DIGITAL SIMULATION

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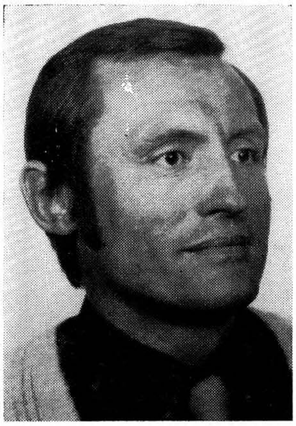
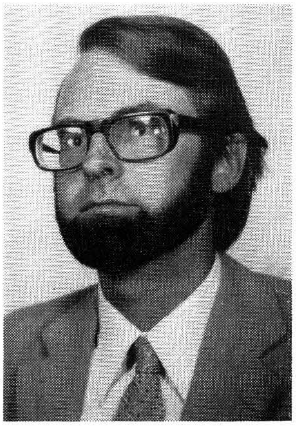
CONVENTIONAL CHEMICAL engineering laboratory courses are often found to be unsatisfactory owing to their routine, predictable nature and lack of challenge. The normal steady state approach can cause difficulties when one is confronted with real-life variable operating conditions. At present, there is a growing realization of the importance of process dynamics, even at the preliminary design stage, in order to optimize design and to implement optimal control strategies. This interest is reflected by the rapidly increasing number of new texts dealing with the mathematical modelling, simulation and control of chemical plants [1-5]. This growing interest in the dynamic state should, we consider, be reflected by a changed emphasis in the method of teaching chemical engineering. Today at least one recent text is available in which unsteady state formulations are used at the onset to introduce students to chemical engineering analysis [6]. Based on the concept that "simulation makes you think" the present course has been developed to bring process dynamics (via the use of mathematical modelling and digital simulation programming) into the chemical engineering laboratory.

In developing the laboratory course, we were motivated by the conviction that the best way to understand the physical processes is through the use of dynamic modelling techniques. Often transient processes are more easily visualized than the steady state. Perhaps it is a matter of daily ex-





Jiri E. Prenosil was educated at the Prague Institute of Chemical Technology and received his Ph.D. degree in Chemical Engineering from the Czechoslovak Academy of Science. He has four years teaching experience at the University of Baghdad and since 1971 he has been at the Chemical Engineering Department of the Federal Institute of Technology, Zurich. His teaching and research interests are in the fundamentals of mixing and diffusion. (left)

John Ingham was educated at the University of Leeds (B.Sc. 1957) and received his Ph.D. degree at the University of Bradford (1970). After several years spent in industry he is presently lecturer in chemical engineering at Bradford where his present research interests lie in the hydrodynamics of solvent extraction columns and computer simulation. This paper was prepared during a one year leave of absence from Bradford spent at the ETH Zurich (1971-72). (center)

Irving J. Dunn studied chemical engineering at the University of Washington in Seattle (B.S. degree, 1960) and at Princeton University (Ph.D., 1963). After periods spent at the Physical Chemistry Institute in Munich, the University of Idaho, and Robert College (now Bosphorus University), Istanbul, Turkey. Dr. Dunn is now at the ETH, Zurich. Present interests lie within the development of research programs in biochemical engineering. Current research includes oxygen transfer in fermenters, tubular loop fermenter design, on-line computer use and the control of biological sewage treatment systems. (right) perience which allows the student to understand the physical meaning of the rates of accumulation of mass and energy within a system rather easily. Steady state conditions can then be presented as a special case in which input rates exactly balance output rates.

