UNIT I BASICS OF MODELING:

1.INTRODUCTION

Analysis of the cognition methods which have been used since early times reveals that the general methods created in order to investigate life phenomena could be divided into two groups: (i) the application of similitude, modeling and simulation, (ii) experimental research which also uses physical models. These methods have always been applied to all branches of human activity all around the world and consequently belong to the universal patrimony of human knowledge. The two short stories told below aim to explain the fundamental characteristics of these cognition methods.

First story. When, by chance, men were confronted by natural fire, its heat may have strongly affected them. As a result of these ancient repeated encounters on cold days, men began to feel the agreeable effect of fire and then wondered how they could proceed to carry this fire into their cold caves where they spent their nights. The precise answer to this question is not known, but it is true that fire has been taken into men's houses. Nevertheless, it is clear that men tried to elaborate a scheme to transport this natural fire from outside into their caves. We therefore realize that during the old times men began to exercise their minds in order to plan a specific action. This cognition process can be considered as one of the oldest examples of the use of modeling research on life.
So we can hold in mind that the use of modeling research on life is a method used to analyze a phenomenon based on qualitative and quantitative cognition where only mental exercises are used.

Second Story. The invention of the bow resulted in a new lifestyle because it led to an increase in men's hunting capacity. After using the bow for the first time, men began to wonder how they could make it stronger and more efficient. Such improvements were repeated continually until the effect of these changes began to be analyzed. This example of human progress illustrates a cognition process based on experimentation in which a physical model (the bow) was used. In accordance with the example described above, we can deduce that research based on a physical model results from linking the causes and effects that characterize an investigated phenomenon. With reference to the relationships existing between different investigation methods, we can conclude that, before modifying the physical model used, modeling research has to be carried out. The modeling can then suggest various strategies but a single one has to be chosen. At the same time, the physical model used determines the conditions required to measure the effect of the adopted strategy. Further improvement of the physical model may also imply additional investigation.

If we investigate the scientific and technical evolution for a random selected domain, we can see that research by modeling or experimentation is fundamental. The evolution of research by modeling and/or experimentation (i.e. based on a physical model) has known an important particularization in each basic domain of science and techniques. Research by modeling, by simulation and similitude as well as experimental research, have become fundamental methods in each basic scientific domain . However, they tend to be considered as interdisciplinary activities. In the case of modeling simulation and similitude in chemical engineering, the interdisciplinary state is shown by coupling the phenomena studied with mathematics and computing science.

1.1 CLASSIFICATION OF MODELS

The advances in basic knowledge and model-based process engineering methodologies will certainly result in an increasing demand for models. In addition, computer assistance to support the development and implementation of adequate and clear models will be increasingly used, especially in order to minimize the financial support for industrial production by optimizing global production processes. The classification of models depending on their methodology, mathematical development, objectives etc. will be a useful tool for beginners in modeling in order to help them in their search for the particular model able to solve the different and variable products synthesis.
Highly-diversified models are used in chemical engineering, consequently, it is not simple to propose a class grouping for models. The different grouping attempts given here are strongly related to the modeled phenomena. In the case of a device model or plant model, the assembly of the model parts creates an important number of cases that do not present any interest for class grouping purposes. In accordance with the qualitative process theory to produce the class grouping of one phenomenon or event, it is important to select a clear characterization criterion which can assist the grouping procedure. When this criterion is represented by the theoretical base used for the development of models, the following classification is obtained:

. mathematical models based on the laws of transport phenomena
. mathematical models based on the stochastic evolution laws
. mathematical models based on statistical regression theory
. mathematical models resulting from the particularization of similitude and dimensional analysis.

When the grouping criterion is given by the mathematical complexity of the process model (models), we can distinguish:

. mathematical models expressed by systems of equations with complex derivatives
. mathematical models containing one equation with complex derivatives and one (or more) ordinary system(s) of differential equations.
.mathematical models promoted by a group of ordinary systems of differential equations
. mathematical models with one set of ordinary differential equations complete with algebraic parameters and relationships between variables
. mathematical models given by algebraic equations relating the variables of the process.

For the mathematical models based on transport phenomena as well as for the stochastic mathematical models, we can introduce new grouping criteria. When the basic process variables (species conversion, species concentration, temperature, pressure and some non-process parameters) modify their values, with the time and spatial position inside their evolution space, the models that describe the process are recognized as models with distributed parameters. From a mathematical viewpoint, these models are represented by an assembly of relations which contain partial differential equations The models, in which the basic process variables evolve either with time or in one particular spatial direction, are called models with concentrated parameters.

