ChE classroom

A SYSTEMATIC APPROACH TO MODELING

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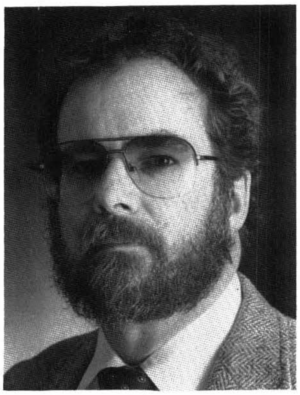
IT IS INTERESTING to note that much of the chemical engineering curriculum is devoted to developing a quantitative description of physico-chemical systems, yet there is little attention given to the subject of modeling. There is usually some discussion of dynamic modeling as an introduction in process control courses, and some departments offer elective courses in process modeling; but, in general, the chemical engineering graduate does not have a good foundation in the fundamentals of modeling. This paper is designed to present a framework for model development that, when used, will help the student (or professor) avoid the major pitfalls associated with modeling: *i.e.*, not properly identifying the controlling factors, lack of model validation, developing a model that is incompatible with its end use, *etc.* A model is defined by *The Random House Dictionary* as

> ***MOD • EL . . . -n. 1. a standard or example for imitation or comparison. 2. a representation, generally in miniature, to show the structure or serve as a copy of something. 3. . . .***



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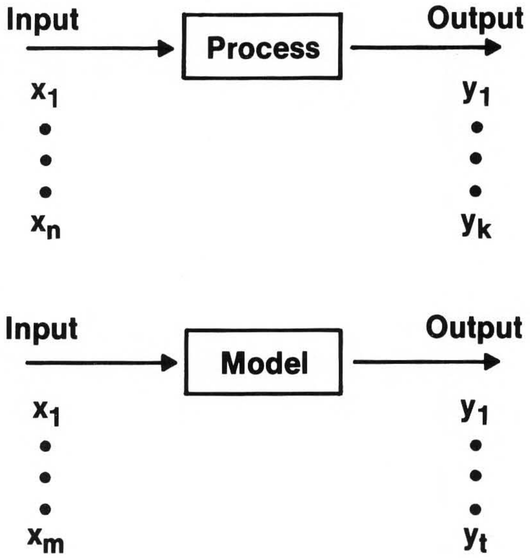

FIGURE 1. Comparison of input/output for a process and its model. Note that n>m and k>t.

With regard to chemical engineering applications, models are used to *approximate* certain characteristics of a process given the input to the process (see Figure 1). Also, remember that a process can range from an entire oil refinery to a single drop falling through a gas. A model can never be a "true" or an exact representation of a process because it would have to be the *same* process, or an exact replica, in order to accomplish that.

A useful model provides reliable information about a process from the operating conditions of the process using a "relatively easy" procedure. Models are used for the following applications:

- **Process control**
- **Process design (scale-up)**
- **Process optimization**

In addition, process models and the development of process models can lead to an overall understanding of the process; *i.e.*, an understanding of the complex interactions within a process.

Models can be categorized into one of the following classes:

- **Empirical models**
- **Scale models**
- **Analog models**
- **Phenomenological models**

An empirical model assumes the form of the functional relationship between the input and output variables of a process. Then, using data from the process, parameters or constants in the functional relationship are determined. The usefulness of an empirical model depends upon a judicious choice for the assumed functional relationship and upon whether the model is to be used outside of the range of data upon which it is based. That is, empirical models are best when used in an interpolative manner, but are dangerously unreliable when used for extrapolation. The application of transfer functions in process control represents a commonly used empirical model.

Scale models are smaller-scale versions of a system which is usually designed to study one factor. Scale models have the same geometric proportions as the full-scale system but on a smaller scale. A classical example is a wind tunnel in which aircraft designers can analyze the drag of a particular aircraft design using a scale version (model) of the aircraft under specific conditions. The conditions used are such that the dimensionless flow equations are the same for both the scale model and the full-scale aircraft. In this manner, a variety of aircraft designs can be analyzed without having to construct and test the full-scale aircraft. Other applications of scale models involve flow modeling and include reservoir modeling, pilot-scale reactors, small-scale distillation columns, *etc.*

When a physical system is used to predict the behavior of the system of interest, it is referred to as an analog model. For example, an electrical circuit can be used as an analog model of a mass-spring-dashpot system. In this analog, an electrical resistor represents the resistance to displacement, an inductor represents the inertia of the mass, and a capacitor represents the storage of potential energy. In this manner, the behavior of the electrical analog can be used to predict the behavior of the mechanical system. This approach is similar to that used by an analog computer in which the solution of sets of linear or nearly linear differential equations is obtained by constructing electrical circuits that are equivalent to the differential equations and then monitoring the time responses of the appropriate voltages and currents.

