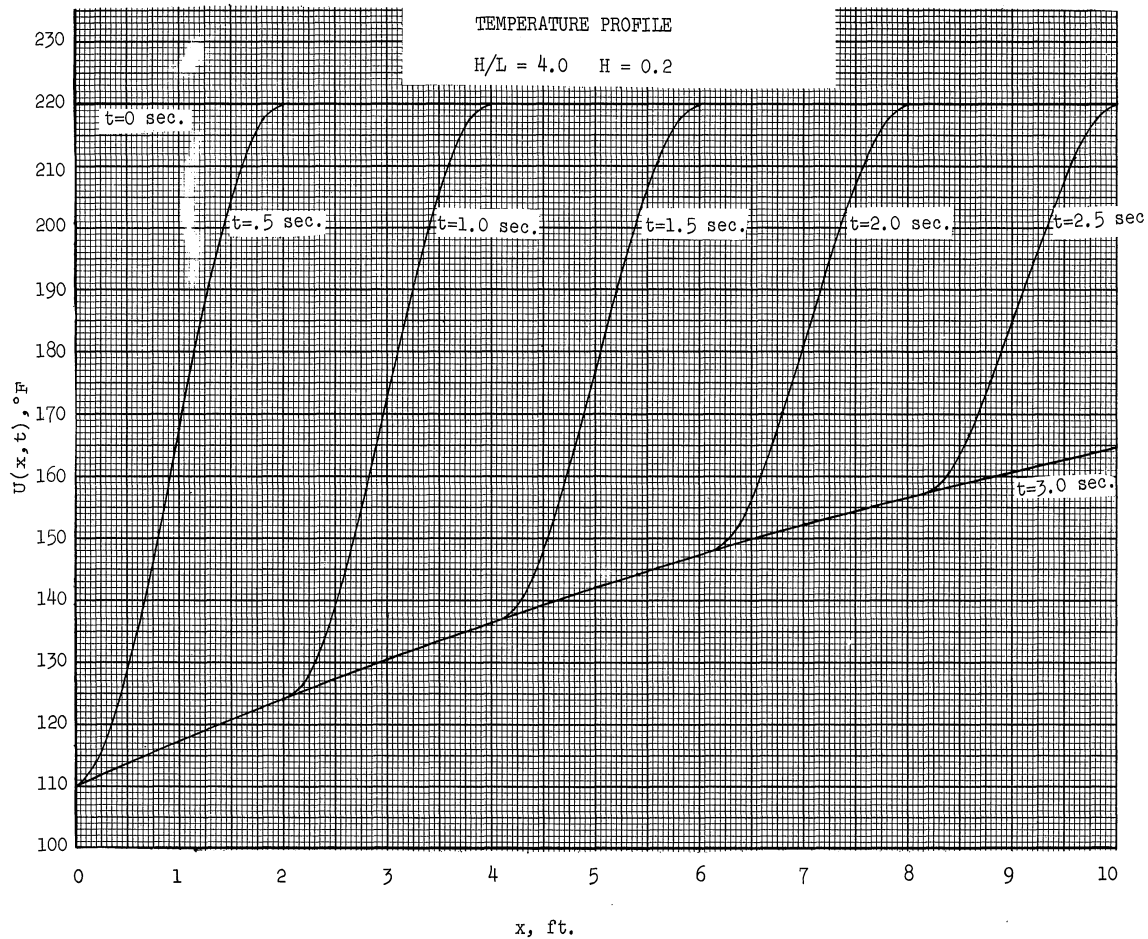
TEMPERATURE PROFILE IN EXCHANGER AT T=10.00 SECS. AT X=0,H,2H,...,XMAX

110.000	111.763	114.006	116.689	119.765	123.178	126.864
130.754	134.777	138.859	142.927	146.909	150.738	154.351
157.693	160.713	163.374	165.644	167.502	168.938	169.952
170.552	170.756	170.593	170.096	169.308	168.275	167.049
165.683	164.235	162.760	161.312	159.945	158.708	157.644
156.793	156.187	155.851	155.803	156.055	156.608	157.458
158.593	159.996	161.640	163.496	165.531	167.705	169.979
172.310	174.656					

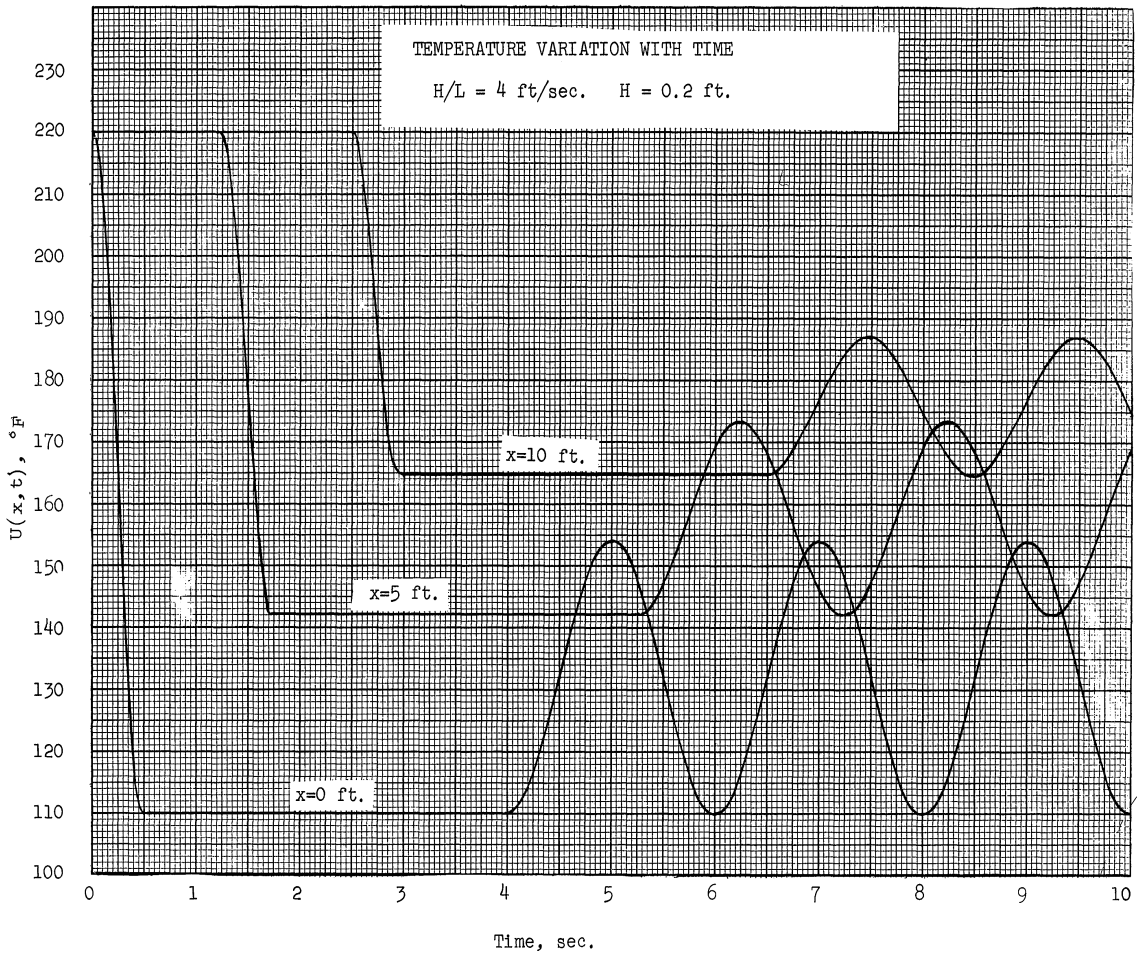
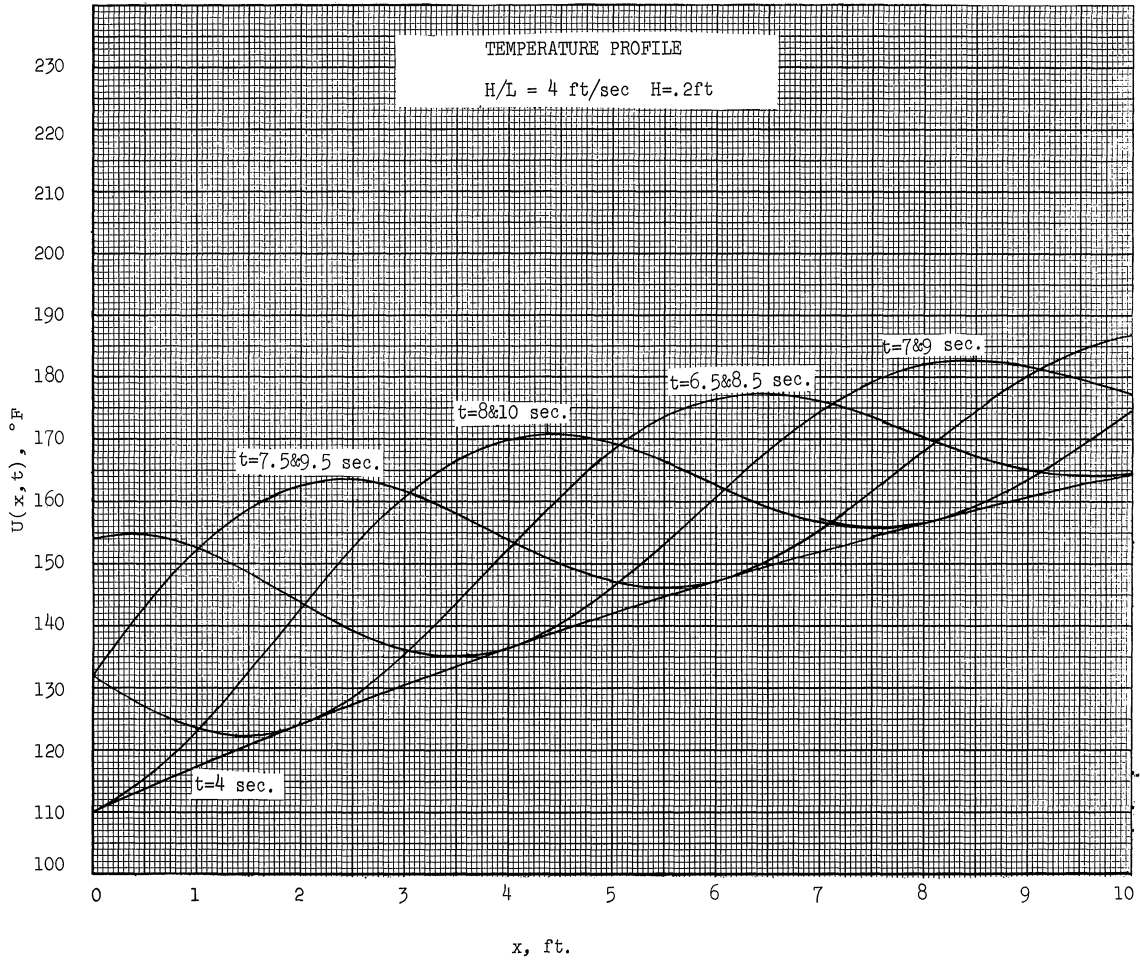
Discussion of Results

The numerical solution of the difference equation is obtained as a series of temperature profiles at various times. The temperature scale is in degrees Fahrenheit and results are printed for  $x = 0, 0.2, 0.4, \dots, 10$  ft.

Sample temperature profiles are plotted below.



Dynamic Heat Exchange





An estimate of the accuracy of the method is obtained by comparing the steady state solution of the difference equation with the exact solution of the steady state differential equation.

The original differential equation is,

$$\frac{\partial U}{\partial x} + \frac{1}{v} \frac{\partial U}{\partial t} + \frac{ZS}{cDAv} (U - U_{st}) = 0$$

For steady state operation,  $\partial U / \partial t = 0$ , and the equation becomes,

$$\frac{dU}{dx} + \frac{ZS}{cDAv} (U - U_{st}) = 0$$

This equation may now be written in terms of

$$\begin{aligned} \tau &= U_{st} - U \\ \Phi &= ZS/cDAv \end{aligned}$$

to yield,

$$\frac{d\tau}{dx} + \Phi \tau = 0$$

which can be integrated to give

$$\ln \tau = -\Phi x + \ln \beta$$

where  $\beta$  is a constant of integration.

The steady state solution sought is the one corresponding to an inlet fluid temperature of 110°F, therefore the constant  $\ln \beta$  can be evaluated from the condition,

$$\tau = 110^\circ\text{F} \quad @ \quad x = 0 \text{ ft.}$$

Substitution into the solution yields,

$$\ln \beta = \ln 110$$

and the complete solution,

$$\ln \frac{\tau}{110} = -\Phi x$$

or,

$$\tau = 110 e^{-\Phi x}$$

Using the data suggested in the problem statement,

$$\Phi = \frac{1}{14.4}$$

and

$$\tau = 110 e^{-\frac{x}{14.4}}$$

## Dynamic Heat Exchange

The solutions of this equation together with computed solutions of the difference equation are tabulated below for comparison.

TABLE OF STEADY STATE SOLUTION,  $U(x)$  °F

X ft.	STEADY STATE DIFFERENTIAL EQUATION	DIFFERENCE EQUATION TEMPERATURE PROFILE 4 sec.
0	110.000	110.000
1	117.38	117.331
2	124.24	124.173
3	130.69	130.559
4	136.68	136.519
5	142.27	142.083
6	147.48	147.275
7	152.35	152.122
8	156.89	156.645
9	161.12	160.868
10	165.58	164.808

### Critique

The study of the dynamic behaviour of process equipment has been avoided in most undergraduate curricula primarily because of the limited mathematical background of the students. However, the rapid development of high speed computers has given impetus to the use of numerical procedures which are well within the grasp of undergraduate engineers. Application of these numerical procedures, or numerical analysis, allows the study of problems which have hitherto been reserved for graduate work. The problem discussed in this report falls into this category.

In addition to exhibiting a mathematical method for solving partial differential equations, the students were exposed to the technique of replacing an actual physical situation by a simplified model which is amenable to mathematical analysis. Known physical laws were then employed to set up the partial differential equation describing the behaviour of this model.

The actual programming was left to the student and no class time was devoted to this aspect of the problem. The problem was somewhat more difficult to program than previous ones which the students had solved in the required course, "Introduction to Computing Techniques", taught in the Math Department and in earlier chemical engineering courses. However, this was desirable. Programming assistance was offered to the students in the form of personal consultation with the instructor. The MAD language was used which proved to be very suitable, and, in the opinion of the author, has removed programming as an obstacle to machine utilization.

Example Problem No. 120

Although an honest attempt was made to prevent the computer problem from interfering with other course material, this was not entirely possible. During the period allotted to the computer problem the normal assignment of problems in the course had to be reduced. This was necessary because of the large amount of time needed by most students for programming, key punching, and debugging.

Some students commented that although this problem was somewhat difficult, they appreciated the fact that this was a practical heat transfer problem.

USE OF COMPUTERS IN AN UNDERGRADUATE CHEMICAL ENGINEERING DESIGN COURSE

by

Dale F. Rudd

Department of Chemical and Metallurgical Engineering

The University of Michigan

Course: Chemical Engineering Process Design      Credit Hours: 3      Level: Senior

In the fall semester of 1960, problems requiring the use of both the analog and digital computer were introduced for solution in the undergraduate chemical engineering course in process design, CM 481. This section contains an analysis of the computer background of the students, a description of the problems, and the response of the students to the problems. Based on the experience gained by this and other experiments, recommendations are made concerning methods of integrating computers into a design course.

#### The Design Course

CM 481 is taught as a senior level chemical engineering design course. Several relatively extensive design problems are assigned which call upon the student's background in unit operations, thermodynamics, rate processes, and economics, as well as upon his ability to make engineering decisions.

Ordinarily two or possibly three design problems are assigned during a semester. Examples of typical problems are; the preliminary design of a butane isomerization unit, the design of a gas gathering system, or a study of helium production. The work is performed in groups of about three students and an extensive report is required when the design is complete.

The class meets regularly and lectures are given related to the process under consideration, basic economic principles, report writing and any new engineering concepts which need to be introduced. All the design work is done out of class. The students are given the responsibility to allocate their time to complete the assigned task by the required due date.

#### Background of the Students

At this level the students have completed the bulk of their fundamental chemical engineering requirements (thermodynamics, unit operations, rate processes, etc.), and commonly are taking concurrently with this process design course such courses as unit operations laboratory, equipment design, or courses in cognate and elective fields.

The students' exposure to digital computer methods began at or before their sophomore year. A one-credit hour course offered by the Mathematics Department (Math 373) on elementary computer methods is required of all chemical engineering students. This is followed by the use of computers in problem assignments in their normal course work. Ability in organization and programming of problems for the computer is expected on the part of the students.

The computer language taught is the problem-oriented MAD (Michigan Algorithm Decoder) language. In the MAD language a program is written in a pseudo-algebraic form and translation is done automatically by the MAD translator with the aid of an executive system called the Monitor.

The operation of the Computing Center is closed shop with regard to actual operation of the computer. The students write the MAD program, punch it on cards, supply the command cards (often referred to as \$-cards since a dollar sign is in column 1) for the executive system and deliver the package to the Computing Center. The staff submits the package to the computer and returns the results to the student. With this arrangement it is possible for the student to make use of the computer with a minimum of technical skill with computing machines. The availability of a problem-oriented language and a computer executive system makes the mass introduction of digital computer methods to the students possible.

In summary, the average student has been exposed to computer programming in the MAD language for about two years, and has programmed approximately a half dozen elementary problems in his chemical engineering course work.

In general, the students have had no prior experience with an electronic analog computer. Lectures were given in class on the theory of the computer, programming manuals were distributed, and the solution of an example problem was demonstrated on the computer. This provided the background necessary for the student groups to formulate their problems for the analog computer. The instructor was available to answer questions of a specific nature. An analog computer containing six integrators, and ten summers was available.

#### The Design Problems

The first design problem assigned to the students did not require the use of the computer. It was the design of a plant to produce styrene monomer. The second problem was the design of a continuous, stirred-tank, reactor-separator system for the continuous nitration of benzene. The computers were used in the last phase of this problem. The students had their choice of either optimizing the design of the nitrator-separator unit or investigating the automatic control of the nitrator on the analog computer.

No specific reference was made to the use of the digital computer to perform the calculations in the optimum-design problem. Of the seven groups in the class, four chose the optimization problem. Three of these four asked permission to use the digital computer to aid in their calculations.

Three groups chose to study the control system analysis. Several lectures were given on control theory and process simulation using the linearized process equations and associated control-system equations. Those who chose the control problem understood that the analog computer was to be used.

1. Optimum Design Problem

The process to be designed is a continuous, stirred-tank nitrator with associated product-separation and reactant-recycle equipment for the production of mononitrobenzene from benzene using mixed acid. Fresh benzene, nitric acid, and sulfuric acid are introduced into a continuous stirred-tank reactor along with a recycle stream of the same main constituents. The benzene is partially converted to nitrobenzene in the reactor and the stream leaving the reactor (containing the feed constituents plus nitrobenzene and water) is fed into a separation device from which the nitrobenzene product is removed. The unreacted material (the acids and benzene) are recycled back to the reactor. The design problem involves the selection of the reactor, heat exchange, separation, and other equipment to achieve the nitration. Once the decisions as to choice of basic equipment are made, the optimum design is obtained by sizing the equipment to achieve the most profitable operation. A comparison of optimum designs for various types of equipment was not expected. A detailed design produced by a student group is presented later.

2. The Control System Analysis

The control system analysis involved the experimental determination of the response of the analog-computer-simulated-nitration-reactor to disturbances when under the control of the feedback control system. The class had no background in control theory and process simulation. Hence, it was necessary first to present the methods of process simulation, the linearized transient material and energy balance equations for a process, and the elementary concepts of feedback control theory. It was not possible to present the powerful analytical tools available for the analysis and synthesis of stable control systems. Only the concepts of proportional and integral feedback control were presented. Control parameters necessary to provide a stable and responsive control system were to be determined experimentally by the simulation experiments on the analog computer. The details of the process-control-system simulation on the analog computer are included with the student solution.

The Response of the Students

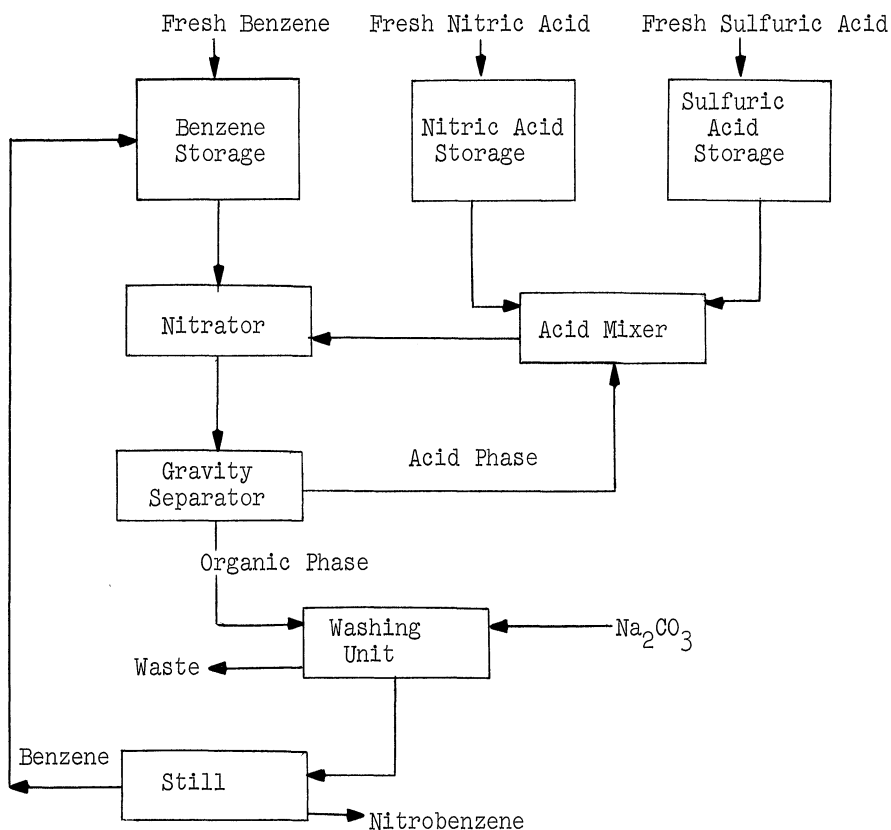
The response of the students to the computer problems can best be presented by the discussion of final reports submitted for each of the two problems. The reports were selected on the basis of quality.

1. Solution to the Optimization Problem

The report of a group consisting of M. Lamont and David Grow follows, in greatly condensed form, with comments by the editor. The report presents the results of their investigations into the optimum design of the nitrator-separation system. Particular emphasis is placed on the use of the digital computer to perform the routine calculations.

a. Description of the Flow Process

A flow diagram of the process is shown below.



At the beginning of the process, there are three large storage tanks containing the raw materials: benzene, nitric acid, and sulfuric acid. The tank holding the benzene is to be constructed of plain carbon steel, and the remaining two are to be constructed of stainless steel. The two acid tanks feed into a large mixing tank which adds the stream from the acid recovery system and brings the mixed acid up to the desired composition of 39%-53%-8%. This stream is then pumped by a centrifugal pump into the nitrator where it is mixed with a similarly-pumped stream of benzene. The nitration takes place almost immediately with high rates of agitation and the resulting product, containing benzene, nitrobenzene, water, nitric acid, and sulfuric acid, is pumped into a separator where the benzene and the nitrobenzene are separated from the spent acid by gravity. This method is rather crude, but still entirely satisfactory since the densities are very different. This piece of equipment, like the nitrator, should be constructed of stainless steel since the temperature will be high and nitric acid is present in the product stream.

Two streams leave the separator, one which contains the spent acid and one which has the resulting product. The spent acid stream is recycled into a short-tube, vertical evaporator where the excess water of nitration and the residual hydrocarbons are removed. The stream leaving contains a somewhat more concentrated acid and is pumped directly into the acid mixing tank, where it will be reused.

The product stream, which contains only benzene, nitrobenzene and a small amount of spent acid, is pumped into a large agitated washing tank where the acid present is neutralized with  $\text{Na}_2\text{CO}_3$ . The actual amount of  $\text{Na}_2\text{CO}_3$  required is about 20 pounds per ton of nitrobenzene. High rates of agitation are not necessary in this wash tank, so a small motor is used.

The crude nitrobenzene along with the neutralized acid is then pumped into a series of three settling tanks where the crude nitrobenzene is separated from the water. Three tanks are used because the hold-up time is sufficiently long to warrant the use of three tanks rather than one large one. This also eliminates the necessity of having to shut down the process while the tank is drained.

The product stream is then pumped from the settling tanks and into the still where the final separation is carried out. The still, as designed, contains only ten plates for the complete separation, which is more than enough. However, the same separation could probably be carried out satisfactorily using a steam distillation apparatus, with additional separation. A large storage tank is needed for the pure nitrobenzene and the benzene is recycled back to the benzene storage tank.

#### b. Methods of Analysis

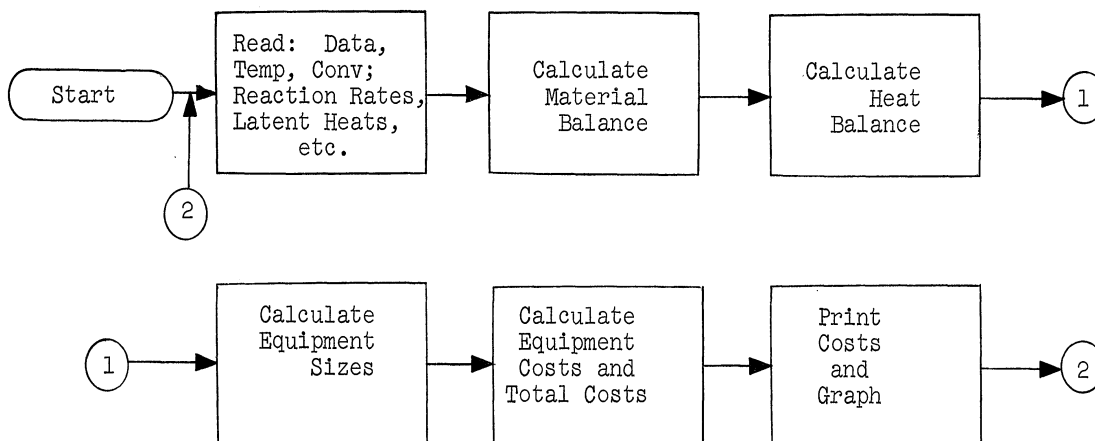
To facilitate the analysis and the extensive amount of calculation required for a process optimization of this type, it was decided to use the IBM 704 computer. Although the complete optimization would require an extensive program and the difficult task of converting the process variables into computer language, it was felt that it would be much more satisfactory and reduce the total computational labor involved. The actual preparation of the program was somewhat simplified by the use of cost curves, previous rate data, and numerous graphs which appeared in earlier reports.