When one or more input process variable and some process and non-process parameters are characterized by means of a random distribution (frequently normal distributions), the class of non-deterministic models or of models with random parameters is introduced. Many models with distributed parameters present the state of models with random parameters at the same time.

The models associated to a process with no randomly distributed input variables or parameters are called rigid models. If we consider only the mean values of the parameters and variables of one model with randomly distributed parameters or input variables, then we transform a non-deterministic model into a rigid model.

The stochastic process models can be transformed by the use of specific theorems as well as various stochastic deformed models, more commonly called diffusion models. In the case of statistical models, we can introduce other grouping criteria.

1.1.1 Type of model Criterion of classification

Mechanistic	- Based on mechanisms/underlying phenomena
Empirical	- Based on input-output data, trials or experiments
Stochastic	- Contains model elements that are probabilistic in nature
Deterministic	- Based on cause-effect analysis
Lumped parameter	- Dependent variables not a function of spatial position
Distributed parameter	- Dependent variables are a function of spatial position
Linear	- Superposition principle applies
Nonlinear	- Superposition principle does not apply
Continuous	-Dependent variables defined over continuous space-time
Discrete	- Only defined for discrete values of time and/or space
Hybrid	- Containing continuous and discrete behavior

Type of model	Equation types	
	Steady-state problem	Dynamic problem
Deterministic	Nonlinear algebraic	ODEs/PDEs
Stochastic	Algebraic/difference equations	Stochastic ODEs or difference equations
Lumped parameter	Algebraic equations	ODEs
Distributed parameter	EPDEs	PPDEs
Linear	Linear algebraic equations	Linear ODEs
Nonlinear	Nonlinear algebraic equations	Nonlinear ODEs
Continuous	Algebraic equations	ODEs
Discrete	Difference equations	Difference equations

1.2 MATHEMATICAL MODEL

Mathematical Model (Eykhoff, 1974)

"a representation of the essential aspects of an existing system (or a system to be constructed) which represents knowledge of that system in a usable form"

Everything should be made as simple as possible, but no simpler.

General Modeling Principles

- The model equations are at best an approximation to the real process.
- *Adage*: "All models are wrong, but some are useful."
- Modeling inherently involves a compromise between model accuracy and complexity on one hand, and the cost and effort required to develop the model, on the other hand.
- Process modeling is both an art and a science. Creativity is required to make simplifying assumptions that result in an appropriate model.
- Dynamic models of chemical processes consist of ordinary differential equations (ODE) and/or partial differential equations (PDE), plus related algebraic equations.

1.3 USES OF MATHEMATICAL MODELS

- to improve understanding of the process
- to optimize process design/operating conditions
- to design a control strategy for the process
- to train operating personnel

The most important result of developing a mathematical model of a chemical engineering system is the understanding that is gained of what really makes the process "tick." This insight enables you to strip away from the problem the many extraneous "confusion factors" and to get to the core of the system. You can see more clearly the cause-and-effect relationships between the variables.

Mathematical models can be useful in all phases of chemical engineering, from research and development to plant operations, and even in business and economic studies.

- Research and development: determining chemical kinetic mechanisms and parameters from laboratory or pilot-plant reaction data; exploring the effects of different operating conditions for optimization and control studies; aiding in scale-up calculations.
- Design: exploring the sizing and arrangement of processing equipment for dynamic performance; studying the interactions of various parts of the process, particularly when material recycle or heat integration is used; evaluating alternative process and control structures and strategies; simulating start-up, shutdown, and emergency situations and procedures.
- Plant operation: troubleshooting control and processing problems; aiding in start-up and operator training; studying the effects of and the requirements for expansion (bottleneck-removal) projects; optimizing plant operation. It is usually much cheaper, safer, and faster to conduct the kinds of studies listed above on a mathematical model than experimentally on an operating unit. This is not to say that plant tests are not needed. As we will discuss later, they are a vital part of confirming the validity of the model and of verifying important ideas and recommendations that evolve from the model studies.

1.4 SCOPE OF COVERAGE

We will discuss in this subject only deterministic systems that can be described by ordinary or partial differential equations. Most of the emphasis will be on lumped systems (with one independent variable, time, described by ordinary differential equations). Both English and SI units will be used. You need to be familiar with both.