Phenomenological models apply conservation equations (mass, energy, and momentum) in order to develop relationships between process input and output variables. In order to apply the conservation equations, a number of constitutive relations may be required; *e.g.*, equations of state, chemical and phase equilibrium relationships, and chemical kinetic expressions. Phenomenological models range from microscopic models (distributed parameter models) to macroscopic models (lumped parameter models). Phenomenological models are the most commonly used models by chemical engineers, and the remainder of this discussion is primarily aimed at this approach to modeling.

This paper presents a framework for model development that, when used, will help the student . . . avoid the major pitfalls associated with modeling; *i.e.*, not properly identifying the controlling factors, lack of model validation, developing a model that is incompatible with its end use, . . .

The recommended procedure for model development is

- **Define the problem**
- **Identify the controlling factors**
- **Evaluate the data for the problem**
- **Develop a set of model equations**
- **Implement a solution procedure**
- **Validate the model**

Define the problem. Here you determine what you want to predict from what input data. In addition, you must also determine how the results of the model are to be used.

Identify the controlling factors. In order to accomplish this task, you must develop a physical understanding of how the process works; *i.e.*, what factors control the behavior of the process. This is obviously one of the most important steps in the model development process. It is usually helpful to develop a physical description of how the process operates. Then, by reviewing the physical description, you can identify the controlling factors of the process.

Evaluate the data for the problem. There are two types of data that you must analyze for a modeling problem: parameter data and process data. Parameters such as dispersion coefficients, diffusion coefficients, and thermal conductivities are typically required in the development of models. The uncertainty associated with parameters used by a model should also be estimated because this will have a direct effect upon overall reliability of the model. In some cases, you may be unable to obtain independently measured values for parameters you need. In that case, you must either use a predictive technique for obtaining the parameter or you must use process data for that purpose. When process data is used, you must recognize that you are moving away from a phenomenological model toward an empirical model. Even if you do not use empirically determined parameters, you may need to estimate the uncertainty associated with the process data if it is to be used in the model validation process.

Develop a set of model equations. The first step is to explicitly define the location and type of system boundaries. That is, you must determine what the system you are modeling is and what are its boundaries. Then equations can be developed which describe the key variables within the defined boundaries—these equations are the model equations.

A major problem with developing the model equations is to determine what degree of detail you should include in order to meet your objectives. Usually, the more detail you include the more complicated the model equations become and the more difficult they are to solve. In addition, when more detail is used, more parameters are required. The flow characteristics of the process usually determine the degree of detail required. For example, if a vessel is well mixed, a macroscopic model will usually provide a good approximation of the process. On the other hand, if the vessel is not well mixed, a more detailed model would be required. In cases where the properties of the process change spatially throughout the system, a microscopic model is usually required. There are models that are intermediate to the macroscopic and microscopic models: models based upon plug flow of the fluid or models based upon plug flow with dispersion. In fact, you can consider that there is a continuum of models of the real process ranging from submolecular to macroscopic, depending upon the simplifying assumptions used.

In choosing the degree of detail to use, you will make simplifying assumptions that must be verified during the validation procedure. The simplifying assumptions come from knowledge of the controlling factors and definition of the problem.

Usually, chemical engineering model equations come from the application of material, momentum, and energy balances to the process with some type of simplifying assumptions associated with the flow behavior. In addition, equations of state, chemical and phase equilibrium, and reaction kinetics are at times combined with the material and energy balance equations in the model development process.

Implement the solution procedure. Not only should the numerical solution procedure reliably solve the equations to yield the desired output, but it should do so in accordance with the overall objectives of the problem. For example, if the model is to be used for control purposes, the solution procedure must be fast enough for the control system to respond quickly enough to control the process. Also, the numerical solution procedure must be selected to operate with the storage and software capabilities of the computer that will be used.

