COMPUTERS IN CHEMICAL ENGINEERING EDUCATION

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The advent of computers has enabled the engineer to broaden his horizons with respect to the types of problems he may study and solve in a given amount of time. As an educational tool, the computer also proves very useful in that it takes over the routine calculations once an appropriate algorithm or procedure has been established for the problem at hand.

Students can investigate problems using numerical methods which before were not presented to them until they were able to solve them by compact analytical techniques. These methods are usually not presented in an undergraduate curriculum. One must, however, choose problems carefully so that the students avoid the numerous pitfalls present when numerical methods of solution are used.

Computers and Engineering Science

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 (engineers who may well be working as engineers in the year 2000) will have occasion to use computers in their technical work. Considering his probable imminent involvement with computers as part of his engineering work, the engineer must know a great deal more about computers than he can learn from the "giant brain" articles so prominent in the Sunday supplements. The question which comes to mind first is, Where should he learn about them? On the job or in the engineering school?

Those who feel that on-the-job training is adequate, usually claim that computer programming and computer-related work involves primarily techniques rather than engineering principle. Those who feel that the engineering school is a proper place for such training agree that there is a significant amount of technique (technique which will incidentally be useful in the student's future engineering work) but that the primary justification for such training, particularly at the undergraduate level, is based on the computer as an educational tool useful in the training of problem solvers. Viewed as an educational tool the computer can be considered a language for communicating as well as a machine for solving problems. A better understanding of principles can be attained because of the rigor required when communicating with the computer. This understanding is also reinforced because the student has a broader experience with solved problems.

Some features of a computer experience which seem to be related to the educational aspect of problem solving are:

a. Precise Definition: The computer is a rather rigid task master 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) and an ability to synthesize (bring together solutions of individual parts as the solution of the whole). Preparing algorithms (problem solving procedures, flow diagrams) for a computer requires just such analysis and synthesis abilities.

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.

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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, some assumptions necessary to permit hand computation may 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 a specific problem in a specific problem situation. This necessitates an essentially symbolic approach to problem solving and is rather different from the customary solution techniques 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 (essential) to work at least one example problem in detail by hand for checkout purposes.

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 logical, essentially non-numeric problems.

Computers and Engineers in Industry

Computers, both digital and analog, have wide acceptance in production, design and research. This trend, although still in its infancy, is making rapid strides. For example, the high degree of sophistication in some applications is illustrated in a recent announcement that complete engineering drawings fro roads are being turned out by computers. A recent survey for the American Petroleum Institute indicated that 86 of 127 responding refineries used off line computers, and several larger refineries have several computers working full time.

Today a large percentage of the "green light time" can be attributed to accounting and scheduling type functions in those computers associated with production units. More and more time is being used, however, by engineering groups to do repetitive computations and optimization studies. Several on line control computers are operating with some success. In a number of processes, where the reaction scheme is complex, for example, co-polymerization, there appears to be great incentive to use either open or closed loop computer control.

In research organizations computers are widely used in a number of areas. Although Esso Research Laboratories may not be typical because we are fortunate to have access to a great variety of computers, it is not atypical with respect to computer utilization. Therefore, we would like to take the liberty of using this organization as a basis for discussing the needs of the engineer vis-a-vis computers in industry.

A very brief look at the organization with particular emphasis on computers, as shown in Figure1, will help to orient the discussion. The Laboratory is one of the major development groups affiliated with Esso Research & Engineering Co. and does bench scale exploratory work as well as operate small and large pilot plants. To fulfill its mission it has several research groups, an engineering group and an applied mathematics group. Three digital computers are available, an IBM 1620 in the applied math group, an IBM 7074 in the Baton Rouge Refinery, and an IBM 7090 in Florham Park accessible by transceiver. The latter two installations are closed shop and the in-house facility is open shop. FORTRAN and symbolic assembly programs are available for all machines.

Almost all of the professional employees are involved with computers to some degree. Computers are used in two primary areas in our technical computing, data work-up and engineering studies. For the former some of the pilot plants are tied to a data gathering system. The data tape is used, along with data picked up from a daily analytical results tape, as input to any one of several unit data work-up programs. Much of the logic for these operations has been handled by experienced non-engineer programmers. The engineers must, however, supply algorithms for the unit work-ups. The programmers in the applied mathematics group are available to program the algorithms. It is usually more efficient, however, for the engineers to write and debug their own programs especially when, as is usually the case, program requirements change frequently.

