INTRODUCTION TO CHE ANALYSIS

T. W. F. RUSSELL and M. M. DENN
University of Delelware
Newark, DE 19711

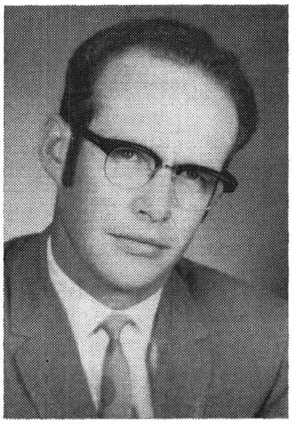
The transition of chemical engineering education during the past two decades from an empirically based, design oriented curriculum to the so-called "engineering science" approach has been neither smooth nor totally successful. Today's curricula have been justifiably criticized for failing to teach applications of principles, and the new trend appears to be a "return to design." A principle-based curriculum *can* be oriented towards practical engineering application and provide the necessary blending of design and engineering science. The resolution lies in imaginative use of the introductory course in chemical engineering, usually taught at the sophomore level.

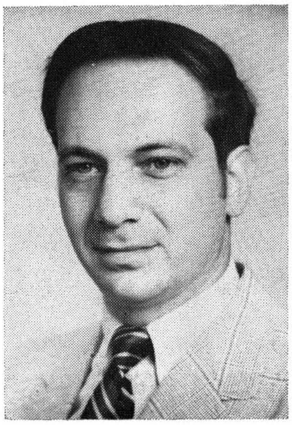
The sophomore course in *Industrial Stoichiometry* has changed little during the era of major modification of upper-class undergraduate and graduate curricula. Though "modernized" at times by introduction of the digital computer to assist in the solution of large problems, the course content remains by-an-large the solution of steady state mass and energy balances for existing processes. Skills are haphazardly developed through many example problems and little attention is paid to the development of a consistent logical approach to engineering problem solution. Recent developments which have greatly improved and expanded high school and university freshman courses are ignored. The student's mathematical skills are not adequately reinforced with practice in engineering problems and almost no attention is paid to his improved abilities in elementary calculus and basic chemistry. In an attempt to "simplify" problems for the sophomore level many concepts, particularly in basic thermodynamics, are introduced incorrectly and a re-learning must take place in the courses which follow. *Considerations of design are never included because the concept of a rate is usually not introduced.* The type of problem considered has little to do with the creative aspects of traditional chemical engineering practice or the extension of chemical engineering skills to a broader class of problems.

The inadequacy of the traditional sophomore course is compounded by the lack of continuity between it and the "engineering science" courses which immediately follow: There is a difference in approach, type of problem, and analytical level. The transition is a difficult one for many students, and in 1965 the Chemical Engineering Department at Delaware initiated a program to study, modify, and if necessary, reorganize the introductory course in the curriculum. This study has resulted in our present "Introduction to Chemical Engineering Analysis" course, which meets the following three objectives:

> To reinforce, amplify, and apply in an engineering environment the material covered in basic chemistry, physics, and mathematics.
> To develop the basic skills needed as a sound foundation for upper level courses.
> To develop an early appreciation for design by involving the student in simple but significant chemical engineering design problems.

Because of the considerable discussion in the profession about the proper direction for undergraduate education it seems to us that it is useful to recount our approach and the evolution of the course and our thinking. We do this because what seemed to us and many colleagues to be obvious remedies for the deficiencies noted above were not successful at all, and the final course outline differs considerably in content and tone from our first attempts. The course in its present form is a result of some five years experience teaching the subject to sophomore students in both the regular and extension programs. Some portions of the material have also been used with engineers and chemists who participated in AIChE continuing education courses at both the national (Today Series) and local levels. For three years we taught the course together at the same hour, each with a section of about twenty-five students. The material was coordinated on a lecture to lecture basis and its impact on students was evaluated after each lecture and again after each major topic had been covered. Substantial stu-