Essentially, the method of analysis consisted of determining the total purchased equipment cost for a number of different possible conversion percentages. In each case the calculations consisted of evaluating the cost of several pieces of "variable" equipment (equipment which varied in cost with percentage conversion) and adding to this the cost of the pieces of equipment whose cost was independent of percent conversion. It was the computer's job to utilize the data, and then evaluate the equations giving the resulting purchased equipment cost as a percentage of conversion. A plotting subroutine (with entries PLOT1., PLOT2., PLOT3., and PLOT4.) was then used to display the curve of cost versus conversion.



c. The Computer Program

A rough flow diagram of the computer program is shown below.



To aid the reader, a detailed step-by-step explanation of the computer program is given below:

1. Read densities of nitric acid, sulfuric acid, water, benzene, and nitrobenzene (DN, DS, DW, DB, and DNB, respectively), latent heats of benzene and nitrobenzene (HB and HNB), conversion rate in percent, CONV, rates for water, nitric acid and sulfuric acid, X(1), X(2), and X(3), and production rate of nitrobenzene, PROD, in pounds per hour.
2. Calculate the material balance from the following equations.
 
$$\text{BENZ} = \text{PROD} \times 1.05 \times 78 / (\text{CONV} \times 123) = \text{benzene feed to reactor (lb./hr. of benzene).}$$

$$\text{NIT} = \text{BENZ} \times 1.025 \times 63 / 78 = \text{nitric acid feed to reactor (lb./hr.)}$$

$$\text{SUL} = \text{NIT} \times 98 \times X(1) / (X(2) \times 63) = \text{sulfuric acid feed to reactor (lb./hr.)}$$

$$\text{WAT} = \text{NIT} \times 18 \times X(3) / (X(2) \times 63) = \text{water feed to reactor (lb./hr.)}$$
  - \* PNBENZ = PROD × 1.05
  - \* PNIT = NIT - PNBENZ × 63/123
  - \* PSUL = SUL
  - \* PWAT = WAT + PNBENZ × 18/123
  - \* PBENZ = BENZ - PNBENZ × 78/123

\* The P preceding the above names refers to the product stream from the reactor.
3. Calculate the heat balance from the following equation.
 
$$Q = 790.6 \times \text{PROD} \times 1.05 = \text{total heat given off by the reaction (BTU/hr.)}$$

The heat of dilution was neglected to simplify the analysis because it is small compared with Q.
4. Calculate the reactor volume from the following equation.
 
$$\text{RV} = \text{PROD} \times 7.49 / (123 \times R) = \text{reactor volume (gallons)},$$

where R = reaction rate (nitrobenzene/hr.ft<sup>3</sup>).
5. Determine the separator volume, SV, from the volume of product leaving the reactor, VP. A thirty minute hold up time was used.
 
$$\text{VP} = \text{PNIT} / \text{DN} + \text{PSUL} / \text{DS} + \text{PWAT} / \text{DW} + \text{PBENZ} / \text{DB} + \text{PNBENZ} / \text{DNB} \text{ (cubic ft./hr.)}$$

The divisor of each product is the density of the respective compound.

$$\text{SV} = \text{VP} \times 7.49 / 2 \text{ (gallons)}.$$

6. The length of the cooling coils can be calculated from the following heat transfer equations.  
 $HI = 150 \times (1. + 0.11 \times TW) \times V^{0.8} / DI^{0.2}$  = tube side heat transfer coefficient (BTU/hr.ft.<sup>2</sup>°F).  
 where TW = average water temperature. (An inlet water temperature of 70°F was assumed.)

V = water velocity (ft./sec.). (10 ft. per second was assumed.)

DI = inside tube diameter (ft.). A one-inch outer diameter tube was used.

$$HC = 0.00265 \times L^2 \times N \times RS / VIS$$

where HC = kettle side heat transfer coefficient (BTU/hr.ft.<sup>2</sup>°F).

L = length of the stirring paddle (assumed 1.5 ft.)

N = revolutions per hour of the stirrer (assumed 7200 rph).

VIS = viscosity of fluid in the kettle (lb.mass/hr.).

A "dirt" factor of 0.002 was used in calculating the over-all heat transfer coefficient from the following equation.

$$U = 1 / (1/HI + 1/HC + RD)$$

where U = overall heat transfer coefficient (BTU/hr.ft.<sup>2</sup>°F).

RD = dirt factor.

The required heat transfer area can be found by the following equation.

$$HTA = Q / (U \times DTl)$$

where HTA = required heat transfer area (ft.<sup>2</sup>).

DTl = log-mean temperature difference (°F) (20°F assumed).

The length of the cooling coils can then be determined since a tube diameter has been specified in previous calculations.

7. The neutralization tank volume can now be found if a residence time is chosen. In this particular piece of equipment a fifteen minute hold-up time was used.

$$PNT = (PNBENZ / DNB + PBENZ / DB) \times 7.49 = \text{feed to neutralization tank (gal./hr.)}$$

$$NTV = PNT / 4 = \text{neutralization tank volume (gal.)}$$

8. The volume of the separator required to remove the water and salt solution from the organic product after neutralization is calculated using a thirty minute residence time.

$$NSV = PNT / 2 = \text{neutralization separator volume (gal.)}$$

9. The distillation tower size is calculated from the following equation.

$$AT = \frac{10.7 \times G}{0.9} \left( \frac{T \times P}{M} - \frac{1}{24} \right)^{0.5} = \text{required tower area (ft.<sup>2</sup>)}$$

where T = temperature of vaporization (620°R).

G = vapor flow rate (lb./sec.) = (PBENZ + PNBENZ) / 3600.

M = molecular weight of fluid being distilled.

P = distillation pressure (psig).

H = tray spacing (in.).

$$D = (4 \times AT / 3.14)^{1/2} = \text{tower diameter (ft.)}$$

10. The reboiler and condenser duties are calculated. Steam was decided upon as the heating medium for the reboiler and a reflux ratio was used in determining the condenser duty.

$$RHTA = (PBENZ \times HB + PNBENZ \times HNB) / 4000 = \text{reboiler heat transfer area (ft.<sup>2</sup>)}$$

HB and HNB = latent heats of vaporization of benzene and nitrobenzene, respectively (BTU/lb.).

4000 = overall U × Temperature difference (U=200 and ΔT=20 °F).

$$CHTA = (PNBENZ \times HNB \times RR) (U \times DTLM) = \text{condenser heat transfer area (ft.<sup>2</sup>)}$$

where RR = Reflux ratio (assumed value = 4).

U = overall heat transfer coefficient (assumed value = 200).

DTLM = log-mean temperature difference (assumed value = 30°F).

Example Problem No. 121

11. The mixed acid tank volume, MATV, was calculated using a tank large enough to hold a two-hour supply of mixed acid.

$$\text{MATV} = (\text{NIT}/\text{CN} + \text{SUL}/\text{DS} + \text{WAT}/\text{DW}) \times 7.49/2 \text{ (gal.)}.$$

12. The size of the evaporator required for the acid recovery system was determined from the following equations.

$$Q = 240 \times \text{CONV} + 60 = \text{heat required to evaporate the excess water (BTU/lb. feed to reactor)}.$$

This equation was derived by calculating several heat duties required for different conversion rates and plotting a line through the points.

$$\text{FEED} = \text{SUL} + \text{NIT} + \text{WAT} = \text{feed to reactor (lb./hr.)}.$$

$$\text{EHTA} = \text{FEED} \times Q/7000 = \text{evaporator heat transfer area (ft.}^2\text{)}.$$

where 7000 = overall heat transfer coefficient times log-mean temperature difference.

13. The storage tanks were required to hold a one-week supply.

$$\text{STV} = 168 \times 7.49 \times \text{VFR}/\text{DFR} = \text{storage tank volume of material in question (gal.)}.$$

where VFR = volume of feed to reactor of material in question (lb./hr.).

$$\text{DFR} = \text{density of material in question (lb./ft.}^3\text{)}.$$

The volume of each of the following tanks was calculated by the above equation.

Nitric acid tank

Benzene tank

Nitrobenzene tank

Sulfuric acid tank

14. The costs of the various pieces of equipment were calculated as follows. The equations of the lines from plotted values of the cost of various pieces of equipment from Aries and Newton are shown.

$$\text{Stirred tank} = 222.2 (\text{tank volume})^{.447} \text{ for stainless steel.}$$

$$\text{Storage tank} = 15.27 (\text{tank volume})^{.447} \text{ for stainless steel.}$$

$$\text{Storage tank} = 5.27 (\text{tank volume})^{.447} \text{ for carbon steel.}$$

$$\text{Tower cost} = 9.20 (\text{diameter})^{1.18} \times \text{number of plates.}$$

$$\text{Tubing cost} = 6.0 \times \text{tube length.}$$

$$\text{Condenser cost} = 149 \times (\text{heat transfer area}) \times .453.$$

$$\text{Reboiler cost} = 78 (\text{heat transfer area})^{0.621}.$$

$$\text{Evaporator cost} = 600 (\text{heat transfer area})^{0.5}.$$

$$\text{Pumping cost} = 1.7 \times \text{water rate}/483.$$

$$\text{Water cost} = .0173 \times \text{water rate (lb./hr)} - \text{yearly basis } (\$.02/1000 \text{ gal.}).$$

MAD Program

```

DIMENSION TC(5),XC(3),DUMMY(870)
EXECUTE PLOT1.(0.,4.,12.,5.,20.)
EXECUTE PLOT2.(DUMMY,100.,0.,10.,3.)
-----
READ FORMAT F0,DM,DS,DM,DB,DNB,HB,HNB
READ FORMAT F2,XC(1),XC(2),XC(3),PROD
START READ FORMAT DATA,CONV,B,TC(0)
PRINT FORMAT HEAD,CONV
-----
R = B*28.3/454.0
RR = 4.0
-----
DI = 0.75/12.
BENZ = PROD*1.05*78.0/(CONV*123.0)
NIT =BENZ*1.025*63.0/78.0
SUL = NIT*98.0*XC(1)/XC(2)*63.0)
-----
WAT =NIT*18.0*XC(3)/XC(2)*63.0)
PNBENZ = PROD*1.05
PNIT = NIT-PNBENZ*63./123.
PSUL = SUL
-----
PWAT = WAT + PNBENZ*18.0/123.0
PBENZ = (BENZ-PNBENZ*78./123.)
-----
PNT = (PNBENZ/DNB + PBENZ/DB)*7.49
RV = PROD*7.49/(123.0*R)
VP = PNIT/DN +PSUL/DS +PWAT/DW +PBENZ/DB +PNBENZ/DNB
SV = VP*7.49/2.
-----
TC(1) = TC(0)*1.8+32
TC(2) = TC(1)-15.
-----
V = 10.
TW = (TC(2)+70.)/2.
HI = 150.*(1.+0.11*TW)*V.P.0.8/DI.P.0.2
M = 7200.
RS = 62.4
L = 1.3
-----
VIS = 4.84
HC = .00265*L.P.2.*N*RS/VIS
HD = 500.
U = 1./((1./HC+1./HI+1./HD)
DT1 = 20.
Q = 790.6*PROD*1.05
HTA=Q/((CU*DT1)
DO = 1/12.
L = HTA/(3.14*DO)
VT = 3.14*DO.P.2.*L/4.
TRV = RV + VT
RHTA = (PBENZ*HB+PNBENZ*HNB)/4000.
DTLM = 30.
CHTA = (PNBENZ*HNB*RR)/(200.*DTLM)
MATV = (NIT/DN + SUL/DS + WAT/DW)*7.49/2.0
NATV =168.*(NIT - PNIT)*7.43/DN
DT = (TC(2)-70.)
RW= PROD*790./DT
DT2 = .50.
CW = HB*PBENZ*RR/DT2
T = 620.
P = 1.0
G = (PBENZ + PNBENZ)/3600.
M = 78.0
-----
AT = 10.7*G*(CT/(CM*P)-1./24.3.P.0.5/0.9
D = (4.*AT/3.14).P.0.5
NF = 10.
NTV = PNT/4.
NSV = PNT/2.
MATV = (NIT/DN + SUL/DS + WAT/DW)*14.98
NATV=(NIT - PNIT)*168.*7.49/DN
ETV = 168.*(BENZ - PBENZ)*7.49/DB
TOWC = (9.20*D.P.1.18)*NF
CR =222.2*TRV.P.0.477
CT = 6.0*L
PC = 1.7*RW/483.3)
SC =15.27*SV.P.0.66
NATC =15.27*NATV.P.0.66

```

Example Problem No. 121

MAD Program, Continued

```

MATC = 222.2*MATV.P.O.477
NTC = 222.2*NTV.P.O.477
-----
SNC = 15.27*NSV.P.O.66
BTC = 15.27*BTV.P.O.66
-----
CC = 149.*CHTA.P.O.453
RC = 78.*RHTA.P.O.621
-----
FEED = SUL + WAT + HIT
Q = 240.*CONV + 60.
-----
EHTA = FEED *Q/7000.
EC = 600.*EHTA.P.O.50
-----
PC = 1.7*(CRW+CW)/483.3
WC = .0173*(CW+RW)
-----
CTOT = TOWC +SC+SNC+MATC+PC+NTC+NATC+BTC+CC+RC+EC+WC+CT+RC
PRINT FORMATF1,TOWC,SC,SNC,MATC,PC,NTC,NATC,BTC,CC,RC,EC,WC,C
TR,CT,CTOT
-----
CON = CONV*100.
CTO = CTOT/100000
EXECUTE PLOT3,(%$,CON,CTO,1.,0.)
-----
WHENEVER CONV.E.O.99,TRANSFER TO THAT
TRANSFER TO START
-----
VECTOR VALUES HEAD=$1H1,530,28H DAVID GROW AND LARRY LAMONT//
1540,15H CHEM. MET. 130///520,19H CONVERSION RATE = 1F7.2*$
-----
VECTOR VALUES F0 = $7F9.3*$
VECTOR VALUES F2 = $4F6.2*$
-----
VECTOR VALUES DATA = $3F9.2*$
VECTOR VALUES F1 = $///530,27H EQUIPMENT COSTS IN DOLLARS,////
1510,12H TOWER COST=1F9.0//,510,18H SEPERATOR COST = 1F9.0//,5
210,36H NEUTRALIZATION SEPERATOR TANK COST=1F9.0//,510,18H MIX
3ING TANK COST=1F9.0//510,15H PUMPING COST =1F9.0//,510,27H NE
4UTRALIZATION TANK COST =1F9.0//,510,24H NITRIC ACID TANK COST
5 =1F9.0//,510,20H BENZENE TANK COST =1F9.0//,510,17H CONDESEE
6R COST =1F9.0//,510,16H REBOILER COST =1F9.0//,510,18H EVAPO
7RATOR COST =1F9.0//,510,13H WATER COST =1F9.0//,510,15H REACT
8OR COST =1F9.0//,510,14H TUBING COST =1F9.0//,510,13H TOTAL C
9OST =1F15.2*$
-----
VECTOR VALUES BOTTOM = $///535,16H CONVERSION RATE*$
VECTOR VALUES MARGIN = % TOTAL EQUIPMENT COST IN
1 100,000 DOLLARS*$
-----
THAT PRINT FORMAT HEAD
EXECUTE PLOT4,(DUMMV,MARGIN,9.,0.,0.)
PRINT FORMAT BOTTOM
END OF PROGRAM
-----

```

Computer Output

A result sheet with a typical design-cost summary, and a computer plot of the equipment cost as a function of percent conversion, are shown below.

EQUIPMENT COSTS IN DOLLARS	
CONVERSION RATE =	0.10
TOWER COST =	2833.
SEPERATOR COST =	58656.
NEUTRALIZATION SEPARATOR TANK COST =	33435.
MIXING TANK COST =	129816.
PUMPING COST =	775.
NEUTRALIZATION TANK COST =	41431.
NITRIC ACID TANK COST =	205433.
BENZENE TANK COST =	116173.
CONDESSER COST =	2177.
REBOILER COST =	4199.
EVAPORATOR COST =	17131.
WATER COST =	3809.
REACTOR COST =	910.
TUBING COST =	17913.
TOTAL COST =	637977.95



2. Solution to the Control Problem

The control-system-analysis problem was preceded by two lectures and a demonstration period covering the uses of the analog computer, three lectures on the fundamentals of process linearization and simulation, and five lectures on elementary control theory. This preparation for the problem was necessary since all of these fields were new to the students. Obviously only the most elementary concepts could be presented in this limited time, but enough background was given to enable the students to understand clearly the principles and to obtain an empirical or experimental solution to the problem.

The problem involves the experimental determination of the transient behavior of the nitrator when under control of certain basic feedback control systems (proportional, integral, proportional-plus-integral), and the selection of a satisfactory control system. This experimental study was performed on an analog computer simulation of the nitrator. The simulation is achieved by the use of the linearized energy and material balances. The control variable is the cooling water temperature and the measured variable is the temperature in the reactor. The exact details of the simulation and control study again are presented using the greatly edited form of one student group's report. The report is that of Peter Lamont and Wayne Allen.

a. Method

Control mechanisms for the production of nitrobenzene in a continuous, stirred-tank reactor were investigated by system simulation with an analog computer. The equations used were linearized differential equations based on the unsteady-state heat and mass balances. The reactor's response to small disturbances from the steady state were noted for several control combinations and for no control. Evaluation of the system with and without control was based on the time required for the system to return to steady state and the manner in which the temperature and concentration settled down.

The linearized differential equations for the simulation of the nitrator shown in the figure are shown on the next page.

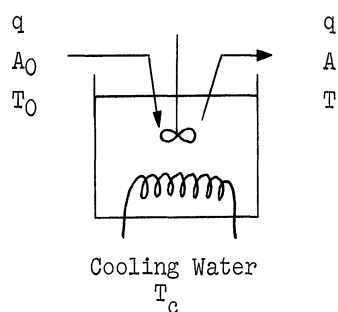




Table of Symbols

$A_0, A$  = concentration of benzene (lb.mol./ft<sup>3</sup>)  
 $q$  = flow rate (ft<sup>3</sup>/hr.)  
 $T_c, T_0, T$  = temperature (°F)  
 $V$  = reactor volume (ft<sup>3</sup>)  
 $r(A, T)$  = reaction rate (lb.mol./ft<sup>3</sup>.hr.)  
 $\rho$  = density (lb./ft<sup>3</sup>)  
 $u$  = heat transfer coefficient (BTU/hr.ft<sup>2</sup>°F)  
 $a$  = heat exchange area (ft<sup>2</sup>)  
 $c$  = specific heat (BTU/lb.°F)  
 $t$  = time (hr.)  
 $\theta$  = nominal holding time (hr.)  
 $-\Delta H$  = heat of reaction

The equations governing the transient behavior of the nitrator for small disturbances are:

$$\frac{d(A-A_s)}{dt} = \frac{\delta F_1}{\delta A}(A-A_s) + \frac{\delta F_1}{\delta T}(T-T_s)$$

$$\frac{d(A-A_s)}{dt} = \frac{\delta F_2}{\delta A}(A-A_s) + \frac{\delta F_2}{\delta T}(T-T_s) + \frac{\delta F_2}{\delta T_c}(T_c-T_{cs})$$

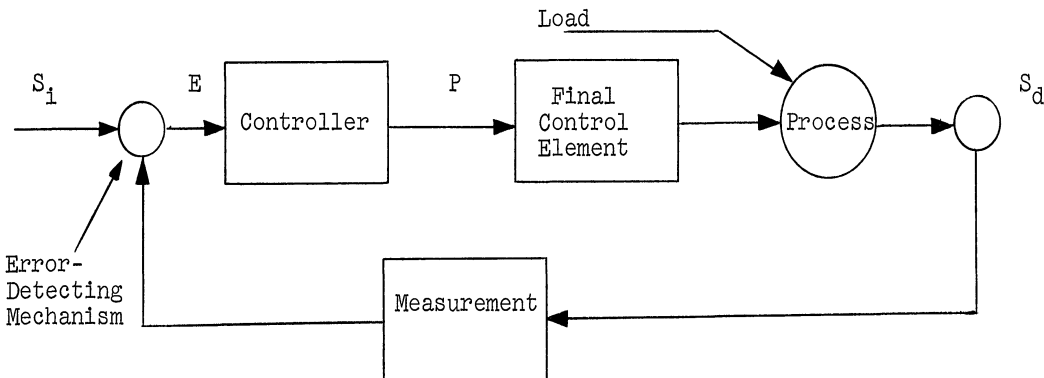
where

$$F_1 = \frac{A_0 - A}{\theta} - r(A, T)$$

$$F_2 = \frac{T_0 - T}{\theta} + \frac{ua(T_c - T)}{V\rho c} + r(A, T) \frac{(-\Delta H)}{\rho c}$$

where partial derivatives are evaluated at the steady state conditions,  $T_s, A_s, T_{cs}$ .

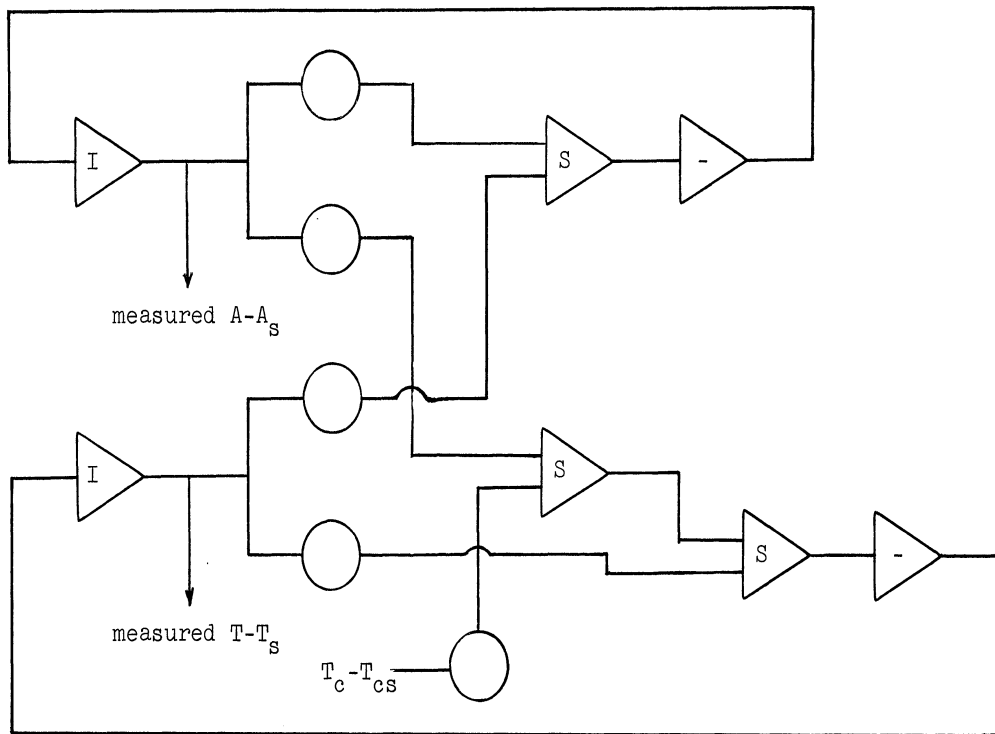
These equations (properly scaled) are programmed on the analog computer, resulting in the following diagram developed by the group.







- $S_i$  = steady state temperature
- $S_d$  = temperature deviation
- $E$  = error
- $P$  = controller output signal

Signal Flow Diagram

A circuit diagram for the analog computer solution is shown below.

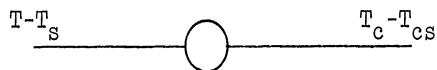


-  = integration plus sign inversion
-  = summation plus sign inversion
-  = sign inversion
-  = potentiometer

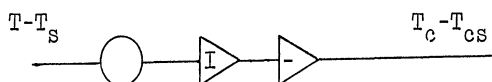
The dynamic performance of the nitrator is then simulated by programming the analog computer and setting the potentiometers to values determined by the design.

The feedback control system was added to the circuit by the additional subprograms which were placed between the  $(T-T_s)$  measured and the  $(T_c - T_{cs})$ , thus forcing  $(T_c - T_{cs})$ , the control variable, to be a function of the measured temperature derivative  $(T-T_s)$ .

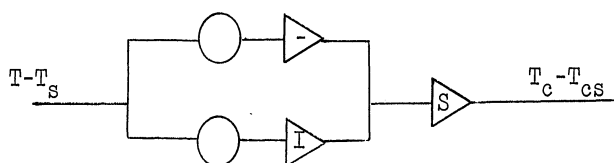
1. Proportional Control Circuit:



2. Integral Control Circuit:



3. Integral Plus Proportional Control Circuit



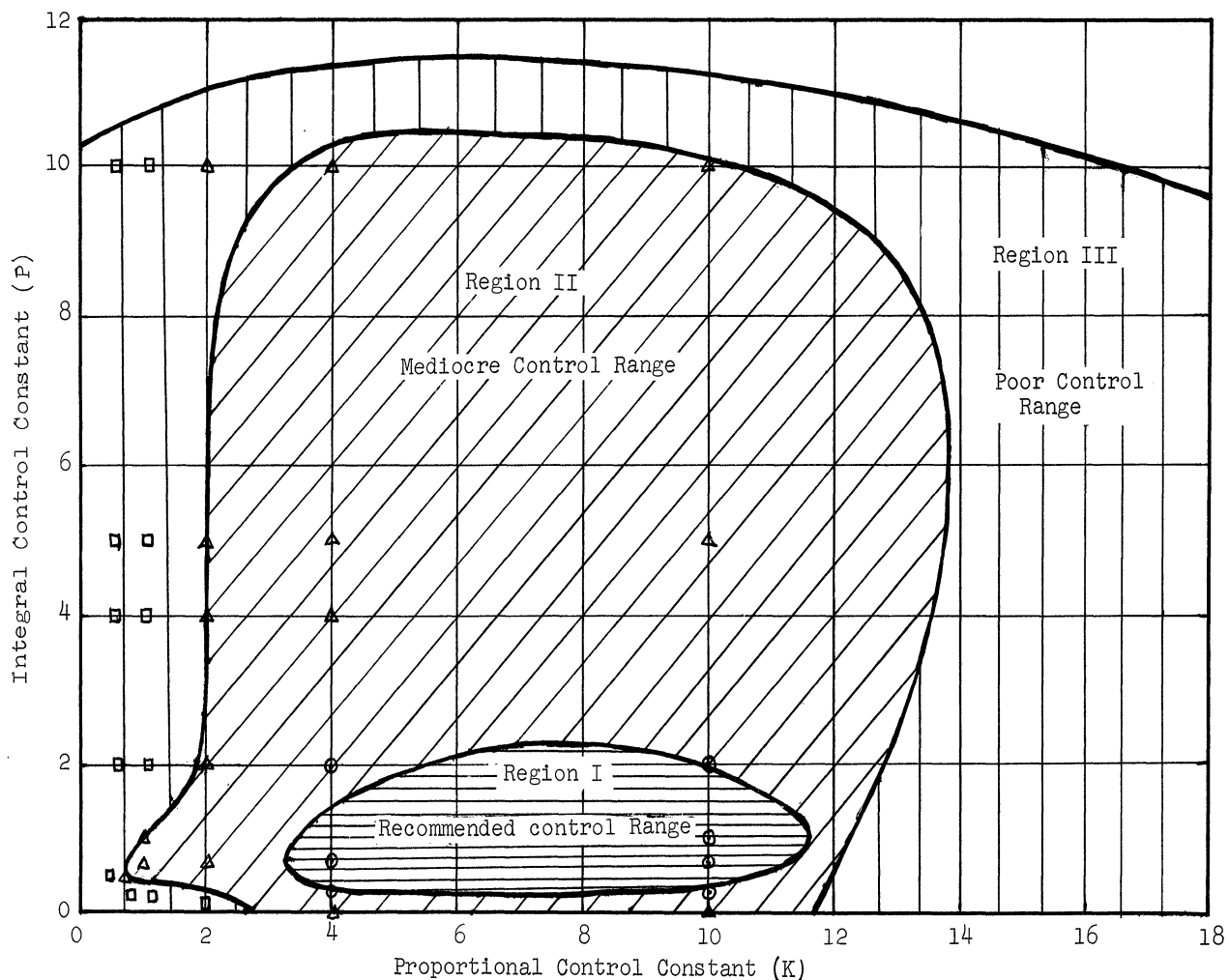
The response of these systems to an initial disturbance in the concentration  $A-A_s$  was then investigated.

b. Results

The findings of this investigation will be reported in an arbitrary sense, as the method does not lend itself to exact numerical results. The initial disturbance placed on the simulated system is to be regarded as a small displacement from steady-state conditions. After a short time lag the temperature departs from the steady state, the displacement being related to the change in concentration initially imposed. The system then responds and returns to steady state, the time required being proportional to the magnitude of the initial disturbance in concentration. But the values of the constants for proportional and integral control are independent of the magnitude of the error in concentration, i.e., no matter what magnitude is assigned to the initial disturbance in concentration, the control mechanism acts in the same manner to return the system to steady state. Therefore, the proportional and integral control constants are as specified, no matter what value is assigned to the initial disturbance in concentration. Since the object is to specify control regarding type and range of control constants, it is justifiable to report the findings in an arbitrary sense.