The engineering studies include process optimization, reactor stability, control, reaction mechanism and similar studies which require the use of chemical engineering and related sciences together with a knowledge of mathematics and computer sense to bring them to a successful conclusion. This type of problem has increased in importance and will continue to take a greater share of the engineering talent and computer time in the future.

The demands on the engineer using computers in industry are many even though specialized help is usually close at hand. To maximize the information obtained from extensive pilot plant operations he must decide when computer data reduction with or without automatic data gathering is warranted, keeping in mind programming time required and computer cost. It is helpful if he can write and test his own programs because this cuts down lead time, often one of the greatest costs of research, and allows him to make any changes with the least delay.

This class of problems does not usually require extensive application of advanced mathematical techniques. It does demand a degree of rigor which we as chemical engineers were not able to exhibit before the computer era. Often the algorithms for this class of problems are simplified by use of simple matrix manipulation.

Engineering studies are becoming much more sophisticated and more encompassing in their scope. Engineers today should have a better understanding of the advanced mathematical techniques used to solve partial differential equations. In this area the computer is a great help, and at the same time its own worst enemy. Many engineers are not aware of the pitfalls which round off errors and non-convergence present. In addition to learning sound problem analysis and efficient algorithm construction, it is important that the engineer be made aware of the pitfalls involved in numerical methods and approximations so often used in digital computation.

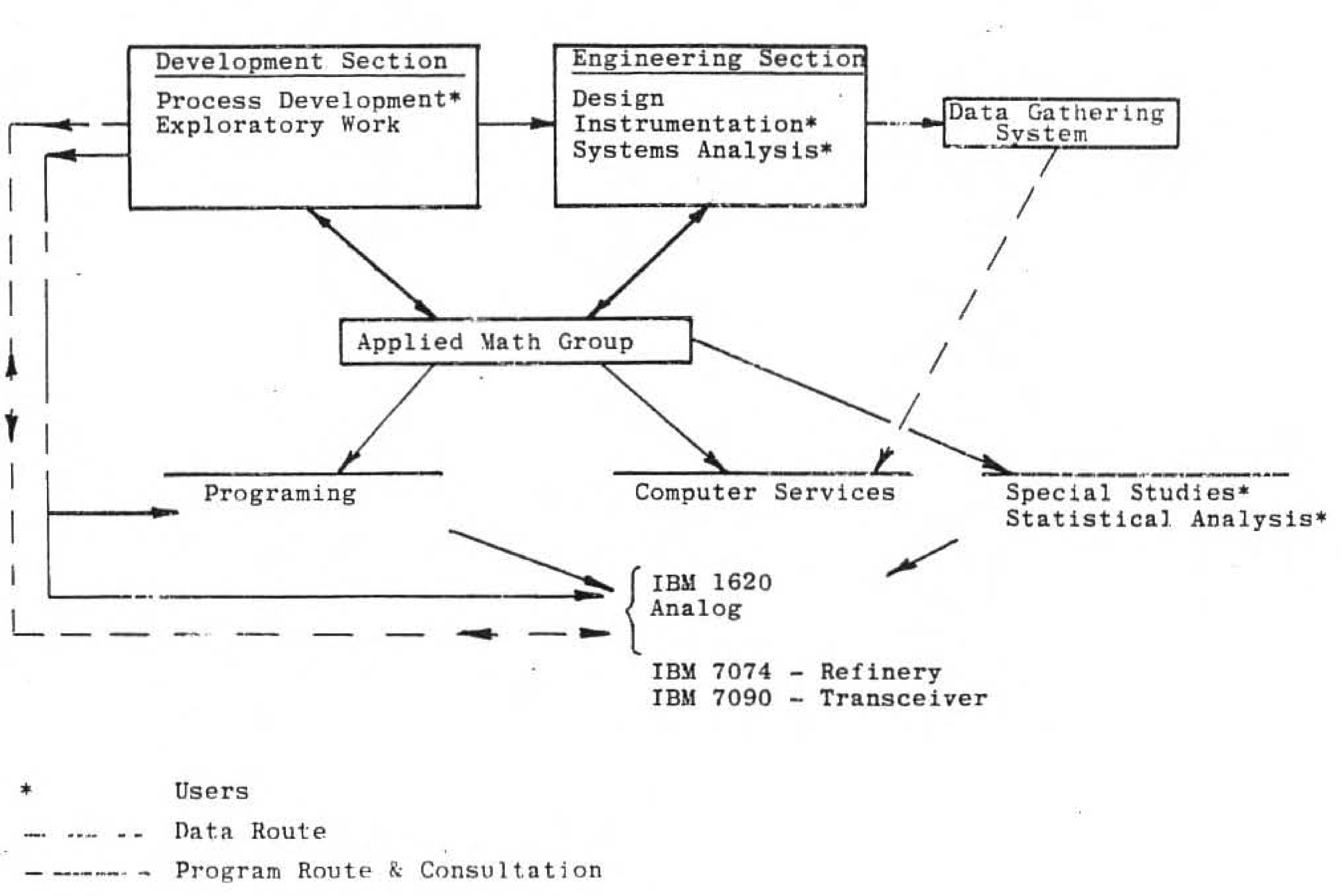
A third area where the chemical engineer and the computer have found common cause is in scheduling and economic optimization. This, of course, requires a knowledge of linear (or, in general, mathematical) programming. Today there is a need to develop a logic which can be used for ultimate design optimization by welding together and exercising supervisory control over independent routines representing a series of interdependent moduli or operations. Here again there is a need for a sound foundation in logic.

