Lecture (9)

Reactor Sizing

1.Introduction

Chemical **kinetics** is the study of chemical reaction rates and reaction mechanisms. The study of chemical reaction engineering (CRE) combines the **study** of chemical kinetics with the reactors in which the reactions occur. Chemical kinetics and reactor design are at **the** heart of producing almost all industrial chemicals.

It is **primarily a** knowledge of chemical kinetics and reactor design that distinguishes the chemical engineer from other engineers. The selection of a reaction system that operates in the safest and most efficient manner can be the **key** to the economic success or failure of n chemical plant.

Design of the reactor is no routine matter, and many alternatives can be proposed for a process. In searching for the optimum it is not just the cost of the reactor that must be minimized. One design may have low reactor cost, but the materials leaving the unit may be such that their treatment requires a much higher cost than alternative designs. Hence, the economics of the overall process must be considered. Reactor design uses information, knowledge, and experience from a variety of areas-thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer, and economics. Chemical reaction engineering is the synthesis of all these factors with the aim of properly designing a chemical reactor.

To find what a reactor is able to do we need to know the kinetics, the contacting pattern and the performance equation. We show this schematically in Figure (1).

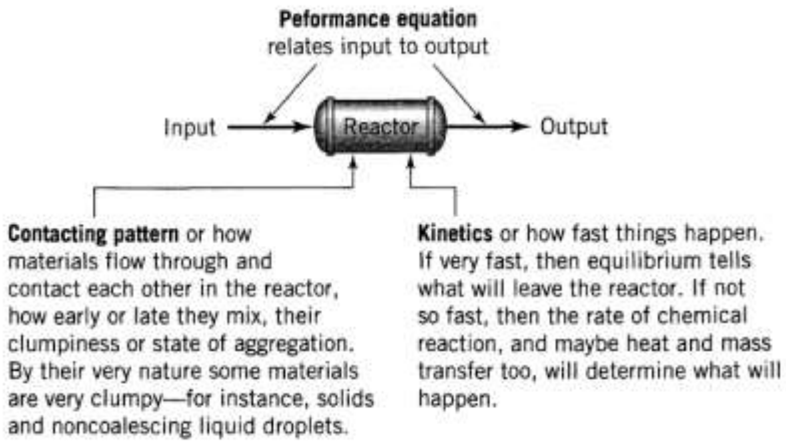


Figure (1). Information needed to predict what a reactor can do.

Much of this lectures deals with finding the expression to relate input to output for various kinetics and various contacting patterns, or

output = f [input, kinetics, contacting] ………………**(1)**

This is called the *performance equation*. Why is this important? Because with this expression we can compare different designs and conditions, find which is best, and then scale up to larger units.

2.Type of Reactors.

mical reactors are vessels designed to contain chemical chemical reactor deals with multiple aspects of chemical engineering. Chemical engineers design reactors to maximize net present value for the given reaction. Designers ensure that the reaction proceeds with the highest efficiency towards the desired output product, producing the highest yield of product while requiring the least amount of money to purchase and operate. Normal operating expenses include energy input, energy removal, raw material costs, labor, etc.

There are a couple main basic vessel types:

- A tank
- A pipe or tubular reactor (laminar flow reactor(LFR))

Both types can be used as continuous reactors or batch reactors. Most commonly, reactors are run at steady-state, but can also be operated in a transient state. When a reactor is first brought back into operation (after maintenance or inoperation) it would be considered to be in a transient state, where key process variables change with time. Both types of reactors may also accommodate one or more solids (reagents, catalyst, or inert materials), but the reagents and products are typically liquids and gases.

There are three main basic models used to estimate the most important process variables of different chemical reactors:

- *Batch Reactor*
- *Continuous Stirred-Tank Reactor (CSTR)*
- *Plug Flow Reactor (PFR)*