T. W. Fraser Russell received the Bachelors and Masters Degrees at the University of Alberta. He worked as a research engineer for the Research Council of Alberta and as a design engineer at Union Carbide Canada before receiving the PhD ('64) from Delaware. He is on leave for 1972-73 at ETH Zurich. Professor Russell received a University of Delaware Excellence in Teaching Award in 1968. His primary research interest is on two phase system analysis and design, and he has a book in progress in the area. (left)

Morton M. Denn received the Bachelors Degree at Princeton University and the PhD (64) at Minnesota. He has been at the University of Delaware since 1964 and was a Guggenheim Fellow in 1971-72. Professor Denn's major research areas are the fluid mechanics and rheology of polymeric liquids and optimization and optimal control.

dent feedback has been received, and several undergraduates and graduate students have worked with us for extended periods in evaluation and revision. This method of teaching has allowed us to experiment with various ways of organizing and presenting the material, and we feel that we have found a very effective way to introduce students to chemical engineering.

In the first year, we taught a slightly modified industrial stoichiometry course, followed by an applied mathematics course which concentrated on solutions of various types of differential equations encountered in chemical engineering. This latter course replaced the more classical course in differential equations taught by the mathematics department. It quickly became apparent that the major problem the student faced was developing the equations that described a particular situation. Since he did not feel adequately trained in this skill, there was a strong tendency to separate the mathematical description and its behavior from the situation which it described. This had two equally undesirable effects. Some students concentrated on the mathematical manipulation and thought little about the relationship to the physical situation, while others became confused as to the role of mathematics and tended to dismiss the material as being an academic exercise unrelated to physical reality. (This is not unlike what has happened outside the University in professional practice. It has been our experience in continuing education activities that the greatest number of engineers who profess a need for "more mathematics" are really in need of a better understanding of model development).

Today's curricula have been justifiably criticized for failing to teach applications of principles and the new trend appears to be a "return to design."

In an attempt to overcome these serious problems and also to revise what we considered to be inadequate or incorrect presentation in the standard stoichiometry course, we decided to restructure both courses and to concentrate on developing the skills which would enable the student to see clearly the relationship between mathematical description and physical reality. We attempted to meet this goal the first time we taught the integrated course by developing mathematical models for a series of increasingly complex physical situations. This "case study" approach was moderately successful and, although it did not

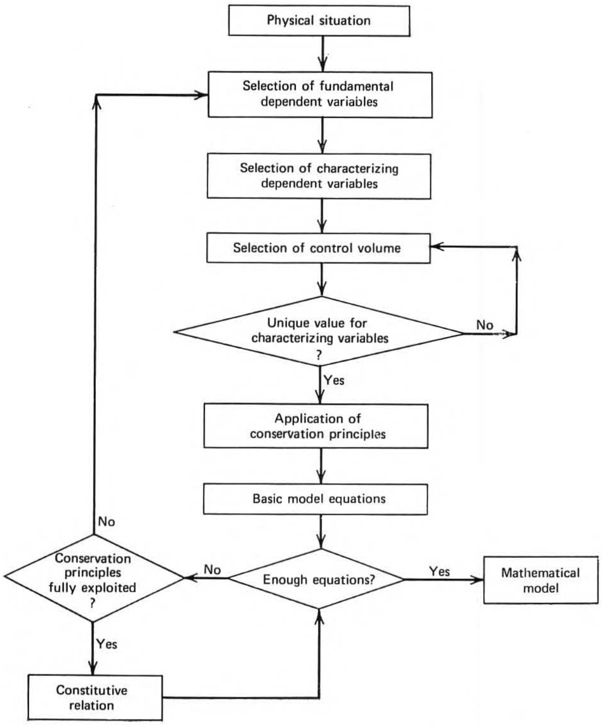


Fig. 1. Model development for any physical situation.

meet our goal of developing a systematic procedure for model development, the students did develop some facility for seeing the proper role of mathematics in the study of engineering.