The use of computers by engineers in an industrial organization would not be complete without discussing communication between man and the computer. This has been very much simplified in the past few years at Michigan because of an excellent executive routine and a very versatile Algol language, MAD, with superb diagnostics. Due to the multiplicity of demands on most large industrial computers -- they do payrolls, accounting and complex engineering calculations -- and the limitations of the smaller computers such as the IBM 1620, communication is usually not quite as simple. This means that precompilation debugging should be more thorough. More important, it is most helpful if the engineer has some knowledge of computer operation or logic so that he can easily adapt to different computers, programming systems and methods of searching for errors.

The use of computers in engineering calculations and their introduction into the engineering sciences curricula is of great benefit to the young engineer. It forces him to be more analytical and rigorous in his approach to problems. It is important that along with the use of computers, numerical analysis, logic and some basic concepts of computer operation be introduced so that the engineer can make wise and efficient use of this powerful tool in an industrial atmosphere.

FIGURE 1

COMPUTERS IN AN INDUSTRIAL RESEARCH ORGANIZATION



Education With Computers

At Michigan there has been some contact with computers for the past 10 years. At first this was rather limited but since 1956 when an IBM 650 became available on an open-shop basis, the use of computers in the chemical engineering science curricula has been ever increasing. At first only limited use was made of the computer in graduate courses because access was rather difficult. With the arrival of a large computer, an IBM 704, and problem oriented languages such as FORTRAN and MAD, the computer became relatively accessible to undergraduates.

A question which arose is where and how the student should be introduced to the computer. If he is to gain a real computer proficiency, it appears that an introduction to computer organization and computer language should come early enough in his training to allow opportunity for extensive use of the machine in solving some engineering problems. Since it seems impractical (and probably unwise) to remove engineering course material to allow insertion of computer work into engineering courses, it would appear that the student should have an independent introductory course which gives him thorough training in the language and a general understanding of computing procedures. If he is not to be lost in the hopeless mire of detail there seems little doubt that the selected computer language should be of the problem-oriented rather than the machine-oriented type. If engineering classroom time is not to be wasted, then he must be trained well enough in the first course to eliminate the need for later retraining in the engineering classroom. The solution to this problem at The University of Michigan has been the introduction of a required one-hour course at the sophomore level which trains the student in the use of a problem-oriented language (MAD) and introduces him to some of the elementary numerical techniques.

At the present time at least one problem whose solution is best obtained with the aid of a high speed computer is presented in most every course in chemical engineering science. As can be seen in Figure 2 this means that students are exposed to computer methods from the beginning of their sophomore year. By applying the techniques learned in the course "Elementary Computer Techniques" immediately we find that students get a better appreciation of computer techniques. In each succeeding course one or more computer oriented problems are presented to the students. These problems, chosen by the individual instructor, are coordinated so that they illustrate many facets of computer programming and use.

Problems which arise in the assignment of computer problems as part of the engineering coursework homework load include timing. While there seems little doubt that a project-type assignment involving a time period of perhaps two weeks or more causes no significant difficulty, homework assignments done on a day-to-day basis do present some problems. Because of the nature of computer languages, i.e., the necessity for very precise grammar and punctuation, it is unusual for an undergraduate student to solve completely correctly an engineering problem on the first approach to the computer. The average may be three or four tries before success. The turn-around time, i.e., the elapsed time between submission of a program to the computer and its return for checking and possible resubmission in case of error, must consequently be fairly short if problems are to be completed between class meetings.

