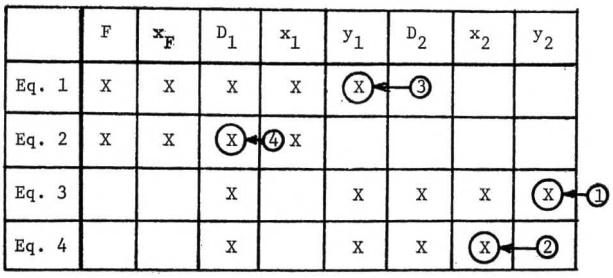

Fig. 2. Structural Array Matrix of the Example

variable and delete Eq. 3 and y_2 from the matrix. This enables us to assign the 7th column (x_2) to Eq. 4 and delete these, and so on.

Assigning a variable to an equation as its output variable means that this equation is solved for the variable. If a variable appears only in one equation, this variable must either by solved from the equation or be given as design variable. We prefer to assign such a variable as an output variable to simplify the information flow structure. Fortunately for our example, we could eliminate all of the equations in the following order.

1st—Assign y_2 to Eq. 3, and delete them
2nd—Assign x_2 to Eq. 4, and delete them
3rd—Assign y_1 to Eq. 1, and delete them
4th—Assign D_1 to Eq. 2, and delete them

When alternate choices of output variable assignment are available, we can incorporate our judgment into the procedure. For example, for the last assignment above, we have assigned D_1 to Eq. 1. However, we could have assigned x_1 to Eq. 1. The reason that we have selected D_1 over x_1 is that it is easier to solve Eq. 1 for D_1 than for x_1. For instance, Eq. 1 can be explicitly expressed for D_1, whereas not for x_1. In digital computers, this means straight computation for D_1 vs. iterative calculation for x_1. This argument has been generalized, which resulted in the concept of **difficulty scores**[3] to account for relative difficulty of solving an equation for a variable.

Step 3: By definition, the variables not assigned yet are design variables, and the order of computation is the reverse order of the elimination in Step 2.

For our example, this technique has found one of the acyclic structure, and hence these equations can be solved one by one in the following order. Assume values of x_F, F, x_1, and D_2 (these are design variables). This will enable us to solve the equations in the following order:

1st—Eq. 2 is solved for D_1 and substitute this value to other equations.
2nd—Eq. 1 is solved for y_1, and substitutions.
3rd—Eq. 2 is solved for x_2, and substitutions.
4th—Eq. 3 is solved for y_2

CONCLUSION

The method of design variable selection has been illustrated with a simple example. Experiences show that this technique is very useful for the analysis of complex systems of equations either in teaching or in industrial research.[4]

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ChE book reviews

Process Analysis and Simulation: Deterministic Systems
D. M. Himmelblau and K. B. Bischoff;
John Wiley and Sons (1968), 348pp.

I wish to mention two points before attempting a review of this excellent book. First, I have not used this book as text in a classroom situation. A review of a textbook without classroom testing is akin to a monk commenting on marriage and should perhaps be discounted fifty cents on the dollar. Second, and somewhat as a result of the first point, I shall adopt a broad and general, rather than detailed and specific, point of view in phrasing my comments. The risk associated with the latter point of view is that of being in error while the former point of view risks saying nothing at all.

This text is divided into three parts plus an introduction discussing the author's overall philosophy of process analysis. Part I discusses and tabulates the mathematical models which are often used in the simulation of physical systems and processes. Chapter 2 of Part I is essentially a resume of the equations of change for mass momentum and energy as formally taught in transport phenomena. A clear distinction is made between the molecular, microscopic (continuum) and macroscopic points of view, although some of this excellent philosophy may be unappreciated by the student who has not completed a formal

