Kinetics and Reactor design-I

CHE-S304

Syllabus

- Introduction and overview
- Kinetics of homogeneous reactions
- Isothermal batch reactor
- Ideal reactor for single reaction
- Reactor design for multiple reactions
- Temperature and pressure effect
- Non-ideal reactors

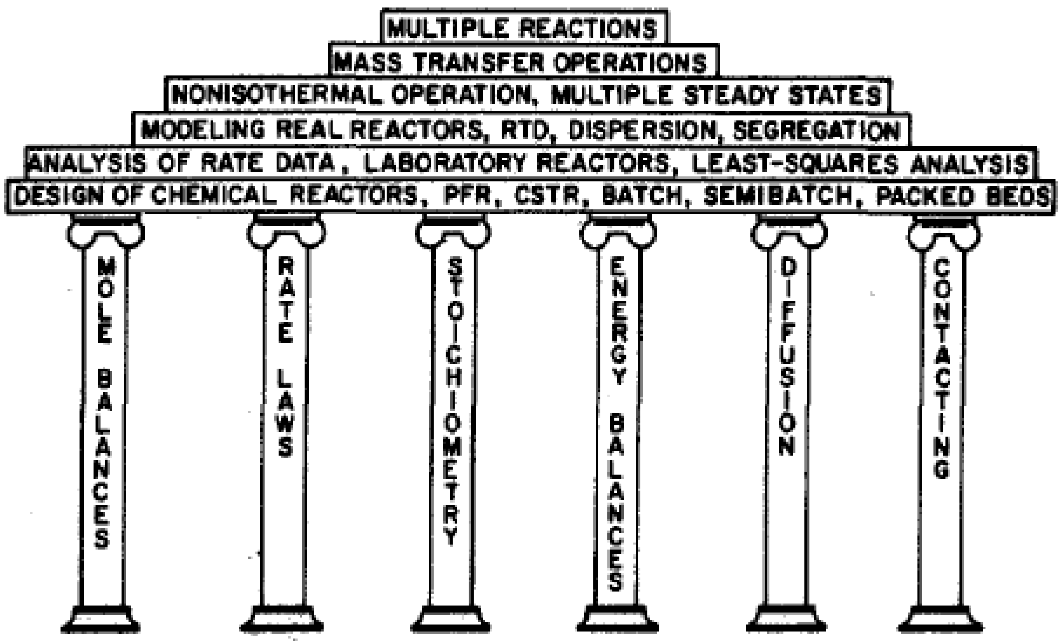
Text books

- O. Levenspiel, Chemical Reaction Engineering, John Willey & Sons

- H. Scott Fogler, Elements of Chemical reaction engineering. Prentice Hall of India

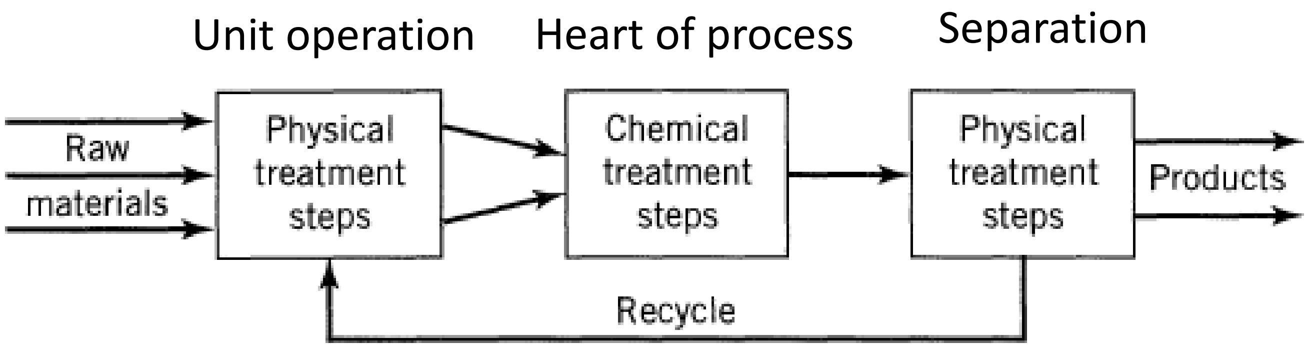
- Charles G. Hill, An Introduction to Chemical Engineering Kinetics & Reactor Design. John Willey & Sons

- Pillars of Chemical reaction Engineering



Overview of Chemical Reaction Engineering

Typical Chemical process



Industrial Chemical process is design to produce economically desired product.