Probably the main reason for avoiding the study of dynamics in the past has been the difficulty in solving the mathematics. Students are easily discouraged and distracted from basic modelling processes when confronted by apparently complicated sets of simultaneous differential equations. The use of a digital simulation programming language can be employed to great advantage in these cases, even when an analytical solution is available. Writing the governing differential equations requires a detailed mathematical description for such component in the process. A clear understanding is necessary and the physical interrelationship and simultaneous nature of the equations must be fully realized. The mathematical model and its derived information flow diagram both contribute to a clearer qualitative picture of the process, as well as providing a means to eventual solution. Our experience has shown that students rapidly obtain a confidence in their mathematical ability and an enjoyment in the description of complex systems, with an increased understanding of the processes actually involved. The lack of formalism in the simulation programming, as compared to conventional computer programming, brings the students into an easy and confident relationship with the computer at a very early stage of development, since the programming is greatly simplified. Thus the student can concentrate on understanding the problem and translating his knowledge into appropriate mathematical terms.

DYNAMIC SIMULATION

THE CHEMICAL ENGINEERING program at the Swiss Federal Institute of Technology (ETH) has undergone considerable development within the last five years [7]. Students receive instruction in unit processes together with chemical reaction engineering, fluid mechanics, process control and process design and planning. A variety of laboratory courses, totalling approximately ten hours per week during one and a half years introduce the students to practical work in the fields of separation techniques, fluid flow, heterogeneous catalysis, heat transfer, measurement methods, chemical reaction engineering and process dynamics. The final eighth half year is devoted to a full-time independent three-month research or design project.

The laboratory course, of which the simulation experiments make up a part, is taken during the first half of the fourth and final year. The students have previously been exposed to the general concepts of transient heat and mass balancing problems, but may have difficulties when confronted by real physical situations, requiring a mathematical description in dynamic terms, although about one quarter of the students take a previous elective course dealing with modelling and simulation. The total time allocated, ten hours per week for a period of four weeks for each experiment includes all aspects of the work: preparation, experiment, computation, interpretation and report writing.

Based on the concept that "simulation makes you think", the present course has been developed to bring process dynamics (via the use of mathematical modelling and digital simulation programming) into the ChE lab.

The students receive a written outline of the experiment, together with references to the underlying theory which is discussed with an instructor. The work is then carried out more or less independently, with only occasional consultation required.

Although few aspects of the experimental equipment as described in the next section and the methods of process analysis are really new, the construction of appropriate mathematical models for real processes and the manipulation of the models on large scale computers represent a new phase in the development of chemical engineering laboratory courses.

The increased educational value is apparent when compared with the conventional steady state approach, as shown in Figure 1. The tasks involved tend to be very routine and with little active thought on the part of the student. On the other hand, the simulation of the dynamic experiments forces a positive interaction between the development of the mathematical model and the experiment. Moreover, the experimental results have their theoretical counterpart which can be used for the instantaneous control of both experiment and model. This is illustrated in Figure 2.

The task of obtaining a solution is very significant in the learning process. All parameters must be defined and any forgotten parameter will be clearly indicated by the computer. The need to define initial conditions forces the student to consider the nature of the physical situation. Any error in any of the parameters will usually lead to results which are physically unreasonable; again forcing the student to analyse the problem with care. Thus, the success of the computer simulation provides a check on the mathematical model. Agreement between experiment and theory greatly improves the students' confidence and ability.

Discussion often arises regarding the correct choice of the factors to be included in the model. These questions often lead to further experiments in order to confirm the assumptions concerning the actual physical situation. Simplifying assumptions in the model may also be suggested.

Although the students have only moderate prior computer experience, they generally have little difficulty in using the MIMIC digital simulation programming language. Thus the step from mathematical model to the numerical solution proceeds with little effort, leaving the students free to concentrate on understanding the nature of the physical system, formulating this into mathematical terms, and determining appropriate numerical parameters. We have found the use of the simulation language to be a significant teaching aid, contributing greatly to student motivation and interest.