The logic procedure outlined in Fig. 1 was introduced on the third try at the course. We emphasized this time the need for experimental verification of constitutive assumptions, as distinct from the application of conservation principles. *This emphasis on the role of experiment in engineering is, paradoxically, the key to a student's understanding of the role of mathematics.* At this time we oriented the course towards liquid phase reactor performance and concentrated on a complete study through design using a single conservation principle (mass) before introducing a second. We also found as we progressed through the third year that it was necessary to drop some of the mathematical skills we had stressed so that the more important aspects of analysis could be properly covered. We eliminated material on differential equations with variable coefficients and reduced our discussion of the Laplace transform.

An initial review of the third year's classroom experience produced a course outline similar to what now exists and pointed out a need for still more emphasis on the experimental aspects of engineering and the use of the mathematical descriptions for simple design. Thus we decided once more to reduce the mathematical content, resulting in total elimination of the Laplace transform. (Students with the need for such mathematical skills learn them in the senior Process Dynamics and Control course).

We concentrated in our fourth year on better organization of the material with respect to the model development step in analysis and we reorganized, using more experimental data, the methods by which constitutive relationships were employed. Our goal was to make sure that *all the relevant material normally covered in the stoichiometry course was introduced in a rational and consistent manner.* Since then the emphasis has been mostly on polishing and minor changes.

The sophomore courses, ChE. 230 and 231, are taught for two shortened semesters, totaling twenty-seven weeks. The relationship of these sophomore courses with other ChE courses at the University of Delaware is shown in Table 1. Since our students are not required to take a separate course in differential equations, but rather study the subject as part of the chemical engineering analysis course, a one-semester course employing a major fraction of our outline is possible. Emphasis is on the analysis of liquid phase systems, for this enables the student to treat meaningful design problems during his first semester of engineering study. He takes this course concurrently with the final semester of calculus and two semesters of physical chemistry. The topics covered follow our book, *Introduction to Chemical Engineering Analysis,* Wiley, New York, 1972.

TABLE 1 Basic Departmental Course Structure

Freshman Year	Introduction to the art and science of engineering	
	EG 125 (Introduction to Engineering) EG 130 (Introduction to Engineering Research)	
Sophomore Year	Aquisition of the basic engineering skill of Analysis-- How to proceed from experiment to design	
	ChE 230, 231 (Introduction to Chemical Engineering Analysis)	
Junior Year	The basic phenomena are studied from an engineering viewpoint	
	Applied Physical Engineering Sciences	Applied Chemical Engineering Sciences
	ChE 341 (Fluid Mechanics) ChE 342 (Heat and Mass Transfer)	ChE 325, 332 (Thermodynamics and Kinetics)
	ChE 345 (Chemical Engineering Lab)	
Senior Year	Skills are integrated by studying complex engineering problems in class, in the laboratory, and by individual thesis.	
	ChE 432 (Chemical Process Analysis-Design) ChE 443 (Transfer Operations) ChE 445 (Chemical Engineering Laboratory) ChE 473,474 (Senior Thesis) ChE 401,466,etc. (Electives in Control, Pollution Abatement, Polymer Processing, Chemical Economics etc.)	

INTRODUCTION. We start with a brief description of three chemical engineering problems, where the emphasis is on "putting together the pieces." We discuss a typical chemical process, the manufacture of ethylene glycol; the operation of an artificial kidney; and the design of a bio-oxidation reactor for sewage treatment. This introduces the idea of reactor, separation process, etc. We then turn to a detailed study of the analysis process, which we define as follows:

1) Description of a physical situation in mathematical symbols.

Student response has been excellent ...

2) Manipulation of the mathematical model to determine expected behavior of the physical situation.
3) Comparison of the model with the true physical situation.
4) Careful study of the **limitations** of the mathematical model.
5) Use of the model for equipment design and prediction of performance.

ANALYSIS. Several days are spent discussing the basic concepts involved in analysis and the total analysis process is described by means of the simple example of an emptying tank.

The model development step is illustrated using real data to develop a relationship between outflow and height of liquid (the orifice equation). Next the laws of conservation of mass, energy, and momentum applied to a well-defined control volume are shown to be the basic source from which mathematical descriptions are derived. A careful distinction is made between general conservation principles, universally applicable, and specific constitutive relations applicable only to certain situations. The necessity of experimental data for the development of constitutive relationships is stressed and dimensional analysis is introduced as one means for planning this needed experimental program. A series of logical procedures is developed to show the student how mathematical descriptions for a physical situation are developed. The ultimate logic is shown in Figure 1.