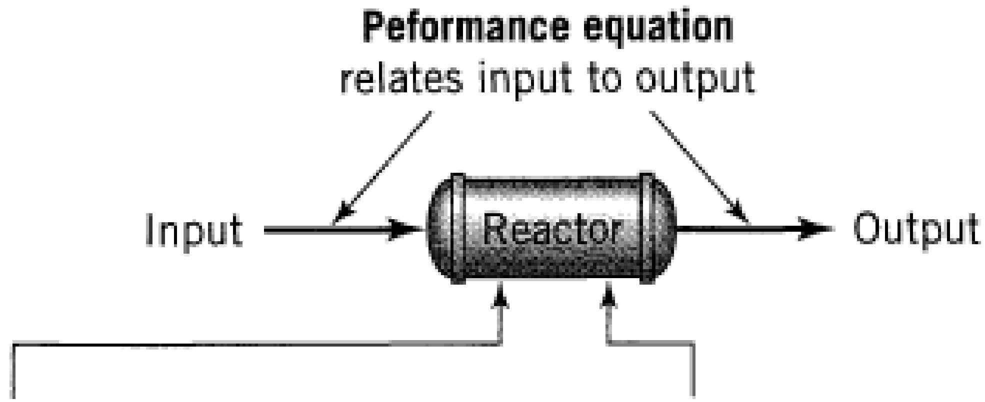
Economical: Overall process must be considered.

Reactor Design

Information:

- Termodynamics
- Chemical kinetics
- Fluid mechanics
- Heat Transfer
- Mass transfer
- Economics

Reactor Design



Contacting Pattern

Kinetics

Materials flow through and contact each other in the reactor. How early or late they mix, state of aggregation

How fast things happen
If very fast, then equilibrium tells what will leave the reactor. If not so fast, then the rate of chemical reaction, and may be heat and Mass transfer too.

Performance Equation

- Finding the expression to relate input and output stream.
- It deals with various kinetics and contacting pattern

$$\text{output} = f\,[\text{input, kinetics, contacting}]$$

Classification of Reactions

Based on the phase present

Homogeneous: one phase only

Heterogeneous: At least two phases

At an interface

- ❖ The reactants and products are distributed among the phases or are all contained within a single phase.
- ❖ All that counts is that at least two phases are necessary for the reaction to proceed as it does.

Classification of Chemical Reactions Useful in Reactor Design

	Noncatalytic	Catalytic
Homogeneous	Most gas-phase reactions	Most liquid-phase reactions
	Fast reactions such as burning of a flame	Reactions in colloidal systems Enzyme and microbial reactions
Heterogeneous	Burning of coal Roasting of ores Attack of solids by acids Gas-liquid absorption with reaction Reduction of iron ore to iron and steel	Ammonia synthesis Oxidation of ammonia to produce nitric acid Cracking of crude oil Oxidation of SO_2 to SO_3

Variables Affecting the Rate of Reaction

Homogeneous systems:

Temperature, Pressure, and Composition

Heterogeneous systems:

Phase to phase movement during reaction;

Rate of mass transfer, Heat transfer

Ddiffusion through the gas film

An exothermic, endothermic reaction

Non-uniform temperature distribution

Definition of Reaction Rate

Rate of reaction:

- All interrelated and all intensive rather than extensive measure. rate in terms of this component i
- Rate of change in number of moles of this component due to reaction is dN_i/dt, Based on unit volume of reacting fluid(HOMOGENEOUS CASE)

$$r_i = \frac{1}{V}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of fluid})\,(\text{time})}$$

- Based on unit mass of solid in fluid-solid systems (HETEROGENEOUS)

$$r_i' = \frac{1}{W}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{mass of solid})\,(\text{time})}$$

- Based on unit interfacial surface in two-fluid systems or based on unit surface of solid in gas-solid systems

$$r_i'' = \frac{1}{S}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{surface})\,(\text{time})}$$

- Based on unit volume of solid in gas-solid systems

$$r_i''' = \frac{1}{V_s}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of solid})\ (\text{time})}$$

