**University of Anbar**

**College of Engineering**

**Chemical and Petrochemical Engineering Department**

# Chemical Reacior Design

## Third Year

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# Lecture No. 14

1-

A reaction with stoichiometric equation $\frac{1}{2}$ A + B = R + $\frac{1}{2}$ S has the following rate expression

$$-r_A = 2C_A^{0.5}C_B$$

What is the rate expression for this reaction if the stoichiometric equation is written as A + 2B = 2R + S?

2-

A certain reaction has a rate given by

$$-r_A = 0.005C_A^2, \qquad \text{mol/cm}^3 \cdot \text{min}$$

If the concentration is to be expressed in mol/liter and time in hours, what would be the value and units of the rate constant?

3-

The pyrolysis of ethane proceeds with an activation energy of about 300 kJ/mol. How much faster is the decomposition at 650°C than at 500°C?

4-

A 1100-K *n*-nonane thermally cracks (breaks down into smaller molecules) 20 times as rapidly as at 1000 K. Find the activation energy for this decomposition.

5-

A 10-minute experimental run shows that 75% of liquid reactant is converted to product by a ½-order rate. What would be the fraction converted in a half-hour run?

6-

In a homogeneous isothermal liquid polymerization, 20% of the monomer disappears in 34 minutes for initial monomer concentration of 0.04 and also for 0.8 mol/liter. What rate equation represents the disappearance of the monomer?

7-

After 8 minutes in a batch reactor, reactant ($C_{A0}$ = 1 mol/liter) is 80% converted; after 18 minutes, conversion is 90%. Find a rate equation to represent this reaction.

8-

The first-order reversible liquid reaction

$$A \rightleftarrows R, \quad C_{A0} = 0.5 \text{ mol/liter}, \quad C_{R0} = 0$$

takes place in a batch reactor. After 8 minutes, conversion of A is 33.3% while equilibrium conversion is 66.7%. Find the rate equation for this reaction.

9-

Aqueous A reacts to form R ($A \rightarrow R$) and in the first minute in a batch reactor its concentration drops from $C_{A0} = 2.03$ mol/liter to $C_{Af} = 1.97$ mol/liter. Find the rate equation for the reaction if the kinetics are second-order with respect to A.

10-

For the elementary reactions in series

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S, \quad k_1 = k_2, \quad \text{at } t = 0 \quad \begin{cases} C_A = C_{A0}, \\ C_{R0} = C_{S0} = 0 \end{cases}$$

find the maximum concentration of R and when it is reached.

11-

At room temperature sucrose is hydrolyzed by the catalytic action of the enzyme sucrase as follows:

$$\text{sucrose} \xrightarrow{\text{sucrase}} \text{products}$$

Starting with a sucrose concentration $C_{A0} = 1.0$ millimol/liter and an enzyme concentration $C_{E0} = 0.01$ millimol/liter, the following kinetic data are obtained in a batch reactor (concentrations calculated from optical rotation measurements):

| $C_A$, millimol/liter | 0.84 | 0.68 | 0.53 | 0.38 | 0.27 | 0.16 | 0.09 | 0.04 | 0.018 | 0.006 | 0.0025 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $t$, hr | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |

Determine whether these data can be reasonably fitted by a kinetic equation of the Michaelis–Menten type, or

$$-r_A = \frac{k_3 C_A C_{E0}}{C_A + C_M} \quad \text{where} \quad C_M = \text{Michaelis constant}$$

If the fit is reasonable, evaluate the constants $k_3$ and $C_M$. Solve by the integral method.

12-

Enzyme E catalyzes the transformation of reactant A to product R as follows:

$$A \xrightarrow{\text{enzyme}} R, \qquad -r_A = \frac{200 C_A C_{E0}}{2 + C_A} \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$

If we introduce enzyme ($C_{E0} = 0.001$ mol/liter) and reactant ($C_{A0} = 10$ mol/liter) into a batch reactor and let the reaction proceed, find the time needed for the concentration of reactant to drop to 0.025 mol/liter. Note that the concentration of enzyme remains unchanged during the reaction.