The control arrangements were evaluated on the basis of the relative times required to return the system to steady state. Critically damped return of temperature and concentration to the steady-state value is desired. The fastest, smoothest control is desirable. It was found that the control which brought the system to steady-state most rapidly was that which produced critical damping of the temperature and concentration. On the other hand, when the concentration was under- or over-damped, there were rapid oscillations in temperature and the system took longer to settle down to steady state conditions. From these correlations it can be seen that the time required for the system to return to steady state provides an excellent means for comparison of the several combinations of control constants.

For integral and proportional control evaluation with respect to combinations of the constants, regions can be differentiated based on the time required for the system to return to steady state. In the figure below, Region I is the recommended control range with relative control times of 0 through 7. Region II is the mediocre control range with relative control times of 7 through 13. Region III is the poor control range with relative control times greater than 13. Control times are given in arbitrary time units. The control in Region I either critically damps or very slightly underdamps the temperature and critically damps the concentration with no "droop" or permanent error. Fast response is experienced with the use of large proportional control constants ( $4 \leq K \leq 10$ ) and droop is adequately corrected with small integral control constants ( $3/10 \leq P \leq 2$ ). Several undesirable responses are found in Region II. For no integral control the permanent error in concentration and temperature does not give good control; for large  $p$ 's, underdamped response leads to oscillations which should be avoided. Of course, these undesirable characteristics are less severe as Region I is approached. Region III is poor in that the time required for the system to return to steady state is excessive either because of slow response with no control or extreme underdamping with large control constants. Extreme underdamping is highly undesirable from the standpoint of the control mechanism in that the large and rapid oscillations overstress the control system.



Regions of control for combination of integral (P) and proportional (K) control constants.

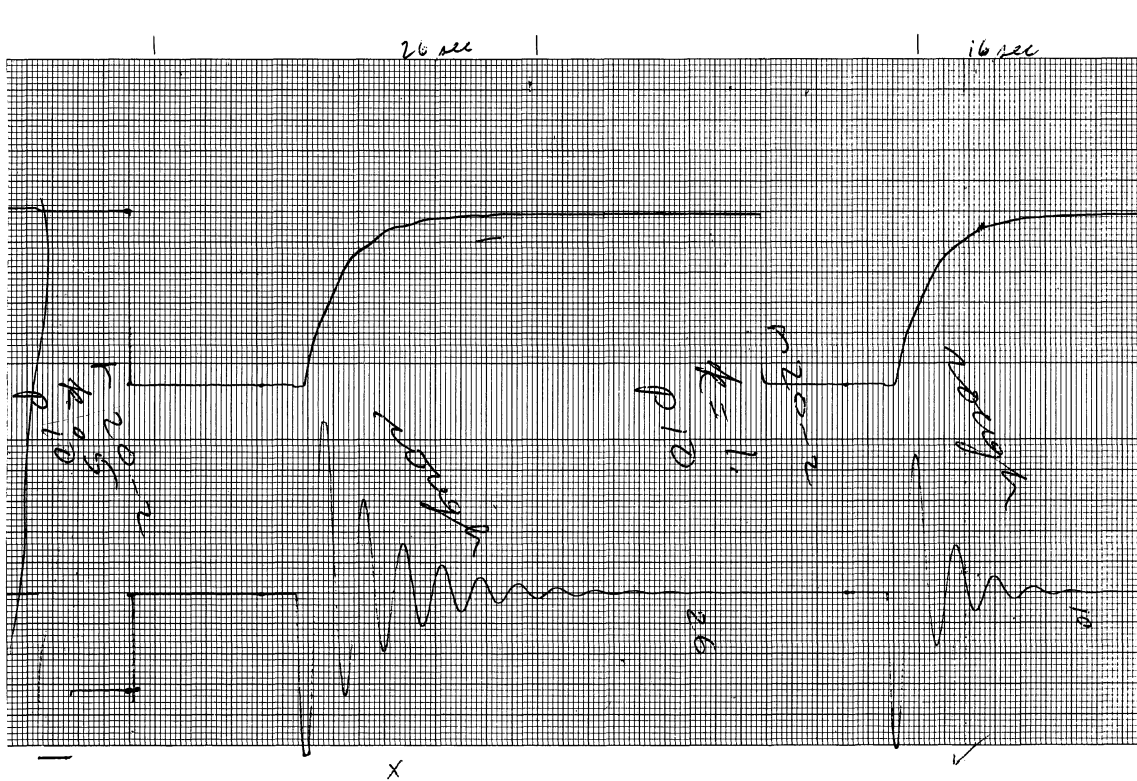
The data from the analog computer are presented below. Concentration and temperature (dimensionless errors) are plotted as functions of time. Plots of dimensionless temperature-error as a function of dimensionless concentration-error (obtained from the parametric data) are presented where each plot is for combinations of a given integral control constant with several proportional control constants. From these plots, control constant combinations can be evaluated by noting that the length of the line is roughly proportional to the time required to bring the system to steady state. Critical damping is signified by the line staying within one quadrant and underdamping by the line oscillating from one quadrant to another. These correlations provide foundation for the control regions explained above.

Example Problem No. 121

Preliminary investigation of rate control did not produce the expected rapid response. Complete results were not obtained, so further research in this regard would be in order. As rate control was not investigated in conjunction with integral or proportional control, definite statements cannot be made against or in favor of employing rate control.

This, then, gives a picture of the students' performance on an analog simulation of a control situation. It should be realized that the group does not have an extensive background in control theory, and hence their analysis of the systems is of an empirical nature.

Typical Computer Output



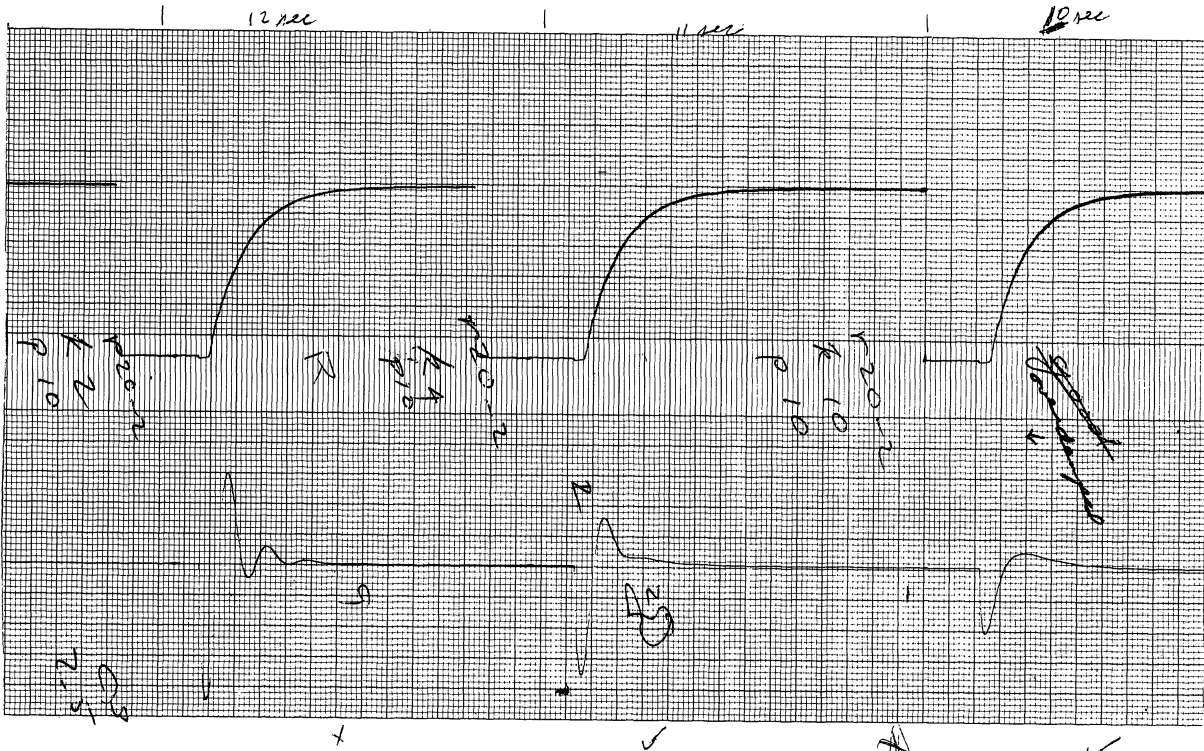
P = 10.  
K = 0.5

P = 10.  
K = 1.0

Integral and Proportional Control

Integral P = 10  
Proportional K, .5-10

Computer Output, Continued

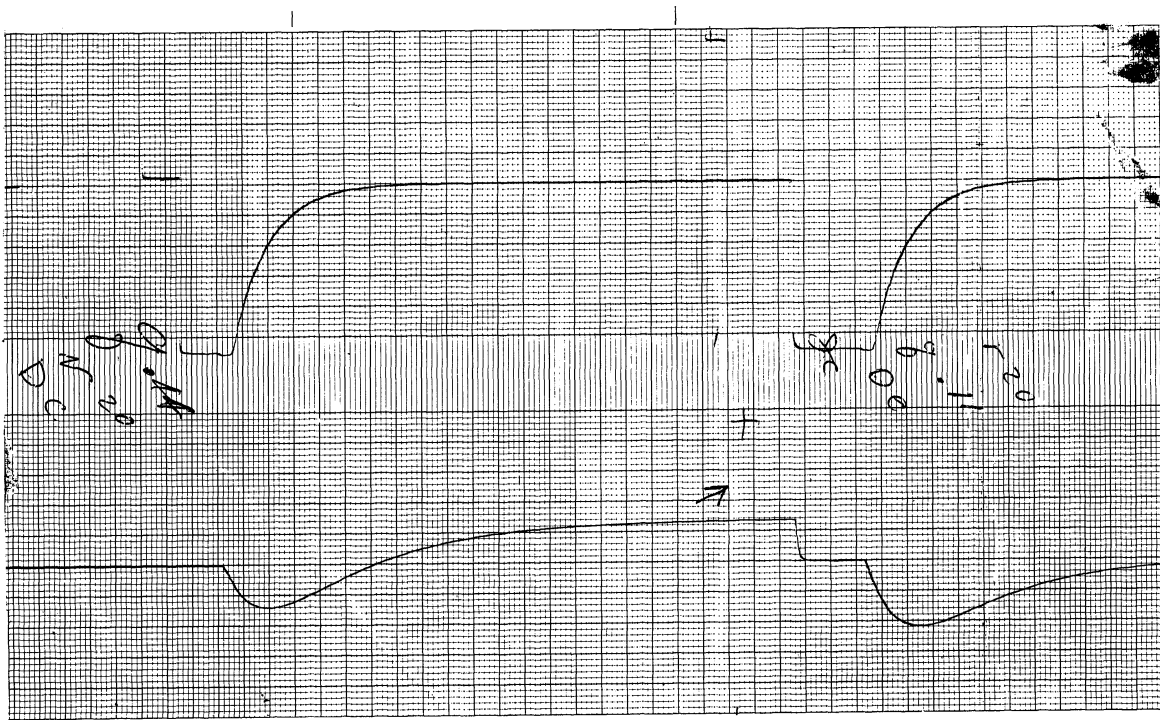


P = 10.  
K = 2.

Integral and Proportional Control,  
Continued

P = 10.  
K = 4.

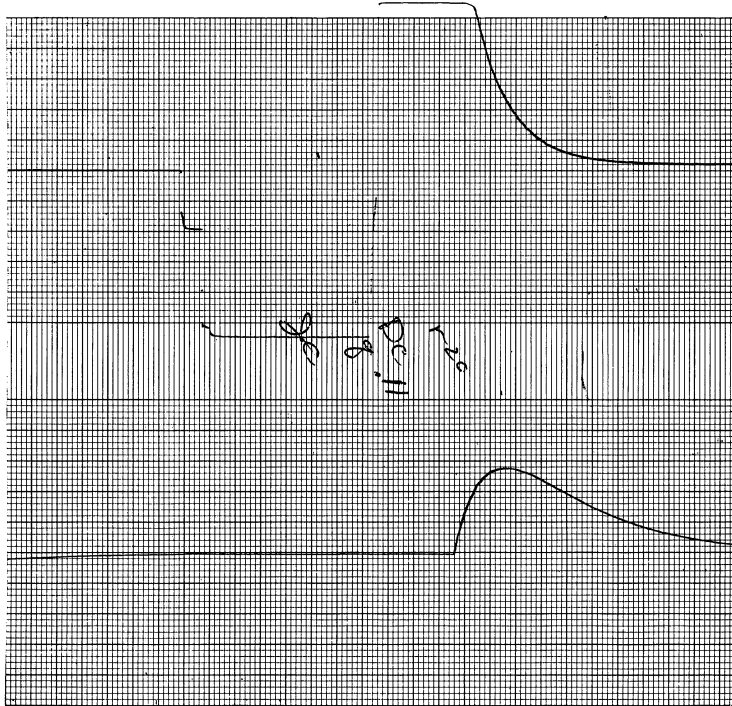
P = 10.  
K = 10.



q = 0.44

(Rate) Differential Control  
Differential control only  
q = .11, .44 (sample)

q = .11



(Rate) Differential Control, Continued

$$q = 0.11$$

Recommendations

Certainly there is no substitute for a strong programming background on the part of the students. In a design course the problems are generally too large to be used as exercises in programming for the students. With digital computer programming, prior experience is necessary; if such experience does not exist it is doubtful that the use of computers will upgrade the level of such a course. Too much class time will be needed to teach the concepts and the technical details of programming. With the digital computer, at least, it appears that gradual introduction of computers beginning at the sophomore level is the answer. The low-level, almost trivial computer problems which are so necessary at the beginning of the student's experience, can be assigned in the beginning chemical engineering courses without detracting from the engineering education of the students. A problem or two assigned in each course over a period of several semesters will give the student adequate experience and confidence to tackle an extensive problem when the need arises.

It should be noted that the experience gained in this work is with a procedure-oriented language, not a machine-oriented language. With such a language, the student's attention may be centered on the logic of the problem-solving technique rather than on the logic of the machine operation. With a machine-oriented language the technical details may be, for the average engineering student, completely overwhelming. The mass introduction of computers to an engineering class by use of a machine language would be very difficult.

## Use of Computers in an Undergraduate Chemical Engineering Design Course

Things are quite different for the electronic analog computer. The programming concepts of the analog computer are more readily assimilated by the students. It was found that it is quite possible to give the students a feel for the analog computer in two or three hours of class time. With a good programming manual, the details of elementary analog programming are well within the reach of the average student. While the digital computer, in a closed-shop situation, remains distant and detached, the analog computer can be as immediate and responsive as a conventional laboratory experiment. This may well make up for its limited problem-solving ability, and make it an educational tool of value equal to that of the digital computer. Both the analog and digital computers should be considered, since they are complimentary, and the effort expended in the introduction of both rather than just one is well rewarded.

The statement is often made that the real educational value of the computer is discipline. The students are forced by the nature of the machine to formulate their problems in an orderly, precise, and logically consistent manner. This is true; but what is orderly, precise, and logically consistent to the machine may be physical nonsense. The computer solution of a formulated problem may be perfect but the physical formulation may well be erroneous. There are numerous examples of foggy thinking which has been properly programmed. For example, in the design course, one group wrote a technically perfect program which solved the equations beautifully and presented the results of the design in a most convenient format. The only trouble was that the equations they solved were not the design equations for the system they thought they were considering. No fault could be found with their computer usage, only with their engineering. Too much emphasis was spent on the details of programming and not enough on engineering fundamentals. Certainly the computer can add to the student's education, but there is no substitute for a knowledge of basic physical fundamentals.



Example Problem No. 122

ECONOMIC DESIGN OF A CONDENSER

by

Dale E. Briggs

Department of Chemical and Metallurgical Engineering

The University of Michigan

Course: Equipment Design

Credit hours: 3

Level: Senior

Statement of Problem

Develop a digital computer program using the MAD language to design a horizontal-tube surface condenser. The program should be sufficiently general to treat any single-component, condensing vapor on the shell side. Water is to be used as the cooling fluid on the tube side. Sub-routines are available for calculating the following:

1. Tube-side pressure drop using water (TUBEDP)
2. Shell-side pressure drop for unbaffled vapor flow (USHEDP)
3. Shell-side pressure drop for baffled vapor flow (BSHEDP)
4. Pertinent economic data (ECON)

Descriptions of the subroutines are given at the end of this problem.

After the program has been written, determine the condenser tube length, number of tube passes, and water velocity which will give the minimum sum of fixed and operating expense for the following conditions:

- |  |   |
|--|---|
| 1. Condensing vapor                        | refrigerant 22                            |
| 2. Amount of condensing vapor              | 40,000 lb./hr.                            |
| 3. Inlet vapor                             | saturated at 105 °F.                      |
| 4. Cooling water                           | cooling tower with treated make-up        |
| 5. Cooling water temperature               | 80°F. summer maximum 70°F. winter minimum |
| 6. Tubes                                   | 3/4 in., 18 BWG, copper                   |
| 7. Tube type                               | plain or finned                           |
| 8. Maximum allowable tube-side $\Delta P$  | 10 lb./sq. in.                            |
| 9. Maximum allowable shell-side $\Delta P$ | 3 lb./sq.in.                              |
| 10. Water cost                             | \$.01/1000 gal.                           |
| 11. Electric power cost                    | \$.008/KWHR                               |
| 12. Amortization rate                      | 3 years                                   |

The factorial search method is recommended for searching for the optimum set of conditions. The normal Tubular Exchanger Manufacturers Association (TEMA) standards should be followed.

Solution

The design of a condenser (as most heat transfer equipment) involves multiple trial-and-error calculations because of the complicated nature of the equations describing heat transfer and pressure drop. Initial values are assigned to all variables, both to those which may be freely chosen and to those which will be fixed by the values assigned to the chosen variables. Iterative procedures are used until calculated values of the "fixed" variables agree with those used in making the calculations.

The general scheme is as follows:

1. Estimate the overall coefficient,  $U_o$ , the logarithmic mean temperature difference, LMTD, and the water velocity,  $v_i$ , and calculate the required heat transfer surface.

$$A_{o\text{total}} = \frac{Q}{U_o * \text{LMTD}}$$

2. Using the tube length,  $L$ , and the heat transfer surface per linear foot,  $A_o$ , calculate the number of tubes required.

$$\text{tubes} = \frac{A_{o\text{total}}}{A_o * L}$$

3. Calculate the tube-side flow area per pass using the inside tube diameter,  $d_i$ , and number of passes, pass.

$$A_{\text{flow}} = \frac{\pi * d_i^2 * \text{tubes}}{4 * \text{pass} * 144}$$

4. Calculate the tube-side (water) flow rate.

$$W = \rho * 3600 * v_i * A_{\text{flow}}$$

5. Calculate the exit water temperature,  $T_{WO}$ , where the inlet temperature is  $T_{WI}$ .

$$T_{WO} = T_{WI} + \frac{Q}{W * C_p}$$

6. Using the inlet and outlet vapor temperatures  $TS_{VI}$  and  $TS_{VO}$ , calculate the logarithmic temperature difference.

$$\text{LMTD} = \frac{(TS_{VO} - T_{WI}) - (TS_{VI} - T_{WO})}{\ln \left[ \frac{TS_{VO} - T_{WI}}{TS_{VI} - T_{WO}} \right]}$$

7. Using an average water temperature,  $t_w$ , calculate the inside heat transfer coefficient,  $h_i$ , from

$$h_i = 150 (1 + 0.011 t_w) \frac{v_i^{0.8}}{d_i^{0.2}} \quad (\text{water})$$

or

$$\text{Nu} = 0.023 \text{Re}^{0.8} \text{Pr}^{0.4}$$

or

$$\text{Nu} = 0.027 \text{Re}^{0.8} \text{Pr}^{1/3} \left( \frac{\mu}{\mu_w} \right)^{0.14}$$

8. Estimate the temperature drop across the condensing film,  $\Delta T_f$ , determine the correction factor,  $C_n$ , and calculate the condensing coefficient,  $h_m$ , using the Nusselt relationship for multiple horizontal tubes.

$$h_m = 0.725 C_n \left[ \frac{k^3 \rho^2 g_c \lambda}{N_a D_o \Delta T_f \mu} \right]^{1/4}$$

9. Where  $r_o$  and  $r_i$  are the outside and inside fouling resistances, calculate the overall coefficient.

$$\frac{1}{U_{o\text{calc}}} = \frac{1}{h_m} + \frac{A_o}{A_i h_i} + \frac{A_o \Delta x}{A_m k_{\text{metal}}} + r_o + \frac{A_o}{A_i} r_i$$

10. Evaluate the temperature drop across the condensing film from

$$\Delta T_{f\text{calc}} = \frac{U_o * \text{LMTD}}{h_m}$$

Return to step 8 if  $\Delta T_{f\text{calc}}$  differs significantly from  $\Delta T_f$ .

11. Recalculate the area and number of tubes required.

$$A_{o\text{total}} = \frac{Q}{U_{o\text{calc}} * \text{LMTD}}$$

$$\text{tubes} = \frac{A_{o\text{total}}}{A_o * L}$$

12. Whenever the required number of tubes differs by an amount greater than  $\epsilon$  from the number of tubes assumed, assign a new value and return to step 3.

Two design alternatives are possible once the number of tubes required is calculated. If the vapor is condensing at a low pressure, the tubes can be placed in a large enough standard shell size so as to provide essentially un baffled flow of the vapor. The shell side pressure drop is calculated using the pressure drop subroutine for un baffled flow. If the pressure drop affects the condensing vapor temperature, the corrected value of the exit vapor temperature should be used to recalculate the LMTD which is then used to obtain a more accurate solution. Calculation of the tube-side pressure drop and economics information (which is done by sub-routines) completes the required calculation for the selected input data.

A second method of treatment which is applicable to higher condensing pressures involves the selection of the smallest standard shell size which will accommodate the required number of tubes on the specified pitch and layout. Usually there will be room for a few additional tubes. The shell is then completely filled with tubes and the shell-side pressure calculated using the baffled-shell pressure drop subroutine. The exit vapor pressure is used to calculate the exit vapor temperature. A new required tube-side fluid velocity is then calculated. This is required since additional flow area has been provided. After the required velocity is

## Economic Design of a Condenser

calculated, the tube-side pressure drop and economics subroutines are executed to complete the calculations for the data specified.

The four subroutines alluded to earlier were written by the instructor and provided to the students in the form of punched IBM cards. A brief description of each subroutine was given to the students. These subroutines are described in more detail at the end of the problem.

### Student Solution

The computer program presented here was prepared by Andrew Padilla and represents a typical student approach to the problem. Mr. Padilla made use of three of the four available subroutines.

His previous computer experience consisted of attending a series of evening lectures sponsored by the Ford Foundation Computer Project and solving a single computer problem in another Chemical and Metallurgical Engineering course.

### List of Symbols

The following are symbols used in the MAD program with their definitions.