1.5 PRINCIPLES OF FORMULATION

BASIS. The bases for mathematical models are the fundamental physical and chemical laws, such as the laws of conservation of mass, energy, and momentum.
To study dynamics we will use them in their general form with time derivatives included.

ASSUMPTIONS. Probably the most vital role that the engineer plays in modeling is in exercising his engineering judgment as to what assumptions can be validly made. Obviously an extremely rigorous model that includes every phenomenon down to microscopic detail would be so complex that it would take a long time to develop and might be impractical to solve, even on the latest supercomputers. An engineering compromise between a rigorous description and getting an answer that is good enough is always required. This has been called "optimum sloppiness." It involves making as many simplifying assumptions as are reasonable without "throwing out the baby with the bath water." In practice, this optimum usually corresponds to a model which is as complex as the available computing facilities will permit. More and more this is a personal computer.
The development of a model that incorporates the basic phenomena occurring in the process requires a lot of skill, ingenuity, and practice. It is an area where the creativity and innovativeness of the engineer is a key element in the success of the process.

The assumptions that are made should be carefully considered and listed. They impose limitations on the model that should always be kept in mind when evaluating its predicted results.

MATHEMATICAL CONSISTENCY OF MODEL. Once all the equations of the mathematical model have been written, it is usually a good idea, particularly with big, complex systems of equations, to make sure that the number of variables equals the number of equations. The so-called "degrees of freedom" of the system must be zero in order to obtain a solution. If this is not true, the system is underspecified or over specified and something is wrong with the formulation of the problem. This kind of consistency check may seem trivial, but I can testify from sad experience that it can save many hours of frustration, confusion, and wasted computer time. Checking to see that the units of all terms in all equations are consistent is perhaps another trivial and obvious step, but one that is often forgotten. It is essential to be particularly careful of the time units of parameters in dynamic models. Any units can be used (seconds, minutes, hours, etc.), but they cannot be mixed. We will use "minutes" in most of our examples, but it should be remembered that many parameters are commonly on other time bases and need to be converted appropriately, e.g., overall heat transfer coefficients in Btu/h "F ft' or velocity in m/s. Dynamic simulation results are frequently in error because the engineer has forgotten a factor of "60" somewhere in the equations.

SOLUTION OF THE MODEL EQUATIONS. the available solution techniques and tools must be kept in mind as a mathematical model is developed. An equation without any way to solve it is not worth much.

VERIFICATION. An important but often neglected part of developing a mathematical model is proving that the model describes the real-world situation. At the design stage this sometimes cannot be done because the plant has not yet been built. However, even in this situation there are usually either similar existing plants or a pilot plant from which some experimental dynamic data can be obtained. The design of experiments to test the validity of a dynamic model can sometimes be a real challenge and should be carefully thought out.

1.6 FUNDAMENTAL LAWS

1.6.1 Continuity Equations

Total continuity equation (mass balance). The principle of the conservation of mass when applied to a dynamic system says

$$\begin{bmatrix}\text{Mass flow}\\ \text{into system}\end{bmatrix} - \begin{bmatrix}\text{mass flow}\\ \text{out of system}\end{bmatrix} = \begin{bmatrix}\text{time rate of change}\\ \text{of mass inside system}\end{bmatrix}$$

The units of this equation are mass per time. Only one total continuity equation can be written for one system.

Component continuity equations (component balances).

If a reaction occurs inside a system, the number of moles of an individual component will increase if it is a product of the reaction or decrease if it is a reactant. Therefore the component continuity equation of the jth chemical species of the system says

$$\begin{bmatrix}\text{Flow of moles of jth}\\ \text{component into system}\end{bmatrix} - \begin{bmatrix}\text{flow of moles of jth}\\ \text{component out of system}\end{bmatrix} + \begin{bmatrix}\text{rate of formation of moles of jth}\\ \text{component from chemical reactions}\end{bmatrix} = \begin{bmatrix}\text{time rate of change of moles of jth}\\ \text{component inside system}\end{bmatrix}$$

The units of this equation are moles of component j per unit time. The flows in and out can be both convective (due to bulk flow) and molecular (due to diffusion). We can write one component continuity equation for each component in the system. If there are NC components, there are NC component continuity equations for any one system. However, the one total mass balance and these NC component balances are not all independent, since the sum of all the moles times their respective molecular weights equals the total mass. Therefore a given system has only NC independent continuity equations. We usually use the total mass balance and NC - 1 component balances. For example, in a binary (two-component) system, there would be one total mass balance and one component balance.

