CHAPTER 2

PROCESS MODELING

2.1 Introduction

This chapter contains a brief introduction to modeling the dynamic behavior of processes. The best model that can reliably represent each real process is developed from the difference proper approach. Thus, many several theories are used and applied to develop the process models of the system, and computational basis approach are also presented.

2.2 Process modeling

A model is nothing more than a mathematical abstraction of a real process. The equation or set of equations that comprise a model are at best an approximation to the true process. Hence, the model cannot incorporate all of the features, both macroscopic and microscopic, of the real process. The engineer normally must seek a compromise involving the cost of obtaining the model, this is, the time and effort required to obtain and verify it. These considerations are related to the level of physical and chemical detail in the model and the expected benefits to be derived from its use. The necessarily model accuracy is intertwined in this compromise and the ultimate use of the model influences how accurate it needs to be.

A dynamic system can be conceptually described as in Figure 2.1. The system is driven by input variables $u(t)$ and disturbances $d(t)$. The $u(t)$ can be controlled but the $d(t)$ cannot be controlled. The output $y(t)$ signals are variables which provide useful information about the system. It depends on input values, disturbance values, and the dynamic behavior of the system or the relation between input, disturbance, and output variables. In chemical processes, the relation between input, disturbance, and output variables is very important in several activities such as predicting the future output $y(t)$ that corresponding with current input $u(t)$ or disturbance $d(t)$, planning and design because it is the basic knowledge for process planning, process optimization, and control system design.

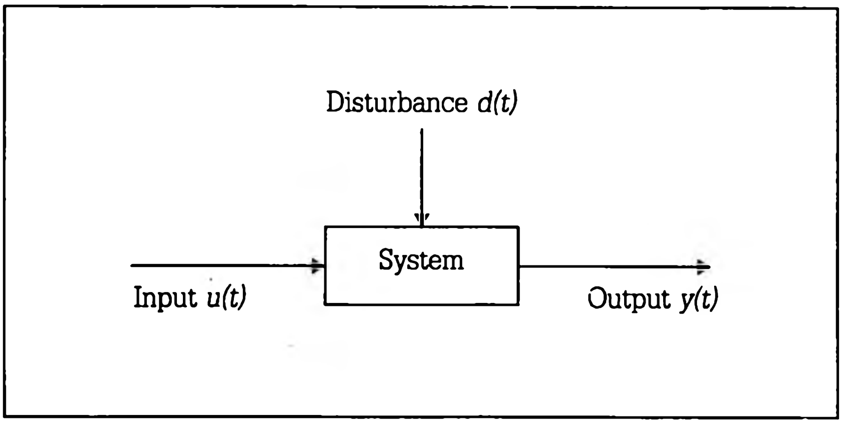

Figure 2.1 A dynamic system with input $u(t)$, output $y(t)$ and disturbance $d(t)$, where t denotes time

The following examples of dynamic systems illustrate the need for mathematical models.

Example 2.1 A stirred tank

Consider the stirred tank shown in Figure 2.2. The reactant concentration in each flow can vary. The flow F_1 and F_2 can be controlled with valves. The signals $F_1(t)$ and $F_2(t)$ are the inputs to the system. The output flow $F(t)$ and the concentration $c(t)$ in the tank constitute the output variables. The input concentration $c_1(t)$ and $c_2(t)$ cannot be controlled and are viewed as disturbances.

Suppose we want to design a regulator which acts on the flow $F_1(t)$ and $F_2(t)$ using the measurements of $F(t)$ and $c(t)$. The purpose of the regulator is to ensure that $F(t)$ and $c(t)$ remain as constant is possible even if the concentrations $c_1(t)$ and $c_2(t)$ vary considerably. For such a design we need some form of mathematical model which describes how the input, the output and the disturbances are related.