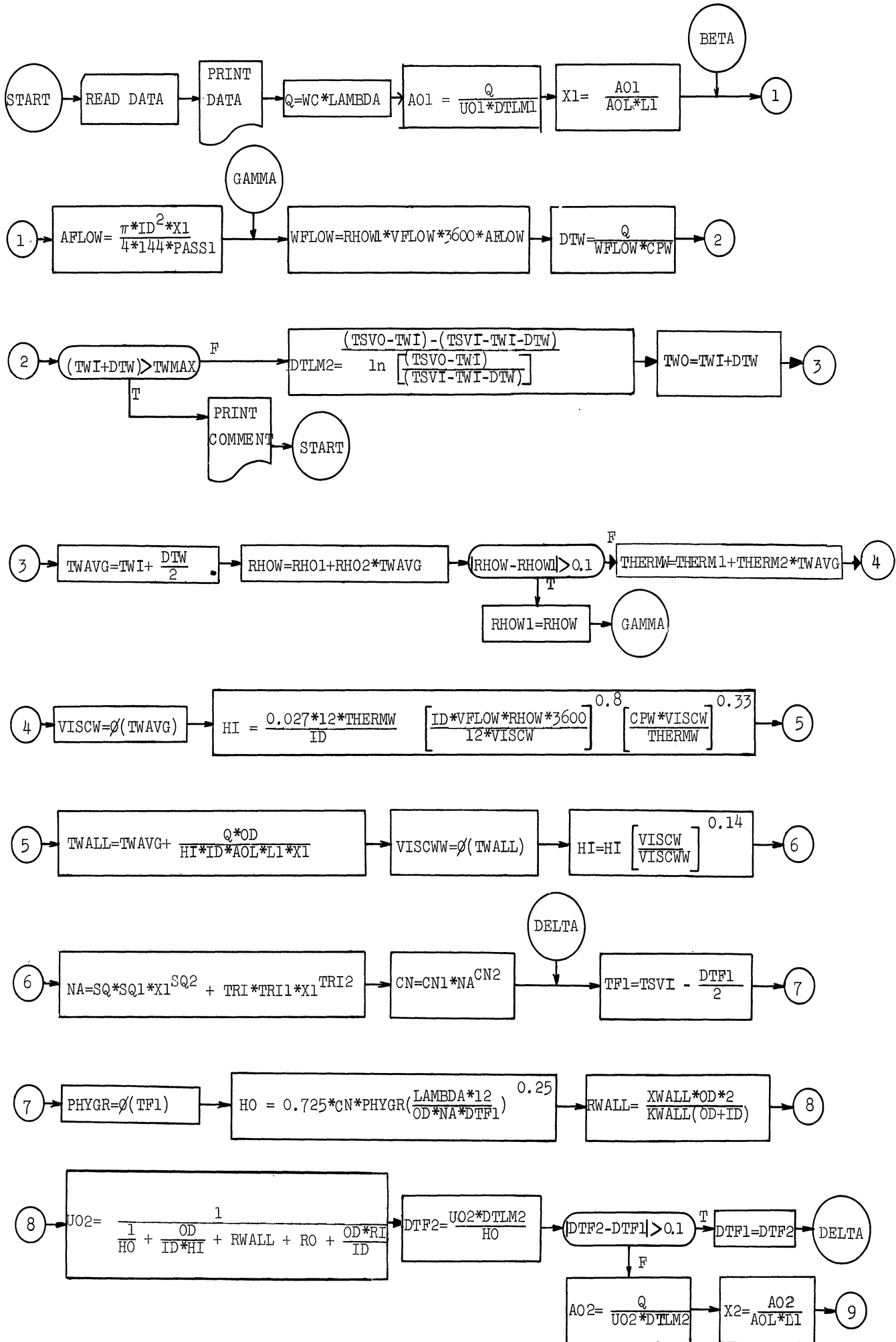
AFLOW2, AFLOW	water flow area per pass, sq. ft.
AO1, AO2, AO	total outside tube area, sq. ft.
AOL	outside surface area per unit length of tube, sq. ft./ft.
CN, CNO	correction factor for Nusselt equation
CN1, CN2	constants in the equation, $CN = (CN1)(NA)^{CN2}$ $CND = (CN1)(NA2)^{CN2}$
CPW	heat capacity of tube-side fluid, Btu/lb. °F.
DOTL1, DOTL2	outer tube limit diameter, ft.
DTF1, DTF2, DTF3	temperature drop across condensing film, °F.
DTLM1, DTLM2, DTLM3, DTLM4	logarithmic mean temperature difference between tube-side and shell-side fluids, °F.
DTW, DTW2	total temperature rise of tube-side fluid, °F.
HL, HL2	heat transfer coefficient for tube-side fluid, Btu/hr.-sq. ft. - °F.
HO, HO2	heat transfer coefficient for shell-side fluid, Btu/hr.-sq. ft.- °F.
ID	inside tube diameter, in.
IDSH	standard shell size inside diameter, in.
IDS	shell size inside diameter, in.
KWALL	thermal conductivity of tube wall, Btu/sq. ft.-hr.- °F./ft.
L1	tube length, ft.

Example Problem No. 122

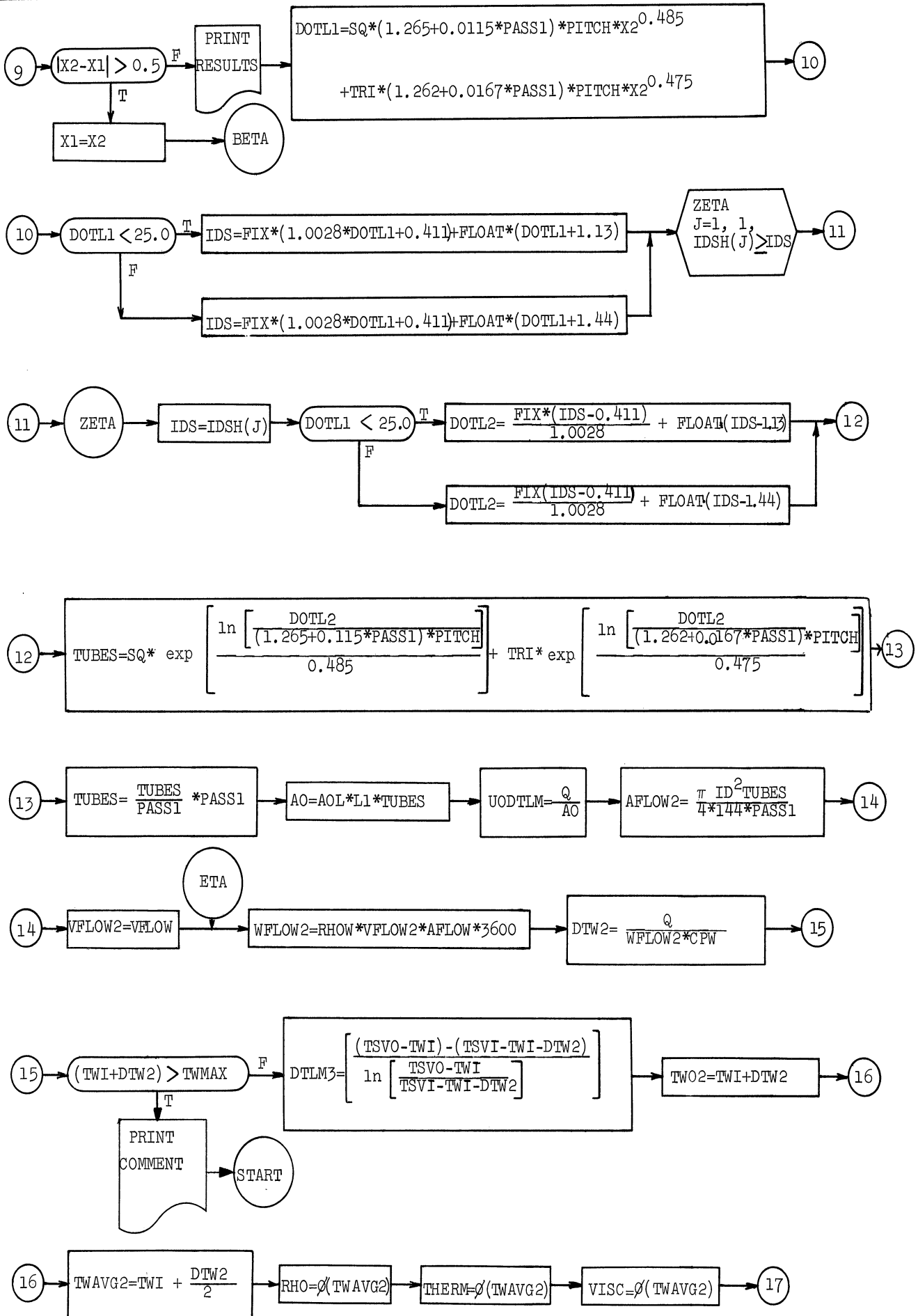
LAMBDA	heat of vaporization of shell-side fluid, Btu/lb.
NA, NA2	average number of tubes in a vertical row
OD	outside tube diameter, in.
PASST	number of passes
PHYGR, PHYGRP	temperature dependent properties of the condensate film defined by $\left[ \frac{k^3 \rho^2 g}{\mu} \right]^{1/4}$
PHYGR1, PHYGR2	constants in the equations: $PHYGR = PHYGR1 + (PHYGR2)(TF1)$ $PHYGRP = PHYGR1 + (PHYGR2)(TF2)$
PITCH	tube pitch, in.
Q	total heat load, Btu/hr.
RHO, RHOW1, RHOW	density of tube-side fluid, lb./cu. ft.
RHO1, RHO2	constants in the equation $RHOW = RHO1 + (RHO2)(TAVG)$
RWALL	thermal resistance of tube wall, hr.-sq.ft.-°F./Btu.
SQ, SQ1, SQ2	constants in the equation $NA = (SQ)(SQ1)(X1)^{SQ2} + (TRI)(TRI1)(X1)^{TRI2}$
TF, TF1	average temperature of the condensing film, °F.
THERM, THERMW	thermal conductivity of tube-side fluid. Btu/sq.ft.-hr.-°F./ft.
THERM1, THERM2	constants in the equation $THERMW = THERM1 + (THERM2)(TAVG)$
TRI, TRI1, TRI2	constants in the equation $NA = (SQ)(SQ1)(X1)^{SQ2} + (TRI)(TRI1)(X1)^{TRI2}$
TSVI	inlet temperature of the condensing vapor, °F.
TSVO	outlet temperature of the condensing vapor, °F.
TUBES	number of tubes for a filled standard shell
TWALL	temperature of tube-side fluid at the tube wall, °F.
TWAVG, TWAVG2	average temperature of tube-side fluid, °F.
TWI	inlet temperature of tube-side fluid, °F.
TWMAX	maximum allowable temperature for tube-side fluid, °F.
TWO, TWO2	outlet temperature of tube-side fluid, °F.
UO1, UO2, UO	overall heat transfer coefficient based on outside tube area, Btu/hr.-sq.ft.-°F.
UODT, UODTLM	product of overall coefficient and log mean temperature difference Btu/hr.-sq. ft.
VFLOW, VFLOW2	tube-side fluid velocity, ft/sec.
VISC, VISCW, VISCWW	viscosity of tube-side fluid, lb./ft.-hr.
VISC1, VISC2, VISC3, VISC4, VISC5	constants in the equations to determine tube-side fluid viscosity
WC	condensing load, lb./hr.
WFLOW, WFLOW2	tube-side fluid mass flow rate, lb./hr.
WINTER	inlet tube-side fluid temperature during winter, °F.
X1, X2	number of tubes required
XWALL	tube wall thickness, in.
Z	compressibility factor of vapor, dimensionless

Economic Design of a Condenser

Flow Diagram

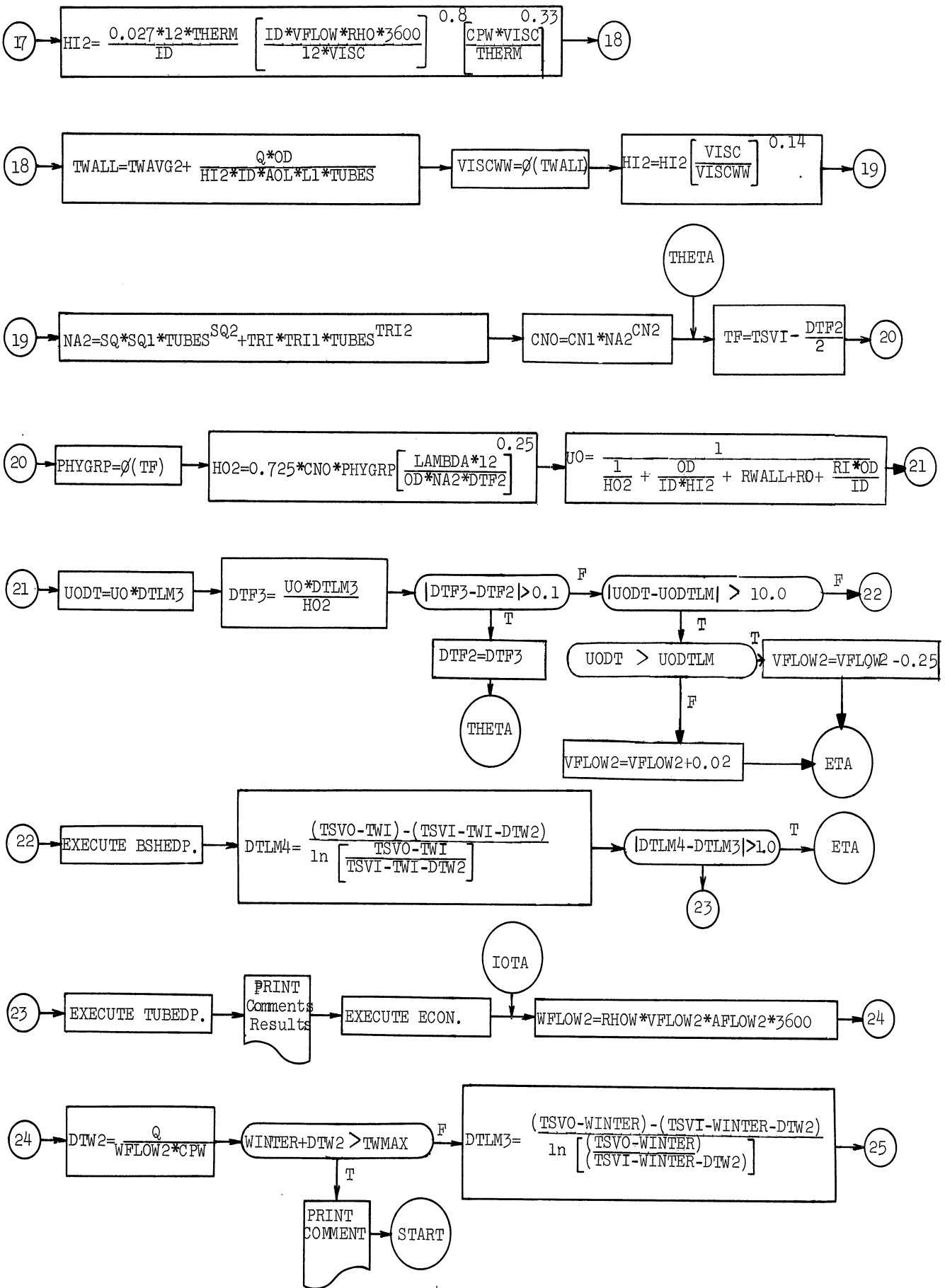


Flow Diagram (continued)



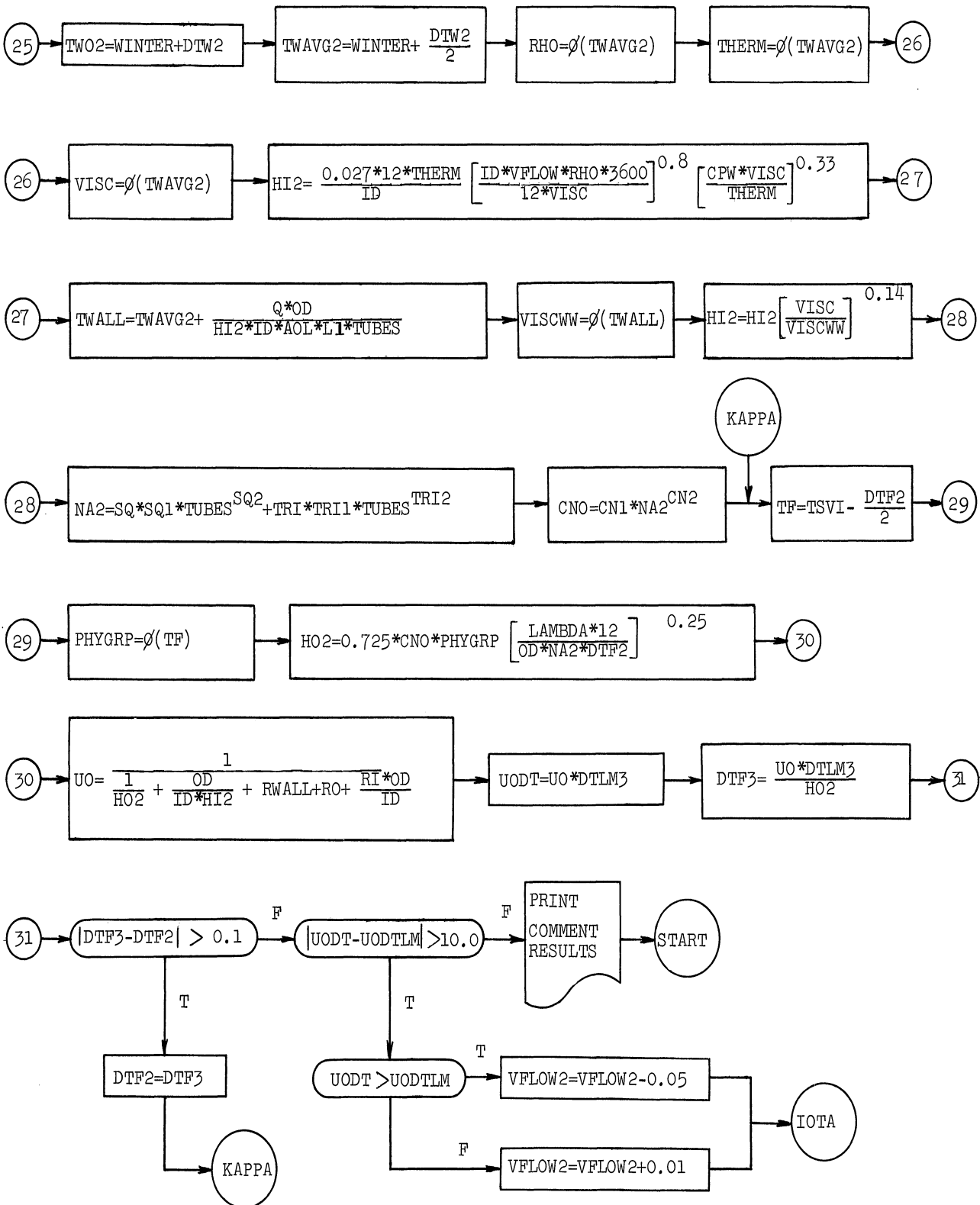
Economic Design of a Condenser

Flow Diagram (continued)





Flow Diagram (continued)



Economic Design of a Condenser

MAD Program and Data

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PADILLA                                X113E 1                                005 030 000
$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT
START  PRINT COMMENT $1CONDENSER DESIGN$
      READ DATA
      INTEGER J,TUBES,PASS1,TRI,SQ,HEAD,FIN,STWPS,STWPT,KTS,KSC,
      1KCFH
      DIMENSION IDSH(22)
      PRINT RESULTS WC, LAMBDA,CN1, CN2, PHYGR1, PHYGR2,
      1TSVI, TSV0, U01, DTLM1, DTF1,
      2SQ1, SQ2, TRI1, TRI2, OD, ID, XWALL, KWALL,
      3L1, AOL, PASS1, RO, RI, SQ, TRI, VFLOW, TWI, RHOW1, CPW,
      4RHO1, RHO2, THERM1, THERM2, VISC1, VISC2,
      5VISC3, VISC4, VISC5, BAFSP, FIN, TOTALL, HEAD, DEQ, Z,
      6MWT, PRTEMA, PRTEMB, VISGA, VISGB, VISGC, PRDALL,
      7STWPS, STWPT, KTS, KSC, KCFH, DAYS, AMORT, BASE, BASES,
      8TWMAX,WINTER,
      9TCSTI, CSTIND,CTGAL,INSTPC,WTFTS,WFTF,ELEC,MCSTF
      Q = WC*LAMBDA
      A01 = Q/(U01*DTLM1)
      X1 = A01/(AOL*L1)
BETA  AFLOW = 3.14*ID*ID*X1/(4.0*144.0*PASS1)
GAMMA WFLOW = RHOW1*VFLOW*3600.0*AFLOW
      DTW = Q/(WFLOW*CPW)
      WHENEVER (TWI+DTW).G.TWMAX
      PRINT COMMENT $EXCESSIVE EXIT WATER TEMPERATURE$
      TRANSFER TO START
      END OF CONDITIONAL
      DTLM2 = ((TSVO-TWI)-(TSVI-TWI-DTW))/ELOG.((TSVO-TWI)/
      1(TSVI-TWI-DTW))
      TWO = TWI+DTW
      TWAVG = TWI+(DTW/2)
      RHOW = RHO1+RHO2*TWAVG
      WHENEVER .ABS.(RHOW-RHOW1).G.0.1
      RHOW1 = RHOW
      TRANSFER TO GAMMA
      END OF CONDITIONAL
      THERMW = THERM1+THERM2*TWAVG
      VISCW = EXP.(VISC1+VISC2/TWAVG+VISC3/TWAVG.P.2.0+
      1VISC4/TWAVG.P.3.0+VISC5/TWAVG.P.4.0)
      HI = 0.027*12.0*(THERMW/ID)*(ID*VFLOW*RHOW*3600.0/(12.0*
      1VISCW)).P.0.8*(CPW*VISCW/THERMW).P.0.33
      TWALL = TWAVG+Q/(HI*(ID*AOL/OD)*L1*X1)
      VISCWW = EXP.(VISC1+VISC2/TWALL+VISC3/TWALL.P.2.0+
      1VISC4/TWALL.P.3.0+VISC5/TWALL.P.4.0)
      HI = HI*(VISCW/VISCWW).P.0.14
      NA = SQ*SQ*X1.P.SQ2+TRI*TRI1*X1.P.TRI2
      CN = CN1*NA.P.CN2
DELTA  TF1 = TSVI-(DTF1/2)
      PHYGR = PHYGR1+PHYGR2*TF1
      HO = 0.725*CN*PHYGR*(LAMBDA*12.0/(OD* NA* DTF1)).P.0.25
      RWALL = XWALL*OD*2.0/(KWALL*(OD+ID))
      U02 = 1/(1/HO+(OD/(ID*HI))+RWALL+RO+OD*RI/ID)
      DTF2 = U02*DTLM2/HO
      WHENEVER .ABS.(DTF2-DTF1).G.0.1
      DTF1 = DTF2
      TRANSFER TO DELTA
      END OF CONDITIONAL
      A02 = Q/(U02*DTLM2)
      X2 = A02/(AOL*L1)
      WHENEVER .ABS.(X2-X1).G.0.5

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Example Problem No. 122

MAD Program and Data (continued)

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X1 = X2
TRANSFER TO BETA
END OF CONDITIONAL
PRINT COMMENT $1THE REQUIRED CONDITIONS ARE$
PRINT RESULTS X2,VFLOW,TWO,UO2,HO,HI,DTLM2
DOTL1 = SQ*(1.265+0.0115*PASS1)*PITCH*X2.P.0.485 +
1TRI*(1.262+0.0167*PASS1)*PITCH*X2.P.0.475
WHENEVER DOTL1.L.25.0
IDS = FIX*(1.0028*DOTL1+0.4.1) + FLOAT*(DOTL1+1.13)
OTHERWISE
IDS = FIX*(1.0028*DOTL1+0.411) + FLOAT*(DOTL1+1.44)
END OF CONDITIONAL
THROUGH ZETA, FOR J=1,1,IDSH(J).GE.IDS
ZETA CONTINUE
IDS = IDSH(J)
WHENEVER DOTL1.L.25.0
DOTL2 = FIX*(IDS-0.411)/1.0028 + FLOAT*(IDS-1.13)
OTHERWISE
DOTL2 = FIX*(IDS-0.411)/1.0028 + FLOAT*(IDS-1.44)
END OF CONDITIONAL
TUBES = SQ*EXP.((ELOG.(DOTL2/((1.265+0.115*PASS1)*PITCH)))/
10.485) + TRI*EXP.((ELOG.(DOTL2/((1.262+0.0167*PASS1)*
2PITCH)))/0.475)
TUBES = (TUBES/PASS1)*PASS1
AO = AOL*L1*TUBES
UODTLM = Q/AO
AFLOW2 = 3.14*ID*ID*TUBES/(4.0*144.0*PASS1)
VFLOW2 = VFLOW
ETA WFLOW2 = RHO*VFLOW2*AFLOW2*3600.0
DTW2 = Q/(WFLOW2*CPW)
WHENEVER (TWI+DTW2).G.TWMAX
PRINT COMMENT $UEXCESSIVE EXIT WATER TEMPERATURE$
TRANSFER TO START
END OF CONDITIONAL
DTLM3 = ((TSVO-TWI)-(TSVI-TWI-DTW2))/ELOG.((TSVO-TWI)/
1(TSVI-TWI-DTW2))
TWO2 = TWI+DTW2
TWAVG2 = TWI+(DTW2/2)
RHO = RHO1+RHO2*TWAVG2
THERM = THERM1+THERM2*TWAVG2
VISC = EXP.(VISC1+VISC2/TWAVG2+VISC3/TWAVG2.P.2.0+
1VISC4/TWAVG2.P.3.0+VISC5/TWAVG2.P.4.0)
HI2 = 0.027*12.0*(THERM/ID)*(ID*VFLOW*RHO*3600.0/(12.0*
1 VISC)).P.0.8*(CPW*VISC/THERM).P.0.33
TWALL = TWAVG2+Q/(HI2*(ID*AOL/OD)*L1*TUBES)
VISCWW = EXP.(VISC1+VISC2/TWALL+VISC3/TWALL.P.2.0+
1VISC4/TWALL.P.3.0+VISC5/TWALL.P.4.0)
HI2 = HI2*(VISC/VISCWW).P.0.14
NA2 = SQ*SQ1*TUBES.P.SQ2+TRI*TRI1*TUBES.P.TRI2
CNO = CN1*NA2.P.CN2
THETA TF = TSVI-(DTF2/2)
PHYGRP = PHYGR1+PHYGR2*TF
HO2 = 0.725*CNO*PHYGRP*(LAMBDA*12.0/(OD*NA2*DTF2)).P.0.25
UO = 1/(1/HO2+OD/(ID*HI2)+RWALL+RO+RI*OD/ID)
UODT = UO*DTLM3
DTF3 = UO*DTLM3/HO2
WHENEVER .ABS.(DTF3-DTF2).G.0.1
DTF2 = DTF3
TRANSFER TO THETA
END OF CONDITIONAL
WHENEVER .ABS.(UODT-UODTLM).G.10.0
WHENEVER UODT.G.UODTLM
VFLOW2 = VFLOW2-0.25
TRANSFER TO ETA
OTHERWISE
VFLOW2 = VFLOW2+0.02
TRANSFER TO ETA
END OF CONDITIONAL
END OF CONDITIONAL
EXECUTE BSHPDP. (IDS, PASS1, OD, L1, BAFSP, TRI, TUBES,FIN,
1TOTAL, PITCH, HEAD, DEQ, Z, WC, MWT, TSVI, PRTEMA, PRTEMB,
2VISGA, VISGB, VISGC, TOTPD, TSVO, START)
DTLM4 = ((TSVO-TWI)-(TSVI-TWI-DTW2))/ELOG.((TSVO-TWI)/

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Economic Design of a Condenser

MAD Program and Data (continued)

