University of Anbar

College of Engineering

Chemical and Petrochemical Engineering Department

Chemical Reacior Design

Third Year

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Lecture No. 1

Introduction:

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 Fig. 1.2.

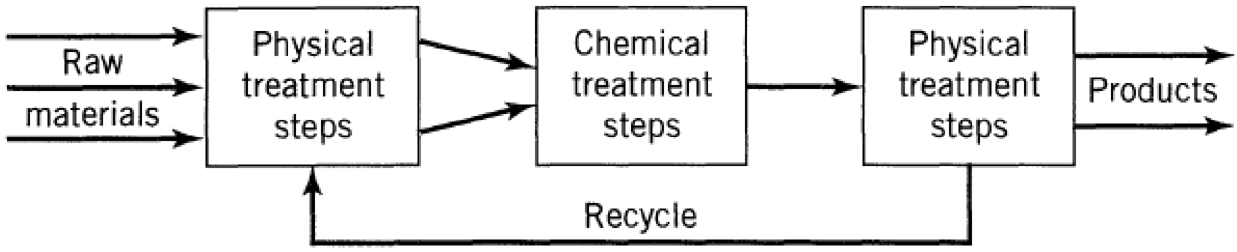

Figure 1.1 Typical chemical process.

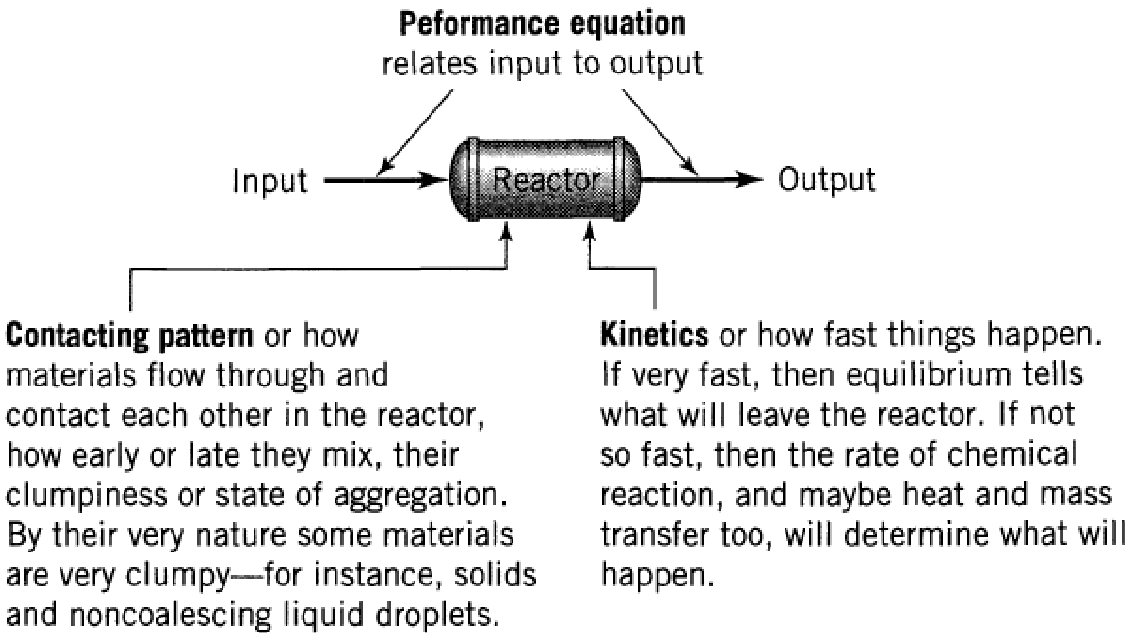

Figure 1.2 Information needed to predict what a reactor can do.

$$\text{output} = f[\text{input, kinetics, contacting}] \qquad \textbf{(1)}$$

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.

Definition of Reaction Rate:

If the rate of change in number of moles of this component due to reaction is dN_i/dt, then the rate of reaction in its various forms is defined as follows. Based on unit volume of reacting fluid,

$$r_i = \frac{1}{V}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of fluid})\ (\text{time})} \quad (2)$$

Based on unit mass of solid in fluid-solid systems,

$$r'_i = \frac{1}{W}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{mass of solid})\ (\text{time})} \quad (3)$$

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

$$r''_i = \frac{1}{S}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{surface})\ (\text{time})} \quad (4)$$

Based on unit volume of solid in gas-solid systems

$$r'''_i = \frac{1}{V_s}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of solid})\ (\text{time})} \quad (5)$$

Based on unit volume of reactor, if different from the rate based on unit volume of fluid,

$$r''''_i = \frac{1}{V_r}\frac{dN_i}{dt} = \frac{\text{moles } i \text{ formed}}{(\text{volume of reactor})\ (\text{time})} \quad (6)$$

In homogeneous systems the volume of fluid in the reactor is often identical to the volume of reactor. In such a case V and Vr are identical and Eqs. 2 and 6 are used interchangeably. In heterogeneous systems all the above definitions of reaction rate are encountered, the definition used in any particular situation often being a matter of convenience.

EXAMPLE 1.1 ***THE ROCKET ENGINE***

A rocket engine, Fig. E1.1, burns a stoichiometric mixture of fuel (liquid hydrogen) 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.

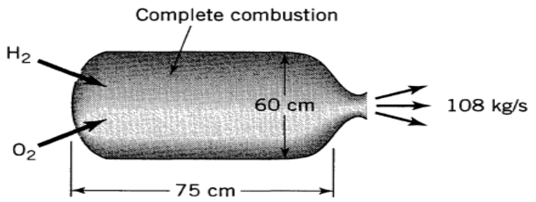

Figure E1.1

SOLUTION

We want to evaluate

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

Let us evaluate terms. The reactor volume and the volume in which reaction takes place are identical. Thus,

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

Next, let us look at the reaction occurring.

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \qquad \textbf{(i)}$$

molecular weight: 2gm 16 gm 18 gm

Therefore,

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

So from Eq. (i)

$$H_2 \text{ used} = 6 \text{ kmol/s}$$
$$O_2 \text{ used} = 3 \text{ kmol/s}$$

and the rate of reaction is

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

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

EXAMPLE 1.2 THE LIVING PERSON

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

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

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.

SOLUTION

We want to find

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

Let us evaluate the two terms in this equation. First of all, from our life experience we estimate the density of man to be

$$\rho = 1000 \frac{\text{kg}}{\text{m}^3}$$

Therefore, for the person in question

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

Next, noting that each mole of glucose consumed uses 6 moles of oxygen and releases 2816 kJ of energy, we see that we need

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

Inserting into Eq. (i)

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