1.6.2 Energy Equation

The first law of thermodynamics puts forward the principle of conservation of energy. Written for a general "open" system (where flow of material in and out of the system can occur) it is

$$\begin{bmatrix}\text{Flow of internal, kinetic, and} \\ \text{potential energy into system} \\ \text{by convection or diffusion}\end{bmatrix} - \begin{bmatrix}\text{flow of internal, kinetic, and} \\ \text{potential energy out of system} \\ \text{by convection or diffusion}\end{bmatrix} + \begin{bmatrix}\text{heat added to system by} \\ \text{conduction, radiation, and} \\ \text{reaction}\end{bmatrix} - \begin{bmatrix}\text{work done by system on} \\ \text{surroundings (shaft work and} \\ \text{PV work)}\end{bmatrix} = \begin{bmatrix}\text{time rate of change of internal, kinetic,} \\ \text{and potential energy inside system}\end{bmatrix}$$

1.6.3 Equations of motion

The equation which links acceleration, initial and final velocity, and time is the first of the equations of motion.

These equations are used to describe motion in a straight line with uniform acceleration. You must to be able to:

- select the correct formula
- identify the symbols and units used
- carry out calculations to solve problems of real life motion
- carry out experiments to verify the equations of motion.

You should develop an understanding of how the graphs of motion can be used to derive the equations. This is an important part of demonstrating that you understand the principles of describing motion, and the link between describing it graphically and mathematically.

$a = \frac{v - u}{t}$

a = acceleration in metres per second per second (m s^{-2})
v = final velocity in metres per second (m s^{-1})
u = initial velocity in metres per second (m s^{-1})
t = time in seconds (s)

$v = u + at$ Equation of motion 1

$s = ut + ½at^2$

s = displacement in metres (m)
u = initial velocity in metres per second (m s^{-1})
t = time in seconds (s)
a = acceleration in metres per second per second (m s^{-2})

$s = ut + ½at^2$ Equation of motion 2

The third equation of motion is derived from with Equation 1.

Equation 1 $v = u + at$
square each side to give $v^2 = (u + at)^2$
$v^2 = u^2 + 2uat + a^2t^2$

$v^2 = u^2 + 2a(ut + ½at^2)$
substitute in Equation 2 $v^2 = u^2 + 2as$

$v^2 = u^2 + 2as$ Equation of motion 3

1.7 REGRESSION AND CORRELATION ANALYSIS

Suppose we have a set of 30 students in a class and we want to measure the heights and weights of all the students. We observe that each individual (unit) of the set assumes two values – one relating to the height and the other to the weight. Such a distribution in which each individual or unit of the set is made up of two values is called a bivariate distribution. The following examples will illustrate clearly the meaning of bivariate distribution.

(i) In a class of 60 students the series of marks obtained in two subjects by all of them.
(ii) The series of sales revenue and advertising expenditure of two companies in a particular year.
(iii) The series of ages of husbands and wives in a sample of selected married couples.

Thus in a bivariate distribution, we are given a set of pairs of observations, wherein each pair represents the values of two variables. In a bivariate distribution, we are interested in finding a relationship (if it exists) between the two variables under study.

The concept of ‘correlation’ is a statistical tool which studies the relationship between two variables and Correlation Analysis involves various methods and techniques used for studying and measuring the extent of the relationship between the two variables.

“Two variables are said to be in correlation if the change in one of the variables results in a change in the other variable”.

1.7.1 Types of Correlation

There are two important types of correlation. They are (1) Positive and Negative correlation and (2) Linear and Non – Linear correlation.

Positive and Negative Correlation

If the values of the two variables deviate in the same direction i.e. if an increase (or decrease) in the values of one variable results, on an average, in a corresponding increase (or decrease) in the values of the other variable the correlation is said to be positive.

Some examples of series of positive correlation are:

(i) Heights and weights;
(ii) Household income and expenditure;
(iii) Price and supply of commodities;
(iv) Amount of rainfall and yield of crops.

Correlation between two variables is said to be negative or inverse if the variables deviate in opposite direction. That is, if the increase in the variables deviate in opposite direction. That is, if increase (or decrease) in the values of one variable results on an average, in corresponding decrease (or increase) in the values of other variable.

Some examples of series of negative correlation are:

(i) Volume and pressure of perfect gas
(ii) Current and resistance [keeping the voltage constant
(iii) Price and demand of goods.

