pms- unit :-1

DATE
PAGE

* Importance of Modus

↳ development of sets of quantitative expressions.

↳ Assist in understanding the complex physical interactions in the system and causes and effects I/O system variable.

↳ Mathematical models are valuable tools since they abstract equations that can be solved and analyzed using computer calculations.

* Incentives for process Modeling

In chemical engineering field, models can be useful in all phases, from research and development to plant operation.

Models and their simulation are tools utilized by chemical engineer to help him analyse the process in following ways:-

* Better understanding the process —
Model used to study & investigate the effect of various process parameters and operating conditions.

* Process synthesis and design:-

Model simulation can be utilized in evaluation

of equipment's size and arrangments.

3. Plant operators training :-

Models can be used to train plant personnel to simulate startup and shutdown procedures to operate complex processes. & to handle emergency situations.

4. controlling design and tuning

↳ Practise To determine the optimum values of the controller settings through dynamic ~~situations~~. simulation.

↳ Process optimization :-

It is desirable from economic standpoint to conduct process optimization before plant operation

Process optimization is also performed during process operation to account for variations in feed-stock & utilities market for changing environmental regulations.

* System:

A System is whole consisting of elements or subsystems. The system has boundaries that distinguish it from the surrounding environment.

* Classification based on thermodynamic principle

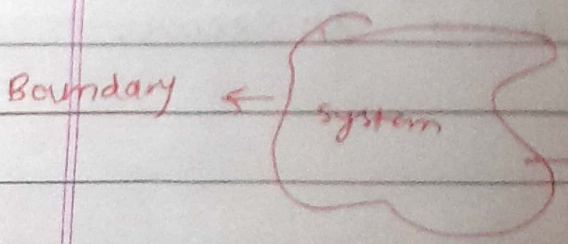
1. Isolated system:- This type of system does not exchange matter nor energy with the surrounding.
Ex- Adiabatic batch reactor.

2. Closed system :- This type of system does not exchange matter with the surrounding but it does exchange energy.

Ex - Non - Adiabatic batch reactor.

3. Open system :- This system exchanges both matter and energy with external environment.

Ex - CSTR (Continuous - stirred tank Reactor).



Classification based on no. of phases :-

1) Homogeneous phase system
↳ This system that involves only one phase such as gas phase or liquid phase.

2) Heterogeneous system.
↳ This system that involves more than one phase.
exist in multi phase reaction.

↳ Classification of Models

- Theoritical Model
- Empirical Model
- Semi - empirical Model.

★ Theoritical Model

These are models that are obtained from fundamental principles, such as law of conservation of mass, energy, momentum along with other chemical principles such as chemical reaction kinematics thermodynamic equilibrium.

Theoretical model are generally difficult to obtain & sometime hard to solve.

DATE
PAGE

★ Empirical Models :-

These models are developed using data fitting techniques such as linear and non linear regression

Provide a description of dynamic relationship b/w inputs and outputs

Models obtained exclusively from experimental plant data are also known as **black - box models**

State variable :- most comman variables, density, concentration, temp, pressure, flow rate are state variable.

Classification of Theoritical Modal

DATE
PAGE

Steady Vs Unsteady state:

Steady State	Unsteady State
↳ When physical state of processing system remains constant with time	When the process state (dependent variable changes with time.
Also called time variant or station-ary models.	also called dynamic transient model.

* They are useful for process control & design & development.

Lumped	Distributed
Lumped parameters are those models which the state variable and other parameter assumed to be no dependence on time & position.	distributed parameters models are those in which state & other variable are function of both time & position.
Ex- CSTR distillation column.	Ex- Heat Exchanger Packed column.

* These models are essential for writing Macroscopic balances eqn.

Linear Vs non linear

Linear	Non Linear.
Have property of superposition	do not ✗
All dependent variables or their derivatives appear in the model equation only to the first power in Linear Model	✗

continious / discrete

continious	discrete.
when dependent variable can assume any values within an interval the model is continious.	Several variable assume to take discrete value. this model called discrete.

Deterministic / Probalistics.

Those model in which each variable can be assigned a definite fixed no. for given set of condition.	Probalistics models used to describe the system are not precisely known,

Building Steps for Mathematical Model.

General procedure for building up mathematical model include the following steps:-

(1) Identification of system configuration its surrounding enviroment & modes of interaction b/w them. Identification of state variables.

(2) Introduction of necessary simplifying Assumptions.

(3) Formulation of model equation based on principles of mass, energy & momentum balances.

(4) Determination of solvability of model using degree of freedom Analysis.

(5) Development of necessary numerical algorithms for the solution of model equations.

(6) Validation of model against experimental results to ensure its reliability and to revaluate the simplifying assumptions.

Component Balance :-

flow of moles (A) in + Rate of Generation of moles of (A) = flow of moles of (A) out

+ Rate of Accumulation of moles of (A)

Degree of freedom

Consistency or Solvability (existence of exact soln) checking done by degree of freedom of model.

$F = N_v - N_e$.

$f = 0$ (system is exactly specified)
eqn has finite no. of soln.

$F < 0$ = system is over determined
f eqn have to be removed for the system to have a solution.

$F > 0$ = system is under determined.
eqn has infinite no. of solution.