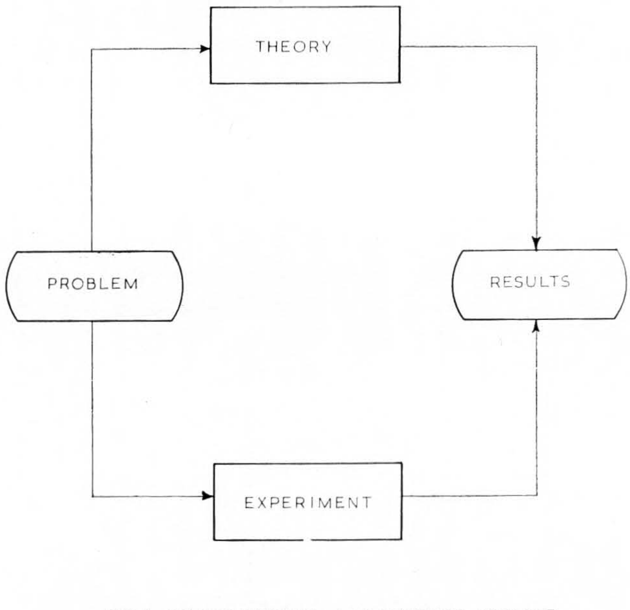


FIG. I CONVENTIONAL LABORATORY COURSE

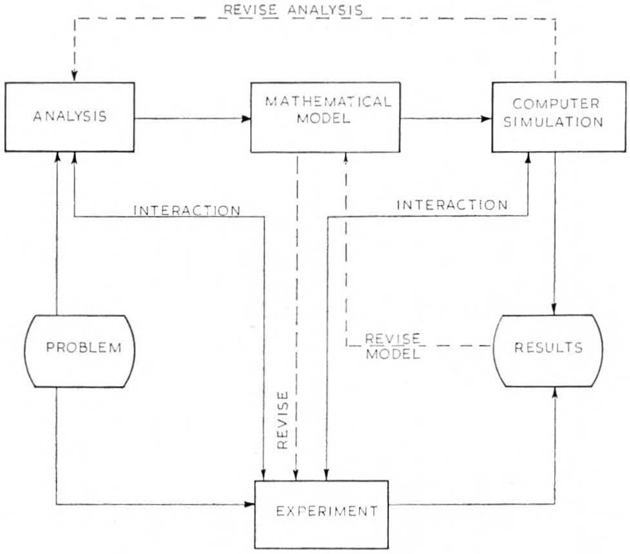


FIG. 2. SIMULATION LABORATORY COURSE

THE EXPERIMENTS

A SERIES OF SIX experiments are presently employed. These involve the study of the dynamic response characteristics of:—

- **a cascade of stirred tank reactors,**
- **a tubular chemical reactor,**
- **a liquid level control system,**
- **a batch distillation,**
- **the transient heating and cooling of a batch reactor vessel and contents,**
- **the control of a continuous stirred tank heating system.**

All have the characteristics of requiring a minimum of expensive apparatus, being easy to carry out experimentally, being easy to model and to simulate on the computer and providing insight into ChE fundamental processes.

EXAMPLE: TRANSIENT HEATING

THE APPARATUS IS shown in Figure 3. A 400 litre capacity stainless steel stirred pressure vessel is heated with steam, using an external jacket. Cooling is provided by an internal water-cooled coil. Temperatures are recorded continuously as a function of time for the tank contents, and for the inlet and outlet cooling water. The steam jacket pressure is measured and also the flow of cooling water. The students are required to measure the dynamics of heating and cooling the tank contents. Starting at ambient conditions, the tank is heated to the maximum temperature