NON-REACTING LIQUID SYSTEMS. Model development for well-mixed tank-type liquid systems in transient and steady state isothermal operation is illusrated in detail, with an experimental check of the perfect mixing assumption and a critical appraisal of the role of the density-concentration constitutive equation. The purpose is to give the student practice in the model development step of analysis with simple problems, so that he can clearly see the relationship between the mathematical description and the physical situation. The simpler aspects of basic calculus are employed to determine model behavior and, as a secondary aim, practice with manipulation of the mathematical description to determine model behavior is stressed. As one example to meet this latter aim we exploit the draining tank problem and design a simple feed back controller. This also shows the student something about the design aspect of analysis.

REACTION RATE. Reacting, well-stirred single phase liquid systems are studied next. The reaction rate arises naturally in the component mass balance and reasonable phenomenological forms are deduced. Emphasis is on the use of batch reactor data to determine the validity of constitutive assumptions for the rate and to find the values of the parameters. Real batch data are used in all cases.

REACTOR DESIGN. The steady state model equations for a well-stirred continuous flow reactor are used for two design problems. In the first, a reactor is sized to meet production requirements for a single, irreversible first order reaction, taking capital and operating costs and depreciation of the reactor and separation unit into account. (The economics are obviously simplified). The other is the problem of sizing a reactor to obtain a required distribution of mono–,di–, and tri-ethylene glycol (a process introduced earlier). The sophomores take this material nicely in stride and take pride in their ability to use the mathematical descriptions. We introduce the plug flow tubular reactor here for comparison.

MASS TRANSFER RATE. Two-phase, well-stirred systems are studied to introduce the concept of mass transfer and to further develop modeling skills. The rate of inter-phase mass transfer arises naturally in the component balances and, like the reaction rate, reasonable phenomenological forms are deduced. Batch data are used to study the approach to equilibrium. For a continuous flow process the equilibrium stage is shown to be a good approximation for typical mass transfer data. Stage efficiency and reaction in a two-phase system are briefly examined.

STAGED PROCESSES. Multistage solvent extraction is studied analytically and graphically (McCabe-Thiele). Calculations are done for minimum solvent requirements and numbers of ideal stages. The triangular diagram is used for single stage calculations. The material nicely illustrates the use of graphical techniques in the model behavior step of analysis.

This is roughly the end of our first semester, together with some mathematical topics as needed, including least squares fitting to data. The student deals routinely with dynamical situations as well as the steady state, but he never requires mathematical concepts not already used in his calculus course. The interplay between laboratory experiment (measuring reaction rates, mass transfer coefficients, equilibrium constants, etc.), mathematical modeling, and engineering design calculations is brought home. This works because there is simply no easier practical problem in chemical engineering than the sizing of a liquid phase reactor with uncomplicated chemistry. The student is motivated to go on to engineering science courses and learn, for example, why a mass transfer coefficient is of a given order, or how to estimate one in the absence of an experiment. Most important, he has learned a systematic approach to solving problems.

At this point we turn to non-isothermal systems. In some curricula it might be desirable in a one semester course to skip some or all of the material on mass transfer processes and include some of the non-isothermal material. Emphasis is on the operational definition of thermodynamic quantities and, to avoid the complication of compressibility, liquid phase systems are studied first.

CONSERVATION OF ENERGY. Internal energy is introduced and the principle of conservation of energy applied to a flowing system. The square root orifice equation is derived using the energy balance. Internal energy and enthalpy are related to temperature by defining the heat capacity. Partial molar enthalpy is defined and used to define the heat of solution and the heat capacity of a mixture. Students are prepared to deal with partial molar quantities at this level because it comes sufficiently soon after seeing partial differentiation in the calculus course.

The student is continually referred back to relevant sections of his calculus and chemistry texts, developing, in his eyes, a logical continuity between his basic secience courses and creative engineering. Physical chemistry laboratory experiments are often discussed in our classroom.