1.7.2 Regression Equation

Suppose we have a sample of size ‘n’ and it has two sets of measures, denoted by x and y. We can predict the values of ‘y’ given the values of ‘x’ by using the equation, called the REGRESSION EQUATION.

y* = a + bx

where the coefficients a and b are given by

$$b=\frac{n\sum xy-(\sum x)(\sum y)}{n(\sum x^2)-(\sum x)^2}$$

$$a=\frac{\sum y-b\sum x}{n}$$

The symbol y* refers to the predicted value of y from a given value of x from the regression equation.

Simulation:

Key words : Executive Program, unit computation and Information flow Diagram.

The Executive Program

This transmits information through streams and store the calculated results. It can plan the sequence in which calculation are to be done.

Several UWOPs, CHIPS, PACWR, CHEVRON, POWER FACTS etc.

Unit Computations

A set of calculations that predicts what occurs within an equipment unit is called Unit computation.

A heat exchanger has the following Unit computations

$$q = UA\,(\Delta T_{min}) \qquad 1.1$$

$$\frac{1}{U} = \left(\frac{1}{h_i} + \frac{1}{h_{id}}\right) \cdot \frac{d_o}{d_i} + \frac{d_o l_n (d_o / d_i)}{2k_w} + \frac{1}{h_o} + \frac{1}{h_{od}} \qquad 1.2$$

How to create a Simulation:

To create a simulation the engineer writes Unit computations. Following figure shows a strategy for solving the problem.