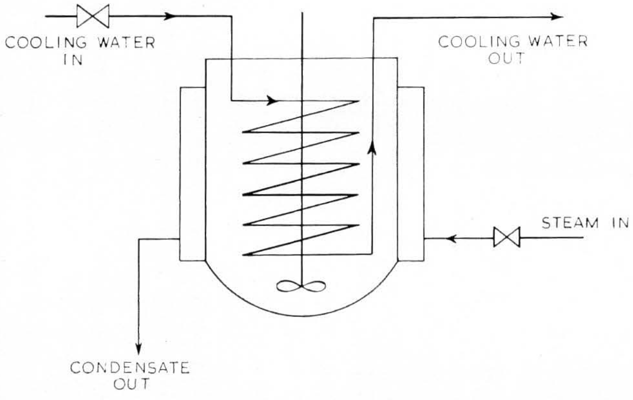


FIG. 3. TRANSIENT HEATING OF A REACTOR VESSEL

provided by the low pressure steam supply. From this stage, the system is cooled to cooling water temperature. A steady state heat balance is made by comparing the heat supplied by the steam to the heat removed in the cooling water.

A heat balance on the well mixed vessel contents is as follows:—

$$M_w C_w \frac{dT_w}{dt} = Q_w$$

Allowing for the rate of accumulation of heat in the thick vessel walls

$$M_m C_m \frac{dT_m}{dt} = Q_s - Q_w$$

The heat transfer relations determine the heat quantities

$$Q_w = U_w A_w (T_m - T_w)$$

$$Q_s = U_s A_s (T_s - T_m)$$

The steam temperature depends on the steam pressure (saturated steam). The steam pressure depends on the mass of steam in the jacket, the jacket volume, and the jacket temperature. Thus a mass balance is required for the steam jacket.

$$\frac{dM_s}{dt} = F_s - Q_s/\Delta H$$

The term $(Q_s/\Delta H)$ is the condensate rate, and F_s is the inlet mass flow rate given by the relation

$$F_s = K\, A_v \sqrt{P_o - P_s}$$

where

$$P_s = \frac{M_s R T_s}{V}$$

and

$$T_s = f_{eq}(P_s)$$

Determining the steam pressure involves an algebraic loop between the data in steam tables and the ideal gas law, as shown in the information flow diagram Figure 4.

CONCLUSIONS

A ChE laboratory course based on the modelling and computer simulation of dynamic experimental conditions has been found to have many advantages over the conventional steady state approach in terms of increased interest and motivation on the part of the student. The use of a digital simulation language forms a considerable aid to the learning process in addition to providing a