If computer integration into engineering classrooms is to be successful, the student's overall computer ability is certainly a major factor. The instructor's ability is probably even more important, particularly for undergraduate training. The selection of appropriate problems and the illustration (by example) of good computer habits (pointing out inadequacies or places where the computer should probably not be used, as well as where it should be) is essential.

In an attempt to help develop a better appreciation of the computer and computer techniques, a set of problems for use in an undergraduate chemical engineering curriculum is described in the Appendix. It is expected that the student will have had prior to or concurrently with the first of these problems a basic course in programming, as too much time taken from course content would be required to learn basic programming techniques.

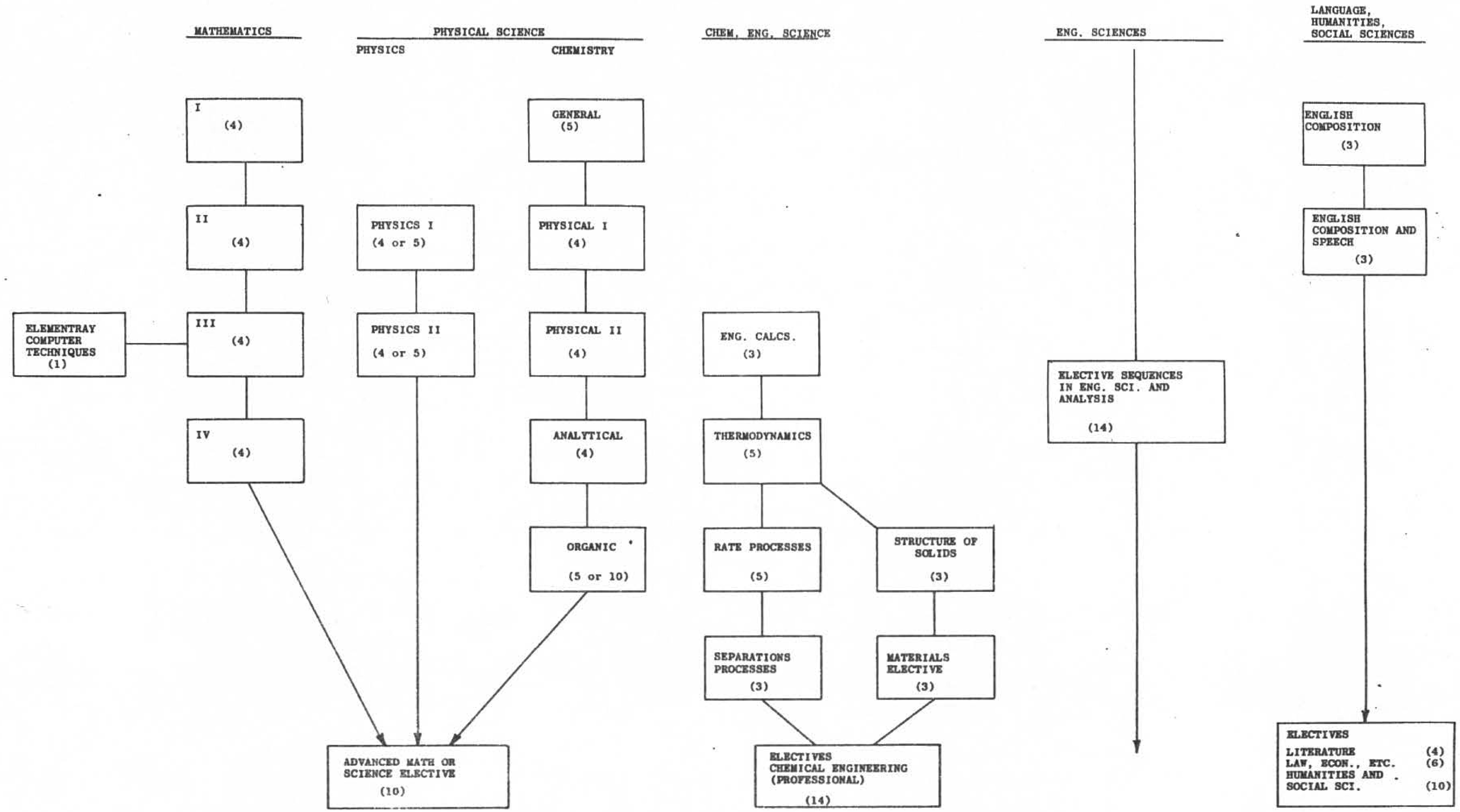
Conclusion

It is not wise to attempt to justify the use of a computer as a time saving device when one deals with a single problem operation, common to introductory educational endeavors. It is much better to look at the computer and program as a method of introcuding a tool which will enable the student, after some experience, to solve complex problems and will force the student into habits of careful, detailed problem analysis and logical solution methods. If exposure to computers and computer programming does nothing else it will be well worth the time and effort required if our students think more logically and precisely.