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1(TSVI-TWI-DTW2))
WHENEVER .ABS.(DTLM4-DTLM3).G.1.0
TRANSFER TO ETA
END OF CONDITIONAL
EXECUTE TUBEDP.(L1, PASS1, VFLOW2, ID, IDS, TWAVG2,TUBES,
1PRDALL, PRDRT, GPM, POWER, START)
PRINT COMMENT $8THE CONDITIONS FOR A FULL SHELL ARE$
PRINT RESULTS IDS,TUBES,VFLOW2,TWO2,UO,HO2,HI2,DTLM3
EXECUTE ECON.(STWPS,STWPT,KTS,KSC,KCFH,OD,L1,IDS,PASS1,
1HEAD,DAYS,GPM,AMORT,BASE,BASES,CSTIND,TCSTI,CTGAL,INSTPC,
2WTFTS,WTFTELEC,POWER,MCSTF,AOL,TUBES,START)
IOTA
VFLOW2 = RHOV*VFLOW2*AFLOW2*3600.0
DTW2 = Q/(VFLOW2*CPW)
WHENEVER (WINTER+DTW2).G.TWMAX
PRINT COMMENT $8EXCESSIVE WINTER EXIT WATER TEMPERATURE$
TRANSFER TO START
END OF CONDITIONAL
DTLM3=((TSVO-WINTER)-(TSVI-WINTER-DTW2))/
1ELOG(((TSVO-WINTER)/(TSVI-WINTER-DTW2))
TWO2 = WINTER+DTW2
TWAVG2 = WINTER+(DTW2/2)
RHO = RHO1+RHO2*TWAVG2
THERM = THERM1+THERM2*TWAVG2
VISC = EXP.(VISC1+VISC2/TWAVG2+VISC3/TWAVG2.P.2.0+
1VISC4/TWAVG2.P.3.0+VISC5/TWAVG2.P.4.0)
HI2 = 0.027*12.0*(THERM/ID)*(ID*VFLOW*RHO*3600.0/(12.0*
1 VISC)).P.0.8*(CPW*VISC/THERM).P.0.33
TWALL = TWAVG2+Q/(HI2*(ID*AOL/OD)*L1*TUBES)
VISCW = EXP.(VISC1+VISC2/TWALL+VISC3/TWALL.P.2.0+
1VISC4/TWALL.P.3.0+VISC5/TWALL.P.4.0)
HI2 = HI2*(VISC/VISCW).P.0.14
NA2 = SQ*SQ1*TUBES.P.SQ2+TRI*TRI1*TUBES.P.TRI2
CNO = CN1*NA2.P.CN2
KAPPA
TF = TSVI-(DTF2/2)
PHYGRP = PHYGR1+PHYGR2*TF
HO2 = 0.725*CNO*PHYGRP*(LAMBDA*12.0/(OD*NA2*DTF2)).P.0.25
UO = 1/(1/HO2+OD/(ID*HI2)+RWALL+RO+RI*OD/ID)
UODT = UO*DTLM3
DTF3 = UO*DTLM3/HO2
WHENEVER .ABS.(DTF3-DTF2).G.0.1
DTF2 = DTF3
TRANSFER TO KAPPA
END OF CONDITIONAL
WHENEVER .ABS.(UODT-UODTLM).G.10.0
WHENEVER UODT.G.UODTLM
VFLOW2 = VFLOW2-0.05
TRANSFER TO IOTA
OTHERWISE
VFLOW2 = VFLOW2+0.01
TRANSFER TO IOTA
END OF CONDITIONAL
END OF CONDITIONAL
PRINT COMMENT $8THE WINTER CONDITIONS ARE$
PRINT RESULTS VFLOW2,TWO2,UO,HO2,HI2,DTLM3
VECTOR VALUES IDSH(1) = 5.047, 6.065, 8.071, 10.02, 12.09,
2 13.375, 15.25, 17.25, 19.25, 21.25, 23.0, 25.0, 27.0, 29.0,
3 31.0, 33.0, 35.0, 37.0, 39.0, 42.0, 44.0, 47.0
TRANSFER TO START
END OF PROGRAM

$DATA
WC=40000.0, LAMBDA=70.52, CN1=0.86, CN2=0.2116, PHYGR1=223.0,
PHYGR2=-0.591, TSVI=105.0, TSVO=105.0,UO1=150.0, DTLM1=20.0, DTF1=10.0,
VFLOW=6.0, TWI=80.0, RHO1=62.22, CPW=0.999,
SQ1=0.815, SQ2=0.52, TRI1=0.481, TRI2=0.505,
OD=0.750, ID=0.652, XWALL=0.049, KWALL= 217.0,
PITCH=0.9375, FIX=1.0, FLOAT=0.0,
L1=12.0, AOL=0.1963, PASS1=2, RO=0.002,RI=0.001, SQ=0, TRI=1,
RHO1=63.13, RHO2=-0.0117, THERM1=0.3145, THERM2=-0.000475,
BAFSP=24.0, FIN=0, TOTALL=3.0, HEAD=0, DEQ=0.750, Z=0.765, MWT=86.48,
PRTEMA=12.9145, PRTEMB=-4230.0, VISGA=-3.245, VISGB=-20.04,VISGC=160.0,
PRDALL=10.0, STWPS=300, STWPT=300, KTS=1, KSC=3, KCFH=3, DAYS=350.0,
AMORT=3.0, BASE=0.7188, BASES=0.360, CSTIND=1.0, TCSTI=1.0,
CTGAL=0.00001, INSTPC=10.0, WTFTS=0.592, WTFTE=0.418, ELEC=0.008,
MCSTF=1.0, TWMAX=100.0, WINTER=70.0,
VISC1=-0.21968738E01, VISC2=0.54722744E03,VISC3=-0.41363282E05,
VISC4=0.16141324E07, VISC5=-0.24764542E08*
L1=8.0, VFLOW=6.0, PASS1=2*
L1=16.0, VFLOW=6.0, PASS1=2*
L1=20.0, VFLOW=6.0, PASS1=2*
L1=8.0, VFLOW=6.0, PASS1=4*
L1=12.0, VFLOW=6.0, PASS1=4*
L1=16.0, VFLOW=6.0, PASS1=4*
L1=20.0, VFLOW=6.0, PASS1=4*

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Computer Output

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CONDENSER DESIGN
WC = 4.00000E 04, LAMBDA = 70.520000, CN1 = .860000, CN2 = .211600
PHYGR1 = 223.000000, PHYGR2 = .591000, TSVI = 105.000000, TSVO = 104.944206
UC1 = 150.000000, DILM1 = 20.000000, DIF1 = 9.335316, SQ1 = .815000
SQ2 = .520000, TRI1 = .481000, TRI2 = .505000, OD = .750000
ID = .652000, XWALL = .049000, KWALL = 217.000000, LI = 20.000000
ACL = .196300, PASS1 = 2, RD = 2.000000E-03, RI = 10.000000E-04
SG = C, TRI = 1, VFLOW = 6.000000, TWI = 80.000000
RHOW1 = 62.220000, CPW = .999000, RH01 = 63.130000, RH02 = .011700
JHERM1 = 314500, JHERM2 = 4.750000E-04, VISC1 = -2.196874, VISC2 = 547.227440
VISC3 = 4.136328E 04, VISC4 = 1.614132E 06, VISC5 = -2.476454E 07, RAESP = 24.000000
FIN = C, ICIAL1 = 3.000000, HEAD = 0, DEG = .750000
Z = .765000, NAI = 86.480000, PRIEMA = 12.914500, PRIEMB = -4230.000000
VISA = -3.245000, VISGB = -20.040000, VISGC = 160.000000, PRDALL = 10.000000
SLWPS = 300, SLWPI = 300, KIS = 1, KSC = 3
KCFH = 3, DAYS = 350.000000, AMGT = 3.000000, BASE = .718800
BASCS = 360000, TWAX = 100.000000, WINTER = 70.000000, IC5II = 1.000000
CSLIND = 1.000000, CICAL = 10.000000E-06, INSTIPC = 10.000000, WTEIS = .592000
WTEJ = 418000, FLEC = 8.000000E-03, MGSIF = 1.000000

THE REQUIRED CONDITIONS ARE
X2 = 254.802340, VELGW = 6.000000, IWO = 87.113179, UO2 = 132.882399
HO = 316.455669, HI = 1181.554291, DILM2 = 21.220281

```

SHELL SIDE PRESSURE DROP FOR BAFFLED FLOW IS .2143 PSI

EXIT VAPOR TEMPERATURE IS 104.929 F

Economic Design of a Condenser

Computer Output, Continued

TUBE SIDE PRESSURE LOSS IS .316 PSI			
THE CONDITIONS FOR A FULL SHELL ARE			
U.S. = 15.25000	TUBES = 316	VELOW2 = 2.31000	IWC2 = 94.826378
U.S. = 136.71610	HC2 = 337.48220	HI2 = 1198.996674	DILM3 = 16.469527
TUBE SHEET AND RAFFLE MATERIAL			
SHELL AND COVER MATERIAL	1-1/4 CR	ADMIRALTY	
CHANNEL AND FLOATING HEAD COVER	1-1/2 MC		
STANDARD WORKING PRESSURE THICKNESS - PSI	300		
STANDARD WORKING PRESSURE SHELLSIDE - PSI	300		
TUBE O.D. - IN.		.7500	
NUMBER OF TUBES		316	
SHELL INSIDE DIAMETER - IN.		19.250	
TUBE OUTSIDE SURFACE AREA - SQ/FT		.1963	
TUBE LENGTH - FT		20.00	
DAYS OPERATION PER YEAR		350.0	
AMORTIZATION RATE - YEARS		3.00	
COST INDEX		1.0000	
TUBE COST INDEX		1.00000	
STEEL TUBE COST - D/LR		.36000	
TUBE COST - D/LR		.71800	
ELECTRICITY COSTS - D/KWHR		.00000	
MAINTENANCE COST - D/YEAR-SQFT		1.0000	
INSTALLED COST - PLX. CNT		.6500	
MECHANICAL EFFICIENCY		.00010	
TUBESIDE FLUID COSTS - D/GAL		382.25	
TUBESIDE LIQUID FLOWRATE - GPM		1926.52	
LIQUID COST - D/YEAR		15.76	
POWER COST - D/YEAR		1248.47	
MAINTENANCE COST - D/YEAR		3190.76	
YEARLY OPERATING EXPENSE - D		1910.92	
TUBE COST - D		9089.78	
TOTAL CONDENSER COST - D		508.98	
INSTALLATION COST - D		9998.76	
INSTALLED CONDENSER COST - D		3332.92	
YEARLY FIXED CAPITAL EXPENSE - D		6523.67	
TOTAL YEARLY COST - D			
THE MINER CONDITIONS ARE			
VELOW2 = 1.190000	IWC2 = 98.780023	UO = 136.297531	HC2 = 336.258636
HI2 = 1144.55110	DILM3 = 16.636992		

Discussion of Results

The results of a factorial search to obtain the optimum plain-tube length, tube passes, and water velocity are presented in the table below.

Summary of Results for Plain Tubes

Tube Length ft.	Tube Passes	Shell I.D. in.	Number of Tubes	Water Velocity ft./sec.	Installed cost \$	Annual cost \$/year
8	2	27.00	658	2.02	14220.99	9271.33
12	2	23.00	466	2.18	12196.26	7840.88
16	2	19.25	318	5.00	9578.35	8480.47
20	2	19.25	318	2.31	9998.76	6523.67
8	4	27.00	624	6.00	14082.15	10838.11
12	4	23.00	440	6.00	12093.14	8757.54
16	4	21.25	372	4.56	11149.93	7216.18
20	4	19.25	300	5.52	9816.60	6795.89

The optimum plain-tube design has the following specifications:

tube length	20 ft.
tube passes	2
shell inside diameter	19.25 inches
tubes	3/4 in., 18 BWG, copper
number of tubes	318
water velocity	2.31 ft./sec.
installed cost	\$9998.76
annual cost	\$6523.67

The engineering results obtained with a digital computer are superior to those obtained by hand calculations because the weak points and assumptions indigenous to hand calculations are eliminated while utilizing the latest and most comprehensive design procedures. Although a finned-tube design would be more economical, the conclusions regarding a plain-tube design are as good as the economic data upon which they are based.

The program was run on an IBM 709 digital computer. The compilation of the MAD language to machine language took 1.03 minutes. The execute time for the eight trials was 2.33 minutes.

Instructors Comments and Critique

In teaching a course in equipment or process design, the instructor is concerned with presenting the latest and best design methods and with presenting the economics of the process in order to effect an optimum design. The selection of an appropriate problem for the students to solve with a digital computer should, therefore, reflect the aims of the course. Furthermore, the techniques and procedures required to solve the problem should be common to a wide class of problems. A simple problem requires little time but at the same time offers very little. On the other hand, to solve a comprehensive problem in which economics are involved requires more time than can be expected of the student.

## Economic Design of a Condenser

To permit the student to do a complete condenser design (a rather involved problem) in a minimum time, considerable preliminary preparation was necessary. Four subroutines were written for the student's use. These included such things as tube-side and shell-side pressure drop programs which, although needed in the complete program, are sufficiently unique to be suitable for subroutines. When treated in this way, a complete problem consists of a small main program with the appropriate peripheral programs included to make the total package complete. The student's responsibility is to write the main program which computes the necessary heat transfer coefficients and which utilizes the subroutines to obtain information necessary for the final solution. This method offers the advantage of short problems for time required while offering the advantages of comprehensive and complete problems for maximum learning.

Several mathematical relations and a major portion of the physical property data were also given to the students. The mathematical relations included such things as the diameter of the outer tube limit for a heat exchanger bundle as a function of the number of tubes, number of passes, tube pitch, and tube arrangement and the inside diameter of the shell as a function of the diameter of the outer tube limit and the type of heat exchanger. The physical property data were presented in most part in the form of equations directly adaptable for computer use.

Two lectures were given on computer programming. These covered the logic involved in the problem and a flow diagram which represented a solution to the problem in the broadest sense. Information was also given on sorting, convergence in trial-and-error problems, and the use of subroutines. Handouts were given to the students describing how to use the subroutines. The subroutines were duplicated and given to the students in the form of IBM cards ready for use in the computer.

Having given similar problems for the past three semesters, it has been found that students with limited computer experience generally have greater success if they attempt to write a simple program at first. After the elementary program is checked out for accuracy, it is an easy task to make alterations to improve the value of the program. To encourage this approach and to offer an incentive to do additional work, the following grading procedure was employed:

Task Accomplished	Grade
1. Calculation of the number of tubes required for a given set of data.	60-70
2. Task 1 and the calculation of the standard shell size and the tube-side pressure drop.	70-80
3. Task 2 and calculate the inside heat transfer coefficient using the Sieder-Tate equation which involves $(\mu/\mu_w)^{0.14}$	80-90
4. Task 3 and the consideration of finned tubes.	90-100



## Example Problem No. 122

Most of the students were able to complete task 3 successfully in approximately seven weeks. (They were also working on an extensive non-computer problem simultaneously.) The computer problem should be started early in the semester to allow the student to proceed as far as possible. There is probably as much benefit from making economic studies with the finished program as the preparation of the program itself. By providing the subroutines, various necessary relations and data, the programming time was reduced by approximately a factor of five.

The advantages of using the computer in design courses are:

1. Optimization studies can be made.
2. Practice can be given in writing complex programs.
3. Introduction to industry practice can be given.
4. Organization of multiple trial-and-error problems by computer or by hand can be taught.

The problem assigned had all the above advantages and was considered satisfactory.

### Description of Tube-side Pressure Drop Subroutine for Water

The method of calling the subroutine is:

EXECUTE TUBEDP. (TUBEL, PASS, TVEL, ID, IDS, TAVG, TUBES, PRDALL, PRDRT, GPM, POWER, START)

The arguments required for TUBEDP. are:

TUBEL	tube length, ft.
PASS	number of tube passes (integer)
TVEL	tube-side velocity, ft./sec.
ID	tube inside diameter, in.
IDS	shell inside diameter, in.
TAVG	average water temperature, °F.
TUBES	actual number of tubes used (integer)
PRDALL	allowable tube-side pressure drop, lb./sq.in.
*PRDRT	actual calculated pressure drop, lb./sq. in.
*GPM	calculated flow rate of water, gallons/min.
*POWER	calculated power required based on 65% eff., kw.
START	transfer location for error return

The arguments marked with "integer" must be in integer mode and declared as such by an integer declaration in the main program.

The subroutine takes the argument values and calculates the pressure drop in the headers due to sudden expansions, reversals, and contractions and in the tubes.

The procedures outlined in McAdams, Heat Transmission 3rd Ed., McGraw-Hill, are followed.

Outputs from the subroutine (in the form of arguments) are PRDRT, GPM and POWER.

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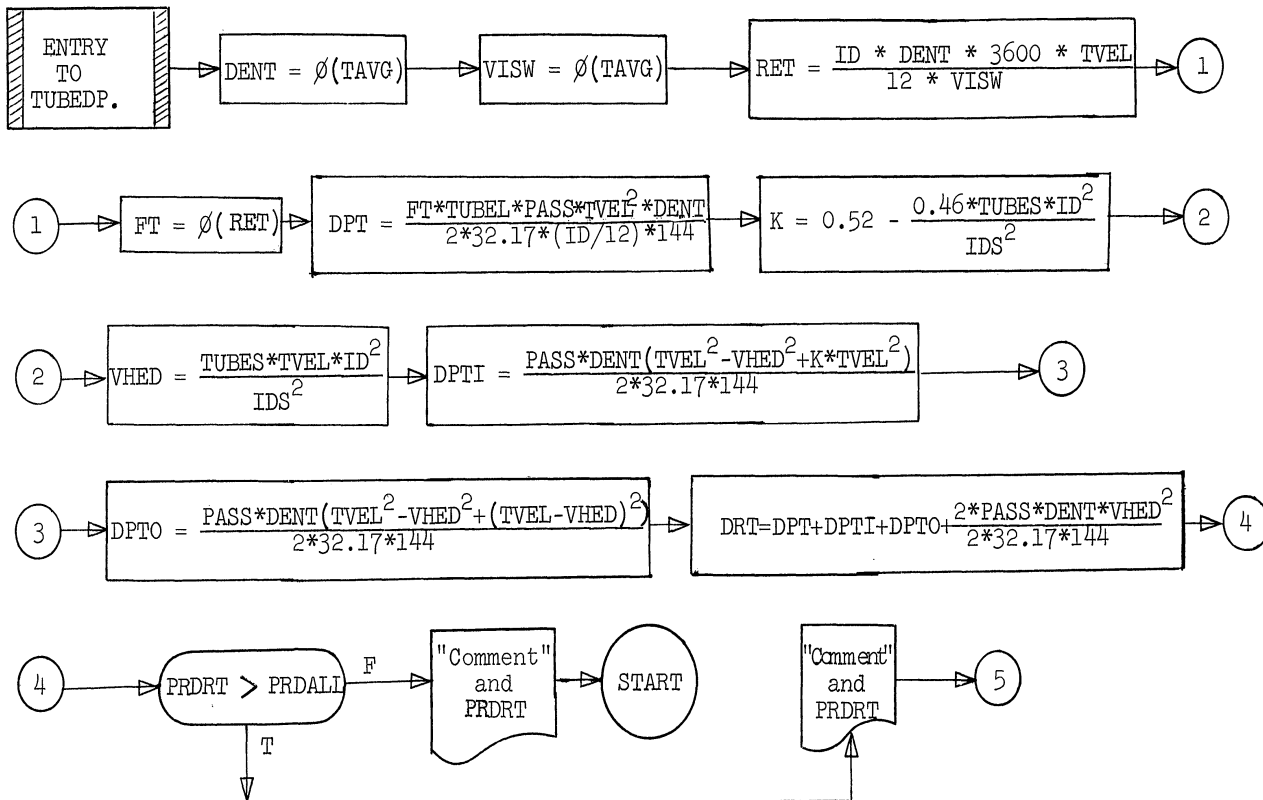
\* The values of PRDRT, GPM, and POWER need not have definite values prior to execution. Values will be calculated in the subroutine and can be used in the main program after execution of the subroutine.

Economic Design of a Condenser

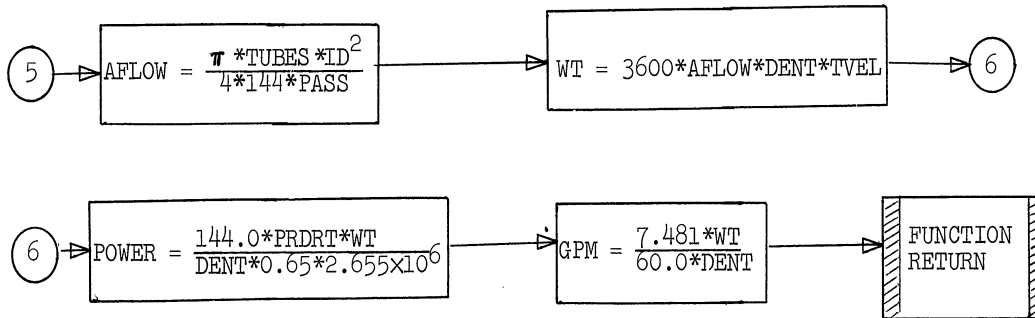
The following variables are used in the MAD language version of the tube-side pressure drop subroutine, but are not arguments for the subroutine.

- AFLOW total tube-side flow area per pass, sq. ft.
- DENT density of water, lb./cu. ft.
- DPTI pressure drop due to sudden contraction from headers to tubes, lb./sq. in.
- DPTO pressure drop due to sudden expansion from tubes to headers, lb./sq. in.
- DPT pressure drop in tubes, lb./sq. in.
- FT tube side friction factor, dimensionless
- K orifice coefficient used in calculating DPTI, dimensionless
- RET Reynolds number  $\frac{D_1 G}{\mu}$ , dimensionless
- VHED water velocity in headers, ft./sec.
- VISW viscosity of water, lb./ft.-hr.
- WT water flow rate, lb./hr.

A flow diagram of the tube-side pressure drop subroutine is shown below.



Flow Diagram, Continued



The MAD listing of the subroutine is shown below.

