Models and their Classification

Keywords: Models, Classifications, Transport Phenomena Based Model

PROCESS ANALYSIS

Process analysis includes

- Mathematical specifications of the problem for the given physical situation.
- Detailed analysis to obtained mathematical model.
- Synthesis and presentation of results to ensure full comprehension.

Process analysis involves an examination of the overall process, alternative process and economics.

General Process Analysis Principles:

To plan for, organize, evaluate, and control complex process in modern technology we must understand the factors which influence the performance of the process. One way of doing this is to build an actual or small scale replica of the process and study the effect of process and study the effect of changes in the input variables on process functions. Such a technique is not only time consuming and experience but actually may be impossible to carry out. Actually may be impossible to carry out. Given a process and a problem, the analyst tries to construct a set of mathematical relations together with boundary conditions that are isomorphic to the relationships between the process variable.

Because of the complexity of the real process and limitations of mathematics, whatever model is developed is poured to be highly idealized and generally gives a faithful representation of only a few of the properties of the process of only a few of the properties of the process. The first model is often simple but unrealistic on the basis of the first model, the analyst tries to diagnose its principal deficiencies and construct another model that will correct selected deficiencies and yet will still be simple enough to manipulate mathematically. The engineer tries several models before finding one that satisfactorily represents those particular attributes of the process that are of interest.

The general strategy of analysis of complex processes follows the following step:

- Formulation of problems and establishments of objectives and criteria of value; delineation of performance requirements.
- Preliminary inspection and classification of the process to break it down into elements.
- Preliminary determination of the relationship among the subsystems.
- Analysis of the variables and relationship to provide as simple and consistent set as possible.
- Mathematical modelling of the relationship in terms of the variables and parameters.
- Description of elements that can only be is completely represented by mathematical models.
- Evaluation of how well the model represents the real process.
- Application of the model; interpretation and analysis of the results

These steps are designed to develop an approach of structuring and analyzing processes wherever possible through mathematical models. This approach provides for more rigorous analysis and trends to make subjective judgments, more formal and thorough. Following fig. indicates the cyclical nature of these steps.

One of the major premise involved in all such process analysis is that the entire process can be broken down into distinguishable subsystems which, when assembled into a whole, can simulate the process. For example, a model of reactor can be developed by considering successive well stirred sub reactors, although in reality no such units exists in the actual reactor.

MODEL AND MODEL BUILDING

Models are used in all fields-engineering, physics, biology, economics, chemistry, biochemistry etc. It is impossible to include all the valid connotations of word model. Models means;

- Physical models: ship models, pilot plants and scale models of buildings.
- Analog models: electronic, electric and mechanical models
- Provisional theories: Liquid drop model of the nuclei.
- Drawings and maps
- Mathematical models.

We are concerned with the mathematical models. There are three types of models and their components;

- Transport Phenomena models (Use of physiochemical principles)
- Population balance models (Use of population balances)
- Empirical Model (use of empirical data, fitting)

Examples of transport phenomena type models are the phenomenological equations of change i.e. the continuum equations describing the conservation of mass, momentum and energy.RTD and other age distributions are examples of population balance models. Finally examples of typical empirical models are those polynomials used to fit empirical data by the method of least squares.

The basic principle that lies behind the models are nothing more than the concepts of the balance of mass, momentum and energy. Each balance can be expressed as follows;

$$\begin{bmatrix} \text{Net Accumaation} \\ \text{in the system volume} \end{bmatrix} = \begin{bmatrix} \text{Net transport in the system} \\ \text{through system space} \end{bmatrix} - \begin{bmatrix} \text{Net transport out of the system} \\ \text{through system space} \end{bmatrix} + \begin{bmatrix} \text{Net generation} \\ \text{in the system volume} \end{bmatrix} - \begin{bmatrix} \text{Net consumption} \\ \text{in the system volume} \end{bmatrix}$$

…7.1

The general objective in model building is to replace these words with the mathematical expressions that are rigorous as possible and involve as few unknown parameters as possible.