Key process variables include

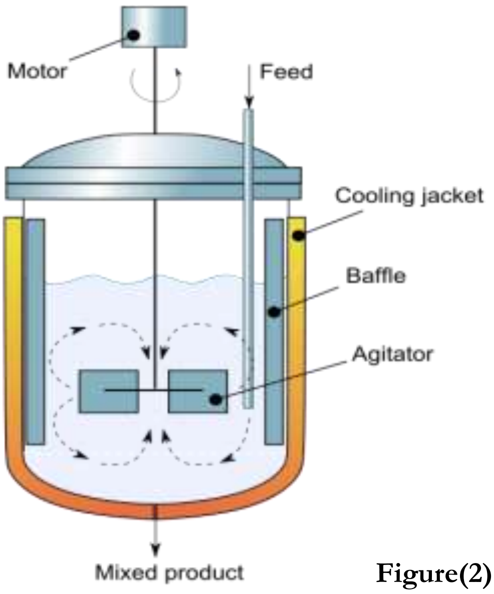
- Residence time (τ) , Volume (V) , Temperature (T) , Pressure (P) , Concentrations of chemical species (C_1, C_2, C_3, ... C_n) ,Heat transfer coefficients (h, U)

Chemical reactions occurring in a reactor may be exothermic, meaning giving off heat, or endothermic, meaning absorbing heat. A chemical reactor vessel may have a cooling or heating jacket or cooling or heating coils (tubes) wrapped around the outside of its vessel wall to cool down or heat up the contents.

2.1 Batch Reactor

Type of Reactor	• Batch Reactor
Characteristics	• Reactor is charged (i.e., filled) through the holes at the top ; while reaction is carried out. • Nothing else is put in or taken out until the reaction is done; tank easily heated or cooled by jacket

Kinds of Phases Present	Usage	Advantages	Disadvantages
1. Gas phase 2.Liquid phase 3.Liquid Solid	1. Small scale production 2. Intermediate or one shot production 3.Testing new process that have not been fully developed 4.Manufacture of expensive products. 5.Pharmaceutical, Fermentation	1. High conversion per unit volume for one pass 2.Flexibility of operation-same reactor can produce one product one time and a different product the next 3. Easy to clean	1. High operating cost 2. Product quality more variable than with continuous operation 3.Difficalty of large scale production .

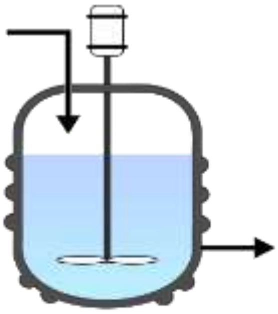


Figure(2) simple batch reactor .

Semi-batch reactors operate much like batch reactors in that they take place in a single stirred tank with similar equipment . It modified allow reactant addition and/or product removal in time. A semi-batch reactor, however, allows partial filling of reactants with the flexibility of adding more as time progresses. Semi-batch reactors **are** used primarily for liquid-phase reactions , **two-phase** reactions in which a **gas** usually is bubbled continuously through **the** liquid , and also for biological and polymerization reaction.

2.2. Continuous-Flow Reactors

2.2.1 Continuous-Stirred Tank Reactor CSTR



Type of Reactor

- Continuous-Stirred Tank Reactor CSTR

Characteristics

- Run at steady state ,the flow rate in must equal the mass flow rate out, otherwise the tank will overflow or go empty (transient state).
- The feed assumes a uniform composition throughout the reactor, exit stream has the same composition as in the tank.
- The reaction rate associated with the final (output) concentration.
- Reactor equipped with an impeller to ensure proper mixing.
- Dividing the volume of the tank by the average volumetric flow rate through the tank gives the *residence time*, or the average amount of time a discrete quantity of reagent spends inside the tank.

Kinds of Phases Present	Usage	Advantages	Disadvantages
1. Gas phase **2. Liquid phase** **3. Liquid Solid**	1. When agitation is required 2. Series configurations for different concentration streams	1. Continuous operation 2. Good temperature control 3. Easily adapts to two phase runs 4. Simplicity of construction 5.Low operating (labor) cost 6. Easy to clean	1. Lowest conversion per unit volume, **very large** reactors are necessary to obtain high conversions 2. By-passing and channeling possible with poor agitation

Some important aspects of the CSTR:

- It is economically beneficial to operate several CSTRs in series. This allows, for example, the first CSTR to operate at a higher reagent concentration and therefore a higher reaction rate. In these cases, the sizes of the reactors may be varied in order to minimize the total capital investment required to implement the process.