```

SCOMPILE MAD, EXECUTE, DUMP, PUNCH OBJECT
R TUBE SIDE PRESSURE DROP ROUTINE FOR WATER
EXTERNAL FUNCTION (TUBEL, PASS, TVEL, ID, IDS, TAVG, TUBES,
1 PRDALL, PRDRT, GPM, POWER, START)
ENTRY TO TUBEDP.
INTEGER TUBES, PASS
STATEMENT LABEL START
DENT = 63.13 - 0.0117*TAVG
VISW = EXP.(-0.21968738E 1 + 0.54722744E03/TAVG
1 -0.41363282E05/TAVG.P.2 + 0.16141324E07/TAVG.P.3
1 -0.24764542E08/TAVG.P.4)
RET = ID*DENT*TVEL*3600.0/(12.0*VISW)
FT = EXP.( 0.90677323E01 - 0.35722616E01*ELOG.(RET)
1 + 0.39637844E0*(ELOG.(RET)).P.2 -0.20815594E-01*
1 (ELOG.(RET)).P.3 + 0.41355033E-03*(ELOG.(RET)).P.4)
DPT=(FT*TUBEL*PASS*TVEL*TVEL*DENT)/(ID*32.17*24)
K = 0.52 - ((0.46*TUBES*ID*ID)/(IDS*IDS))
VHED = (TUBES*ID*ID*TVEL)/(IDS*IDS)
DPTI=(PASS*DENT*(TVEL*TVEL-VHED*VHED+K*TVEL*TVEL))/(288*32.17
1)
DPTO=(PASS*DENT*(TVEL*TVEL-VHED*VHED+(TVEL-VHED).P.2))/(288*3
12.17)
PRDRT=DPT+DPTI+DPTO+(2*PASS*DENT*VHED*VHED)/(288*32.17)
WHENEVER PRDRT .G. PRDALL
PRINT FORMAT COMM2
PRINT FORMAT INFO, PRDRT
TRANSFER TO START
OTHERWISE
PRINT FORMAT INFO, PRDRT
END OF CONDITIONAL
AFLOW = (3.1416*TUBES*ID*ID)/(576.0*PASS)
WT = 3600.0*AFLOW*DENT*TVEL
POWER = (144.0*PRDRT*WT)/(DENT*2.655*10.P.6*0.65)
GPM = (WT*7.481)/(60. *DENT)
FUNCTION RETURN
VECTOR VALUES INFO = $ 28H4TUBE SIDE PRESSURE DROP IS F7.3,
1 4H PSI *$
VECTOR VALUES COMM2 = $ 86H0CALCULATION WAS TERMINATED BECAUS
1E TUBE-SIDE PRESSURE DROP EXCEEDED ALLOWABLE LIMIT *$
END OF FUNCTION
  
```

Economic Design of a Condenser

Description of Economics Subroutine for Calculating Heat Exchanger Fixed and Operating Expenses

The method of calling the subroutine is:

EXECUTE ECON. (STWPS, STWPT, KTS, KSC, KCFH, OD, TUBEL, IDS, PASS, HEAD, DAYS, GPM, AMORT, BASE, BASES, CSTIND, TCSTI, CTGAL, INSTPC, WTFTS, WTFT, ELEC, POWER, MCSTF, AO, TUBES, START)

The arguments required for ECON. are:

STWPS	standard working pressure for shell side, lb./sq. in. (integer)
STWPT	standard working pressure for tube side, lb./sq. in. (integer)
KTS	material index for tube sheet (integer)
KSC	material index for shell and cover (integer)
KCFH	material index for channel and floating head cover (integer)
OD	tube outside diameter, in.
TUBEL	tube length, ft.
IDS	a standard shell inside diameter, in.
PASS	number of tube passes (integer)
HEAD	HEAD = 0 if fixed head, HEAD = 1 if floating point (integer)
DAYS	full days operation per year
GPM	tube-side flow rate, gal./min.
AMORT	amortization period, years
BASE	base cost of alloy tubes, \$/lb.
BASES	base cost of steel tube, \$/lb.
CSTIND	cost index for heat exchanger less tubes
TCSTI	cost index for tubes
CTGAL	tube-side liquid cost, \$/gal.
INSTPC	installation cost as per cent of installed cost, per cent
WTFTS	steel tube weight, lb./ft.
WTFT	alloy tube weight, lb./ft.
ELEC	electric power cost, \$/kwhr.
POWER	power required for tube-side pumping, kw.
MCSTF	maintenance cost, \$/sq.-ft.
AO	heat transfer surface, sq. ft./ft.
TUBES	actual number of tubes used (integer)
START	transfer location for error return

The TEMA class R standard working pressures are 150, 300, 450, and 600 psi. Only these values can be used for STWPS and STWPT.

The arguments marked with "integer" must be in the integer mode and declared as such by an integer declaration statement in the main program.

The subroutine takes the argument values and computes and prints out all the economic data. NO additional print statements are required.

An error return to statement labeled START occurs when a non-standard shell size is specified.

KTS, KSC, and KCFH specify the materials to be used.

	admiralty	=	1
	monel	=	2
1- $\frac{1}{4}$ %	chrome	=	3
4-6 %	chrome	=	4
11-13%	chrome	=	5
304	stainless	=	6

Example Problem No. 122

For example, if the tube sheets are admiralty,

$$KTS = 1$$

If the shell and cover are 4-6% chrome,

$$KSC = 4$$

If the floating head is monel

$$KCFH = 2$$

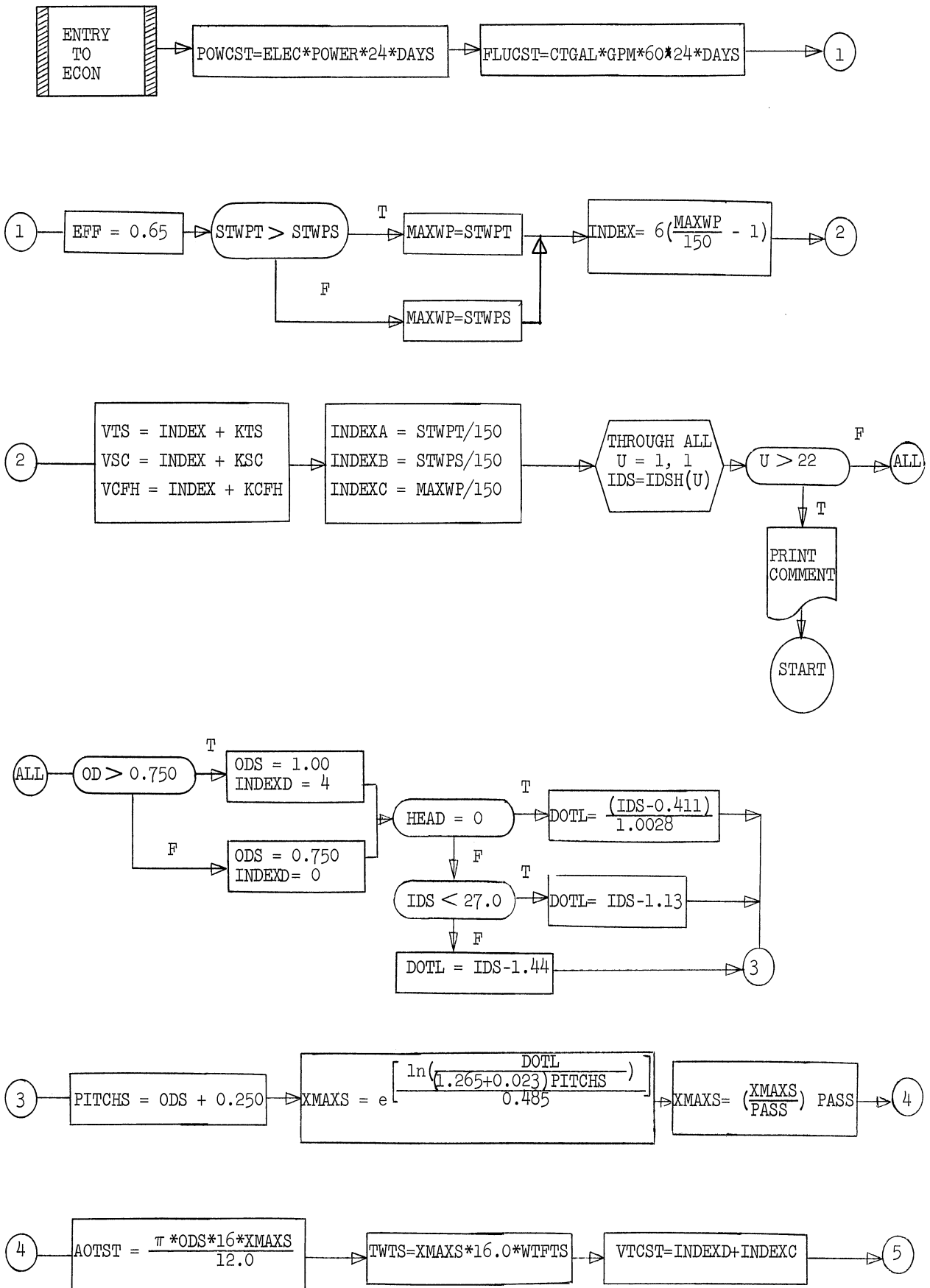
The method is based on the procedure of Sieder, E. H. and Elliott, G. N., "How to Check Costs When Selecting Material for Heat Exchangers," Petroleum Refiner, Vol. 39, No. 5 (1960). A digital computer adaptation was presented by Briggs, D. E., "Economic Design of Heat Transfer Equipment," A.I.Ch.E. Regional Meeting, Detroit, Michigan, April 27, 1962.

The following variables are used in the MAD language version of the Economics subroutine, but are not arguments for the subroutine.

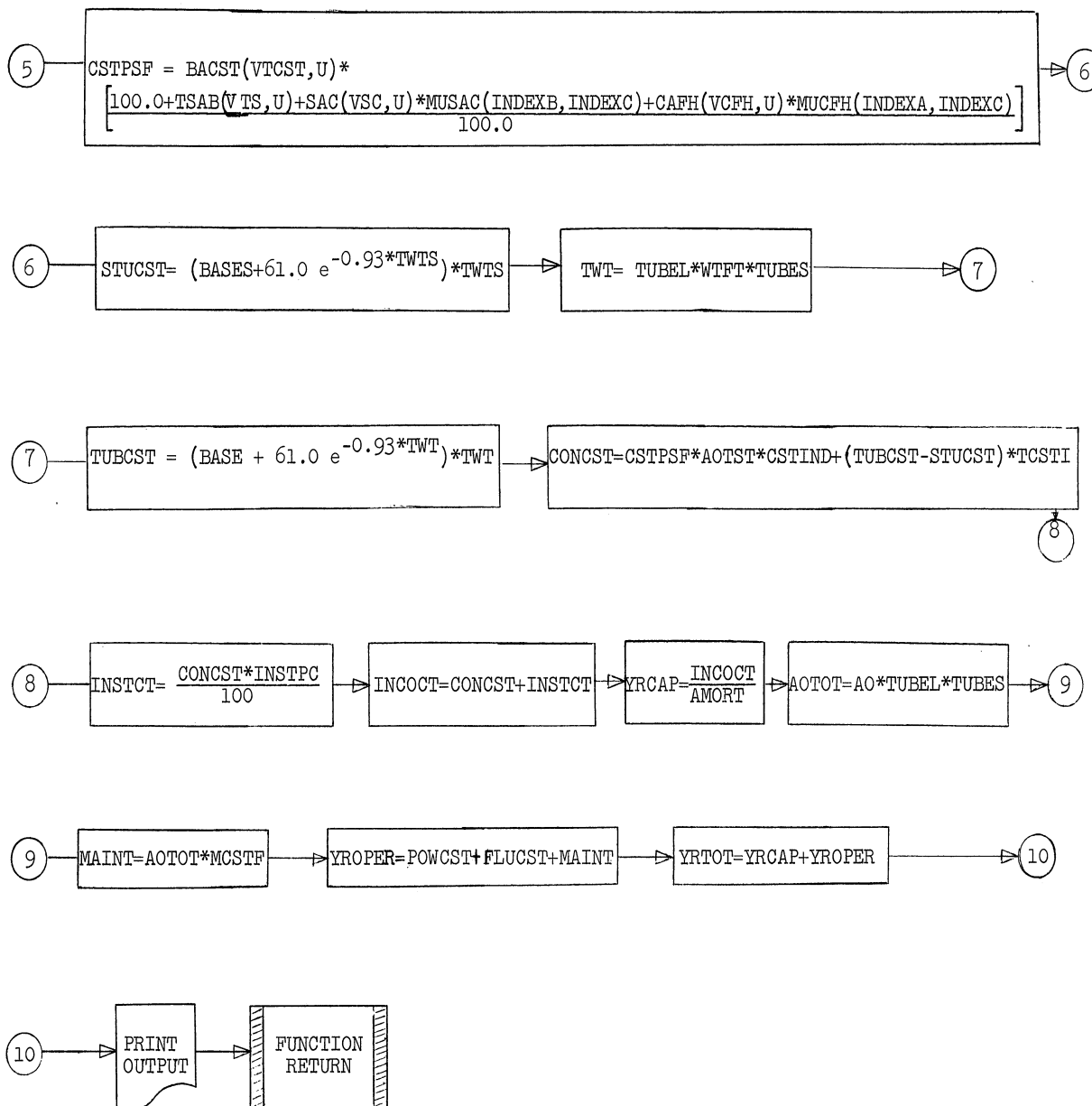
AOTOT	total heat transfer area, sq. ft.
AOTST	total area of steel tubes (based on 16 -ft. tube length), sq. ft.
BACST(VTCST, U)	basic cost of all-steel heat exchanger, \$/sq. ft. heat transfer surface
CAFH(VCFH, U)	per cent extra for alloy channel and floating head
CONCST	heat exchanger cost, dollars
CSTPSF	cost of alloy constructed heat exchanger containing steel tubes, \$/sq. ft. heat transfer surface
DOTL	diameter of outer tube limit, in.
EFF	mechanical efficiency of pump system, fraction
FLUCST	tube side fluid cost, \$/year
IDSH(U)	inside diameter of shell, in.
INCOCT	installed heat exchanger cost, dollars
INDEX	variable used in calculating array indices
INDEXA	index used in array for multiplying factor for channel and floating head
INDEXB	index used in array for multiplying factor for shell and cover
INDEXD	variable used in calculating an array index for basic cost of all-steel heat exchanger
INSTCT	installation cost of heat exchanger, dollars
MAINT	maintenance cost, \$/year
MAXWP	maximum working pressure for exchanger, lb./sq. in.
METAL	an array containing alphabetic names of alloy materials
MUCFH(INDEXA,INDEXC)	multiplying factor for channel and floating head extra cost when tube-side working pressure is less than shell-side pressure
MUSAC(INDEXB,INDEXC)	multiplying factor for shell and cover extra cost when shell-side working pressure is less than tube-side pressure
ODS	steel tube outside diameter, in.
PITCHS	steel tube pitch, in.
POWCST	electric power cost, \$/year
SAC(VSC, U)	extra cost for alloy shell and cover, percent
STUCST	steel tube cost, dollars
TSAB(VTS, U)	extra cost for alloy tube sheets and baffles, percent
TUBCST	alloy tube cost, dollars
TWT	total weight of alloy tubes, lbs.
TWTS	total weight of steel tubes, lbs.
U	an array index which designates shell size
VCFH	an array index which designates channel and floating head alloy and working pressure
VSC	an array index which designates shell and cover alloy and working pressure
VTCST	an array index which designates the steel tube outside diameter and working pressure
VTS	an array index which designates the tube sheet and baffle alloy and working pressure
XMAXS	number of steel tubes that can be placed inside of shell on a specified layout
YRCAP	total fixed-capital expense on a yearly basis, \$/year
YROPER	total yearly operating cost, \$/year
YRTOT	total yearly cost (fixed and operating), \$/year

Economic Design of a Condenser

A flow diagram of the economics subroutine is shown below.



Flow Diagram, Continued



The MAD listing of the subroutine is shown below.

```

SCOMPILE MAD, EXECUTE, DUMP, PUNCH OBJECT
R ECONOMICS SUBROUTINE
EXTERNAL FUNCTION (STWPS, STWPT, KTS, KSC, KCFH, OD, TUBEL,
1 IDS, PASS, HEAD, DAYS, GPM, AMORT, BASE, BASES, CSTIND,
1 TCSTI, CTGAL, INSTPC, WTFTS, WTFT, ELEC, POWER, MCSTF, AO,
1 TUBES, START)
ENTRY TO ECON.
DIMENSION IDSH(23),METAL(30)
STATEMENT LABEL START
INTEGER MAXWP, STWPT, STWPS, VTS, VSC, VCFH, INDEX, INDEXA,
1 PASS, TUBES, DIM, DIME,
1 INDEXB, INDEXC, KTS, KSC, KCFH, XMAXS, INDEXD, U, HEAD,VTCST
DIMENSION MUSAC(16,DIME), MUCFH(16,DIME)
VECTOR VALUES DIME = 2,1,4
DIMENSION TSAB(528,DIM), SAC(528,DIM), CAFH(528,DIM),
1BACST(176,DIM)
VECTOR VALUES DIM = 2,1,22
POWCST=ELEC*POWER*24*DAYS
FLUCST=CTGAL*GPM*60*24*DAYS
EFF = 0.65
WHENEVER STWPT .G. STWPS
MAXWP = STWPT
OTHERWISE
MAXWP = STWPS
  
```

MAD Program, Continued