FIGURE 2

CHEMICAL ENGINEERING BSE PROGRAM

UNIVERSITY OF MICHIGAN



( ) SEMESTER HOURS REQUIRED.

BLOCKS ARE IN VERTICAL ORDER OF SEMESTERS IN WHICH COURSES ARE TAKEN.

It is true that this is a relatively new area in our curricula, but a very essential one. At this stage we have and should raise more questions than we can answer but by proper choice of problems the advantages of the computer will be well demonstrated. The student will gain new insight into many more problems and will become quite at home with the computer, a valuable tool for the engineer.

Acknowledgement

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APPENDIX

A SERIES OF GRADED CHEMICAL ENGINEERING COMPUTER PROBLEMS

This series of computer problems is typical of those used during the past four years in the chemical engineering curricula at the University of Michigan. No attempt has been made to be all inclusive as this set, it is hoped, will merely serve as a guide. Complete solutions for many of these problems -- mainly written in MAD -- may be found in the various reports issued by the Ford Foundation Project on Computers in Engineering Education (2).

PROBLEM FOR A FIRST COURSE IN STOICHIOMETRY

A typical first problem after some basic programming experience might be a detailed mass balance as follows:

Problem Statement:

A countercurrent multiple-contact extraction system is to treat 100 tons per hour of tailings with fresh water as a solvent. The composition of the tailings fed to the extration unit is

Component	Mass Fraction
Water	0.48
Gangue	0.40
Salt	0.12

The strong solution leaving the system is to contain 0.15 mass fraction salt. A 99 per cent recovery of the salt is anticipated. Calculate the number of equilibrium stages required as a function of the solution retained by the gangue.

Solution:

This problem may be solved by a number of methods, including the method of linear differences. The basic material stage-wise balance method of solution is discussed in detail by Brown (1) and a computer solution for a similar problem may be found in the First Annual Report of the Project on the Use of Computers in Engineering Education sponsored by the Ford Foundation at the University of Michigan. (2)

Basically, the solution requires that an overall balance around the extraction be made and then stage-wise calculations be made until the raffinate from the last stage meets the required concentration specifications. Once the basic program is written, it may be easily enlarged to include either variable solution retention (as a function of the solution composition) or a series of solution retention values.

The problem is not difficult to program but does require the use of subscripts. Students have programmed a similar problem in 15 steps and with relatively little expenditure of time. It has the added advantage of illustrating the effect of solution carry-over.

A SECOND PROBLEM IN STOICHIOMETRY OR A FIRST PROBLEM IN THERMODYNAMICS

A second problem in Stoichiometry which could also serve as a first problem in Thermodynamics is the computation of the adiabatic flame temperature as a function of the fuel and fuel to air or oxygen ratio.

Solution:

The solution to this problem requires writing a material balance for the components involved and then making a thermal balance assuming a flame temperature. If the amount of sensible heat out equals heat of combustion plus the sensible heat in the correct flame temperature has been established. If the heat in and out do not balance, a new flame temperature must be chosen; the Newton-Raphson (3) method for estimating the successive values for the flame temperature will allow for quick convergence on the correct answer.

This problem is quite simple to program for a given fuel and fuel to air ratio and should require even less time than the problem discussed above. If it is desired to investigate the effect of fuel to air ratio or type of fuel, a little more thought is required to successfully program the problem. It is still a reasonable problem for people with a minimum of computer experience.

A PROBLEM IN THERMODYNAMICS

A number of thermodynamic calculations lend themselves readily to solution by the computer. The study of non-ideality and physical equilibria are probably two of the areas which are often neglected in beginning courses and which with the aid of the computer may be studied quantitatively. A typical request of students might be to require them to determine the degree of non-ideality and the per cent vaporization of a ternary mixture of hydrocarbons as a function of pressure and temperature.

Solution:

The instructor must supply an equation of state which is to be used to compute the properties of the non-ideal gases. This equation should be used to obtain densities and fugacities as a function of pressure and temperature. Once this has been programmed successfully, the students may use the equation of state in subroutine form.