$$c(t) = \text{function}(F_1, F_2, c_1, c_2) \quad (2.1)$$

$$F(t) = \text{function}(F_1, F_2, c_1, c_2) \quad (2.2)$$

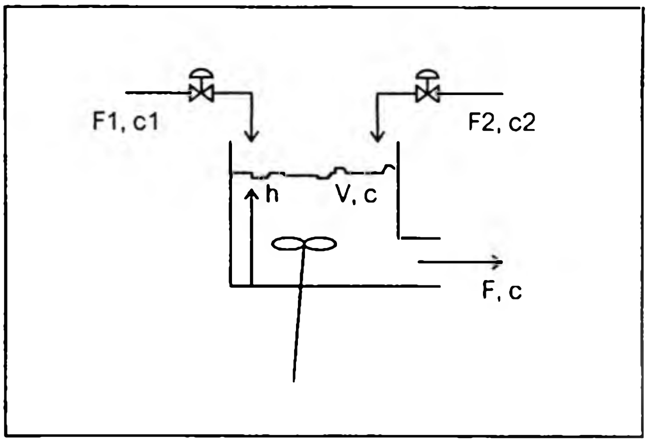

Figure 2.2 A stirred tank

In many cases, the primary aim of modeling is to aid in design. In other cases the knowledge of a model can itself be the purpose, as for if the models can explain measured data satisfactorily, they might also be used to explain and understand the observed phenomena. In more general sense, modeling is used in many branches of science as an aid to describe and understand reality. Also in such a case the purpose of modeling is to gain insight into and knowledge of the dynamic behavior of the system, an example is a large space structure, where the dynamic behavior cannot be deduced by studying structure on earth, because of gravitational and atmospheric effects. For examples like this, the modeling must be based on theory and priori knowledge, since experimental data are not available.

Mathematical models can be helpful in process analysis and control in the following ways :

1. To improve understanding of process.

   Process models can be analyzed or used in a computer simulation of the process to investigate process behavior without the expense and, perhaps, without the unexpected hazards of operating the real process. This approach is necessary when it is not feasible to perform dynamic experiments in the plant or before the plant is actually constructed.

2. To train plant operating personal

   Plant operators can be trained to operate a complex process and to deal with emergency situations by use of a process simulator. By interfacing a process simulator to standard process control equipment, a realistic environment can be created for operator training without the cost or exposure to dangerous conditions that might exist in a real plant situation.

3. To design the control strategy and select controller setting for a new process or new system

   A process model allows alternative control strategies to be evaluated, for example, the section of the variables that are to be measured(controlled) and those that are to be manipulated. Moreover, a dynamic model of the process may be used to develop appropriate controller settings, either via computer simulation or by direct analysis of the dynamic model. Prior to start-up of a new process it is desirable to have reasonable estimates of the controller settings. For some operating processes it may not be feasible to perform experiments that would lead to better controller setting

4. To design control law.

   Advance control techniques use the process model as base of control law. Such techniques are called model-based control or model-predictive control.

5. To optimize process operating conditions.

   In most processing plants there is an incentive to adjust operating conditions periodically so that the plant maximizes profits or minimizes costs. For example, blending operations for production of gasoline, fuel oil, and jet fuel in a refinery need to be modified in response to changes in the physical properties of the crude oil feed-stock, market conditions, and product inventory capacity. A steady-state model of the process and appropriate economic information can be used to determine the most profitable process condition, as in supervision control.

2.2.1 Types of model

The models of dynamic systems can be of many kinds, including the following :

1. Mental, intuitive or verbal model. For example, this is the form of model we use when driving a car (turning the wheel causes the car to turn, pushing the brake decreases the speed, etc.)
2. Graphs and tables. In some application, the models of systems are presented in graphical and tubular forms. For example, a bode plot of a servo system is a typical example of a model in a graphical form. The step responses, i.e. the output of a process excited with a step as input, is another type of model in graphical form.
3. Mathematical models, a mathematical equation or a set of mathematical equations that can represent the relation between input and output of the system. Although graphs may also be regarded as mathematical models. Mathematical models of dynamic systems are useful in many areas and applications. Mathematical models are useful because they are very well suited to the analysis, prediction and design of dynamic systems. They can provide a description of a physical phenomenon or a process, and can be used as a tool for the design of a regular or a filter.

The mathematical model can be typed into two types as follow

1. Empirical model or system identification.

   System identification is the field of modeling dynamic system from experimental data or plant data. This is an experimental approach. Some experiments are performed on the system, a model is then fitted to the recorded data by assigning suitable numerical values to its parameters.
2. Theoretical model.