```

END OF CONDITIONAL
INDEX = 6*(MAXWP/150 - 1)
VTS = INDEX + KTS
VSC = INDEX + KSC
VCFH = INDEX + KCFH
INDEXA = STWPT/150
INDEXB = STWPS/150
INDEXC = MAXWP/150
THROUGH ALL, FOR U = 1, 1, IDS .E. IDSH(U)
WHENEVER U .G. 22
PRINT COMMENT $SHELL SIZE TOO LARGE FOR STANDARD SIZE $
TRANSFER TO START
OTHERWISE
CONTINUE
ALL END OF CONDITIONAL
WHENEVER OD .G. 0.750
ODS = 1.00
INDEXD = 4
OTHERWISE
ODS = 0.750
INDEXD = 0
END OF CONDITIONAL
WHENEVER HEAD .E. 0
DOTL = (IDS-0.411)/1.0028
OR WHENEVER IDS .L. 27.0
DOTL = IDS-1.13
OTHERWISE
DOTL = IDS-1.44
END OF CONDITIONAL
PITCHS = ODS + 0.250
XMAXS = EXP.(ELOG.(DOTL/((1.265 + 0.023)*PITCHS)))/0.485)
XMAXS = (XMAXS/PASS)*PASS
AOTST = ODS*3.1416*16.0*XMAXS/12.0
TWTS = XMAXS*16.0*WTFTS
VTCST = INDEXD + INDEXC
CSTPSF = BACST(VTCST,U)*(100.0 + TSAB(VTS,U) + SAC(VSC,U)*
1MUSAC(INDEXB,INDEXC) + CAFH(VCFH,U)*MUCFH(INDEXA,INDEXC))
1/100.0
STUCST = (BASES + 61. *EXP.(-0.93*TWTS))*TWTS
TWT = TUBEL*WTFT*TUBES
TUBCST=(BASE+61*EXP.(-0.93*TWT))*TWT
CONCST = CSTPSF*AOTST*CSTIND + (TUBCST - STUCST)*TCSTI
INSTCT = (CONCST*INSTPC)/100.0
INCOCT = CONCST + INSTCT
YRCAP = INCOCT/AMORT
AOTOT = AO*TUBEL*TUBES
MAINT = AOTOT*MCSTF
YROPER = POWCST + FLUCST + MAINT
YRTOT = YRCAP + YROPER
PRINT FORMAT TITLE
PRINT FORMAT OUTA, METAL(3*KTS-2),
1METAL(3*KTS-1), METAL(3*KTS), METAL(3*KSC-2), METAL(3*KSC-1),
1METAL(3*KSC), METAL(3*KCFH-2), METAL(3*KCFH-1),
1 METAL(3*KCFH), STWPT, STWPS
PRINT FORMAT OUTAA, OD, TUBES, IDS, AO, TUBEL
PRINT FORMAT TITLEG
PRINT FORMAT OUTF, DAYS, AMORT, CSTIND, TCSTI, BASES, BASE,
1ELEC, MCSTF, INSTPC, EFF
PRINT FORMAT OUTFA, CTGAL, GPM, FLUCST, POWCST, MAINT,
1YROPER, TUBCST, CONCST, INSTCT
PRINT FORMAT OUTFB, INCOCT, YRCAP, YRTOT
FUNCTION RETURN
VECTOR VALUES TITLEG = $ 43H1CONDENSER OPTIMIZATION - OUTPUT
1CONTINUED //// *$
VECTOR VALUES OUTA = $ 32H TUBE SHEET AND BAFFLE MATERIAL
1 S12, 3C6 /
126H SHELL AND COVER MATERIAL S18, 3C6 /
133H CHANNEL AND FLOATING HEAD COVER S11, 3C6 /
142H STANDARD WORKING PRESSURE TUBESIDE - PSI S15, I5 /
143H STANDARD WORKING PRESSURE SHELLSIDE - PSI S14, I5 //*$
VECTOR VALUES OUTAA = $ 16H TUBE O.D. - IN S41, F10.4 /

```



MAD Program, Continued

117H NUMBER OF TUBES S33, I12 /  
 128H SHELL INSIDE DIAMETER - IN S28, F10.3 /  
 137H TUBE OUTSIDE SURFACE AREA - SQFT/FT S20, F10.4 /  
 118H TUBE LENGTH - FT S37, F10.2 //// \*\$  
 VECTOR VALUES TITLE = \$ 32H1CONDENSER OPTIMIZATION - OUTPUT  
 1 //// \* \$  
 VECTOR VALUES OUTF = \$ 25H DAYS OPERATION PER YEAR S29, F10.1/  
 127H AMORTIZATION RATE - YEARS S28, F10.2 /  
 112H COST INDEX S44, F10.3 /  
 117H TUBE COST INDEX S41, F10.5 /  
 124H STEEL TUBE COST - D/LB S34, F10.5 /  
 118H TUBE COST - D/LB S4 , F10.5/  
 128H ELECTRICITY COSTS - D/KWHR S30, F10.5 /  
 132H MAINTENANCE COST D/YEAR-SQFT S25, F10.4 /  
 127H INSTALLED COST - PER CENT S30, F10.4 /  
 123H MECHANICAL EFFICIENCY S34, F10.4 / \*\$  
 VECTOR VALUES OUTFA = \$ 30H TUBESIDE FLUID COSTS - D/GAL  
 1 S30, F10.7 /  
 132H TUBESIDE LIQUID FLOWRATE - GPM S23, F10.2 /  
 122H LIQUID COST - D/YEAR S33, F10.2 /  
 121H POWER COST - D/YEAR S34, F10.2 /  
 127H MAINTENANCE COST D/YEAR S28, F10.2 /  
 135H YEARLY OPERATING EXPENSE - D/YEAR S20, F10.2 /  
 115H TUBE COST - D S4 , F10.2 /

126H TOTAL CONDENSER COST D S29, F10.2 /  
 123H INSTALLATION COST - D S32, F10.2 / \*\$  
 VECTOR VALUES OUTFB = \$ 30H INSTALLED CONDENSER COST - D  
 1 S25, F10.2 /  
 134H YEARLY FIXED CAPITAL EXPENSE - D S21, F10.2 /  
 128H TOTAL YEARLY COST - D/YEAR S27, F10.2 / \*\$  
 VECTOR VALUES BACST(1) = 24.00,20.00,16.00,13.00,10.00,8.05,  
 16.70,5.88,5.40,5.10,5.15,4.80,4.55,4.30,4.15,4.00,3.90,3.80,  
 13.70,3.52,3.49,3.30, 25.00,21.00,17.00,14.00,10.70,8.63,  
 17.30,6.42,5.98,5.68,5.51,5.23,4.98,4.75,4.60,4.46,4.32,4.25,  
 14.18,4.05,4.00,3.75, 26.00,22.00,18.00,15.00,11.90,9.68,  
 18.15,7.20,6.68,6.20,6.30,6.00,5.70,5.50,5.32,5.20,5.05,4.95,  
 14.90,4.72,4.65,4.40, 28.00,24.00,20.00,16.00,12.90,  
 110.68,9.10,8.03,7.33,6.94,6.90,6.60,6.30,6.10,5.90,5.75,  
 15.60,5.50,5.40,5.25,5.15,5.00  
 VECTOR VALUES BACST(89) = 27.00,23.00,19.00,15.40,11.90,9.30,  
 17.55,6.50,5.80,5.48,5.40,5.10,4.80,4.55,4.40,4.20,4.10,4.00,  
 13.90,3.80,3.70,3.60, 28.00,24.00,20.00,16.20,12.50,  
 19.85,8.08,6.95,6.30,5.95,5.95,5.60,5.34,5.10,4.90,4.75,4.63,  
 14.52,4.47,4.35,4.25,4.10, 29.00,25.00,21.00,17.30,14.00,  
 111.00,9.05,7.82,7.18,6.8 6.90,6.55,6.25,6.00,5.80,5.62,5.50,  
 15.40,5.27,5.15,5.10,4.90, 30.00,26.00,22.00,18.20,15.10,  
 112.15,10.05,8.67,7.93,7.60,7.70,7.33,7.00,6.70,6.50,6.30,  
 16.18,6.00,5.86,5.70,5.60,5.50  
 VECTOR VALUES TSAB(1) = 5.0, 7.0, 9.0, 11.0, 13.0, 15.0,  
 118.0, 20.0, 21.0, 21. , 21.0, 21.0, 21.0, 21.0, 21.0, 21.0,  
 121.0, 21.0, 22.0, 22. , 22.0, 22.0, 10.,13.,16.,19.,23.,  
 131.,34.,36.,37.,38.,39.,39.,39.,39.,39.,39.,39.,38.,38.,38.,  
 138.,38., 4.,5.,6.,6.,6.,6.,7.,7.,7.,8.,8.,8.,8.,9.,9.,9.,  
 19.,9.,9.,9.,9.,9., 8.,11.,14.,17.,19.,22.,24.,25.,26.,26.,  
 126.,25.,25.,25.,25.,25.,24.,24.,24.,24.,24.,24., 9.,13.,  
 116.,19.,21.,23.,25.,26.,27.,27.,27.,27.,27.,26.,26.,26.,26.,  
 126.,26.,26.,26.,26., 1 .,13.,16.,19.,22.,26.,28.,30.,30.,  
 131.,31.,31.,30.,30.,3 .,30.,29.,29.,29.,29.,29.,29.,  
 VECTOR VALUES TSAB(133) = 6.,8.,10.,12.,14.,17.,19.,21.,  
 122.,22.,22.,22.,22.,22.,22.,23.,24.,24.,24.,25.,25.,25.,  
 111.,14.,17.,20.,24.,31.,35.,37.,39.,39.,40.,40.,40.,41.,41.,  
 141.,41.,41.,41.,42.,42.,42., 4.,5.,6.,6.,6.,6.,7.,7.,7.,8.,8.,  
 18.,8.,8.,9.,9.,10.,10.,1 .,10.,11.,11.,11., 8.,11.,14.,  
 117.,19.,22.,24.,25.,26.,26.,26.,26.,25.,25.,25.,25.,25.,26.,26.,  
 126.,26.,26.,26., 9.,13.,16.,19.,21.,24.,26.,27.,27.,27.,  
 127.,27.,27.,27.,27.,27.,27.,27.,27.,28.,28.,28., 10.,13.,  
 116.,19.,22.,27.,29.,3 .,31.,31.,31.,31.,31.,30.,30.,30.,30.,  
 131.,31.,31.,31.,  
 VECTOR VALUES TSAB(265) = 6.,8.,10.,12.,14.,17.,19.,21.,22.,  
 122.,22.,22.,23.,23.,23.,24.,25.,25.,26.,27.,27.,27., 11.,  
 114.,17.,20.,24.,31.,35.,37.,39.,39.,40.,40.,41.,41.,42.,42.,  
 142.,42.,42.,43.,43.,43., 4.,5.,6.,6.,6.,6.,7.,7.,7.,8.,8.,8.,  
 19.,9.,10.,10.,10.,11.,11.,11.,12.,12.,12., 8.,11.,14.,17.,  
 119.,22.,24.,25.,26.,26.,26.,26.,25.,26.,26.,26.,26.,27.,  
 127.,27.,26., 9.,13.,16.,19.,21.,24.,26.,27.,27.,27.,27.,  
 127.,27.,27.,27.,28.,28.,28.,28.,29.,29.,29., 10.,13.,16.,  
 119.,22.,27.,29.,30.,31.,31.,31.,31.,31.,30.,30.,30.,30.,  
 131.,31.,31.,31.,  
 VECTOR VALUES TSAB(397) = 6.,8.,10.,12.,14.,17.,19.,21.,22.,  
 122.,22.,22.,23.,23.,23.,24.,25.,25.,26.,27.,27.,27., 11.,  
 114.,17.,20.,23.,31.,34.,35.,36.,37.,39.,39.,40.,41.,41.,42.,  
 143.,43.,43.,43.,43.,43.,4.,5.,6.,6.,6.,6.,6.,7.,7.,7.,7.,8.,  
 18.,9.,9.,10.,10.,10.,11.,12.,12.,12., 8.,11.,14.,17.,19.,

MAD Program, Continued

121.,23.,24.,24.,24.,25.,25.,25.,25.,25.,25.,26.,27.,27.,28.,  
 128.,28.,8.,11.,14.,17.,19.,20.,22.,24.,25.,26.,26.,26.,26.,  
 127.,27.,27.,28.,29.,29.,30.,30.,30., 9.,13.,16.,19.,21.,  
 125.,27.,29.,29.,29.,29.,29.,30.,30.,30.,30.,31.,32.,33.,33.,  
 133.,33.,  
 VECTOR VALUES SAC( 23 ) = 26.,30.,34.,38.,42.,46.,49.,51.,  
 152.,52.,51.,50.,49.,47.,44.,44.,41.,40.,39.,38.,38.,37.,  
 18.,10.,13.,16.,19.,22.,23.,25.,24.,24.,23.,22.,21.,19.,18.,  
 118.,17.,17.,16.,16.,16.,15., 16.,18.,21.,24.,27.,30.,  
 133.,34.,35.,34.,33.,32.,30.,29.,26.,26.,25.,24.,23.,23.,23.,  
 122., 18.,21.,24.,27.,30.,33.,35.,35.,36.,36.,35.,34.,  
 133.,31.,29.,27.,27.,26.,25.,24.,24.,23., 21.,24.,27.,  
 130.,33.,35.,36.,37.,37.,37.,36.,35.,34.,33.,31.,28.,28.,28.,  
 127.,25.,25.,24.,  
 VECTOR VALUES SAC(155) = 33.,36.,39.,42.,45.,48.,51.,52.,53.,  
 153.,52.,51.,51.,49.,47.,47.,45.,44.,44.,44.,43.,43.,  
 112.,14.,16.,18.,20.,22.,24.,25.,25.,25.,24.,22.,20.,20.,19.,  
 119.,18.,17.,17.,17.,16.,16., 16.,19.,22.,25.,28.,31.,  
 133.,35.,35.,35.,34.,32.,30.,30.,28.,28.,27.,26.,26.,26.,25.,  
 125., 17.,20.,23.,26.,29.,33.,35.,36.,36.,36.,35.,34.,  
 132.,32.,30.,30.,28.,27.,27.,27.,26.,26., 20.,23.,26.,  
 129.,32.,34.,36.,37.,38.,38.,37.,35.,33.,33.,31.,31.,30.,29.,  
 128.,28.,27.,27.,  
 VECTOR VALUES SAC(287) = 37.,40.,43.,47.,51.,55.,57.,57.,  
 156.,56.,55.,54.,54.,52.,50.,50.,48.,47.,47.,46.,46.,46.,  
 111.,14.,17.,20.,23.,25.,26.,27.,27.,27.,26.,23.,23.,22.,21.,  
 121.,19.,19.,19.,18.,18.,18., 19.,22.,25.,28.,31.,34.,  
 137.,38.,38.,37.,36.,34.,34.,32.,30.,28.,28.,27.,27.,26.,26.,  
 126., 21.,24.,27.,3 3.,33.,36.,37.,39.,39.,39.,38.,36.,36.,  
 134.,31.,30.,30.,28.,28.,28.,28.,28., 24.,27.,30.,33.,  
 136.,39.,41.,41.,41.,4 3.,39.,37.,37.,35.,33.,31.,31.,30.,30.,  
 130.,30.,30.,  
 VECTOR VALUES SAC(419) = 48.0,50.,52.,54.,56.,56.,55.,55.,  
 155.,54.,54.,53.,53.,51.,49.,49.,48.,47.,47.,46.,46.,46.,  
 29.,12.,15.,18.,21.,24.,25.,25.,26.,25.,25.,23.,23.,21.,20.,  
 120.,19.,18.,18.,18.,18., 19.,22.,25.,28.,31.,34.,36.,  
 137.,37.,36.,35.,33.,33.,31.,29.,29.,28.,27.,27.,26.,26.,26.,  
 1 21.,24.,27.,30.,33.,36.,37.,38.,38.,37.,36.,35.,35.,33.,  
 131.,31.,29.,28.,28.,28.,28.,28., 30.,32.,34.,36.,38.,  
 140.,42.,42.,40.,39.,38.,37.,37.,35.,32.,32.,31.,30.,30.,30.,  
 130.,30.,  
 VECTOR VALUES CAFH(23) = 38.0,39.0,40.,41.,42.,41.,41.,41.,  
 140.,38.,37.,36.,36.,35.,34.,34.,33.,32.,32.,32.,31.,31.,  
 118.,20.,21.,22.,23.,24.,25.,25.,24.,23.,23.,22.,22.,21.,21.,  
 121.,21.,21.,21.,21.,21., 31.,33.,35.,36.,37.,38.,37.,  
 137.,36.,35.,33.,30.,3 2.,29.,27.,27.,28.,27.,27.,26.,26.,26.,  
 1 34.,35.,36.,37.,38.,38.,37.,37.,36.,35.,34.,32.,32.,30.,  
 129.,29.,28.,27.,27.,27.,27., 35.,36.,37.,38.,39.,38.,  
 138.,37.,36.,35.,34.,33.,33.,31.,30.,30.,29.,28.,28.,28.,  
 128.,28.,  
 VECTOR VALUES CAFH(155) = 32.,34.,36.,38.,40.,42.,42.,43.,  
 142.,41.,40.,37.,37.,34.,32.,32.,31.,30.,30.,30.,30.,  
 119.,20.,21.,22.,23.,24.,24.,25.,24.,24.,23.,22.,22.,21.,21.,  
 121.,21.,20.,20.,20.,2 20., 32.,33.,34.,35.,36.,37.,38.,  
 138.,37.,36.,34.,31.,31.,29.,27.,27.,26.,25.,24.,24.,24.,  
 133.,34.,35.,36.,37.,38.,39.,39.,38.,37.,35.,32.,32.,30.,28.,  
 128.,27.,26.,26.,25.,25.,25., 33.,34.,35.,36.,37.,39.,  
 139.,39.,38.,37.,36.,33.,33.,31.,29.,29.,28.,26.,26.,26.,26.,  
 126.,  
 VECTOR VALUES CAFH(287) = 38.,39.,40.,41.,42.,42.,43.,42.,  
 140.,39.,37.,36.,36.,33.,32.,32.,31.,30.,30.,30.,30.,  
 121.,22.,23.,24.,25.,26.,26.,25.,24.,23.,23.,22.,22.,22.,21.,  
 121.,21.,20.,20.,20.,2 20., 34.,35.,36.,37.,38.,39.,39.,  
 139.,37.,35.,33.,31.,31.,29.,27.,27.,26.,25.,25.,25.,25.,  
 134.,35.,36.,37.,38.,4 40.,40.,37.,36.,34.,32.,32.,30.,28.,  
 128.,27.,26.,26.,26.,26.,26., 34.,35.,36.,37.,39.,40.,  
 140.,39.,38.,36.,35.,33.,33.,31.,29.,29.,28.,27.,27.,26.,  
 126.,26.,  
 VECTOR VALUES CAFH(419) = 39.,41.,42.,43.,44.,45.,44.,43.,  
 142.,41.,39.,36.,36.,34.,30.,30.,29.,28.,28.,28.,28.,  
 121.,22.,23.,24.,25.,25.,26.,26.,25.,23.,23.,22.,22.,21.,20.,  
 120.,19.,19.,19.,19.,19., 34.,35.,36.,37.,38.,39.,39.,  
 139.,38.,36.,34.,31.,31.,28.,26.,26.,24.,23.,23.,23.,23.,  
 136.,37.,38.,39.,40.,41.,41.,40.,38.,36.,35.,32.,32.,28.,26.,  
 126.,25.,24.,24.,23.,23.,23., 36.,37.,38.,39.,40.,41.,41.,  
 141.,39.,37.,35.,32.,32.,29.,27.,27.,26.,25.,25.,23.,23.,23.,  
 VECTOR VALUES MUSAC(1) = 1.0, 0.92, 0.81, 0.75, 0.0, 1.0,  
 10.89, 0.83, 0.0, 0.0, 1. , 0.92, 0.0, 0.0, 0.0, 1.0  
 VECTOR VALUES MUCFH(1) = 1.0, 0.92, 0.88, 0.78, 0.00, 1.0,  
 10.95, 0.86, 0.0, 0.0, 1. , 0.92, 0.0, 0.0, 0.0, 1.0  
 VECTOR VALUES METAL(1) = \$ ADMIRALTY MONE  
 1L 1-1/4 CR 1/2 MO 4 6 CR 1/2 MO 11-13 CR 3  
 104 STAINLESS\*\$  
 VECTOR VALUES IDSH(1) = 5.047, 6.065, 8.071, 10.02, 12.09,  
 2 13.375, 15.25, 17.25, 19.25, 21.25, 23.0, 25.0, 27.0, 29.0,  
 3 31.0, 33.0, 35.0, 37.0, 39.0, 42.0, 44.0, 47.0  
 END OF FUNCTION

Description of Baffled Shell-Side Pressure Drop Subroutine

The method of calling the subroutine is:

EXECUTE BSHPEDP. (IDS, PASS, OD, TUBEL, BAFSP, TR, TUBES, FIN,  
TOTALL, PITCH, HEAD, DEQ, Z, W, MWT, TSVI, PRTEMA, PRTEMB,  
VISGA, VISGB, VISGC, TOTPD, TSVO, START)

The arguments required for BSHPEDP. are:

IDS	a standard shell inside diameter, in.
PASS	number of tube passes, (integer)
OD	tube outside diameter, in.
TUBEL	tube length, ft.
BAFSP	baffle spacing, in.
TR	set TR = 1 if triangular pitch; set TR = 0 if square pitch (integer)
TUBES	actual number of tubes used (integer)
FIN	set FIN = 1 if finned tubes; set FIN = 0 if plain tubes (integer)
TOTALL	total allowable shell-side pressure drop, lb./sq. in.
PITCH	tube pitch, in.
HEAD	set HEAD = 1 if floating head; set HEAD = 0 if fixed head (integer)
DEQ	equivalent diameter of tube, in. DEQ = OD for plain tubes
Z	compressibility factor for condensing vapor
W	amount of condensing vapor, lb./hr.
MWT	molecular weight of condensing vapor
TSVI	inlet vapor temperature, °F
PRTEMA	constant A for saturated pressure where $P = \exp.(A+B/T_{\text{abs}})$ lb./sq. in.
PRTEMB	constant B for saturated pressure where $P = \exp.(A+B/T_{\text{abs}})$ lb./sq. in.
VISGA	constant A for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ lb./ft.-hr.
VISGB	constant B for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ lb./ft.-hr.
VISGC	constant C for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ lb./ft.-hr.
*TOTPD	calculated shell-side pressure drop, lb./sq. in.
*TSVO	calculated exit vapor temperature, °F
START	transfer location for error return

The arguments marked with "integer" must be in integer mode and declared as such by an integer declaration in the main program.

The subroutine takes the argument values and computes the shell-side pressure drop based on a modification to the method of D. A. Donohue, "Heat Transfer and Pressure Drop in Heat Exchangers," Industrial and Engineering Chemistry, Nov. 1949. In the modified version the pressure drop is calculated in increments. The tube length is divided by the baffle spacing to obtain the number of increments. For each increment the pressure drop is calculated based on the average amount of vapor flowing across the bundle. The pressure drop through each window is also calculated based on the average amount of vapor flowing through the particular window. The individual pressure drops are summed to give the total pressure drop. Using the exit vapor pressure, the exit vapor temperature is calculated.

An error return to statement labeled START occurs when (1) shell size specified is not a standard size or (2) pressure drop is excessive.

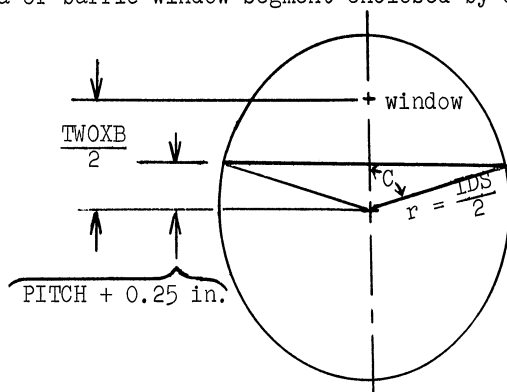
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\* The values TOTPD and TSVO need not have definite values prior to execution of BSHPEDP. Values will be calculated by the subroutine and can be used in the main program after execution of the subroutine.

## Economic Design of a Condenser

The following variables are used in the MAD language version of the baffled shell-side pressure drop subroutine, but are not arguments for the subroutine.

AOTLIM	area enclosed by outer tube limit, sq. in.
BAFCTL	baffle cut expressed as a fraction of diameter of outer tube limit, fraction
BAFCUT	baffle cut expressed as a fraction of shell inside diameter, fraction
COSC	cosine of angle C (see figure below)
DELCON	one-half of the amount of vapor condensed in passing across bundle between baffles, lb./hr.
DENG	density of condensing vapor, lb./cu. ft.
DOTL	diameter of outer tube limit, in.
DPG	pressure drop in passing across bundle between baffles, lb./sq. in.
DPWIND	pressure drop in passing through a baffle window, lb./sq. in.
FFWA	free flow area in window normal to flow, sq. ft.
FSPACL	free flow area at center of bundle normal to flow, sq. ft.
FS	friction factor for shell side, dimensionless
G	mass flow rate, lb/hr.-sq. ft.
IDSH	shell inside diameter, in.
NOREST	number of tube restrictions encountered in crossing bundle from centroid of window to centroid of window
NOTUCL	number of tubes across center of shell normal to vapor flow
PAVGA	calculated average pressure in any section under consideration, lb./sq. in.
PAVG	assumed average pressure in any section under consideration, lb./sq. in.
PIN	inlet pressure to any section under consideration, lb./sq. in.
POUT	outlet pressure from any part of condenser, lb./sq. in.
PROTUA	cross-sectional area of tubes in the baffle window, sq. in.
PTOP	pressure at inlet, lb./sq. in.
RADC	angle C in radians
REG	average Reynolds number of flowing vapor in any section under consideration
SEGFAC	segment factor used to calculate segment area
SINC	sine of angle C
SPACES	number of spaces between baffles available for vapor flow
TAVG	average temperature of vapor in any section under consideration
TOTWIN	total window area, sq. in.
TWOXB	normal distance from centroid of one baffle window to the centroid of an adjacent baffle window, in.
U	index designating shell size
VISG	viscosity of vapor at any point under consideration, lb./ft.-hr.
WAVG	average amount of vapor at any point under consideration, lb./hr.
WINATU	area of baffle window segment enclosed by diameter of outer tube limit, sq. in.

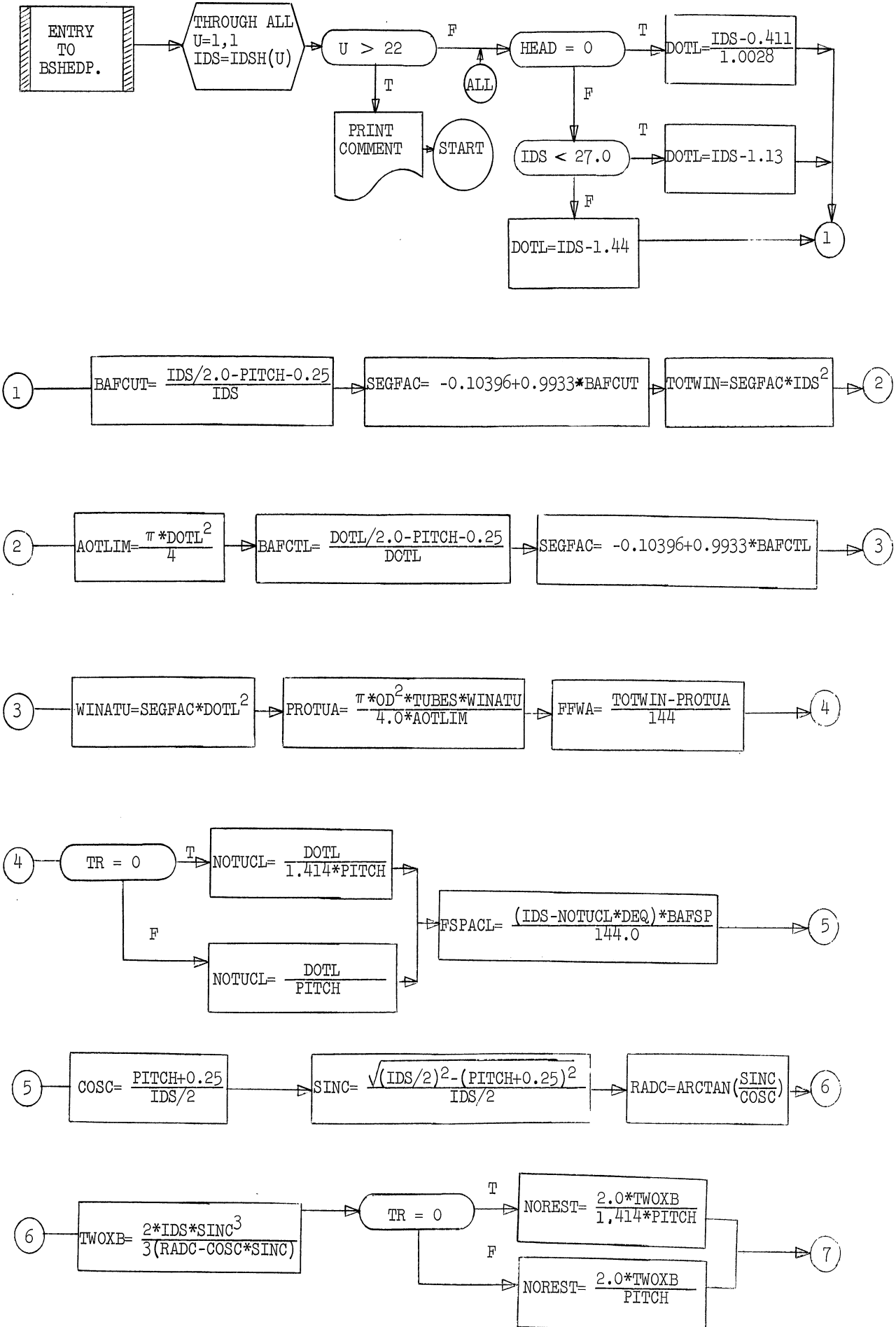


$$\text{window centroid distance from center of circle} = \frac{2/3 r \sin^3 C}{\text{rad } C - \cos C \sin C}$$

A flow diagram of the baffled shell-side pressure drop subroutine is shown on next page.

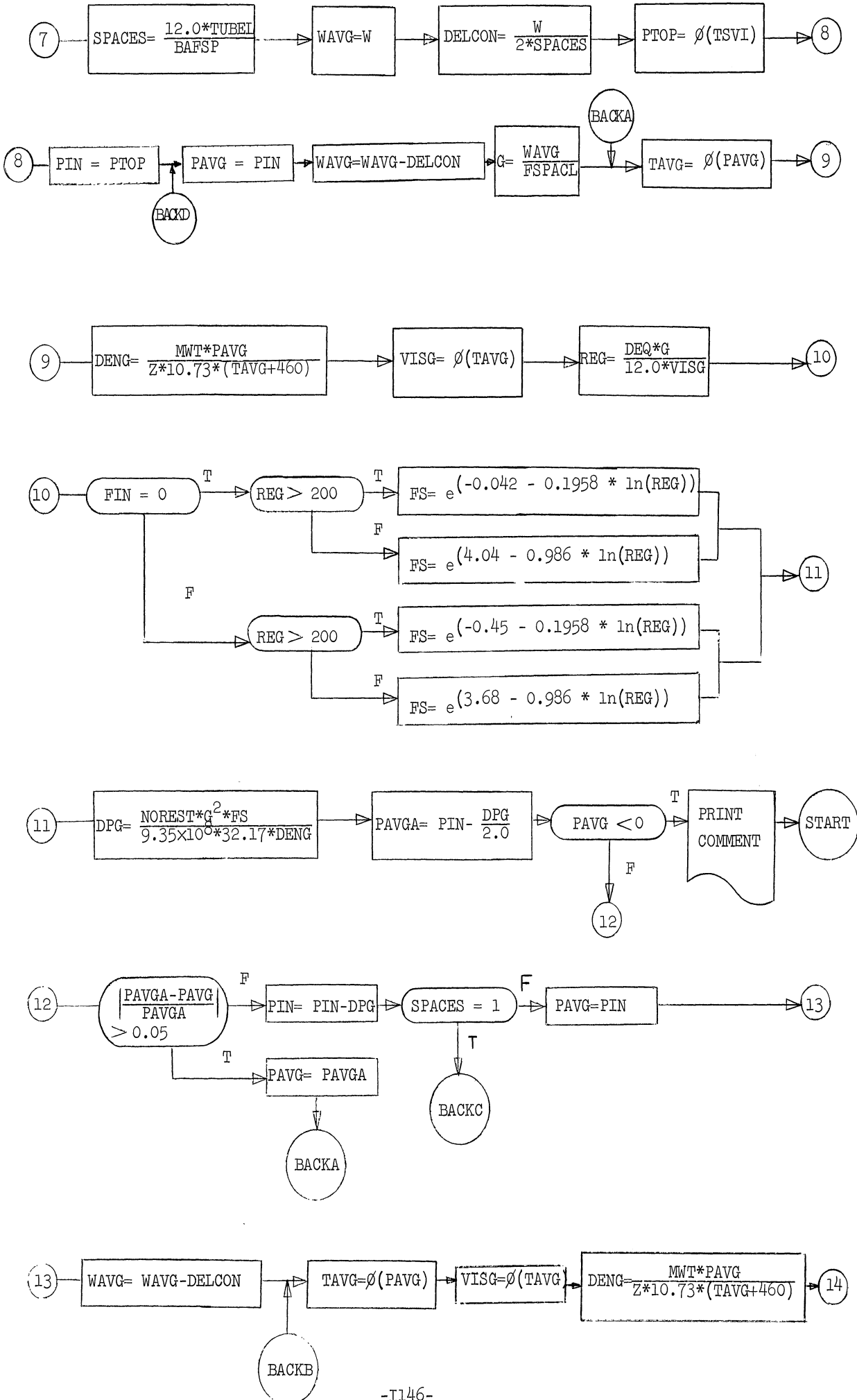
Example Problem No. 122

Flow Diagram

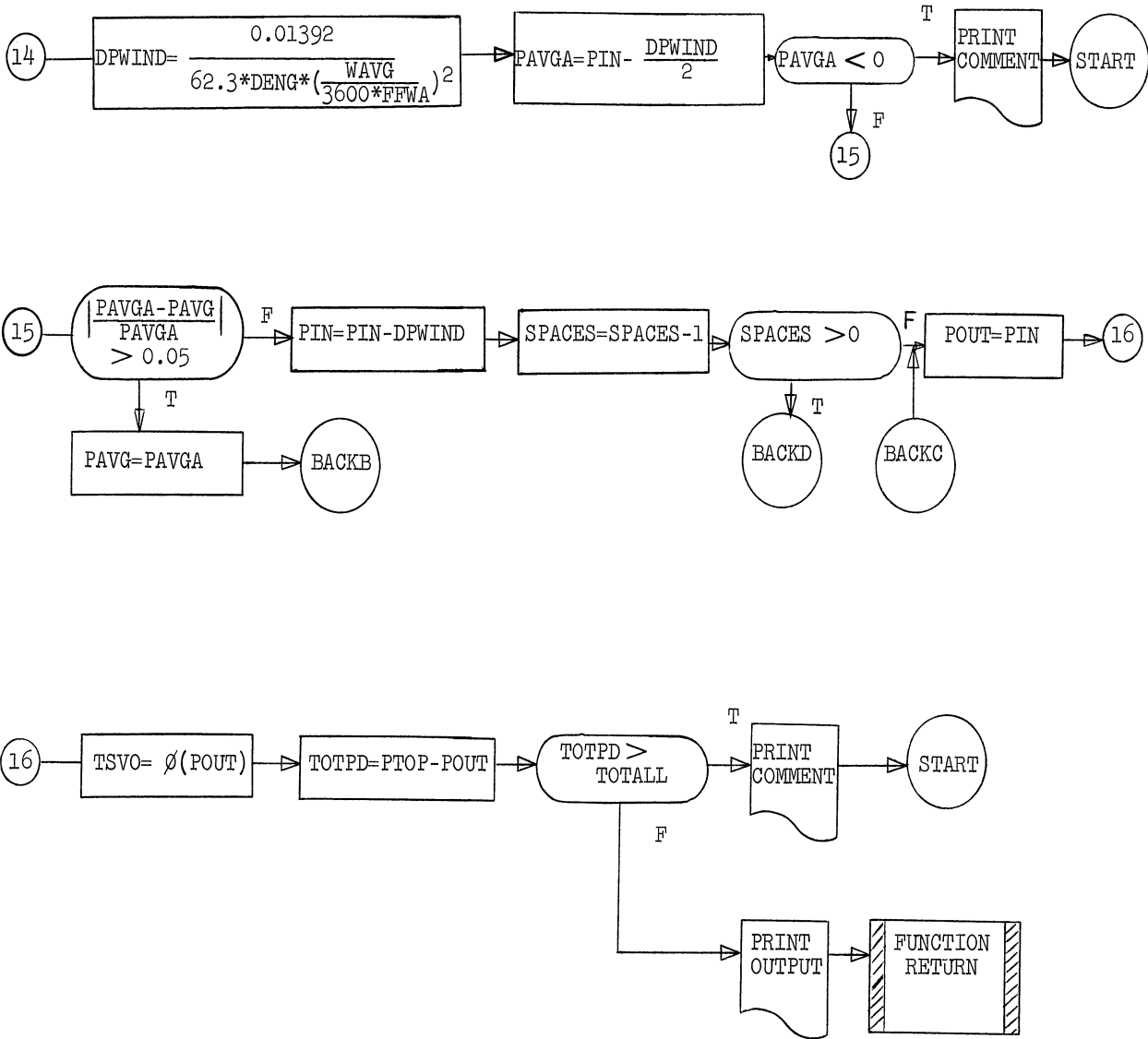


Economic Design of a Condenser

Flow Diagram, Continued



Flow Diagram, Continued



Economic Design of a Condenser

A MAD listing of the subroutine is shown below.

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$COMPILE MAD, EXECUTE, DUMP, PUNCH OBJECT
R  BAFFLED SHELL SIDE PRESSURE DROP FOR A CONDENSER
EXTERNAL FUNCTION(IDS, PASS, OD, TUBEL, BAFSP, TR, TUBES,
1FIN, TOTALL, PITCH, HEAD, DEQ, Z, W, MWT, TSVI,
1 PRTEMA, PRTEMB, VISGA, VISGB, VISGC, TOTPD, TSVO, START)
ENTRY TO BSHPEDP,
DIMENSION IDSH(23)
STATEMENT LABEL START
INTEGER HEAD, TR, SPACES, U, TUBES, FIN
THROUGH ALL, FOR U = 1, 1, IDS .E. IDSH(U)
WHENEVER U .G. 22
PRINT COMMENT $SHELL SIZE TOO LARGE FOR STANDARD SIZE $
TRANSFER TO START
OTHERWISE
CONTINUE
ALL  END OF CONDITIONAL
WHENEVER HEAD .E. 0
DOTL = (IDS-0.411)/1.0028
OR WHENEVER IDS .L. 27.0
DOTL = IDS-1.13
OTHERWISE
DOTL = IDS-1.44
END OF CONDITIONAL
BAFCUT = (IDS/2.0 - PITCH - 0.25)/IDS
SEGFAC = -0.10396 + 0.9933*BAFCUT
TOTWIN = SEGFAC*IDS*IDS
AOTLIM = 3.1416*DOTL*DOTL/4.0
BAFCTL = (DOTL/2.0 - PITCH - 0.25)/DOTL
SEGFAC = -0.10396 + 0.9933*BAFCTL
WINATU = SEGFAC*DOTL*DOTL
PROTUA = (3.1416*OD*OD*TUBES*WINATU)/(4.0*AOTLIM)
FFWA = (TOTWIN - PROTUA)/144.0
WHENEVER TR .E. 0
NOTUCL = DOTL/(1.414*PITCH)
OTHERWISE
NOTUCL = DOTL/PITCH
END OF CONDITIONAL
FSPACL = (IDS - NOTUCL*DEQ)*BAFSP/144.0
COSC = (PITCH + 0.25)/(IDS/2.0)
SINC = (SQRT.((IDS/2.0).P.2 - (PITCH + 0.25).P.2))/(IDS/2.0)
RADC = ATAN.(SINC/COSC)
TWOXB = (2.0*IDS*(SINC).P.3)/(3.0*(RADC - COSC*SINC))
WHENEVER TR .E. 0
NOREST = 2.0*TWOXB/(PITCH*1.414)
OTHERWISE
NOREST = 2.0*TWOXB/PITCH
END OF CONDITIONAL
SPACES = 12.0*TUBEL/BAFSP
WAVG = W
DELCON = W/(2*SPACES)
PTOP = EXP.(PRTEMA + PRTEMB/(TSVI + 460.0))
PIN = PTOP
BACKD  PAVG = PIN
WAVG = WAVG - DELCON
G = WAVG/FSPACL
BACKA  TAVG = PRTEMB/(ELOG.(PAVG) - PRTEMA) - 460.0
DENG = (MWT*PAVG)/(Z*10.73*(TAVG + 460.0))
VISG = EXP.(VISGA + VISGB/TAVG + VISGC/TAVG.P.2)
REG = DEQ*G/(VISG*12.0)
WHENEVER FIN .E. 0

WHENEVER REG .G. 200.0
FS = EXP.(-0.042 - 0.1958*ELOG.(REG))
OTHERWISE
FS = EXP.( 4.04 - 0.986*ELOG.(REG))
END OF CONDITIONAL
OTHERWISE
WHENEVER REG .G. 200.0
FS = EXP.(-0.45 - 0.1958*ELOG.(REG))
OTHERWISE
FS = EXP.( 3.68 - 0.986*ELOG.(REG))
END OF CONDITIONAL
END OF CONDITIONAL
DPG = NOREST*G*G*FS/(9.35*10.P.8*32.17*DENG)

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MAD Program, continued

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PAVGA = PIN - DPG/2.0
WHENEVER PAVGA .L. 0.0
PRINT COMMENT $4PRESSURE DROP IS EXCESSIVE WHEN MAXIMUM NUMBE
1R OF TUBES IS USED.$
TRANSFER TO START
OTHERWISE
CONTINUE
END OF CONDITIONAL
WHENEVER .ABS.((PAVGA-PAVG)/PAVGA) .G. 0.05
PAVG = PAVGA
TRANSFER TO BACKA
OTHERWISE
PIN = PIN - DPG
END OF CONDITIONAL
WHENEVER SPACES .E. 1, TRANSFER TO BACKC
PAVG = PIN
WAVG = WAVG - DELCON
BACKB TAVG = PRTEMB/(ELOG.(PAVG) - PRTEMA) - 460.0
VISG = EXP.(VISGA + VISGB/TAVG + VISGC/TAVG.P.2)
DENG = (MWT*PAVG)/(Z*10.73*(TAVG + 460.0))
DPWIND = (0.01392/(62.3*DENG))*(WAVG/(3600*FFWA)).P.2
PAVGA = PIN - DPWIND/2.0
WHENEVER PAVGA .L. 0.0
PRINT COMMENT $4PRESSURE DROP IS EXCESSIVE WHEN MAXIMUM NUMBE
1R OF TUBES IS USED.$
TRANSFER TO START
OTHERWISE
CONTINUE
END OF CONDITIONAL
WHENEVER .ABS.((PAVGA-PAVG)/PAVGA) .G. 0.05
PAVG = PAVGA
TRANSFER TO BACKB
OTHERWISE
PIN = PIN - DPWIND
END OF CONDITIONAL
SPACES = SPACES - 1
BACKC WHENEVER SPACES .G. 0, TRANSFER TO BACKD
POUT = PIN
TSVO = PRTEMB/(ELOG.(POUT) - PRTEMA) - 460.0
TOTPD = PTOP - POUT
WHENEVER TOTPD .G. TOTALL
PRINT COMMENT $4PRESSURE DROP IS EXCESSIVE WHEN MAXIMUM NUMBE
1R OF TUBES IS USED.$
PRINT FORMAT INFO , TOTPD, TSVO
TRANSFER TO START
OTHERWISE
PRINT FORMAT INFO , TOTPD, TSVO
END OF CONDITIONAL
FUNCTION RETURN
VECTOR VALUES INFO = $ 45H4SHELL SIDE PRESSURE DROP FOR BAFFL
1ED FLOW IS F7.4, 4H PSI/// 27H EXIT VAPOR TEMPERATURE IS
1 F8.3, 3H F *$
VECTOR VALUES IDSH(1) = 5.047, 6.065, 8.071, 10.02, 12.09,
2 13.375, 15.25, 17.25, 19.25, 21.25, 23.0, 25.0, 27.0, 29.0,
3 31.0, 33.0, 35.0, 37.0, 39.0, 42.0, 44.0, 47.0
END OF FUNCTION