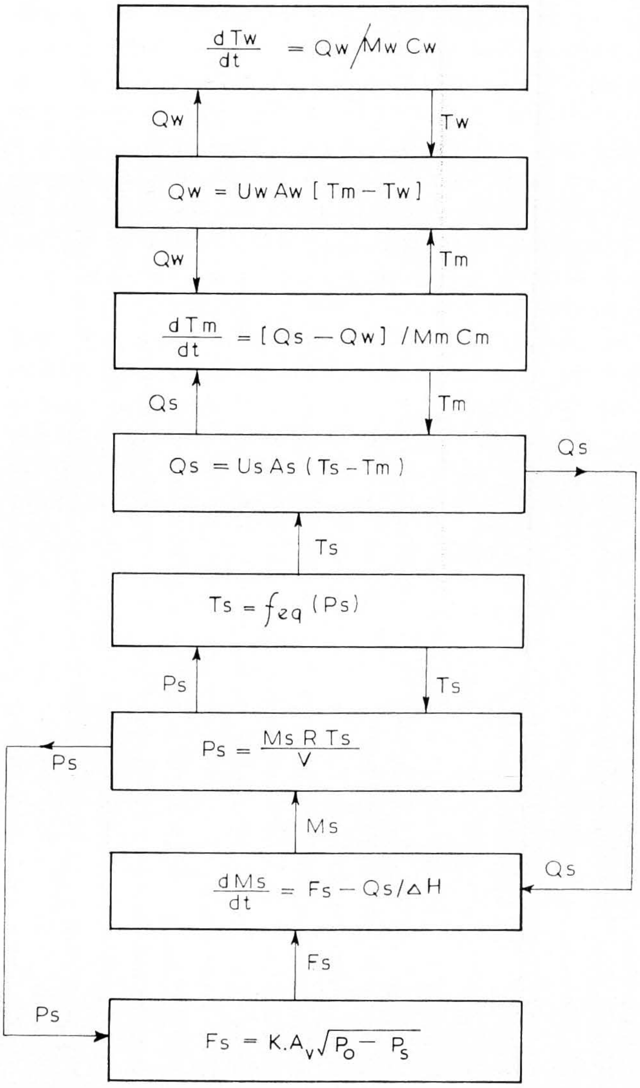


FIG. 4. INFORMATION FLOW DIAGRAM

simple and direct means of solving quite complex problems leaving the student free to concentrate on the actual physical nature of the system. □

ACKNOWLEDGEMENTS

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NOMENCLATURE

A_w	Heat transfer area on water side	L^2
A_s	Heat transfer area on steam side	L^2
A_v	Valve fractional opening	
C_w	Heat capacity of water	$L^2T^{-1}\theta^{-1}$
C_m	Heat capacity of metal	$L^2T^{-1}\theta^{-1}$
F_s	Flow rate of steam	MT^{-1}
ΔH	Latent heat of vapourization	L^2T^{-2}
K	Valve coefficient	LT
M_w	Mass of water in vessel	M
M_m	Mass of metal in jacket wall	M
M_s	Mass of steam in jacket	M
P_o	Pressure of steam source	$ML^{-1}T^{-2}$
P_s	Pressure of steam in jacket	$ML^{-1}T^{-2}$
Q_s	Heat transfer rate from steam	ML^2T^{-3}
Q_w	Heat transfer rate at water side	ML^2T^{-3}
R	Gas constant	$ML^2T^{-2}\theta^{-1}$
T_m	Temperature of metal wall	θ
T_s	Temperature of steam	θ
T_w	Water temperature	θ
U_w	Heat transfer coefficient on water side	$MT^{-3}\theta^{-1}$
U_s	Heat transfer coefficient on steam side	$MT^{-3}\theta^{-1}$
V	Steam jacket volume	L^3

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BOOK REVIEWS

Continued from page 5.

A chapter on power consumption of mixing impellers reviews some of the theory, gives guidance on measuring power on small scale equipment and then extensively covers the prediction of power consumption for various impellers in large scale equipment both for baffled and unbaffled vessels and Newtonian and non-Newtonian fluids.

In the chapter on heat transfer some modifications to common correlations are presented, including additional geometric parameters. These new forms correlate well the published data for turbulent heat transfer which had previously been correlated with equations having differing exponents. Heat transfer from viscous fluids using anchor or helical ribbon impellers is well covered.

Three chapters deal with flow modeling theory, as well as data for calculating mixing times, and circulation rates continuing the balance between theory and practical design information.

Four chapters are devoted to nonhomogeneous agitation operations: solid-liquid, immissible liquid contacting, and gas-liquid processing. Quantitative information is presented, but the correlations are not as well defined and substantiated as those for power and heat transfer.

A final chapter is called "Applications" which is a qualitative overview of the whole subject of mixing. This chapter is a good summary for developing an understanding of the field of mixing, but is void of any quanitative design information.

While I highly recommend this book, it does have limitations, some of which are acknowledged by the author. For a book titled "Mixing" there is no real discussion of pipeline or static mixing techniques, which is presently one of the most active areas of mixing interest. Mixing of very high viscosity materials, greater than about 1000 poise, is also excluded. Lists of nomenclature are found at the end of each chapter, but they are not all inclusive, and symbols and units are a source of confusion throughout the book. Some of the text reads a little rough, which may be due to translation from Japanese. For those looking for accurate design and scale-up methods for all mixing equipment the book will not completely satisfy the need. Mixing operations are very dependent on geometry of the particular system which makes generalizations difficult. There remains a need for considerable judgment among existing methods and techniques. This book can provide a good source from which to exercise that judgment.