course in transport phenomena. Chapter 3 in Part I further discusses an heirarchy in the classification of mathematical models arising from transport phenomena. Thus, the groupings of deterministic vs probabilistic, linear vs nonlinear, steady state vs transient, and lumped parameter vs distributed parameter are discussed. Some illustrative problems are discussed, but this chapter remains essentially an amplification of the philosophy of mathematical model building. Again, this excellent discourse on the philosophy of model structure might well be lost on students who have not had formal courses in transport phenomena and process dynamics. Chapter 4, population balance models, completes Part I. Obviously, this area is the author's forte, and they devote considerable attention to the formalism of description and prediction of residence-time distributions in flow systems. The strength of this chapter is that the population balance-derived equations are laid out for comparison with the transport equations of Chapter 2; the weakness of this chapter is the emphasis on residence-time distributions at the expense of the concept of particle phase space. This latter concept emphasizes the link of population balance equations with the transport equations in the complete description of particulate processes.

Part II commences the "nuts-and-bolts" techniques of process analysis. Students who have completed a first-year graduate transport course together with an undergraduate process control background could start with Part II of this book with perhaps some additional time spent in review of Chapter 4. Part II is introduced by Chapter 5, which chapter presents many of the mathematical techniques appropriate to the process models previously discussed. Again, Chapter 5 is prefaced by an excellent philosophical discussion of the strategy of mathematical techniques as they operate on such process models. Discussed are the techniques of solution of differential equations, analytically and numerically, dynamic response to impulse and step inputs, frequency response and stability. Thus, the techniques of process dynamics are linked with the model equations arising from transport phenomena and population balances. The emphasis of this section is on the simplistic response equations of process dynamics rather than the detailed gradient analysis found in transport texts. The techniques of dimensional analysis, not deserving of an entire chapter, are included at the end of Chapter 5. Chapters 6 and 7 complete Part II. Chapter 6 illustrates the application of population balance-derived models to the study of reactors, including the problem of crystal size distribution analysis in an ideal backmixed single stage crystallizer (reactor). Chapter 7 illustrates the techniques of solution for typical subsystem models arising from transport-based models. The strength of this section is that an heirarchy of simplifying assumptions is used in the formulation of these models and the results are in turn compared to experimental data. The successful trade-off between rigor and simplicity in modeling processes is perhaps the key to this art and the techniques are well illustrated here.

Part III is potentially the most important section of this book in that it attempts to integrate all of the detail presented to this point, models and techniques of analysis, into detailed studies of complete systems. The techniques of decomposition of large-scale systems for a rational attack on the problem of calculating the entire system are demonstrated in Chapter 8. This chapter introduces the subjects of graph theory and their related Boolean matrices; such tools are essential to the rational decomposition of large-scale systems. The techniques of signal flow graphs and sensitivity analysis are also introduced in this chapter. Chapter 9 concludes Part III and the book with specific applications and examples of total systems analysis. The subject of systems analysis is very difficult to teach except by case history and detailed example. Fortunately, Part III is replete with complex and detailed examples, graphically presented, and should present a constructive challenge to the motivated teacher. It is this writer's pessimistic opinion that in a classroom situation, the material in Parts I and II will be emphasized at the expense of Part III. Intentions and motives will be pure, but lack of time and the difficulty of teaching such integrated material will prevail. This is a criticism of academia, not of this text.

It is this writer's opinion that the ideal situation for this text would be a class of second-year graduate students who have taken a graduate course in transport phenomena and have at least an undergraduate background in process control. The issue is not intellectual difficulty of the material, but rather the wide range of ideas and techniques that the integrated into the content of this text. Successful teaching of such integrated material and the meaningful assimilation of the

propounded philosophies of model building requires a certain amount of maturity on the part of the students as well as teacher. The material can certainly be taught in abbreviated form as an undergraduate senior year elective, as the authors themselves do, but it would require a great deal of judgment and experience as well as enthusiasm on their part. Fortunately, the University of Arizona has a second-year graduate course in the area of process simulation, following first-year courses in transport phenomena and process dynamics and control; this text is quite successfully used in this graduate course. The material in this book is as important, or more so, to the terminating MS candidate as to the PhD student. Three semesters are normally required for such MS students and it should not be difficult to enroll them in the course during their final term.