- Based on unit volume of fluid

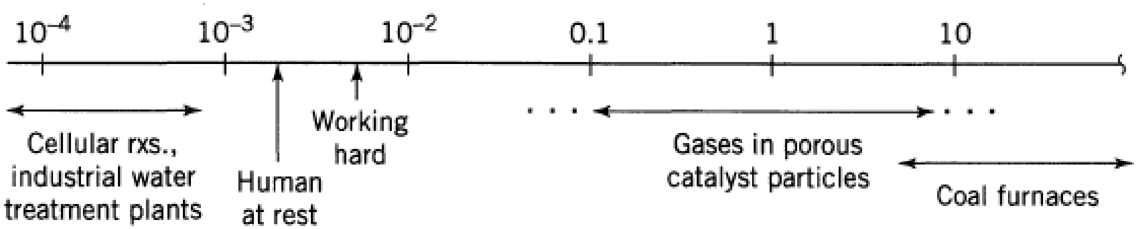
$$r_i'''' = \frac{1}{V_r}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of reactor})\ (\text{time})}$$

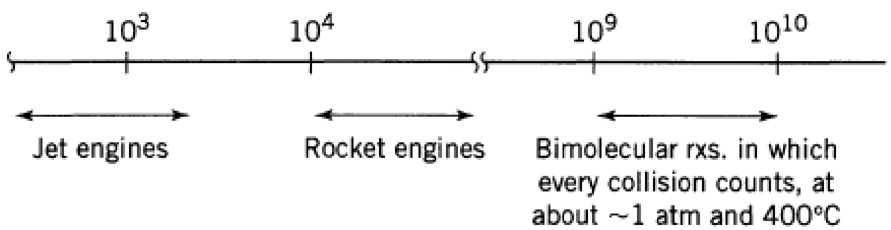
- intensive definitions of reaction rate are related by

$$Vr_i = Wr_i' = Sr_i'' = V_s r_i''' = V_r r_i''''$$

Speed of Chemical Reactions

- Some reactions occur very rapidly; others very, very slowly
- Relative rates at which reactions occur
- With such a large ratio, of course the design of reactors will be quite different in these cases





$$\text{Rate of reactions } -r_A''' = \frac{\text{moles of A disappearing}}{\text{m}^3 \text{ of thing} \cdot \text{s}}$$

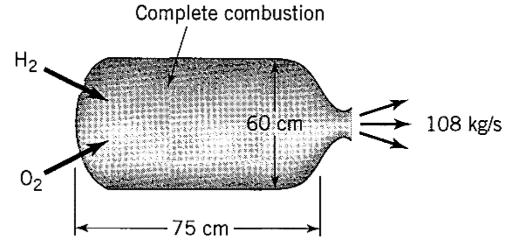
Examples

- A rocket engine, burns a stoichiometric mixture of fuel (liquid hydrogen)

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

$$2\text{gm} \quad 16\text{ gm} \quad 18\text{ gm}$$

- in oxidant (liquid oxygen). The combustion chamber is cylindrical, 75 cm long and 60 cm in diameter, and the combustion process produces 108 kg/s of exhaust gases.



- If combustion is complete, find the rate of reaction of hydrogen and of oxygen.

$$-r_{H_2} = \frac{1}{V}\frac{dN_{H_2}}{dt} \quad \text{and} \quad -r_{O_2} = \frac{1}{V}\frac{dN_{O_2}}{dt}$$

Solution:

- The reactor volume and the volume in which reaction takes place are identical

$$V = \frac{\pi}{4}(0.6)^2(0.75) = 0.2121 \text{ m}^3$$

- Given

$$H_2O \text{ produced/s} = 108 \text{ kg/s}\left(\frac{1 \text{ kmol}}{18 \text{ kg}}\right) = 6 \text{ kmol/s}$$