The information, fugacity and density of the pure components and mixtures, obtained from the equation of state subroutine, may now be used in a larger program which actually calls on the subroutine when required. K's may be evaluated as a function of the fugacity and estimated composition and these may then be used in a flash-vaporization computation to calculate the degree of vaporization of a mixture. In addition gas phase densities may be checked against ideal densities to determine compressibilities factor values, a measure of non-ideality.

This program would be fairly advanced and it may be desirable to first compute the degree of vaporization based on Raoult's Law, that is, using vapor pressures obtained from a Clapyron relationship. This program would be quite simple to write and would serve as a good introduction to the general problems of physical equilibria.

A PROBLEM IN RATE PROCESSES

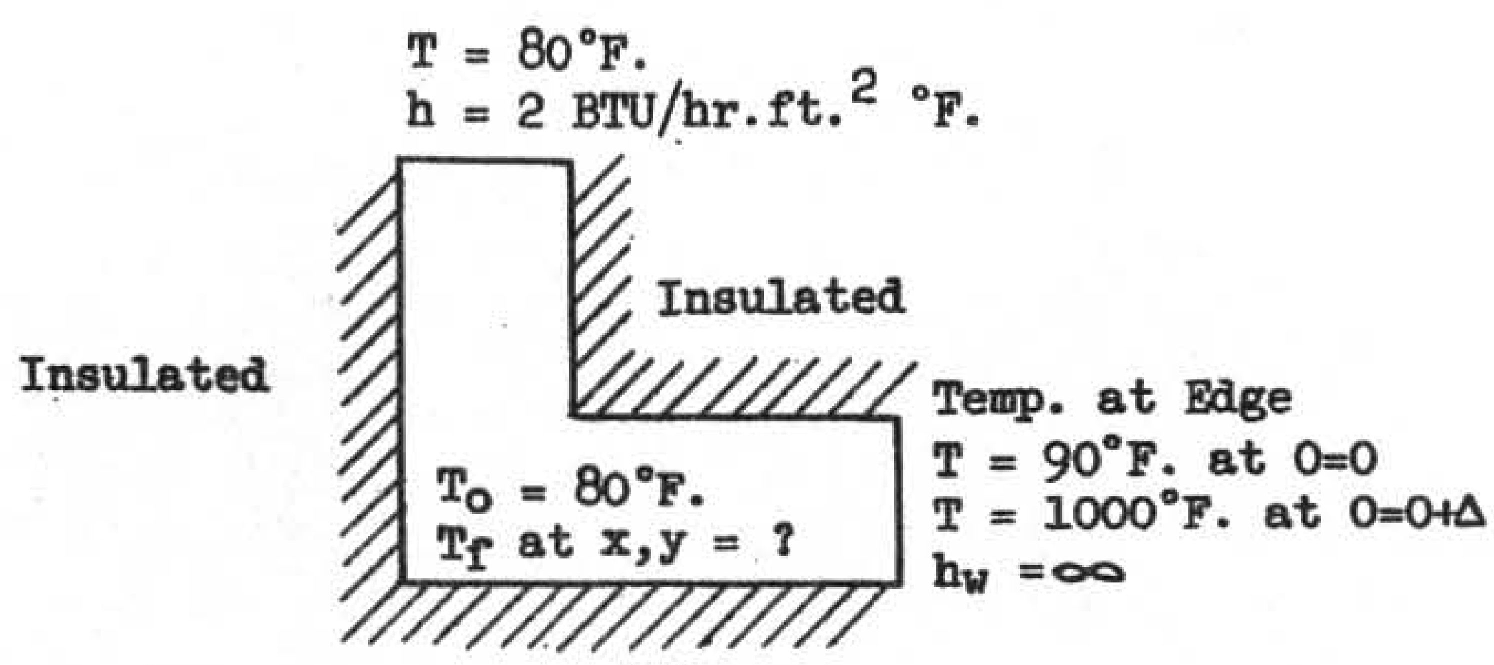
In the area of rate processes, the computer can greatly benefit and enhance the subject matter discussed in a beginning course. Many of the problems involving rates of heat or mass transfer involve partial differential equations which may be reduced to difference equations for numerical solution on the computer. A good elementary discussion of these methods may be found in "Numerical Methods for Science and Engineering" by Ralph G. Stanton.

The first problem in this area which is very suitable for computer solution is an unsteady-state heat transfer problem. The time required to quench an odd shaped bar is to be determined. In order to simplify the geometrical concepts, it is probably good to choose a rectangle with irregular insulation or study the converse problem of heating of a right angle bar at one end and determine the time dependence of the temperature at the other end of the angle iron as indicated in Figure 1 where T_f if a function of time.