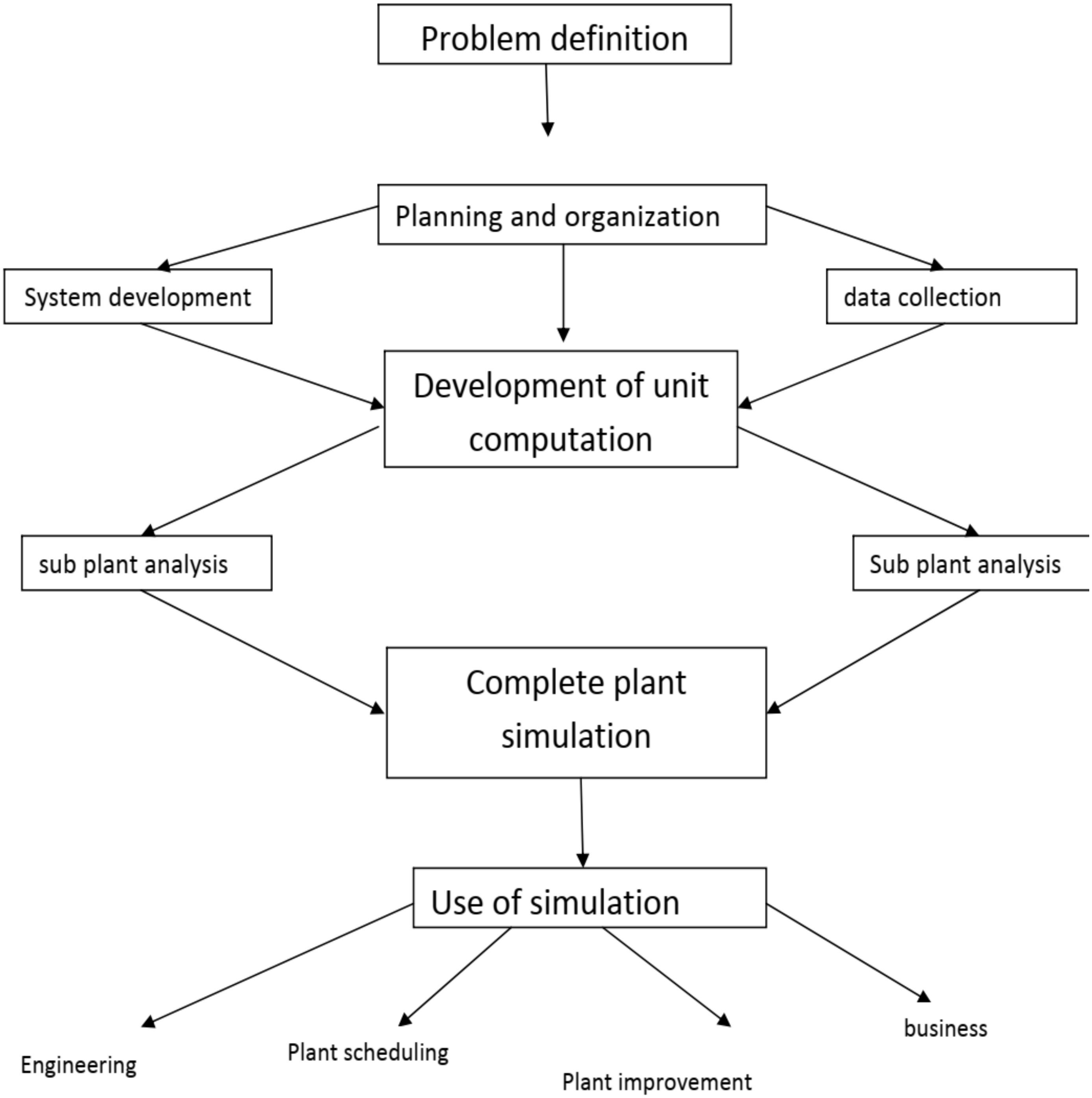

Fig. 1.1 Creation of Simulation of a Plant.

Process simulation requires the following skills:

- A sound understanding of engineering fundamentals
- modeling skills
- computational skills

Chemical process simulation:

- Steady state simulation
- Dynamic simulation

General strategy of process simulation of complex process follows a fairly well defined path consisting of the common sense steps given in the figure 1.2.

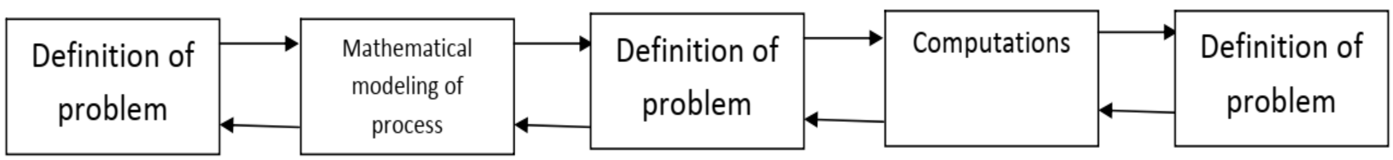

Fig. 1.2 Common steps of process simulation

Limitations of process simulation

- Lack of good data and knowledge of process mechanism.
- Character of the computational tools
- the danger of forgetting the assumptions mode in modeling the process

Development a description of Information flow.

Information is a set of values for the variables of a process needed to describe fully state of a stream at any point in the process. These include flow rate temperature, pressure and composition of a process fluid. Information can flow from place to place not only through actual streams but also through control lines across heat exchanger surfaces. A process flow diagram of a typical plant is given in figure 1.3.

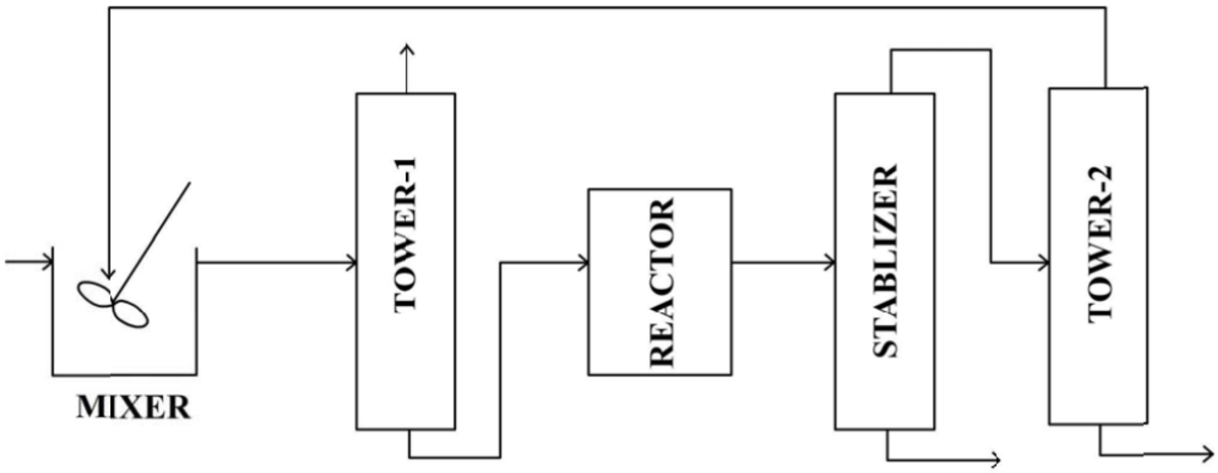

Fig. 1.3 Process Flow Diagram of a Typical Plant

A set of distinctive symbols will be adopted for the various type of unit computation. These are given in figure 1.4.