Validate the model. You can never completely validate a model since you can only check your model with a finite number of tests. That is, just because your model passes certain tests does not guarantee that it is correct. Therefore, the trick is to devise a set of tests that provides the best chance to identify either logic or application errors within the context of the end-use of the model. Following is a list of approaches that are useful in the search for modeling errors:

- **Verify simplifying assumptions**
- **Check that the general model behavior is in accordance with the process behavior**
- **Develop analytical solutions for simplified cases and compare**
- **Compare with other models using a common problem**
- **Perform a sensitivity analysis to evaluate the effects of parameter uncertainty**
- **Compare the model directly with process data**

Verification of the simplifying assumptions involves checking your assumptions using the results of the model, or perhaps even testing the process to examine the accuracy of the assumptions used to formulate the model equations. For example, if you were to assume that a particular side reaction was insignificant, you should take the results of your model and determine the magnitude of the side reaction throughout the process. If the reaction rate is sufficiently low, your assumption is acceptable. As another example, consider the assumption of plug flow through a reactor. This assumption can be checked by measuring the outlet concentration profile to an injected slug of tracer for the actual process.

The model should also be checked against the general behavior of the process. For example, if the conversion in a reactor increases as the feed rate to the reactor is decreased, the model should show the same behavior.

A very useful means of model validation or debugging is to apply your model to a limiting case for which you can obtain an analytical solution. For example, if you developed a model for the non-isothermal effectiveness factors in a spherical catalyst particle, it could be checked against the analytical solution for an isothermal effectiveness factor for a spherical catalyst particle by simply using the model with the heat of reaction set equal to zero. This validation procedure allows you to check for programming errors and unit conversion errors, as well as the overall physics of your model equations.

Similar to the last approach, you can apply your model to a problem for which another model (well established and verified) can also be applied. For example, if you had developed a two-dimensional model for a fixed bed reactor, you could compare it with results for a one-dimensional model of a fixed bed reactor by making the appropriate modifications to the input data for your model.

Next, you should perform a sensitivity study using your model. That is, you should vary each parameter you used over its range of uncertainty and observe the resulting effect upon the model predictions. It is very important to know if your model is especially sensitive to one or more parameters.

Finally, you should compare your model with process data whenever possible. This is always the best test of any model. Unfortunately, process data may not be available; *e.g.*, the process has not yet been constructed or you may be unable to directly measure all the output variables of the process. In the latter case, you should verify your model with process data that are available.

(The material presented here will appear in An Introduction to Numerical Methods for Chemical Engineers, *by James B. Riggs, which will be published in early 1988.*

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REVIEW: Engineering Education

Continued from page 11.

covers four further volumes which may be of interest to those who were stimulated by the initial report.

Engineering in Society is a thoughtful and interesting overview of the evolution of American engineering and its role in society today. The panelists conclude that the engineering profession has responded well to changing societal demand, although they are less confident that the profession can be sufficiently adaptive to rapid changes in the future. They argue for educational programs that are broad and balanced, rather than highly specialized. They suggest that the faculty shortage could be alleviated by a greater use of educational technology in developing alternative methods of instruction and they ask that engineering students be sensitized to the role of engineering in society.

Continuing Education of Engineers focuses on formal, non-credit education of employed engineers. The panel reviews patterns of continuing education in industry, academic and the professional societies. Professional societies are assuming an increasing role in continuing education. Most universities, preoccupied with undergraduate and graduate education and research, have little interest in continuing education. The panel examines reasons for engineers participating (or not participating) in continuing education. The most startling finding is that while most people consider continuing education a good idea, there is little scientific evidence that it actually benefits the participant. Nevertheless, the panel sees an increasing need for continuing education of engineers as the pace of technological change accelerates.

Engineering Employment Characteristics provides considerable data on the engineering work force and its utilization. It draws no conclusions and makes no recommendations. There are few surprises. The numbers of women and minorities are increasing, although the percentage in the engineering work force is still woefully small. Japan graduates more engineers than the United States, with a substantially smaller population. Many of Japan's engineering graduates enter government service. A statistic of interest to academics is that it takes an engineer who continued to the PhD about 20 years to catch up in total earnings with his classmate who went to work after receiving a BS degree.

Engineering Technology Education is probably of limited interest to chemical engineers because there are only a few associate degree programs in chemical engineering technology and no baccalaureate programs. This brief report reviews the history and current status of engineering technology education and employment. It compares and contrasts engineering and engineering technology, as well as industrial technology and engineering technology. Engineering technology enrollments have not grown as fast as engineering enrollments, so the issues in technology education are not so sharply focused. The doctorate isn't typically required for faculty appointment, and industrial experience is highly valued. Hence there aren't the extreme faculty shortages that exist in some engineering fields. On the other hand, the need for state-of-the-art laboratory equipment may be more pronounced in technology programs. ☐