

1.7 Isoprene and acrolein react together according to second order kinetics (first order with respect to both isoprene and acrolein). The stoichiometric coefficient  $b = 1$ . If ratio of moles of acrolein to moles of isoprene in the feed is kept at 5.0 and reaction time is 600 s, which action will result in the least reaction time?

- (1) Increasing temperature from 150 °C to 175 °C, or
- (2) Changing the stoichiometric concentration ratio of acrolein to isoprene from 5.0 to 4.0 keeping the concentration of isoprene constant at 1 mol/L.

- The batch reactor operates at constant volume.
- The following data apply:  
 $k_1 = 2.2 \times 10^{-4} \text{ L}/(\text{mol}\cdot\text{s})$  at  $150 \text{ }^\circ\text{C}$ ,  
 $k_2 = 7.6 \times 10^{-4} \text{ L}/(\text{mol}\cdot\text{s})$  at  $175 \text{ }^\circ\text{C}$

# 1.7 Solution:

- Fractional volume change,  $\varepsilon = 0$ ,
- Stoichiometric concentration ratio of B,  $M_1 = 5.0$
- Reaction time,  $t_b = 600$  s.
- $C_{A0} = 1$  mol/L
- $kbt_b C_{A0} = \frac{1}{M-1} \ln \frac{M-X_A}{M(1-X_A)}$
- $2.2 \times 10^{-4} (1)(600)(1) = \frac{1}{5-1} \ln \frac{5-X}{5(1-X)}$
- $X=0.465$

- First Option:
- Temperature,  $T_2 = 175 \text{ }^\circ\text{C}$
- Reaction rate constant,  $k_2 = 7.6 \times 10^{-4} \text{ mol}/(\text{L}\cdot\text{s})$
- Stoichiometric concentration ratio of B,  $M_1 = 5.0$

$$t_{b1} = \frac{1}{k_2 b C_{A0} (M_1 - 1)} \ln \frac{M_1 - X_A}{M_1 (1 - X_A)}$$

$$t_{b1} = \frac{1}{7.6 \times 10^{-4} (1)(1) (5.0 - 1)} \ln \frac{5.0 - 0.465}{5(1 - 0.465)} = 173.7 \text{ s}$$

- Second Option

- $$t_{b2} = \frac{1}{k_1 b C_{A0} (M_2 - 1)} \ln \frac{M_2 - X_A}{M_2 (1 - X_A)}$$

- $$t_b = \frac{1}{2.2 \times 10^{-4} (1) (1) (4.0 - 1)} \ln \frac{4.0 - 0.465}{4 (1 - 0.465)} = 760.7 \text{ s}$$

- Obviously the first option results in a smaller reaction time.