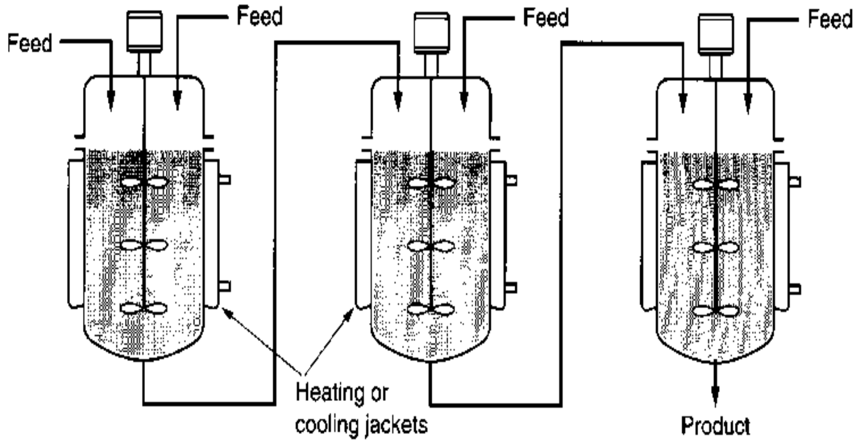
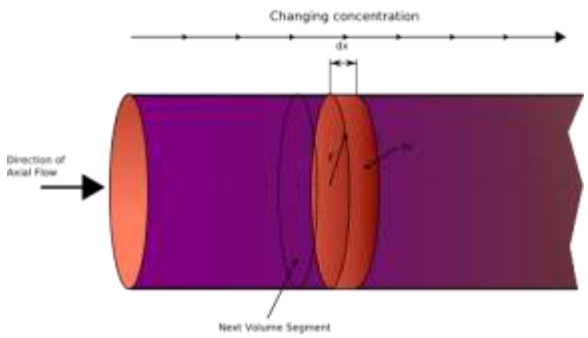


Figure (3) Flow sheet for the manufacture of nitrobenzene from benzene using a cascade of CSTR

2.2.3. Tubular Reactor (PFR)



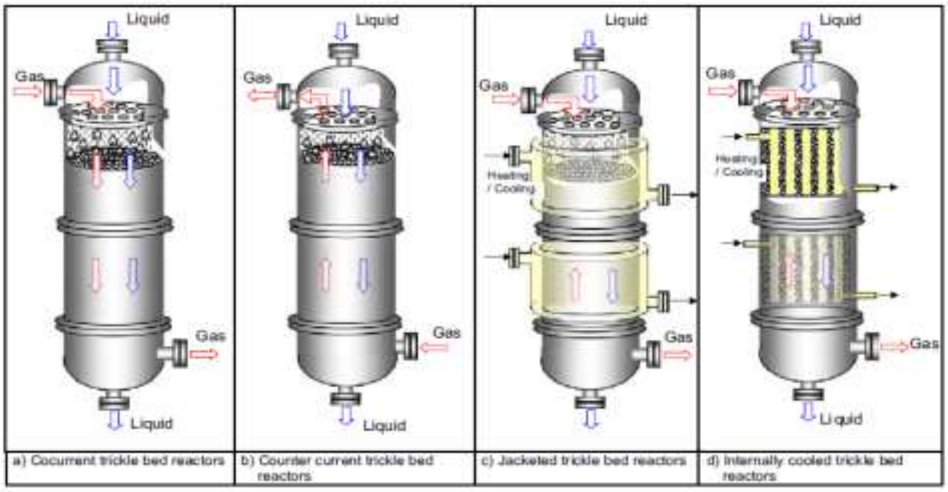
Type of Reactor	• Tubular Reactor (PFR)
Characteristics	•Consists **of** a long cylindrical tube or many short reactors in a tube bank. •Operated at steady state. •The rate is very high at the inlet to the PFR. • No radial variation in reaction rate (concentration) and the reactor is referred to as a plug-fiow rcactor (PFR). • Concentration changes with length down the reactor •As the concentrations of the reagents decrease and the concentration of the product(s) increases the reaction rate slows. •A PFR typically has a higher efficiency than a CSTR of the same volume. That is, given the same space-time, a reaction will proceed to a higher percentage completion in a PFR than in a CSTR.

Kinds of Phases Present	Usage	Advantages	Disadvantages
1. Primarily Gas Phase	1. Large Scale 2. Fast Reactions 3. Homogeneous Reactions 4. Heterogeneous Reactions 5. Continuous Production 6. High Temperature	1. High Conversion per Unit Volume 2. Low operating (labor) cost) 3.Good heat transfer	1. Undesired thermal gradients may exist 2. Difficult temperature control 3. Shutdown and cleaning may be expensive 4.Hot spot occur for exothermic reaction

- Other types of reactors:- Catalytic reactors(packed bed and Fluidized-bed Reactor

Type of Reactor	• Paced bed Reactor (fixed-bed,PBR)
Characteristics	•is essentially a tubular reactor that is packed with solid catalyst particles.

