

系所:化材系

科目: 化工動力學

- 1. In a batch reactor, after operation for 7 minutes, reactant ($C_{A0} = 1 \text{ mol/liter}$) is 70 % converted. However, after 27 minutes, reactant conversion reaches 90 %. Find a rate equation to represent this reaction. (25%)
- 2. The hypophosphorous acid (H₃PO₂) is transformed into phosphorous acid (H₃PO₃) under the influence of oxidizing agent. The kinetics of this transformation present the following features. At a low concentration of oxidizing agent,

$$\gamma_{H3PO3}$$
 = k [oxidizing agent] [H₃PO₂]

At a high concentration of oxidizing agent,

$$\gamma_{H3PO3} = k' [H^+] [H_3PO_2]$$

To explain the observed kinetics, it has been postulated that, with hydrogen ions as catalyst, normal unreactive H₃PO₂ is transformed reversibly into an active form, the nature of which is unknown. This intermediate then reacts with the oxidizing agent to give H₃PO₃.

- (a) Write a two-step mechanism based on the above description. (10%)
- (b) Derive the rate law (γ_{H3PO3}) for the mechanism in (a), stating any assumption made. (15%)
- 3. For a first-order liquid-phase irreversible reaction,
- (a) Show the Damköhler number (Da) in terms of 'space time' for this reaction if Damköhler number is defined as the following equation. (4%)

$$Da = \frac{-r_{A,0} \cdot V}{F_{A,0}} = \frac{\text{Rate of reaction at entrance}}{\text{Entering flow rate of A}}$$

- (b) Express the conversion rate of this reaction in a single CSTR in terms of 'Damköhler number'. (10%)
- (c) Derive the conversion rate of this reaction in terms of 'Damköhler number' if 5 equal-sized CSTRs connected in series with the same volumetric flowrate under the same operating temperature. (10%)
- (d) Considering numerous equal-sized CSTRs connected in series, determine how many reactors are required to reach 80% conversion if (case I) Da = 1.0 and (case II) Da = 0.1. (6%)



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4. Suppose a liquid-phase reaction $(A \rightarrow B + C)$ was carried out isothermally and the data were obtained as following:

Conversion, X	0	0.2	0.4	0.6	0.8
-r _A (kmol/m ³ ·hr)	73	60	25	8	5

The molar flow rate is 20 kmol/hr.

- (a) For a single CSTR, what is the volume necessary to achieve 80% conversion of the entering species A? (4%)
- (b) For the two CSTRs in series, 40% conversion rate is achieved in the first reactor. What is the volume of each of the two reactors necessary to achieve 80% overall conversion of the entering species A? (8%)
- (c) Followed by part (b), determine the volume of PFR if it is used to replace the second CSTR. (8%)