13-

An ampoule of radioactive Kr-89 (half life = 76 minutes) is set aside for a day. What does this do to the activity of the ampoule? Note that radioactive decay is a first-order process.

14-

Find the conversion after 1 hour in a batch reactor for

$$A \rightarrow R, \quad -r_A = 3 C_A^{0.5} \frac{\text{mol}}{\text{liter} \cdot \text{hr}}, \quad C_{A0} = 1 \text{ mol/liter}$$

15-

$$H_2SO_4 + (C_2H_5)_2SO_4 \rightarrow 2C_2H_5SO_4H$$

Initial concentrations of $H_2SO_4$ and $(C_2H_5)_2SO_4$ are each 5.5 mol/liter. Find a rate equation for this reaction.

| $t$, min | $C_2H_5SO_4H$, mol/liter | $t$, min | $C_2H_5SO_4H$, mol/liter |
|---|---|---|---|
| 0 | 0 | 180 | 4.11 |
| 41 | 1.18 | 194 | 4.31 |
| 48 | 1.38 | 212 | 4.45 |
| 55 | 1.63 | 267 | 4.86 |
| 75 | 2.24 | 318 | 5.15 |
| 96 | 2.75 | 368 | 5.32 |
| 127 | 3.31 | 379 | 5.35 |
| 146 | 3.76 | 410 | 5.42 |
| 162 | 3.81 | ∞ | (5.80) |

16-

A small reaction bomb fitted with a sensitive pressure-measuring device is flushed out and then filled with pure reactant A at 1-atm pressure. The operation is carried out at 25°C, a temperature low enough that the reaction does not proceed to any appreciable extent. The temperature is then raised as rapidly as possible to 100°C by plunging the bomb into boiling water, and the readings in Table ¯ are obtained. The stoichiometry of the reaction is $2A \rightarrow B$, and after leaving the bomb in the bath over the weekend the contents are analyzed for A; none can be found. Find a rate equation in units of moles, liters, and minutes which will satisfactorily fit the data.

| $T$, min | $\pi$, atm | $T$, min | $\pi$, atm |
|---|---|---|---|
| 1 | 1.14 | 7 | 0.850 |
| 2 | 1.04 | 8 | 0.832 |
| 3 | 0.982 | 9 | 0.815 |
| 4 | 0.940 | 10 | 0.800 |
| 5 | 0.905 | 15 | 0.754 |
| 6 | 0.870 | 20 | 0.728 |

17-

For the reaction $A \rightarrow R$, second-order kinetics and $C_{A0} = 1$ mol/liter, we get 50% conversion after 1 hour in a batch reactor. What will be the conversion and concentration of A after 1 hour if $C_{A0} = 10$ mol/liter?

18-

For the decomposition A → R, $C_{A0}$ = 1 mol/liter, in a batch reactor conversion is 75% after 1 hour, and is just complete after 2 hours. Find a rate equation to represent these kinetics.

19-

In the presence of a homogeneous catalyst of given concentration, aqueous reactant A is converted to product at the following rates, and $C_A$ alone determines this rate:

| $C_A$, mol/liter | 1 | 2 | 4 | 6 | 7 | 9 | 12 |
|---|---|---|---|---|---|---|---|
| $-r_A$, mol/liter · hr | 0.06 | 0.1 | 0.25 | 1.0 | 2.0 | 1.0 | 0.5 |

We plan to run this reaction in a batch reactor at the same catalyst concentration as used in getting the above data. Find the time needed to lower the concentration of A from $C_{A0}$ = 10 mol/liter to $C_{Af}$ = 2 mol/liter.

20-

The following data are obtained at 0°C in a constant-volume batch reactor using pure gaseous A:

| Time, min | 0 | 2 | 4 | 6 | 8 | 10 | 12 | 14 | ∞ |
|---|---|---|---|---|---|---|---|---|---|
| Partial pressure of A, mm | 760 | 600 | 475 | 390 | 320 | 275 | 240 | 215 | 150 |

The stoichiometry of the decomposition is A → 2.5R. Find a rate equation which satisfactorily represents this decomposition.

21-