

3.9

$$-\ln \left( 1 - \frac{x_A}{x_{Ae}} \right) = (k_1 + k_2) t.$$

How?

$$\frac{k_1}{k_2} = \frac{m + x_{Ae}}{1 - x_{Ae}} = \frac{C_{Re}}{C_{Ae}}$$

$$k_2 = \left( \frac{1 - x_{Ae}}{m + x_{Ae}} \right) k_1$$

$$\begin{aligned} k_1 + k_2 &= k_1 \left[ 1 + \frac{1 - x_{Ae}}{m + x_{Ae}} \right] \\ &= k_1 \left[ \frac{m + 1}{m + x_{Ae}} \right]. \end{aligned}$$

Rev Rate equation

$$-\ln \left( 1 - \frac{x_A}{x_{Ae}} \right) = \left( \frac{m + 1}{m + x_{Ae}} \right) k_1 \times t$$

$$k_1 \left( \frac{m + 1}{m + x_{Ae}} \right) = k_1 + k_2.$$

∴

$$-\ln \left( 1 - \frac{x_A}{x_{Ae}} \right) = (k_1 + k_2) t.$$

$$t = 8 \text{ mins for } x_A = 1/3, \quad x_{Ae} = 2/3$$

$$\therefore -\ln\left(1 - \frac{Y_3}{2/3}\right) = (K_1 + K_2) 8$$

$$\therefore K_1 + K_2 = \frac{\ln^2}{8} = 0.086625 \text{ min}^{-1} \quad \text{--- (1)}$$

$$\frac{K_1}{K_2} = \frac{C_{Re}}{C_{Ac}} = \frac{C_{A0} X_{Ac}}{C_{A0}(1 - X_{Ac})} = \frac{0.5 \times 2/3}{0.5 \times 1/3} = 2$$

$$\therefore K_1 = 2K_2 \quad \text{--- (2)}$$

Solving (1) and (2)

$$K_1 = 0.0577, \quad K_2 = 0.028875$$

$\therefore$

$$-r_A = K_1 C_A - K_2 C_R$$

$$= 0.05775 C_A - 0.028875 C_R$$

3.11

$$C_{A0} = 500$$

From table if  $C_{A0} = 500$   $t_0 = 100 \text{ min}$   
 $\therefore$  For 5 hrs.  $t = 100 + 300 = 400 \text{ min}$

$$\therefore X_A = 1 - \frac{C_A}{C_{A0}} = 1 - \frac{200}{500} = 0.6$$

or

Plot graph, find  $k$ , then find  $C_A$   
 Then find  $X_A$ .

3.15

$$-r_A = \frac{k_3 C_A C_{E0}}{C_A + m}$$

$$- \frac{dC_A}{dt} = \frac{k_3 C_{E0} \cdot C_A}{(C_A + m)}$$

$$- dC_A \left( \frac{C_A + m}{C_A} \right) = k_3 C_{E0} dt$$

Integrating on both sides

$$-dC_A \left[ 1 + \frac{m}{C_A} \right] = k_3 C_{E0} dt$$

$$(C_{A0} - C_A) + m \ln \frac{C_{A0}}{C_A} = k_3 C_{E0} t$$

$$\frac{1}{m} + \frac{\ln \frac{C_{A0}}{C_A}}{C_{A0} - C_A} = \frac{k_3 C_{E0}}{m} \left( \frac{t}{C_{A0} - C_A} \right)$$

Plot graph  $\frac{\ln \frac{C_{A0}}{C_A}}{C_{A0} - C_A}$  vs  $\frac{t}{C_{A0} - C_A}$

$$\text{slope} = \frac{k_3 C_{E0}}{m}$$

$$\text{intercept} = -\frac{1}{m}$$

$$k_3 = 19.7 \text{ hr}^{-1}$$

$$m = 0.197 \frac{\text{mmol}}{\text{lit}}$$

$$3.18 \quad -r_A = \frac{200 C_A C_{E_0}}{2 + C_A} \Rightarrow k_3 = 200.$$

$$n = 2.$$

$$C_{E_0} = 0.001 \text{ mol/lit}$$

$$(C_{A_0} - C_A) + n \ln \frac{C_{A_0}}{C_A} = k_3 C_{E_0} t$$

$$\text{For } C_A = 0.025 \text{ mol/lit \& } C_{A_0} = 10 \text{ mol/lit}$$

$$(10 - 0.025) + 2 \ln \left( \frac{10}{0.025} \right) = 200 \times 0.001 \times t$$

$$9.975 + 11.9829 = 0.2 \times t.$$

$$\frac{21.9579}{0.2} = t$$

$$t = 109.7895 \text{ min}$$

5.

$$C = C_0 e^{-kt} \quad \text{or} \quad \frac{C}{C_0} = e^{-kt}$$

$$\text{or } t = \frac{1}{k} \ln \left( \frac{C_0}{C} \right)$$

$$\frac{C}{C_0} = 0.6 \quad k = 3.546 \times 10^{-4} \text{ hr}^{-1}$$

$$t = \frac{1}{k} \ln \left( \frac{C_0}{C} \right) = \frac{1}{3.546 \times 10^{-4}} \ln \left( \frac{1}{0.6} \right)$$

$$= 1440.56 \text{ hr}$$

$$= 60.02 \text{ days}$$

6.

**Solution:**

First order reaction,  $\ln(C_0/C) = k \cdot t$  or  $k = 1/t \cdot \ln(C_0/C)$  or  $t = (1/k) \cdot \ln(C_0/C)$

At 298 K ( $T_1$ ),  $k_1 = 1/(300 \cdot 24 \cdot 60) \cdot \ln(2) = 1.6045 \times 10^{-6} \text{ min}^{-1}$ .

Using the Arrhenius equation for temperature dependency,

$$\ln(k_2/k_1) = E/R \cdot [1/T_1 - 1/T_2]$$

$$\text{or } k_2 = k_1 \cdot \exp(E/R \cdot [1/T_1 - 1/T_2])$$

where  $T_2 = 523 \text{ K}$ ,  $E = 60,000 \text{ J/mol}$ ,  $R = 8.314 \text{ J/mol-K}$

Plugging in values for the terms on the right hand side of the above equation,

$$k_2 = 0.0537 \text{ min}^{-1}$$

From the 1<sup>st</sup> order rate equation,

$$C/C_0 = \exp(-k_2 \cdot t)$$

Plugging in  $k_2$  and  $t = 30 \text{ min.}$ ,  $C/C_0 = 0.1996$  so **approximately 80% of the initial aspartame is lost after baking for 30 minutes.**