A First Course on Kinetics and Reaction Engineering

Example 21.2

Problem Purpose

This example illustrates the qualitative analysis of a reversible reaction occurring in an adiabatic CSTR.

Problem Statement

An acid, A, is to be hydrated according to the reaction A + W ⇄ P, where W represents water and P, the product. The reaction is exothermic and the rate expression is given in equation (1). If this reaction takes place in a CSTR operating adiabatically, sketch how the temperature and conversion will vary if the space time is varied. How will these plots change if the feed temperature is raised? Do not write any equations in deriving your solution.

$$r = kC_AC_W\left[1 - \frac{C_P}{KC_AC_W}\right] \tag{1}$$

Problem Analysis

The problem specifically states that no equations are to be used, therefore, this problem will be approached using a qualitative analysis. Since the system is adiabatic, both concentration and temperature effects must be considered. The shape of temperature and concentration profiles as a function of space time are expected to be similar to temperature and concentration versus time profiles for a batch reactor.

Problem Solution

Here we have a reversible exothermic reaction that is taking place adiabatically. Let's start by noting that if the space time was zero, no reaction would take place so the conversion would be zero and the temperature would equal the feed temperature.

If the space time was increased just slightly, meaning the reaction would occur for only a very short amount of time, the conversion would increase because a little reaction would take place. A small amount of heat would be released as a consequence of reaction taking place, and since no heat is removed in an adiabatic reactor, the temperature would increase slightly.

If the space time was increased yet a little more, the reaction would take place for a little longer. It would be taking place at a higher temperature than before, at a lower reactant concentration and at a higher product concentration. Since the temperature dependence of the rate is exponential while the concentration dependence is not, the temperature increase is expected to predominate over the concentration changes as long as the concentrations aren't approaching their equilibrium values. Therefore, during the time the reaction takes place, the rate will be higher than at the previous space velocity. As a consequence, the temperature and the conversion will rise more steeply than they did at the lower space velocity.

As the space time continues to increase, the steepness of the conversion versus space time must eventually start to decrease because the system can't progress beyond the equilibrium conversion (the conversion can't keep increasing faster and faster forever). Thus, there must be an inflection point in the conversion versus space time curve. At space times less than the inflection point, the temperature effect is predominating causing the rate to increase whereas at space times greater than the inflection point, the concentration terms are predominating causing the rate to decrease. The temperature increase is proportional to the amount of reaction that takes place (that is, to the conversion), and so the temperature plot will also display an inflection point.

As the space time increases beyond the inflection point, the conversion and temperature will continue to increase, but with decreasing steepness until their values essentially become constant. The final conversion will be less than 100% and will correspond to the equilibrium conversion and the final temperature will be equal to the adiabatic temperature rise.

Figure 1 shows a representative conversion profile and Figure 2 shows a representative

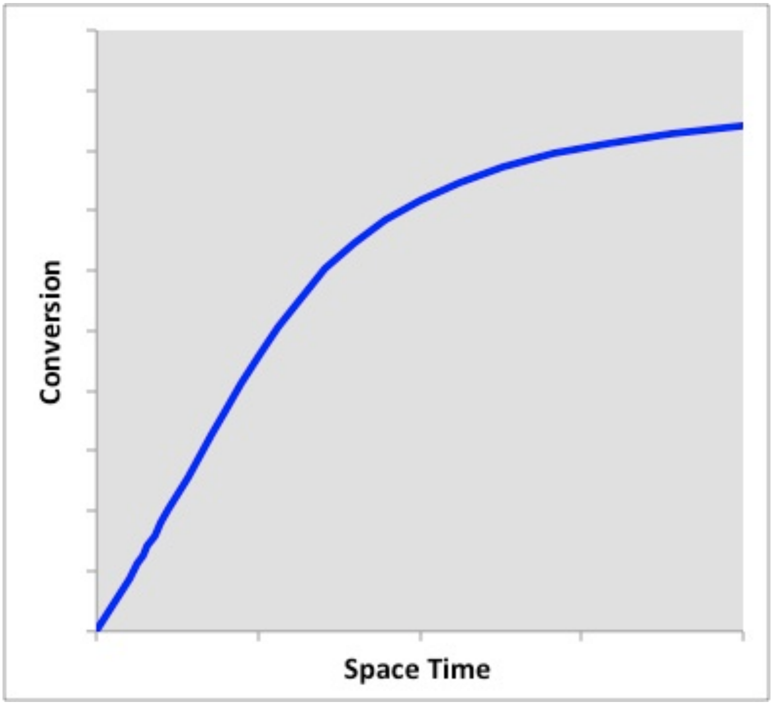

Figure 1. Conversion in a reversible, exothermic reaction as a function of CSTR space time.

