A First Course on Kinetics and Reaction Engineering

Activity 32.1

Problem Purpose

This problem will allow you to practice the analysis of a semi-batch reactor.

Problem Statement

The reaction between A and B produces the desired product, D according to reaction (1), but B also decomposes according to reaction (2), generating the undesired product U. The reactions take place in solution, and the heat of reaction is so small that the reactions are effectively isothermal. Reaction (1) is first order in each of the two reactants, second order overall. Reaction (2) is second order in B. At the process temperature the rate coefficient for reaction (1) is 8×10^{-3} L mol^{-1} min^{-1} and that for reaction (2) is 4×10^{-3} L mol^{-1} min^{-1}. A 2000 L stirred tank reactor will be used, taking its feed from one solution containing A at a concentration of 3 mol L^{-1} and from a second containing B at a concentration of 1 mol L^{-1}. Compare the selectivity (mol D per mol U) that will result from a batch process charged with 500 L of the A solution and 1500 L of the B solution to a semi-batch process where the reactor is charged with 500 L of the A solution after which time the B solution flows into the reactor at a rate of 150 L h^{-1}. In both cases, allow the reaction to proceed to a 95% conversion of B; in the semi-batch system, this may require stopping the flow when the reactor contains 2000 L of solution and allowing it to continue to react as a batch reactor until the desired conversion is reached.

$$A + B \rightarrow D \tag{1}$$

$$2\,B \rightarrow U \tag{2}$$

Worksheet

The analysis of the batch process will be left for you to perform as an exercise. Here it will simply be noted that if the reactor is operated as a batch reactor, it takes 651 minutes for the conversion of B to reach 95%, and at that time, the overall selectivity is equal to 3.2 mol D per mol U.

Before beginning the analysis of semi-batch operation, mentally perform a qualitative analysis and predict whether (a) the semi-batch processing will take more or less time than batch processing and (b) whether the final selectivity in semi-batch processing will be larger or smaller than that in batch processing.

1. Read through the problem statement. Each time you encounter a quantity, write it down and equate it to the appropriate variable. When you have completed doing so, if there are any additional constant quantities that you know will be needed and that can be calculated from the values you found, write the equations needed for doing so.

2. Generate the design equations needed to model the semi-batch reactor by simplification of the general design equations found in Unit 32 or on the AFCoKaRE Exam Handout.

3. Determine whether the design equations can be solved once, covering the entire semi-batch process, or whether they will need to be solved in stages. If they need to be solved in stages, identify the beginning and end of each stage.

4. For each stage of the solution, identify the specific set of equations that needs to be solved and within those equations identify the independent and dependent variables, if appropriate, and the unknown quantities to be found by solving the equations.

5. Assuming that the semi-batch reactor design equations will be solved numerically, specify the information that must be provided and show how to calculate any unknown values for each stage of the solution.

6. Identify what variables will become known upon solving the design equations and show how those variables can be used to answer the questions that were asked in the problem.