MIXING AND HEAT TRANSFER. In parallel with the isothermal system development, we model non-reacting liquid systems. Consideration of temperature effects in batch mixing is followed by construction of the enthalpy-concentration diagram and graphical solution of the same problems. This is then repeated for steady state continuous mixing. The analysis of mixing is done rigorously, using partial molar enthalpies, for otherwise the student learns incorrect procedures which ensure the wrong answer when working with multi-phase systems. Heat transfer between adjacent chambers leads naturally to the rate of heat transfer and definition of the heat transfer coefficient. Area and flow rate calculations are carried out for cooling a tank by a jacket and a coil.

REACTING LIQUIDS. Reacting liquid systems are dealt with after the student has seen how partial molar quantities are used in the simple mixing situation. The heat of reaction is defined in terms of the partial molar enthalpy and the batch reactor equations derived which demonstrate how to measure it. Calculation of the heat of reaction from tabular data is discussed. The Arrhenius temperature dependence of reaction rate is demonstrated and the transient adiabatic batch reactor equations for a single reaction are integrated using numerical quadrature. (This still requires only the calculus course as preparation.) The energy balance for a continuous flow stirred reactor is derived. A numerical solution of the steady state is obtained, and the qualitative behavior of the non-isothermal reactor is discussed using the Van Heerden slope argument and phase plane construction via the method of isoclines. The non-isothermal tubular reactor is touched upon very briefly. By this point the student is becoming quite skilled in making his mathematical skills work for him to understand physical problems.

TRANSIENT REACTOR BEHAVIOR. We include this material as the practical application for linear differential equations, which are included in the course. The section can be omitted without serious loss. The reactor equations are linearized in the neighborhood of the steady state to obtain a linear second order system with constant coefficients. Applications are to the stability of the steady state, response of a stable system to a feed disturbance, and proportional feedback control by coolant flow rate adjustments. Students have no trouble with the notion of linearization. They have seen a number of examples in which the physical problem is severely limited in order to obtain a tractable mathematical model, and they recognize the virtue and limitation of such a trade-off.

GAS SYSTEMS. To show that analysis skills can be readily extended we deal with gas systems as a final topic. Non-reacting and reacting batch systems are re-examined with the compressibility term retained in the energy equation. Constitutive equations are introduced for the ideal gas and several non-ideal gases and the compressibility chart and mixing rules are introduced.

MATHEMATICS. At appropriate times we cover numerical methods for solving algebraic equations, and, towards the end of the course, analytical solution of linear, non-homogeneous differential equations with constant coefficients and elementary numerical solution of nonlinear differential equations.

Student response to the course has been excellent. We feel, with some pride, that this is at least in part a reflection of the course content and organization, particularly chemical engineering courses seem to the student to be a natural outgrowth of the analysis course. There is another factor, however, which helps considerably. The student is continually referred back to relevant sections of his calculus and chemistry texts, developing, in his eyes, a logical continuity between his basic science courses and creative engineering. Physical chemistry laboratory experiments are often discussed in our classroom. This blending is in stark contrast to the nearly total discontinuity which existed under the old program.

Colleagues unfamiliar with the details and student performance often express concern over the level of material and wonder whether sophomores can really handle it. Our emphatic "yes" supported by formal AIChE student chapter and Student Government Association evaluations, is most easily justified by a related fact. Last year we introduced a course for non-majors based on our first semester course. We will discuss that course in detail at another time, but it is quite similar in content and level to the first semester course for chemical engineering majors. We have had participation from students to biology, chemistry, economics, **home economics,** and **secondary education,** among others, some of whom have studied no chemistry. Registration went from eight in the first year to thirty-two in the second, and the course is recommended now by the chemistry department for its undergraduate majors. The students rated the course 4.7 out of a possible 5.0 in the SGA evaluation. It is clear from the performance of the non-engineers that our engineering procedures for problem solving are appreciated by a much larger portion of the student body than we originally anticipated. When the concepts can be grasped by non-majors, it is evident that the material belongs at the sophomore level in a Chemical Engineering curriculum.