   This is an analytic approach. Basic laws from physics, chemistry, or thermodynamic (such as Newton' s laws, material and energy balance equations, reaction rate equations) are used to describe the dynamic behavior of a phenomenon or a process.

A comparison can be made of these two modeling approaches : theoretical model and system identification. In many cases the processes are so complex that they are not possible to obtain reasonable models using only physical insight (using first principles e.g. balance equations). In such cases one is forced to use identification techniques. It often happens that a model based on physical insight contains a number of unknown parameters even if the structure is derived from physical laws. Identification methods can be applied to estimate the unknown parameters. The models obtained by system identification have the following properties, in contrast to models based solely on theoretical model:

- The system identification approach have limited validity. The models are valid for a certain working point such as: a certain type of input, a certain process, a certain parameter or constant parameter of process, and etc.
- The system identification models give little physical insight, become in most cases the parameters of the model have no direct physical meaning. The parameters are used only as tools to give a good description of the system' s overall behavior or macro behavior.
- The system identification models are relatively easy to construct and use.

Identification is not a foolproof methodology that can be used without the interaction from the user. The reasons for this include :

- An appropriate model structure must be found. This can be difficult problem, in particular if complex process and the dynamics of the system nonlinear.
- There are certainly no perfect data in real life. The fact that the recorded data are disturbed by noise must be taken into consideration.
- The process may vary with the time, which can cause problems if an attempt is made to describe it with a time-invariant model.
- It may be difficult or impossible to measure some variables or signals that are of central importance for the model.

Mathematical models of the dynamic systems can be classified in various ways. The ways of classification dynamic models include the following:

1. Single input, single output (SISO) models-multivariable (MIMO) models, the type of model that is classified by using a number of input and output variables. SISO models refer to processes where a description is given of the influence of one input on one output. When more variables are involved a multivariable model results. All of these models, MISO, SIMO, and MIMO are the multivariable models. It should be noted that multi input, single output (MISO) models or single input, multi output (SIMO) models are in most cases as easy to derive as SISO models. The MIMO models are more difficult to determine than SISO models.
2. Linear models-nonlinear models. A model is linear if the output depends linearly on the input and possible disturbances ; otherwise it is nonlinear.
3. Parametric models-nonparametric models, the type of model that is classified by using the characteristic of parameters of models. A parametric model is described by set of parameters.
4. Time invariant models-time varying models. Time invariant models are certainly the more common. For time varying models special identification methods are needed. In such cases where a model has parameters that change with time, one often speaks about tracking or real-time identification when estimating the parameters.
5. Time domain models-frequency domain models. Typical examples of time domain models are differential and difference equations, while a spectral density and a bode plot are examples of frequency domain models.
6. Discrete time models-continuous time models. A discrete time model describes the relation between inputs and outputs at discrete time points. It will be assumed that these points are equidistant and the time between two points will be used as time unit. Continuous time models or analog models, the models which are based on analogies between processes in

different areas. For example, a mechanical and electrical oscillator can be describe by the same second-order linear differential equation, but the coefficients will have different physical interpretation. Analog computers are based on such principles : differential equations constituting a model of some system are solved by using an analog equivalent of electrical network. The voltages at various points in this network are recorded as functions of time and give the solution to the differential equations.

7. Lumped models-distributed parameter models. Lumped models are described by or based on a finite number of ordinary differential or difference equations. If the number of equations is infinite or the model is based on partial differential equations, then it is called a distributed parameter model.
8. Deterministic models-stochastic models. For a deterministic model the output can be exactly calculated as soon as the input signal is known. In contrast, a stochastic model contains random terms that make such an exact calculation impossible. The random terms can be seen as description of disturbances.

Model can be classified in other ways. For example :

- Physical models, which are mostly laboratory-scale units that have the same essential characteristics as the (full-scale) processes they model.
- Theoretical models developed using the principles of chemistry and physics.
- Empirical models obtained from a mathematical (statistical) analysis of process operating data.
- Semiempirical models that are a compromise between theoretical models and empirical models, with one or more parameters to be evaluated from plant data.