This problem has been programmed by students quite successfully before. A detailed discussion of the method may be found in a paper by Rudd (4). In this problem a grid is established over the piece in question and the method of relaxation is employed to determine the temperature distribution over the grid at any given point in time.

FIGURE I

CROSS-SECTION OF RIGHT-ANGLE BAR



ANOTHER RATE PROCESSES PROBLEM

The design of tubular reactors is a very common task undertaken on a computer. In the case usually considered the equations representing the temperature and volume dependence of the system become somewhat complex for analytical solution. It is therefore necessary to use a set of difference equations and iterate down the length of the tube. This problem is well suited to computer solution but one word of caution. The choice of increment size is a difficult one. Care must be taken not to introduce round-off problems when results from preceding segments are used as a basis for computing the next segment.

A typical problem might be: the decomposition of SO_2Cl_2 to SO_2 and Cl_2. The heats of formation and heat capacities for the compounds are

SO_2Cl_2 (g) ΔH_f = -82,040 cal/gm. mole

$C_p = 13.00+24.0\times10^{-3}T-14.4\times10^{-6}T^2$

SO_2 (g) ΔH_f = -70,920 cal/gm. mole

$C_p = 8.12+6.825\times10^{-3}T-2.103\times10^{-6}T^2$

Cl_2 (g) ΔH_f = 0

$C_p = 7.5755+2.4244\times10^{-3}T-0.965\times10^{-6}T^2$

and the rate of decomposition may be expressed as follows:

$$r = A\ e^{E/RT}$$

where

$$A = 6.427\times10^{15} \quad 1/\text{sec}$$

$$E = -50610 \quad °K\ \text{cal/gm. mole}$$

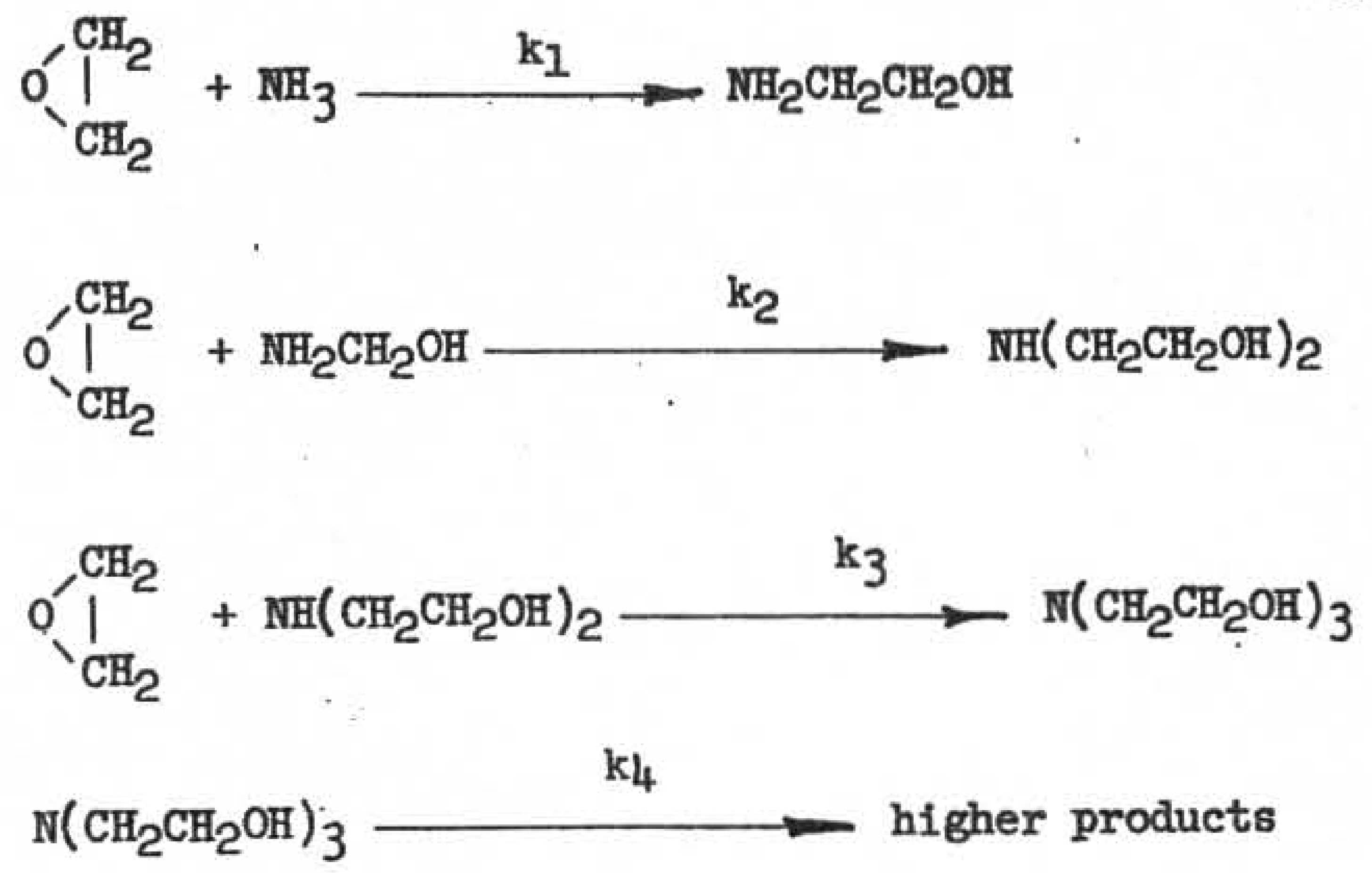
Compute the length of a 1 1/2" I.D. tube required to insure 98% decomposition of 418 pounds per hour of SO_2Cl_2 fed at 200°F. and 1.2 atm, heat is transferred to the tube at the rate of 5000 BTU per square foot per hour.