To form a complete model it is necessary to have both,

A) Mathematical statement of the governing differential equation or algebraic equation

b) The appropriate initial and boundary conditions.

Transport phenomena models can be classified into five groups

1. Molecular and atomic
2. Microscopic
3. Multiple gradient
4. Maximum Gradient
5. Macroscopic

Molecular Description

The most fundamental description of processes would be based on molecular considerations. The molecular descriptions are distinguished by the fact that it treats an arbitrary system as if it were composed of individual entities, each of which obeys certain rules. This approach deal with discrete entities, quantum mechanics, statistical mechanics and kinetic theory.

Microscopic Description

It involves phenomenological approach and assumes that the system can be represented as a continuum. In other words, the detailed molecular interaction can be ignored and certain differential balance equations are formulated for mass, momentum and energy. For non-flow processes or for process in a laminar flow, this approach has many practical uses; although it is often excessive complex.

Consider the volume element $\Delta x \Delta y \Delta z$ as shown in fig.

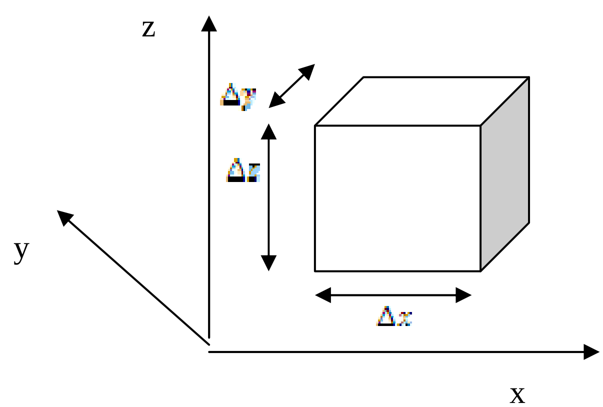

Fig. 7.1: Microscopic Description

We shall follow the following notation

ρ = Mass density of fluid

ρ_A = Mass Density of Component A

j_i^A = mass flux of component A by diffusion

r_A = rate of production of A by chemical reaction

v_i = fluid mass average velocity with respect to stationery coordinates

v_i^A= velocity of species A relative to stationery coordinates.

t=time, sec

In words, the equation of continuity for component A is as follows;

$$\left[Net\ Accumalation\right] = \begin{bmatrix}Input\ through\\ the\ surface\end{bmatrix} - \begin{bmatrix}Output\ through\\ the\ surface\end{bmatrix} + \begin{bmatrix}Generation\ inside\\ Volume\end{bmatrix} - \begin{bmatrix}Consumption\ inside\\ Volume\end{bmatrix} \quad (1) \qquad \ldots 7.2$$

Net transport through the surface consists of transport in by molecular diffusion and transport in by bulk flow, less the transport out by the same two mechanisms for three pairs of surfaces-one in each coordinate direction. The generation or loss of mass inside the elemental volume will be presumed to be due to the chemical reaction, although other effects could be handled similarly.

Accumulation:

$$[\rho_A(\Delta y \Delta z \Delta x)]_{t+\Delta t} - [\rho_A(\Delta y \Delta z \Delta x)]_t$$

Transport by bulk flow:

$$[v_x \rho_A(\Delta y \Delta z)\Delta t]_x - [v_x \rho_A(\Delta y \Delta z)\Delta t]_{x+\Delta x}$$

$$[v_y \rho_A(\Delta x \Delta z)\Delta t]_y - [v_y \rho_A(\Delta x \Delta z)\Delta t]_{y+\Delta y}$$

$$[v_z \rho_A(\Delta y \Delta x)\Delta t]_z - [v_z \rho_A(\Delta x \Delta y)\Delta t]_{z+\Delta z}$$

Transport by molecular diffusion:

$$[J_x^A(\Delta y \Delta z)\Delta t]_x - [J_x^A(\Delta y \Delta z)\Delta t]_{x+\Delta x}$$

$$[J_y^A(\Delta x \Delta z)\Delta t]_y - [J_y^A(\Delta x \Delta z)\Delta t]_{y+\Delta y}$$

$$[J_z^A(\Delta y \Delta x)\Delta t]_z - [J_z^A(\Delta y \Delta x)\Delta t]_{z+\Delta z}$$

Note that J_i^Arepresents the mass diffusion flux w.r.t to the mass average velocity.

