A First Course on Kinetics and Reaction Engineering
Example 12.5

Problem Purpose

This example examines what one needs to do to perform *equivalent* kinetics experiments using different reactor types.

Problem Statement

Someone in your company read an old report that included one batch reactor experiment on the conversion of glucose to fructose. The experiment was run in a 750 mL batch reactor using a 0.5 M aqueous solution of glucose at a pH of 2.5 and at 95 °C. The experimental run lasted 3 hours, with samples being taken every 20 minutes. This resulted in nine experimental data points. You've been asked to generate a data set that can be compared to the results in the report. The conditions do not need to be identical, but they should be similar. You do not have a suitable batch reactor to use, but you do have a 250 mL reactor that has been verified as a perfectly mixed CSTR. Describe how you would perform the necessary experiments using this CSTR.

Problem Solution

Because you are using a CSTR while the original study used a batch reactor, there will be some differences between the two data sets. It appears that the essence of the assignment is to quickly validate the previous study. As such, it makes sense to try to use conditions as similar as possible to those used in the prior work. The data in the report were all generated in a single experimental run that lasted 3 hours; because you are using a CSTR, you will need to make nine separate experimental runs if you want to generate nine data similar data points.

The first data point from the report corresponds to a system that had reacted for 20 minutes. With a CSTR, you start the feed flowing at the desired composition and temperature and wait for steady state to be reached; then you take a sample. Once steady state has been reached, it doesn't matter whether you wait 20 minutes or the full three hours, the composition of the sample will be the same. Put differently, the duration of a steady-state CSTR experiment has nothing to do with how long the reagents have been allowed to react. Instead, it is the average residence time that determines how much time the reactants have had to react. The average residence time, $\overline{t}$, is just the steady state volume of fluid within the reactor, V_{fluid}, divided by the volumetric flow into the reactor, $\dot{V}^0$, as given in equation (1).

$$\overline{t} = \frac{V_{fluid}}{\dot{V}^0} \tag{1}$$

One approach would be to use the same feed composition, pH and reactor temperature as were used in the batch experiment, and to vary the feed rate in the 9 CSTR experiments so that the CSTR residence times matched the sampling times used in the batch reactor experiments. With this approach,

you would like the average residence time to be 20 minutes in your first experiment. Since the fluid volume of your reactor is 250 mL, this means that the volumetric flow rate should be 12.5 mL min^{-1}, as can be found by rearranging equation (1).

$$\dot{V}^0 = \frac{V_{fluid}}{\overline{t}} = \frac{250\ \text{mL}}{20\ \text{min}} = 12.5\frac{\text{mL}}{\text{min}} \qquad (2)$$

The remaining data points from the report represent batch reaction times of 40, 60, 80, 100, 120, 140, 160 and 180 minutes, and you can calculate the corresponding CSTR feed rates as shown in Table 1.

Table 1. CSTR feed rates necessary to match CSTR residence time to batch reaction time.

Batch Reaction Time (min)	***Equivalent CSTR Flow Rate (mL/min)***
20	12.50
40	6.25
60	4.17
80	3.13
100	2.50
120	2.08
140	1.79
160	1.56
180	1.39

There are a couple of shortcomings to this approach. First, the last few data points would require very precisely maintaining very low flow rates, and that might prove challenging experimentally. More significantly, the conversions that would be observed in the CSTR experiments above, would very likely be much smaller than those that were observed in the corresponding batch experiments. The reason for this is that the conversion in the batch experiments represents an integral of the rate over the range of compositions from the initial to the final. During the initial stages, the rate is expected to be high, leading to reasonable conversions. In the CSTR experiments, the composition will not vary during the time of reaction, and for the whole time the reaction takes place, the composition will be the final composition. As a consequence, the conversion is likely to be smaller in the CSTR experiments.

An alternative approach would be to use the same residence time in all the CSTR experiments, perhaps 20 minutes as in the first row of Table 1. The first experiment would use the same feed as in the batch reactor experiments. However, in each successive CSTR experiment, the amount of glucose in the feed (the reactant) would be decreased and replaced with a stoichiometrically equivalent amount of fructose (the product). Doing this simulates increased conversion of glucose. The amounts of glucose replaced in each of the nine experiments could be chosen to match the conversion at each of the batch reactor sampling times. The resulting data still would not be completely equivalent to the batch experiments, but the range of compositions (or conversions) would be closer than if the residence time were varied.