Kinds of Phases Present	Usage	Advantages	Disadvantages
1. Gas-Soli phase 2. Liquid-Solid phase 3. Gas-Liquid - Solid	Heterogeneous reaction	Most reaction gives the highest conversion per weight of catalyst of any catalytic reactor.	1. Difficulties with temperature control. 2. Catalyst is usually troublesome to replace 3. Channeling of the gas or liquid flow occurs, resulting in ineffective use of part of the reactor bed



Figure(4) Packed bed Reactors

Type of Reactor	• Fluidized-bed Reactor
Characteristics	• Is analogous to the CSTR in that its contents. • Heterogeneous reactor, are well mixed.

Kinds of Phases Present	Usage	Advantages	Disadvantages
1. Gas-Solid phase 2. Liquid-Solid phase 3. Gas-Liquid – Solid phase	1.Heterogeneous reaction 2. reactor can handle large amounts of feed	1.Good mixing 2. temperature is relatively uniform throughout 3. Catalyst can be continuously regenerated with	1. Bed-fluid mechanics not well known 2. Severe agitation can result in catalyst destruction and dust

	and solids	the use of an auxiliary loop 4. good temperature control	formation 3. Uncertain scale-up

Figure(5) Fluidized-bed Reactors

3.Classification of Chemical Reaction

it classify according to

- Five traditional types of chemical reactions are

1. Decomposition reactions: single compound decomposes to two or more other substances,decomposition of calcium carbonate by heating it.

   $CaCO_3(s)$ ---> $CaO(s) + CO_2(g)$

2. Combination reactions (Synthesis reactions)
3. Single-replacement reactions (Displacement reactions):copper displaces silver from an aqueous solution of silver nitrate is an example of a single-replacement reaction.

$Cu(s) + 2\ AgNO_3(aq) \dashrightarrow Cu(NO_3)_2(aq) + 2\ Ag(s)$

4. Double-replacement reactions (Metathesis reactions):Precipitation reactions are one type of double-replacement reaction. An example is

$AgNO_3(aq) + NaCl(aq) \dashrightarrow AgCl(s) + NaNO_3(aq)$

5. Combustion reactions: substance reacts with oxygen,butane burns in air as follows.

$2\ C_4H_{10}(g) + 13\ O_2(g) \dashrightarrow 8\ CO_2(g) + 10\ H_2O(l)$

Also Oxidation-reduction reactions (Redox reactions).

- ***phases involved:***
  - *Homogeneous reaction* : it takes place in one phase alone
  - *Heterogeneous reaction* : multiple phases, reaction usually occurs at the interface between phases.

- ***Direction of reaction***
  - ***Irreversible Reaction***: Proceeds in only one direction and continues in that direction until the reactants are exhausted.

    Example :

    Heterogeneous reaction

    Toluene-hydrogenation $C_6H_5CH_{3(L)} + H_{2(g)} \xrightarrow{catalyst} C_6H_{6(g)} + CH_{4(g)}$

    Homogeneous reaction

    Decomposition N_2O $N_2O\ (g) + 2O_2(g) \longrightarrow 2\ N_2(g) + O_2(g)$

    Water gas shift reaction $H_2O\ (g) + CO\ (g) \longrightarrow H_2(g) + CO_2(g)$

  - ***Reversible Reaction***: Can proceed in either direction, depending on the concentrations of reactants and products present relative to the corresponding equilibrium concentration.

    Example :

    Homogeneous reaction

    Ammonia synthesis $2N_{2(g)} + 3H_{2(g)} \Leftrightarrow 2NH_{3(g)}$

    Thermal cracking of ethane : $C_2H_{6(g)} \Leftrightarrow C_2H_{4(g)} + H_{2(g)}$

    Heterogeneous reaction

    Ammonium chloride synthesis or decomposition

$$NH_{3(g)} + HCL_{(g)} \Leftrightarrow \quad NH_4CL_{(s)}$$

Related links and youtubes

Reactor runaway

1)www.che.utexas.edu/course/che360/.../chapter_10.ppt

2)www.youtube.com/watch?v=C561PCq5E1g