Chapter 10: Computer Simulations and Experiments

P10-1B (a) Example 10-1: Site Concentrations, $C_W$, $C_B$ and $C_T$

*Wolfram*

(i) Find the critical value of $K_T$ and $K_B$ at which fraction of vacant sites starts to increase with conversion? Vary only one parameter at a time.

(ii) Find the value of $K_B$ such that fraction of sites occupied by benzene is doubled at 40% conversion of Toluene.

(iii) Find the value $K_B$ where the curve for $\left(\frac{C_{v,S}}{C_v}\right)$ versus conversion $X$ changes from convex to concave and explain why this shape change occurs.

(b) Example 10-2: Catalytic Reactor Design

*Wolfram*

(i) How would the conversion change if the entering pressure were (1) increased to 80 atm or (2) it were reduced 1 atm?

(ii) What if the molar flow rate were reduced by 50%; how would $X$ and $p$ change?

(iii) After reviewing *Generating Ideas and Solutions* on the Web site (http://www.umich.edu/~elements/Se/oc/SCPS_3rdEdBook(Ch07).pdf), choose one of the brainstorming techniques (e.g., lateral thinking) to suggest two questions that should be included in this problem.

(iv) Write two conclusions from your experiments with the sliders in this example.

*Polymath*

(v) What catalyst weight would be required for 60% conversion?

(vi) Which parameter will you vary so that $P_B = P_{H2}$ at the middle of the reactor (i.e., $W = 5000Kg$).

(c) Example 10-3: Hydrogenation Ethylene to Ethane

(1) Use Polymath to learn how your answers would change if the following data for run 10 were incorporated in your regression table.

$$-r'_E = 0.8 \text{ mol/kg-cat \cdot s}, P_E = 0.5 \text{ atm}, P_{EA} = 15 \text{ atm}, P_H = 2 \text{ atm}.$$ 

(2) How do the rate laws (e) and (f) compare with the nonlinear analysis with the other rate laws used to model the data?

(d) Example 10-4: Calculating Conversion with Catalyst Decay

*Wolfram*

(i) What is the maximum conversion that can be achieved if there is no catalyst decay?

(ii) Vary $k$ and $k_d$ and describe what you find. Can you explain why there is no effect of catalyst decay on conversion at a high value of $k$?

(iii) Vary $E$, $E_g$, $k_1$, and $k_2$ and then write a few sentences describing the results of your experiments.

(iv) Explain why conversion with catalyst decay increases with increasing $E_g$ and decreases with increasing $E$.

*Polymath*

(v) Vary the ratio of $(k/k_d)$ and describe what you find.

(vi) Repeat this example (i.e., the plotting of $X$ vs. $t$) for a second-order reaction with $(C_{AO} = 1 \text{ mol/dm}^3)$ and first-order decay and describe the differences from the base case.

(vii) Repeat this example for a first-order reaction and first-order decay and describe the differences from the base case.

(viii) Repeat this example for a second-order reaction $(C_{AO} = 1 \text{ mol/dm}^3)$ and a second-order decay and describe the differences from the base case.

(e) Example 10-5: Catalytic Cracking in a Moving Bed

*Polymath*

(i) Use Polymath to learn what the conversion would be if there is no catalyst decay.

(ii) What if the solids and reactants entered from opposite ends of the reactor? How would your answers change?

(iii) What if the decay in the moving bed were second order? By how much must the catalyst charge, $U_0$, be increased to obtain the same conversion?

(iv) What if $\varepsilon = 2$ (e.g., $A \rightarrow 3B$) instead of zero. How would the results be affected?
Example 10-6: Decay in a Straight-Through Transport Reactor

**Polymath**

(i) What if you varied the parameters $P_{A0}$, $U_e$, $A$, and $k'$ in the STTR? What parameter has the greatest effect on either increasing or decreasing the conversion?

(ii) Ask questions such as: What is the effect of varying the ratio of $k$ to $U_e$ or of $k$ to $A$ on the conversion? Make a plot of conversion versus distance as $U_e$ is varied between 0.5 and 50 m/s.

(iii) Sketch the activity and conversion profiles for $U_e = 0.025, 0.25, 2.5$, and 25 m/s.

(iv) What generalizations can you make? Plot the exit conversion and activity as a function of gas velocity between velocities of 0.02 and 50 m/s.

(v) What gas velocity do you suggest operating at?

(vi) What is the corresponding entering volumetric flow rate?

(vii) What concerns do you have operating at the velocity you selected? Would you like to choose another velocity? If so, what is it? Which parameter will you vary so that conversion increases but activity decreases? Explain, if you can, this unusual behavior.