Generation or Loss:

For the time being let this value be $r_A(\Delta x \Delta y \Delta z \Delta t)$. Now assemble the terms as indicated by eq. 1 and after rearranging and dividing by $\Delta x \Delta y \Delta z \Delta t$ we obtain;

$$\frac{[\rho_A]_{t+\Delta t} - [\rho_A]_t}{\Delta t} + \frac{[v_x \rho_A]_{x+\Delta x} - [v_x \rho_A]_x}{\Delta x} + \frac{[v_y \rho_A]_{y+\Delta y} - [v_y \rho_A]_y}{\Delta y} + \frac{[v_z \rho_A]_{z+\Delta z} - [v_z \rho_A]_z}{\Delta z}$$

$$= -\frac{[J_x^A]_{x+\Delta x} - [J_x^A]_x}{\Delta x} - \frac{[J_y^A]_{y+\Delta y} - [J_y^A]_y}{\Delta y} - \frac{[J_z^A]_{z+\Delta z} - [J_z^A]_z}{\Delta z} \quad \text{...7.3}$$

Now taking limits

$\Delta x \Delta y \Delta z \rightarrow 0$

In Cartesian coordinate term,

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_A v_i}{\partial x_i} = -\frac{\partial J_i^A}{\partial x_i} + r_A \quad \text{...7.4}$$

In vector form,

$$\frac{\partial \rho_A}{\partial t} + \nabla.(\rho_A V) = -\nabla.J^A + r_A \quad \text{...7.5}$$

For component B,

$$\frac{\partial \rho_B}{\partial t} + \nabla.(\rho_B V) = -\nabla.J^B + r_B \quad \text{...7.6}$$

Addition of eq. 7.5 and 7.6 gives the equation of continuity on a total basis.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_i}{\partial x_i} = 0 \quad \text{...7.7}$$

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho V) = 0 \quad \text{...7.8}$$

The exact form of the diffusion flux, J_i, must be found from the molecular considerations.

$$J_i^A = -\rho D_{AB} \frac{\partial w_A}{\partial x_i} \quad \text{...7.9}$$

where D_{AB} is the binary diffusion coefficient , w_A is the mass fraction of A.

Introduction of eq. 9 into eq.4 leads us to,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_i}{\partial x_i} = \frac{\partial \left[\rho D_{AB}\left(\frac{\partial w_A}{\partial x_i}\right)\right]}{\partial x_i} + r_A \qquad \ldots 7.10$$

For constant ρ & D_{AB} eq.10 becomes,

$$\frac{\partial \rho_A}{\partial t} + \rho_A \frac{\partial v_i}{\partial x_i} + v_i \frac{\partial \rho_A}{\partial x_i} = D_{AB} \frac{\partial^2 \rho_A}{\partial x_i \partial x_i} + r_A \qquad \ldots 7.11$$

For fluids with constant density, $\frac{\partial v_i}{\partial x_i} = 0$

$$\frac{\partial C_A}{\partial t} + v_i \frac{\partial C_A}{\partial x_i} = D_{AB} \frac{\partial^2 C_A}{\partial x_i \partial x_i} + r_A \qquad \ldots 7.12$$

If no chemical changes occur, $v_i = 0, r_A = 0$

$$\frac{\partial C_A}{\partial t} = D_{AB} \nabla^2 C_A \qquad \ldots 7.13$$

This equation is known as diffusion equation or Fick’s Seconds law.

Similar derivations may be made for microscopic mass balances for multi component systems and for momentum and energy balances. Some of the compact results of such derivations are presented in Table-2.2-1 on Pg.13 of Process Analysis and Simulation by D.Himmelblau and K.Bishoff.

Source:
http://nptel.ac.in/courses/103107096/7