```

Economic Design of a Condenser

Description of Unbaffled Shell-Side Pressure Drop Subroutine

The method of calling the subroutine is:

EXECUTE USHEDP. (HEAD, IDS, TUBEL, TUBES, TSVI, W, TOTALL, OD, TR, SQ, DEQ, MWT, Z, LATA, LATEB, DENLA, DENLB, VISGA, VISGB, VISGC, PRTEMA, PRTEMB, TSVO, TOTPD, PITCH, START)

The arguments required by USHEDP. are:

HEAD	HEAD = 0 if fixed head; HEAD = 1 if floating head (integer)
IDS	a standard shell inside diameter, in.
TUBEL	tube length, ft.
TUBES	actual number of tubes (integer)
TSVI	temperature of the inlet vapor, °F
W	amount of condensing vapor, lb./hr.
TOTALL	allowable shell-side pressure drop, lb./sq. in.
OD	tube outside diameter, in.
TR	TR = 1 if tubes are on a triangular pitch, otherwise TR = 0 (integer)
SQ	SQ = 1 if tubes are on a square pitch, otherwise SQ = 0 (integer)
DEQ	equivalent diameter of tube, DEQ = OD for plain tube, in.
MWT	molecular weight of condensing vapor
Z	compressibility factor for inlet vapor
LATA	constant A for latent heat where $\lambda = A+B*T$ , Btu./lb.
LATEB	constant B for latent heat where $\lambda = A+B*T$ , Btu./lb.
DENLA	constant A for density of condensed liquid where $\rho_L = A+B*T$ , lb./cu.-ft.
DENLB	constant B for density of condensed liquid where $\rho_L = A+B*T$ , lb./cu.-ft.
VISGA	constant A for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ , lb./ft.-hr.
VISGB	constant B for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ , lb./ft.-hr.
VISGC	constant C for vapor viscosity where $\mu_g = \exp.(A+B/T+C/T^2)$ , lb./ft.-hr.
PRTEMA	constant A for saturated pressure where $p = \exp.(A+B/T_{abs})$ , lb./sq. in.
PRTEMB	constant B for saturated pressure where $p = \exp.(A+B/T_{abs})$ , lb./sq. in.
*TSVO	temperature of saturated vapor leaving, °F
*TOTPD	calculated shell-side pressure drop, lb/sq. in.
PITCH	tube pitch, in.
START	transfer location for error return

The arguments marked with "integer" must be in integer mode and declared as such by an integer declaration in the main program.

The subroutine takes the argument values and computes the shell-side pressure drop based on the method of J. E. Diehl, "Calculate Condenser Pressure Drop," Petroleum Refiner, Vol. 36, No. 10, 1957. The calculated shell-side pressure drop is printed out in the subroutine.

An error return to statement labeled START occurs when (1) shell size is not large enough for the number of tubes specified, (2) shell size is not a standard shell size, or (3) allowable shell-side pressure drop is exceeded.

The following variables are used in the MAD language version of the unbaffled shell-side pressure drop subroutine, but are not arguments for the subroutine.

CL	distance between outermost tube and shell wall, in.
COND	amount of vapor condensing on row R, lb./hr.
CONDT	total amount of condensate at point in question, lb./hr.
DELP	difference in pressure from inlet to point in question, lb./sq. in.
DENG	density of condensing vapor, lb./cu. ft.
DENL	density of condensate, lb./cu. ft.
DOTL	diameter of outer tube limit, in.
DPG	pressure drop for all-gas flow across row R, lb./sq. ft.

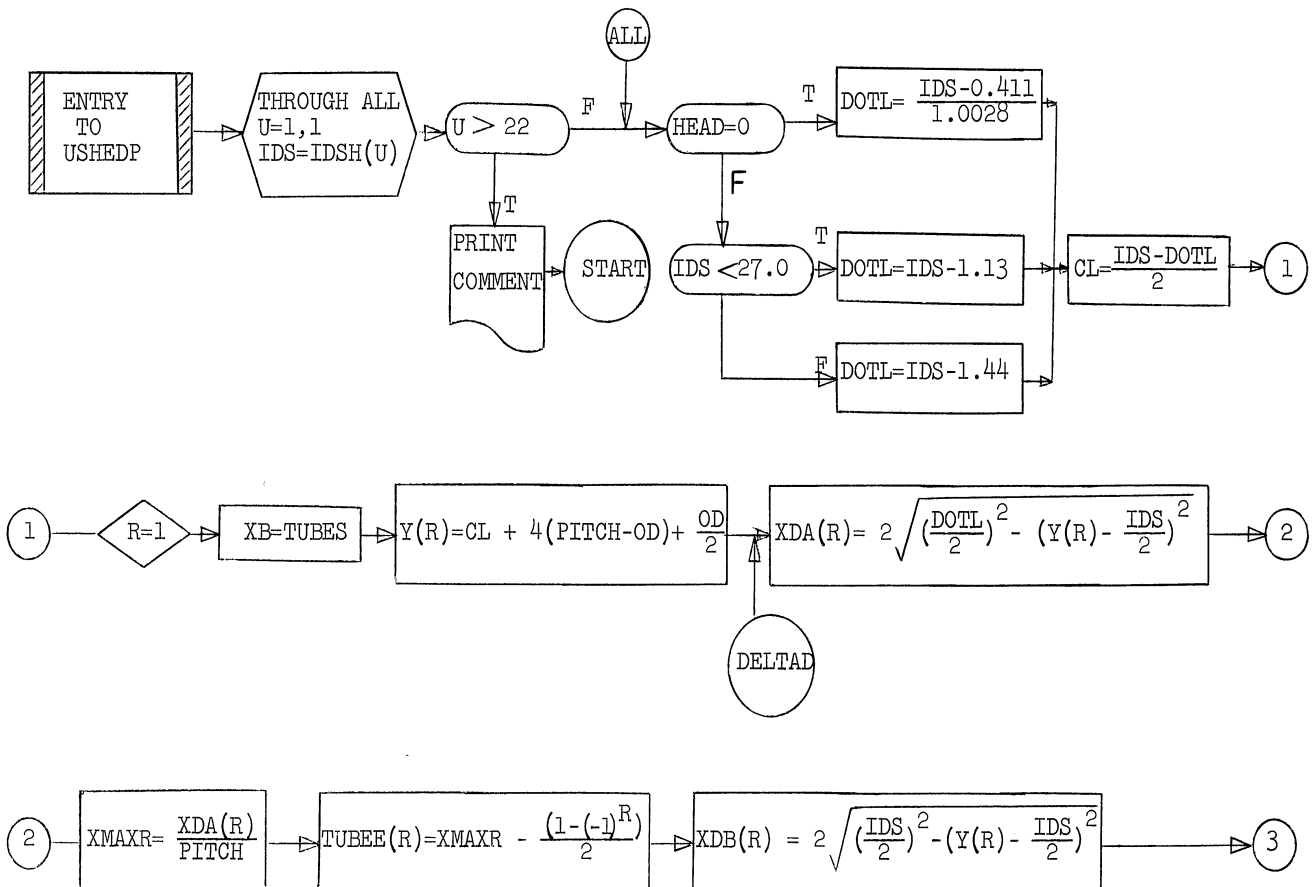
\* The values TSVO and TOTPD need not have definite values prior to execution of USHEDP. Values will be calculated by the subroutine and can be used in the main program after execution of the subroutine.

Example Problem No. 122

DPTP(R) two-phase pressure drop across row R, lb./sq. in.  
 FFA(R) free flow area normal to the vapor flow at row R, sq. ft.  
 FS friction factor based on all-gas flow, dimensionless  
 FUNC defined by  $\frac{(LVF)(DENL)}{(DENG)(R_e)^{0.5}}$   
 GVOL gas volume flowing at point in question, cu. ft./hr.  
 IDSH(U) inside diameter of a standard shell size, in.  
 LAT latent heat of condensing vapor, Btu./lb.  
 LVF liquid volume fraction, dimensionless  
 LVOL liquid volume, cu. ft./hr.  
 PAVG assumed average pressure at point in question, lb./sq. in.  
 PAVGA calculated average pressure at point in question, lb./sq. in.  
 PIN pressure above any row of tubes in question, lb./sq. in.  
 POUT(R) pressure drop across row R, lb./sq. in.  
 PTOP pressure at top of condenser, lb./sq. in.  
 Q total heat load, Btu./hr.  
 RATIO ratio of two-phase pressure drop to all-gas pressure drop defined by  

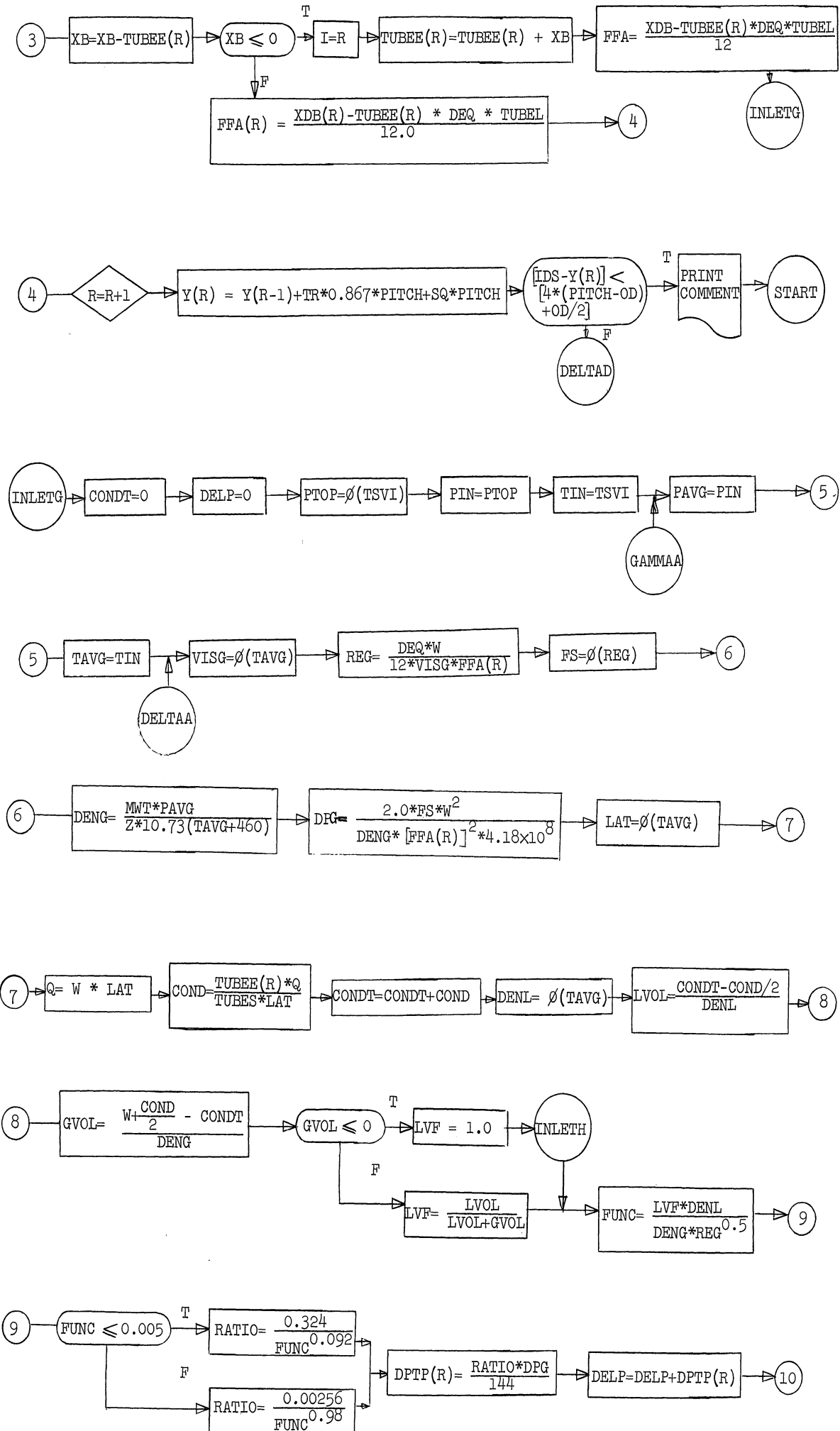
$$\frac{0.324}{(FUNC)^{0.092}} \quad \text{or} \quad \frac{0.00256}{(FUNC)^{0.88}}$$
  
 REG Reynolds number for all-gas flow past row of tubes in question, dimensionless  
 R counter designating tube row; numbered from bottom up  
 TAVG average temperature at point in question, °F  
 TIN temperature above any row of tubes in question, °F  
 TUBEE(R) number of tubes in row R  
 U index which designates a standard shell size  
 VISG viscosity of gas, lb./ft.-hr.  
 XB number of tubes not yet placed in shell  
 XDA(R) horizontal distance between outer tube limits at row R, in.  
 XDB(R) horizontal distance between shell walls at row R, in.  
 XMAXR maximum number of tubes in any row  
 Y(R) vertical distance between bottom of shell and row R, in.

A flow diagram of the un baffled shell-side pressure drop subroutine is shown below.

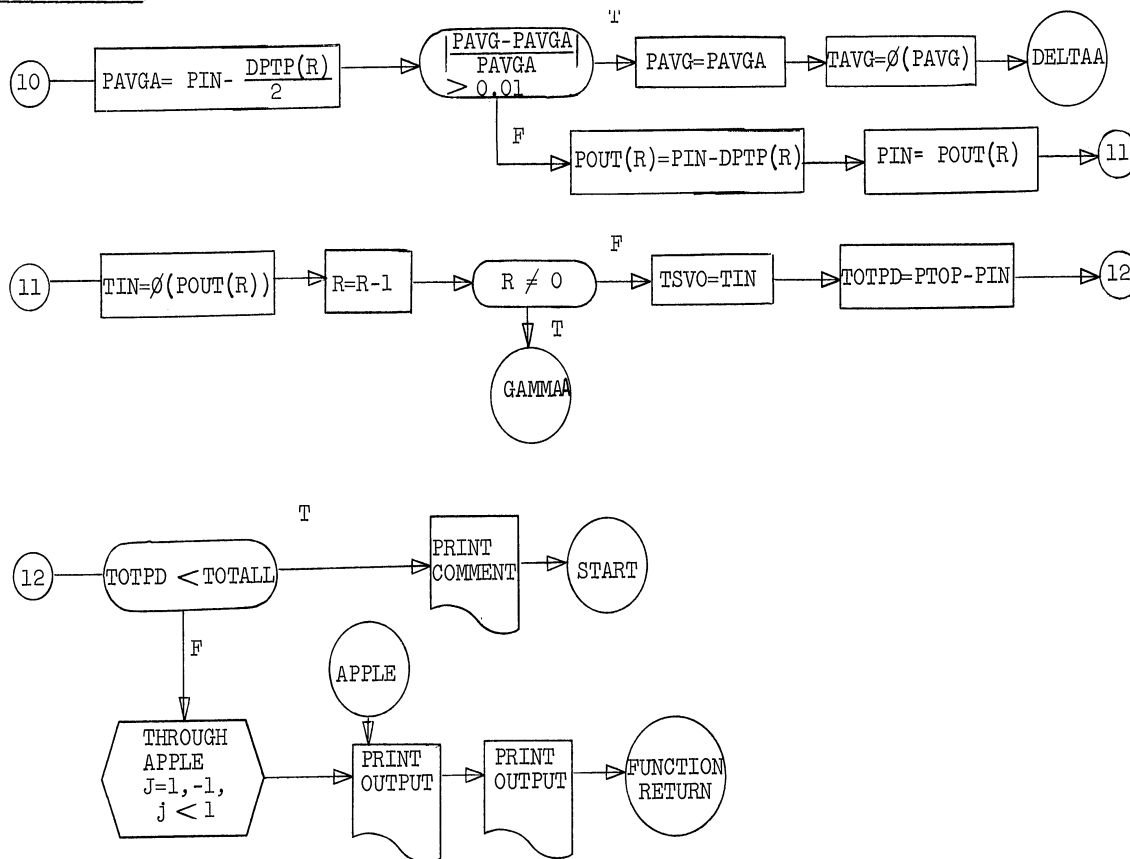


Economic Design of a Condenser

Flow Diagram, Continued



Flow Diagram, Continued



The MAD listing of the subroutine is shown below.

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SCOMPILE MAD, EXECUTE, DUMP, PUNCH OBJECT
R UNBAFFLED SHELL SIDE PRESSURE DROP FOR A CONDENSER
EXTERNAL FUNCTION (HEAD, IDS, TUBEL, TUBES, TSVI, W, TOTALL,
1 OD, TR, SQ, DEQ, MWT, Z, LATA, LATB, DENLA, DENLB, VISGA,
1 VISGB, VISGC, PRTEMA, PRTEMB, TSVO, TOTPD, PITCH, START)
ENTRY TO USHEDP.
STATEMENT LABEL START
INTEGER HEAD, TUBES, I, R, U, TUBES, TUBEE, XMAXR, XB, J,
1 TR, SQ
DIMENSION IDSH( 23), Y(100), XDA(100), TUBEE(100), FFA(100),
1 XDB(100), DPTP(100), POUT(100)
THROUGH ALL, FOR U = 1, 1, IDS *E. IDSH(U)
WHENEVER U *G. 22
PRINT COMMENT $1SHELL SIZE TOO LARGE FOR STANDARD SIZE $
TRANSFER TO START
OTHERWISE
CONTINUE
END OF CONDITIONAL
WHENEVER HEAD *E. 0
DOTL=(IDS-0.411)/1.0028
OR WHENEVER IDS *L. 27.0
DOTL=IDS-1.13
OTHERWISE
DOTL=IDS-1.44
END OF CONDITIONAL
CL=(IDS-DOTL)/2
R=1
XB = TUBES
Y(R)=CL+4*(PITCH-OD)+OD/2
DELTAD XDA(R)=2*SQRT.((DOTL/2)*P.2-(Y(R)-IDS/2)*P.2)
XMAXR=XDA(R)/PITCH
TUBEE(R)=XMAXR-(1-(-1)*P.2)/2
XDB(R)=2*SQRT.((IDS/2)*P.2-(Y(R)-IDS/2)*P.2)
XB=XB-TUBEE(R)
WHENEVER XB *L. 0
I=R
TUBEE(R) = TUBEE(R) + XB
FFA(R)={(XDB(R)-TUBEE(R)*DEQ)*TUBEL}/12
TRANSFER TO INLETG
OTHERWISE
    
```

MAD Program, Continued



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FFA(R)=((XDB(R)-TUBEE(R)*DEQ)*TUBEL)/12
TRANSFER TO INLETG
OTHERWISE
FFA(R)=((XDB(R)-TUBEE(R)*DEQ)*TUBEL)/12
END OF CONDITIONAL
R=R+1
Y(R)=Y(R-1)+TR*0.867*PITCH+SQ*PITCH
WHENEVER (IDS-Y(R))*L*(4*(PITCH-OD)+OD/2)
PRINT COMMENT $1SHELL SIZE NOT LARGE ENOUGH FOR NUMBER OF TUB
IES SPECIFIED.$
TRANSFER TO START
OTHERWISE
TRANSFER TO DELTAD
END OF CONDITIONAL
INLETG
CONDT=0
DELP=0
PTOP = EXP.(PRTEMA + PRTEMB/(TSVI + 460.0))
PIN=PTOP
GAMMAA
TIN=TSVI
PAVG=PIN
DELTA
VISG = EXP.(VISGA + VISGB/TAVG + VISGC/TAVG*P.2)
REG=(DEQ*W)/(12*VISG*FFA(R))
FS = EXP.( 0.11138076E02 - 0.49929705E01*ELOG.(REG) +
1 0.72354022E0*(ELOG.(REG)).P.2 - 0.47569737E-01*
1 (ELOG.(REG)).P.3 + 0.11495005E-02*(ELOG.(REG)).P.4)
DENG=(MWT*PAVG)/(Z*10.73*(TAVG+460))
DPG=(2.0*FS*W*W)/(DENG*FFA(R)*FFA(R)*4.18*10.0.P.8)
LAT = LATA + LATB*TAVG
Q = W*LAT
COND=(TUBEE(R)*Q)/(TUBES*LAT)
CONDT=CONDT+COND
DENL = DENLA + DENLB*TAVG
LVOL=(CONDT-COND/2)/DENL
GVOL=(W+COND/2-CONDT)/DENG
WHENEVER GVOL.LE.0
LVF=1.0
TRANSFER TO INLETH
OTHERWISE
LVF=LVOL/(LVOL+GVOL)
END OF CONDITIONAL
INLETH
FUNC = (LVF*DENL)/(DENG*REG.P.0.5)
WHENEVER FUNC.LE.0.005
RATIO = 0.324/FUNC.P.0.092
OTHERWISE
RATIO = 0.00256/FUNC.P.0.98
END OF CONDITIONAL
DPTP(R)=(RATIO*DPG)/144
DELP=DELP+DPTP(R)
PAVGA=PIN-DPTP(R)/2
WHENEVER .ABS.((PAVG - PAVGA)/PAVGA) .G. 0.01
PAVG=PAVGA
TAVG = PRTEMB/(ELOG.(PAVG) - PRTEMA) - 460.0
TRANSFER TO DELTAA
OTHERWISE
POUT(R)=PIN-DPTP(R)
END OF CONDITIONAL
PIN=POUT(R)
TIN = PRTEMB/(ELOG.(POUT(R)) - PRTEMA) - 460.0
R=R-1
WHENEVER*R.NE.0,TRANSFER TO*GAMMAA*****
TSVO = TIN
TOTPD=PTOP-PIN
WHENEVER TOTPD .G. TOTALL
PRINT FORMAT COMM3
PRINT FORMAT INFO,TOTPD
TRANSFER TO START
OTHERWISE
THROUGH APPLE,FOR J=I, -1, J .L. 1
APPLE
PRINT FORMAT OUTE, J, Y(J), TUBEE(J), DPTP(J)
PRINT FORMAT INFO,TOTPD
END OF CONDITIONAL
FUNCTION RETURN
VECTOR VALUES COMM3 = $ 87HOCALCULATION WAS TERMINATED BECAUS
1E SHELL-SIDE PRESSURE DROP EXCEEDED ALLOWABLE LIMIT *$
VECTOR VALUES TITLEC = $ 40H1 ROW DIST/BOT TUBES PRESSU
1RE DROP / * $
VECTOR VALUES OUTE = $ 15, F10.4, I10, F15.7 *$
VECTOR VALUES INFO = $ 48H4SHELL SIDE PRESSURE DROP FOR UNBAF
1FLED FLOW IS F7.5, 4H PSI *$
VECTOR VALUES IDSH(1) = 5.047, 6.065, 8.071, 10.02, 12.09,
2 13.375, 15.25, 17.25, 19.25, 21.25, 23.0, 25.0, 27.0, 29.0,
3 31.0, 33.0, 35.0, 37.0, 39.0, 42.0, 44.0, 47.0
END OF FUNCTION
$DATA

```