A First Course on Kinetics and Reaction Engineering

Example 18.3

Problem Purpose
This example illustrates the use of a qualitative analysis to predict the effects of a change in the operation of a batch reactor.

Problem Statement
The series reactions given in equations (1) and (2) take place in the liquid phase in an isothermal batch reactor. The concentrations of S, D and U are plotted as a function of reaction time in Figure 1. Suppose the solvent used in the reactor is changed, and doing so has no effect upon the rate coefficient of reaction (1), but it decreases the rate coefficient of reaction 2 to 10% of its value in the original solvent. How would the plot shown in Figure 1 change?

\[ S \rightarrow D \quad (1) \]
\[ D \rightarrow U \quad (2) \]

Figure 1. Concentration versus time plot for Example 18.3
Problem Analysis

This problem shows the concentration profiles for a series reaction network taking place in an isothermal batch reactor and asks how they would change if one of the rate coefficients were to change. A qualitative analysis will indicate the relative changes in the curves, which is all that can be determined with the data given.

Problem Solution

The change in solvent has absolutely no effect upon the concentration of S as a function of time because the rate coefficient for the first reaction remains the same and the reactions are irreversible. The latter can be seen from the long-time behavior in Figure 1; the concentration of S and D both go to zero.

Initially we expect very little effect upon the concentration of D versus time either. This is because at very short times there is so little D present that the effect of the second reaction is negligible. As the concentration of D builds, the effect of reaction (2) will increase. However, with the new solvent, this will take a longer time because the rate of reaction (2) is slower in the new solvent. Consequently, we expect the concentration of D to continue to increase for a longer time when the reaction runs in the new solvent. Eventually, however, the rate of reaction (2) will increase to the point where it equals that of reaction (1). At this point, the concentration of D will reach its maximum, after which it will steadily decline to zero.

In short, we expect the plot of the concentration of D versus time to have a similar shape in both solvents, but in the new solvent we expect it to reach a larger maximum concentration and to do so at a longer reaction time. The concentration of U versus time will also be similar in both solvents, but it will grow more slowly in the new solvent than in the original. The expected behavior is shown in Figure 2 where the dashed lines represent the behavior in the new solvent.

Figure 2. Comparison of concentration profiles in the two solvents.