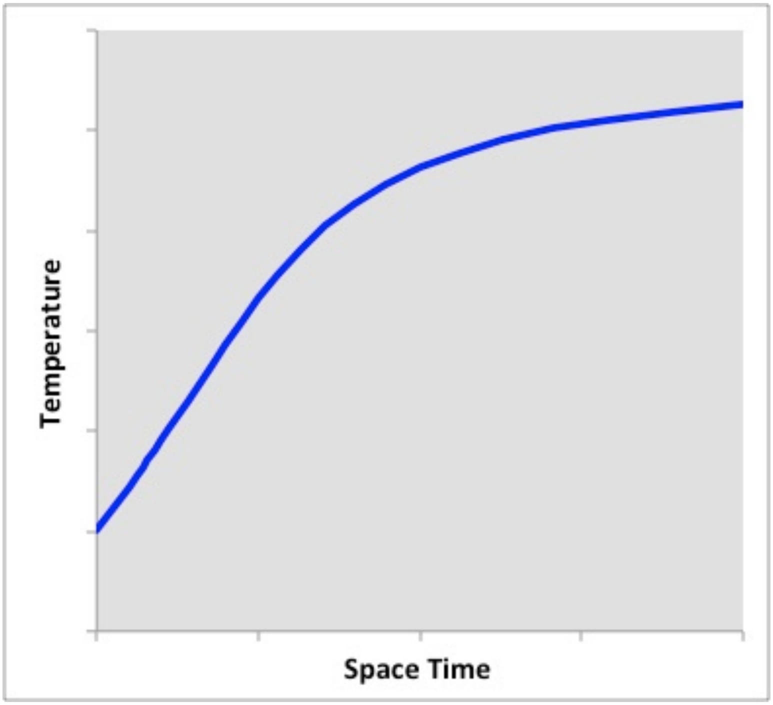

Figure 2. Temperature in a reversible, exothermic reaction as a function of CSTR space time.

temperature profile where the inflection point is very subtle. If the feed temperature was increased, the shapes of curves would be qualitatively the same. Obviously, the temperature profile would lie above that for the lower temperature at all space times. At the higher feed temperature, the rate at lower space times would also be greater, so the conversion would increase more steeply. However, the equilibrium conversion for an exothermic reaction will decrease as the temperature increases. Therefore, the maximum conversion at the higher temperature will be smaller than the maximum conversion at the lower temperature. Consequently, the conversion profile for the higher temperature will start out above that for the lower temperature, but eventually they will cross as shown in Figure 3.

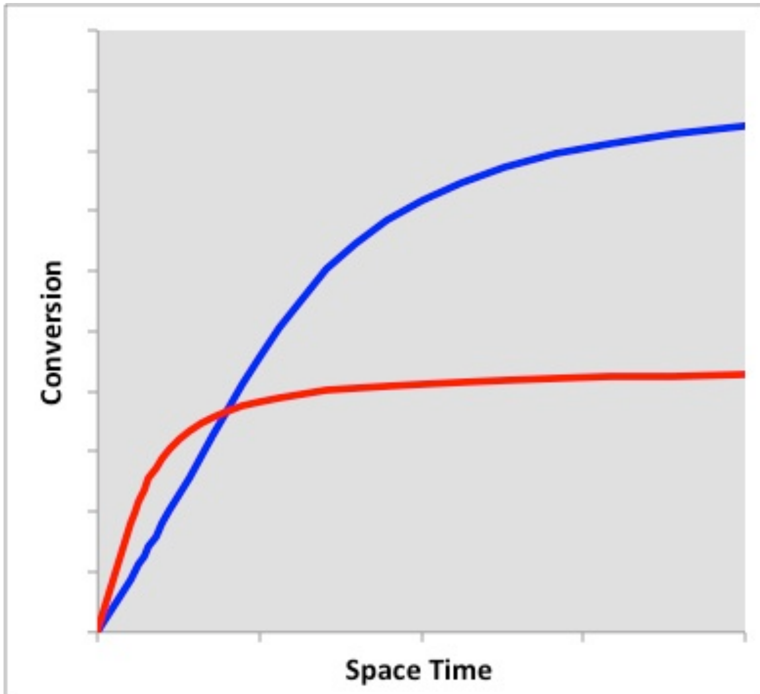

Figure 3. Effect of an increased feed temperature (red curve) on the conversion profile of Figure 1.