- By stoichiometry

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

2gm 16 gm 18 gm

$$H_2 \text{ used} = 6 \text{ kmol/s}$$

$$O_2 \text{ used} = 3 \text{ kmol/s}$$

- Rate of reaction is

$$\underline{\underline{-r_{H_2}}} = -\frac{1}{0.2121 \text{ m}^3} \cdot \frac{6 \text{ kmol}}{\text{s}} = \underline{\underline{2.829 \times 10^4 \frac{\text{mol used}}{(\text{m}^3 \text{ of rocket}) \cdot \text{s}}}}$$

$$\underline{\underline{-r_{O_2}}} = -\frac{1}{0.2121 \text{ m}^3} \cdot 3\frac{\text{kmol}}{\text{s}} = \underline{\underline{1.415 \times 10^4 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}}}$$

Examples

- A human being *(75* kg) consumes about 6000 kJ of food per day. Assume that the food is all glucose and that the overall reaction is

$$\underset{}{C_6H_{12}O_6} + \underset{\text{from air}}{6O_2} \rightarrow \underset{\text{breathed out}}{6CO_2} + 6H_2O, \quad -\Delta H_r = 2816 \text{ kJ}$$

- Find man's metabolic rate (the rate of living, loving, and laughing) in terms of moles of oxygen used per m^3 of person per second

$$-r'''_{O_2} = -\frac{1}{V_{\text{person}}}\frac{dN_{O_2}}{dt} = \frac{\text{mol } O_2 \text{ used}}{(\text{m}^3 \text{ of person})\text{s}}$$

density of man

$$\rho = 1000\,\frac{\text{kg}}{\text{m}^3} \qquad V_{\text{person}} = \frac{75 \text{ kg}}{1000 \text{ kg/m}^3} = 0.075 \text{ m}^3$$

Solution

Each mole of glucose consumed uses 6 moles of oxygen and releases 2816 kJ of energy

$$\frac{dN_{O_2}}{dt} = \left(\frac{6000 \text{ kJ/day}}{2816 \text{ kJ/mol glucose}}\right)\left(\frac{6 \text{ mol } O_2}{1 \text{ mol glucose}}\right) = 12.8 \frac{\text{mol } O_2}{\text{day}}$$

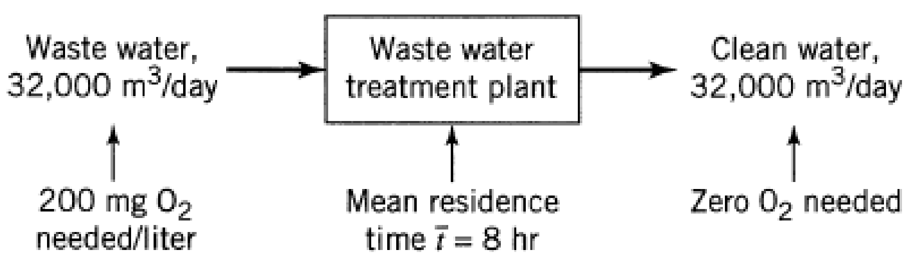
$$-r'''_{O_2} = \frac{1}{0.075 \text{ m}^3} \cdot \frac{12.8 \text{ mol } O_2 \text{ used}}{\text{day}} \frac{1 \text{ day}}{24 \times 3600 \text{ s}} = \underline{0.002 \frac{\text{mol } O_2 \text{ used}}{\text{m}^3 \cdot \text{s}}}$$

Problems

1.1. ***Municipal waste water treatment plant.*** Consider a municipal water treatment plant for a small community (Fig. P1.1). Waste water, 32 000 m^3/day, flows through the treatment plant with a mean residence time of 8 hr, air is bubbled through the tanks, and microbes in the tank attack and break down the organic material

$$\text{(organic waste)} + O_2 \xrightarrow{\text{microbes}} CO_2 + H_2O$$

A typical entering feed has a BOD (biological oxygen demand) of 200 mg O_2/liter, while the effluent has a negligible BOD. Find the rate of reaction, or decrease in BOD in the treatment tanks.



Solution 1.1

- Find the rate of reaction defined as
- ro_2 =mole o_2 used/ sec. m^3 of tank
- Evaluate terms
- t = V/v
- Volume of the treatment tank = (1/3day) (3200 m^3/day) = 10667 m^3

<u>O_2 used</u>

- (200 mg/lit) (1g / 1000mg)(mol/32gm)(1000lit/day)
- $\frac{2\times10^5\, mol\ O_2\ day}{10667 m^3}$= 18.75 mol/ m^3.day
- = 2.17 x 10^{-4} mol/ m^3.s