DESIGN PROBLEM IN REACTION KINETICS

The use of computers in design courses has been quite successful. After a program of problems in earlier courses, the students often ask to have the computing facility made available to them. The choice of material taught or problems assigned to students is very wide so we include an example for illustrative purposes of what can be done.

A typical problem would be to determine the optimum reaction time for a given product if three competing products are formed, that is, mono-, di- and tri- ethanol amine. If one knows the rate constants as a function of temperature, one can write expressions for the concentration of all the species in the system. This results in this case in a system of five simultaneous linear differential equations. These may be readily solved using the standard Runga-Kutta method which is programmed for most large computing facilities and discussed in detail in any of a number of texts in numerical analysis (6).

The original reaction data for the ethanol amine reactions were determined by Ferrero and coworkers (7) and are summarized below with additional data required to solve the problem. The possible reactions are:



The velocity constants for the Arrhenius equation

$$k_i = A_i e^{-E_i/RT} \quad \text{are:}$$

	A gm. mole/liter min.	E
1.	3.58×10^{8}	14,500
2.	9.9×10^{9}	15,600
3.	2.58×10^{9}	15,000
4.	3.93×10^{6}	12,650

It is now possible to determine concentrations of each product in the effluent of an isothermal reactor as a function of the space velocity and the initial concentrations. If sufficient data is available on the heats of reaction and specific heats of the constituents the non-isothermal case may be studied.

This problem and similar problems have been very useful in demonstrating the course of reactions. This and similar problems, it should be mentioned, are also very suitable for analog computer analysis.

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The following list of problems were prepared by various staff members and visiting professors at the University of Michigan under the sponsorship of the Ford Foundation project on "The Use of Computers in Engineering Education" (8). The titles are included to suggest some more areas where computers have been and can be used. Complete descriptions and programs are available from the project at the University of Michigan.

Title	Level[1]
Optimization of Reactor Operation	2
Approach to Steady-State of an Othmer Still	2
Temperatures and Heat Flux in a Radiant Thermal Circuit	2
Heat Balance for an Iron Blast Furnace	2
Three Component, Two Phase, Counter-Current, Liquid Extraction	3
Temperature Distribution in a Three Dimensional Body	3
Solution of a Boundary Value Porblem Using an Initial Value Technique: Temperature Profile in a Circular Transverse Fin	3
Velocity Profiles for Flow in Smooth Pipes	3
Determine Reflux Ratio by McCabe-Thiele Method	3
Temperature Profile in a Longitudinal Fin Using the Analog Computer	3
Diffusion and Slow Chemical Reaction	4
Number of Theoretical Plates in a Multi-Component Distillation Column	4
Multiple Regression Analysis	4
Solvent Allocation in Multi-Stage Crosscurrent Extraction	4-G
Dynamic Heat Exchange	3-4
Storage of Natural Gas in Aquifers	G
Adiabatic Reactor	G
Predicting the Scrap Requirement for the Oxygen-Steel Converting Process	4

(1) Year in which normally used.