Part (c) Solution by hand calculation to perhaps give greater insight and to build on techniques in Chapter 2

We will now integrate Equation (WE11-3.8) using Simpson's rule after forming a table (WE11-3.1) to calculate $(F_{A0}/-r_A)$ as a function of X. This procedure is similar to that described in Chapter 2. We now carry out a sample calculation to show how Table WE11-3.1 was constructed.

For example, for $X = 0.2$, follow the downward arrows for the sequence of the calculations.

(a) First calculate the temperature T, Equation (WE11-3.9):

$T = 330 + 43.4(0.2) = 338.6$ K

(b) Calculate k: Equation (WE11-3.10):

$$k = 31.1 \exp\left[7906 \left(\frac{338.6 - 360}{(360)(338.6)} \right) \right] = 31.1 \exp\left(-1.388 \right) = 7.76 \text{ h}^{-1}$$

(c) Calculate K_C: Equation (WE11-3.11):

$$K_C = 3.03 \exp\left[-830.3 \left(\frac{338.6 - 333}{(333)(338.6)} \right) \right] = 3.03 e^{-0.0412} = 2.9$$

(d) Calculate X_e: Equation (WE11-3.12):

$$X_e = \frac{2.9}{1 + 2.9} = 0.74$$

(e) Calculate $-r_A$: Equation (WE11-3.7):

$$-r_A = \left(\frac{7.76}{\text{h}} \right) (9.3) \frac{\text{mol}}{\text{dm}^3} \left[1 - \left(1 + \frac{1}{2.9} \right)(0.2) \right] = 52.8 \frac{\text{mol}}{\text{dm}^3 \cdot \text{h}} = 52.8 \frac{\text{kmol}}{\text{m}^3 \cdot \text{h}}$$

(f) Dividing $(-r_A)$ into F_{A0}

$$\frac{F_{A0}}{-r_A} = \frac{(0.9 \text{ mol butane}/\text{mol total})(163. \text{ kmol total}/\text{h})}{52.8 \frac{\text{kmol}}{\text{m}^3 \cdot \text{h}}} = 2.78 \text{ m}^3$$

Continuing in this manner for other conversions, we can complete Table WE11-3.2.

TABLE WE11-3.2   HAND CALCULATION

X	T (K)	k (h^{-1})	K_C	X_e	$-r_A$(kmol/m$^3 \cdot$h)	$\frac{F_{A0}}{-r_A}$ (m^3)
0	330	4.22	3.1	0.76	39.2	3.74
0.2	338.7	7.76	2.9	0.74	52.8	2.78
0.4	347.3	14.02	2.73	0.73	58.6	2.50
0.6	356.0	24.27	2.57	0.72	37.7	3.88
0.65	358.1	27.74	2.54	0.718	24.5	5.99
0.7	360.3	31.67	2.5	0.715	6.2	23.29

Use the data in Table WE11-3.2 to make a Levenspiel plot, as in Chapter 2.

(e) The reactor volume for 70% conversion will be evaluated using the quadrature formulas. Because $(F_{A0}/-r_A)$ increases rapidly as we approach the adiabatic equilibrium conversion, 0.71, we will break the integral into two parts

$$V = \int_0^{0.7} \frac{F_{A0}}{-r_A} \, dX = \int_0^{0.6} \frac{F_{A0}}{-r_A} \, dX + \int_{0.6}^{0.7} \frac{F_{A0}}{-r_A} \, dX \qquad \text{(WE11-3.14)}$$

Using Equations (A-24) and (A-22) in Appendix A, we obtain

$$V = \frac{3}{8} \times \frac{0.6}{3} [3.74 + 3 \times 2.78 + 3 \times 2.50 + 3.88] \text{m}^3 + \frac{1}{3} \times \frac{0.1}{2} [3.88 + 4 \times 5.99 + 23.29] \text{m}^3$$

$$V = 1.75 \text{ m}^3 + 0.85 \text{ m}^3$$

$$\boxed{V = 2.60 \text{ m}^3}$$

Analysis: **Part (c)** You probably will never ever carry out a hand calculation similar to the one shown above. So why did we do it? Hopefully, we have given you a more intuitive feel for the magnitude of each of the terms and how they change as one moves down the reactor (i.e., what the computer solution is doing), as well as a demonstration of how the Levenspiel Plots of $(F_{A0}/-r_A)$ versus X in Chapter 2 were constructed. At the exit, $V = 2.6 \text{ m}^3$, $X = 0.7$, $X_e = 0.715$, and $T = 360$ K.