In the last classification, certain theoretical model parameters such as reaction rate coefficients, heat transfer coefficients, and similar fundamental relations usually must be evaluated from physical experiments or from process operating data. Such semiempirical models do have several inherent advantages. They often can be extrapolated over a wider range of operating conditions than purely empirical models which are usually accurate over a very limited range. Semiemprical models also provide the capability to infer how unmeasured or numerable process variables vary as the process operating condition change.

2.3 General modeling principles

Mathematical models of chemical processes invariably consist of one or more differential equations (ordinary differential equations(ODE) and/or partial differential equations (PDE)) often combined with one or more algebraic relation. The dynamic model can be obtained from the application of unsteady-state conservation relations, usually material and energy balances. Force-momentum balances are employed less often. For process with transport systems, such balances should be considered. Algebraic equations in process model can arise from thermodynamic and transport relations. For example, heat transfer coefficient may be a function of fluid velocity (flow rate) equation. The basic equations that are usually involved in the mathematical models are:
The fundamental law for mass conservation that can be written as

[rate of mass accumulation] = [rate of mass in]-[rate of mass out] (2.3)

If the reactions occur in processes, a mass conservation equations can be written as

[rate of mass accumulation] = [rate of mass in]-[rate of mass out]+
[rate of mass generation] (2.4)

The rate of mass generations usually derive from reaction rate equations.

[rate of reaction] = Function(K, concentration of reactants and/or products) (2.5)

For simple example:

$$[\text{rate of reaction}] = K[\text{Reactant}_1]^n[\text{Reactant}_2]^m \qquad (2.6)$$

The general law for energy conservation that can be written as

[rate of energy accumulation] = [rate of energy in by flow or convection]-
[rate of energy out by flow or convection]+
[net rate of heat addition to system] (2.7)

2.4 Degrees of freedom in modeling

To use a mathematical model for process simulation, must ensure that the model equations provide a unique relation among all inputs and outputs. This requirement is analogous to the requirement for a set of linear algebraic equations to have a unique solution, which is that the number of variables must equal the number of independent equations. It is easy to make a similar evaluation for a large, complicated steady-state or dynamic model. However, for such a system of equations to have a unique solution, the number of unknown variables must equal the number of independent model equations. An equivalent way of stating this condition is to require that the degree of freedom be zero, that is

$$N_F = N_V - N_E = 0 \qquad (2.8)$$

Where

N_F = the degrees of freedom

N_V = the total number of variables (unspecified inputs plus outputs)

N_E = the number of independent equations

Hence, a degree of freedom analysis separates modeling problems into three categories.

1. $N_F = 0$: exactly determined process. If $N_F = 0$, then the number of equations is equal to the number of process variables and the set of equations has a unique solution.

2. $N_F > 0$: underdetermined process. For $N_F > 0$, then $N_V > N_E$, so there are more process variables than equations. Consequently, the N_E equations have an infinite number of solutions since N_F process variables can be specified arbitrarily.
3. $N_F < 0$: overdetermined process. For $N_F < 0$, there are fewer process variables than equations and consequently the set of equations has no solution.

Note that $N_F = 0$ is only satisfactory case. If $N_F > 0$, then sufficient inputs have not been identified. If $N_F < 0$, then additional independent model equations must be developed.

For SPEEDUP, the model can be easily checked by checking the number of equations and the unknown variables :

- counting the number of variables in the type section (*NV*).
- counting the number of input stream variables (*NI*).
- counting the number of equations (*NE*).

The SPEEDUP model will solve if

$$NS = NV - (NI + NE) \tag{2.9}$$

NS is the number of set variables that should expect to set for a simulation. For *NS* = 0, the solution of the model can be solved.

2.5 Summary

All of the presented subject in this chapter are the basic knowledge for an application of process modeling. The different process modeling approach is proper with each process or system. The consideration for selecting the approach is depend on the knowledge and the contained data of the process. The details of an application is presented in chapter 5 and 6 that an area of application and the SPEEDUP background is presented in appendix C. The next chapter maintains in an area of theories. It is covered in the data reconciliation subject.