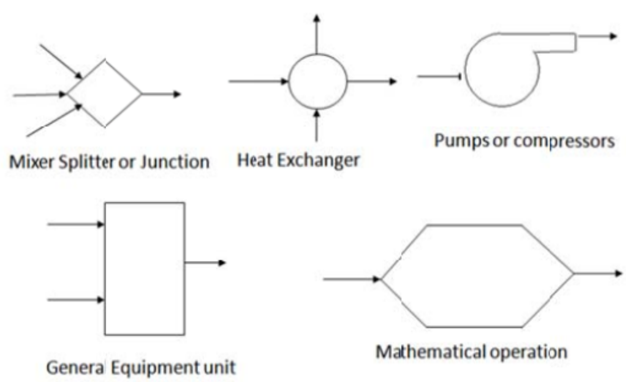

Figure 1.4 : Unit Computation

Modularity:

It means that each unit computation must be written so that the calculation is independent of the source of the input information and the use of output information.

A given unit computation may be used for several different equipment units of the same basic type in the same processing scheme.

From process to Information flow diagram

A process flow diagram depicts the equipment and pipes which make up the plant. The pipes are shown as arrows pointing in the direction of material flow. Such a diagram can be encoded in numerical form for use in computer. This is done in two steps

- Conversion of process flow diagram into information flow diagram.
- Conversion of information flow diagram in to numerical form.

Conversion of process flow diagram into information diagram

The information flow diagram represents the flow of information via streams between unit computations. It is constructed as follows:

(a) Each unit computation is represented by a suitable symbol.
(b) Each symbol is given the name of a unit computation
(c) The flows of information between units are drawn as directed lines (streams) between symbols, with arrows indicating the direction of information flow.
(d) The steams and symbols are separately numbered, usually ascending in the direction of flow. The numbering is arbitrary, but no two symbols or two streams may have the same numbers.

By following the above procedure, the figure 1.3 is converted into information flow diagram as shown in figure 1.5.

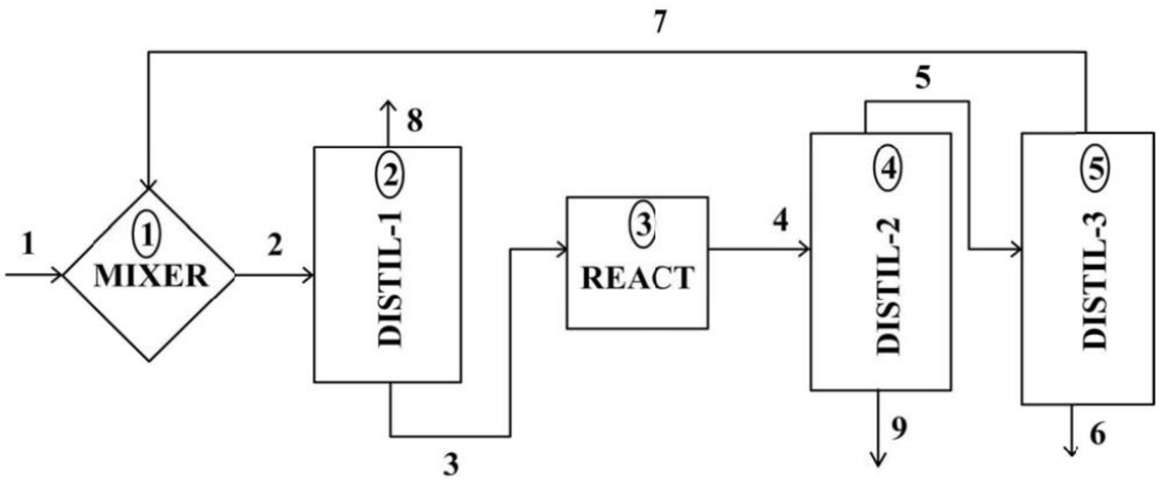

Fig. 1.5 Information Flow Diagram

Although the information flow diagram will generally resemble the process flow diagram, these will be different in some stream and units are not in both diagram. In the case of fig the surge tanks of fig are absent because the process is steady state and capital cost is ignored.