Finally, this book should be on the shelf of every practicing engineer who is even remotely connected with the art of process simulation or must interact with those who are. Some books, by their language and format, widen the gap between the academic establishment and practicing engineers in industry. This book moves the two groups closer together.

University of Arizona
Alan D. Randolph

LETTERS (cont'd from p. 103)

Consider a gas filling an originally empty tank. If we assume the gas in the tank to be well mixed, the total internal energy of the gas is given, at any instant, by

$$U_{total} = m\,u \qquad [1]$$

where m is the total mass, and u the internal energy per unit mass. The internal energy per unit mass may be expressed in the following manner:

$$u - u_o = \int_{T_o}^{T} \left(\frac{\partial u}{\partial T}\right)_v d\,T = \int_{T_o}^{T} c_v\,d\,T \qquad [2]$$

where T_o is a reference temperature and c_v the heat capacity per unit mass, at constant volume. Then

$$U_{total} = m\left[\,u_o + \int_{T_o}^{T} c_v\,dT\,\right] \qquad [3]$$

Differentiating with respect to time

$$\dot{U}_{total} = \dot{m}\,u + m\,\frac{d}{dt}\int_{T_o}^{T} c_v\,d\,T$$

where

$$\frac{d}{dt}\int_{T_o}^{T} c_v\,d\,T = \left(\frac{d}{dT}\int_{T_o}^{T} c_v\,d\,T\right)\frac{dT}{dt} = c_v(T)\,\frac{dT}{dt}$$

by Leibnitz's rule. Hence we finally obtain

$$\dot{U}_{total} = \dot{m}\,u + m\,c_v(T)\,\frac{dT}{dt} \qquad [4]$$

It is thus incorrect to express U total in the form

$$\dot{U}_{total} = \frac{d}{dt}\left\{\,m\,c_v(T)\,(T-T_o)\,\right\} \qquad [5]$$

as noted by Dr. Davidson. In the case where $c_v \neq c_v\,(T)$, eqs. 4 and 5 are equivalent.

University of Florida
R. J. Gordon

ChE News

CACHE Committee Established by National Academy of Engineering . . . Goal Is to Accelerate Integration of Digital Computation into ChE Education

A panel of chemical engineering educators called the CACHE (Computer Aids for Chemical Engineering Education) Committee has been established by the National Academy of Engineering's Commission on Education. The purpose of the committee is to coordinate and encourage the development of computing systems for use in chemical engineering education. The National Science Foundation has provided a grant to support the activities of the CACHE Committee for a two-year period.

The 17 members of the committee are drawn from universities throughout the United States and Canada. Each member is actively concerned with the use of computers in chemical engineering and many of them have been at the forefront of the rapid developments in chemical engineering computing that have taken place during the past decade.

CACHE officers elected at a recent meeting in Ann Arbor are: W. D. Seider (Pennsylvania), chairman; L. B. Evans (MIT), vice chairman; and A. W. Westerberg (Florida), secretary. Other members of the committee are: B. Carnahan (Michigan), J. H. Christensen (Oklahoma), E. Elzy (Oregon State), E. A. Grens (California at Berkeley), E. J. Henley (Houston), R. R. Hughes (Wisconsin), R. V. Jelinek (Syracuse), A. I. Johnson (McMaster), R. L. Motard (Houston) M. J. Reilly (Carnegie-Mellon), J. D. Seader (Utah), P. T. Shannon (Dartmouth), R. E. C. Weaver (Tulane), and I. Zwiebel (Worcester Polytechnic).

The principal goal of the committee will be to accelerate the integration of digital computation into the chemical engineering curriculum by promoting inter-university cooperation in preparation of new courses, teaching aids, and computing systems.

A major stumbling block to widespread use of the computer in engineering education has been the difficulty in transferring computer programs developed at one institution for use at another. Incompatibilities in computer system conventions, data formats, and documentation have been responsible for duplication of effort at different schools. CACHE has established a Standards Subcommittee to devise mechanisms for facilitating easier inter-university interchange of computer programs.