Complex Chemical Engineering Systems

WOOYOUNG LEE and YUICHI OZAWA
Mobil Research and Development Corp.
Paulsboro, N. J. 08066

The analysis of complex systems described by sets of nonlinear simultaneous equations appears frequently in chemical engineering teaching. The method[1,2] proposed here will simplify the computational procedures and provide students with better insight into the problem.

If a set of m-simultaneous equations contain n variables, we have to assign numerical values to at least (n − m) variables to start the computation; these variables are called **design variables.** The selection of a set of design variables may yield the simplest information flow structures in which no feedback loops are involved. (acyclic flow structure). If no acyclic structure is found by the selection of design variables, at least parts of the system of equations must be solved simultaneously.[1] We will illustrate the method of selecting a set of design variables to obtain an acyclic structure:

Q. The binary mixture of A and B forms an ideal solution which has the relative volatility of α. A batch of this mixture containing x_F of A is charged for a batch distillation. A fraction of the initial charge is distilled and the distillate is again charged to a second still, a fraction of which is distilled. (See Fig. 1.) Write a mathematical model for this operation and derive a solution procedure for the model.

A. The material balance equations and Rayleigh's equations for Fig. 1 are:

1st Distillation:

$$F\, x_F = D_1 y_1 + (F - D_1)\, x_1 \tag{1}$$

$$\left(\frac{F}{F - D_1}\right)^{\alpha-1} = \frac{x_F}{x_1}\left(\frac{1 - x_1}{1 - x_F}\right)^{\alpha} \tag{2}$$

2nd Distillation:

$$D_1 y_1 = D_2 y_2 + (D_1 - D_2)\, x_2 \tag{3}$$

$$\left(\frac{D_1}{D_1 - D_2}\right)^{\alpha-1} = \frac{y_1}{x_2}\left(\frac{1 - x_2}{1 - y_1}\right)^{\alpha} \tag{4}$$

where

F = moles of initial mixture charged
x_F = mole fraction of A in initial mixture
D_i = mole distilled
y_i = mole fraction of A in distillates
x_i = mole fraction of A in bottoms
α = relative volatility

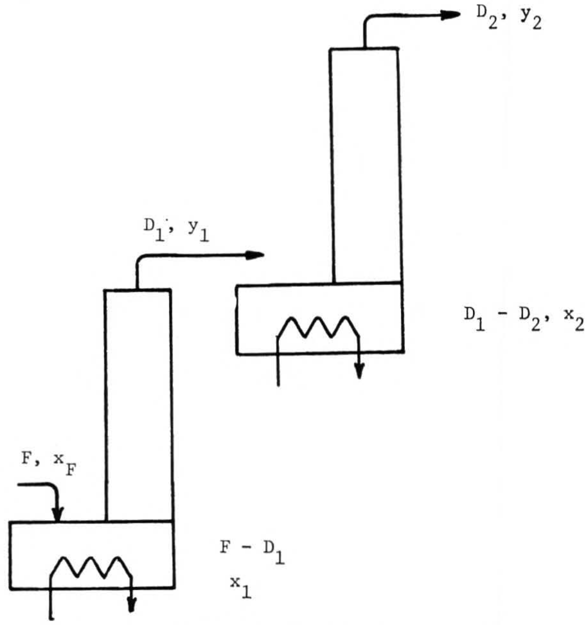

Fig. 1. Two-State Batch Distillation of a Binary Mixture

Notice that we have 4 independent equations and 8 variables; 4 of which must be known to solve the equations for the remaining variables. The step-by-step procedure of the technique[2] is described below.

Step 1: Construct a structural array matrix **of the system as shown in Fig. 2. The rows correspond to equations, and the columns to variables. An X is placed whenever a variable appears in an equation.**

The structural array matrix, compactly revealing the pattern of interconnections of these equations, improves one's insight into the problem considerably. For example, it directly shows which variable appears most frequently in which equations and therefore its relative importance in the system. For systems of large sizes it is extremely useful to employ the structural array representation to systematically analyze their structures.

Step 2: Find a column which has only one X. Assign the variable corresponding to this column to the equation (row) that has this X, and delete this column and row from the matrix. Repeat this procedure of elimination until no further reduction is possible. For example, in Fig. 2, the last column (y_2) has only one X in the third row (Eq. 3); therefore, assign y_2 to Eq. 3 as its **output**

	F	x_F	D_1	x_1	y_1	D_2	x_2	y_2	
Eq. 1	X	X	X	X	(X)←	③			
Eq. 2	X	X	(X)←④	X					
Eq. 3			X		X	X	X	(X)←	①
Eq. 4			X		X	X	(X)←	②	

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]

REFERENCES

1. Lee, W., Christensen, J. H., and Rudd, D. F., **AIChE J. 12**, 1104 (1966).
2. Rudd, D. F. and Watson, C. C., Strategy of Process Engineering, Wiley, 1968, Chapt. 3.
3. Lee, W. and Rudd, D. F., "Design Variable Selection Method and the Concept of Difficulty Scores," to be published.

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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