Web Example 18–1 Equivalency of Models for a First-Order Reaction

Show that $X_{\text{T–I–S}} = X_{\text{MM}}$ for a first-order reaction

$$\text{A} \xrightarrow{k} \text{B}$$

Solution

For a first-order reaction, we already showed in Problem P17-3$_{\text{B}}$ that

$$\boxed{X_{\text{Seg}} = X_{\text{MM}}}$$

Therefore, we only need to show $X_{\text{Seg}} = X_{\text{T-I-S}}$.
For a first-order reaction in a batch reactor the conversion is

$$X = 1 - e^{-kt} \tag{E18-1.1}$$

Segregation Model

$$\overline{X} = \int_0^\infty X(t)E(t)dt = \int_0^\infty (1 - e^{-kt})E(t)dt \tag{E18-1.2}$$

$$= 1 - \int_0^\infty e^{-kt}E(t)dt \tag{E18-1.3}$$

Using Maclaurin's series expansion gives

$$e^{-kt} = 1 - kt + \frac{k^2t^2}{2} + \text{Error} \tag{E18-1.4}$$

Neglecting the error term

$$\overline{X} = 1 - \int_0^\infty \left[1 - kt + \frac{k^2t^2}{2}\right]E(t)dt \tag{E18-1.5}$$

$$\overline{X} = \tau k - \frac{k^2}{2}\int_0^\infty t^2E(t)dt \tag{E18-1.6}$$

To evaluate the second term, we first recall Equation (16-23) for the variance

$$\sigma^2 = \int_0^\infty (t-\tau)^2E(t)dt = \int_0^\infty t^2E(t)dt - 2\tau\int_0^\infty tE(t)dt + \tau^2\int_0^\infty E(t)dt \tag{E18-1.7}$$

$$\sigma^2 = \int_0^\infty t^2E(t)dt - 2\tau^2 + \tau^2 \tag{E18-1.8}$$

Rearranging Equation (E18-1.8)

$$\int_0^\infty t^2E(t)dt = \sigma^2 + \tau^2 \tag{E18-1.9}$$

Combining Equations (E18-1.6) and (E18-1.9), we find the mean conversion for the segregation model for a first-order reaction is

$$\boxed{\overline{X} = \tau k - \frac{k^2}{2}(\sigma^2 + \tau^2)} \tag{E18-1.10}$$

Tanks in Series

Recall from Chapter 4, for n tanks in series for a first-order reaction, the conversion is

$$X = 1 - \frac{1}{\left(1 + \frac{\tau}{n}k\right)^n} \tag{E18-1.11}$$

Rearranging yields

$$X = 1 - \left(1 + \frac{\tau}{n}k\right)^{-n} \tag{E18-1.12}$$

We now expand in a binomial series

$$X = 1 - \left[1 - n\frac{\tau}{n}k + \frac{n(n+1)}{2}\frac{\tau^2 k^2}{n^2} + \text{Error}\right] \tag{E18-1.13}$$

$$= k\tau - \frac{\tau^2 k^2}{2} - \frac{\tau^2 k^2}{2n} + \text{Error} \tag{E18-1.14}$$

Neglecting the error gives

$$X = k\tau - \frac{k^2}{2}\left[\tau^2 + \frac{\tau^2}{n}\right] \tag{E18-1.15}$$

Rearranging Equation (18-12) in the form

$$\frac{\tau^2}{n} = \sigma^2 \tag{18-12}$$

and substituting in Equation (E18-1.15), the mean conversion for the T-I-S model is

$$\boxed{X = \tau k - \frac{k^2}{2}(\tau^2 + \sigma^2)} \tag{E18-1.16}$$

We see that Equations (E18-1.10) and (E18-1.16) are identical; thus, the conversions are identical, and for a first-order reaction we have

Important result

$$\boxed{X_{\text{T-I-S}} = X_{\text{Seg}} = X_{\text{MM}}} \tag{E18-1.17}$$

But this is true only for a first-order reaction.

Analysis: For first-order reactions, we have shown that no matter how the molecules mix (macromixing, micromixing, T-I-S), the conversions predicted for each model are identical.