A First Course on Kinetics and Reaction Engineering Example 18.2

Problem Purpose

This example illustrates the process involved in the qualitative analysis of an adiabatic batch reactor.

Problem Statement

Ten years ago, your company studied a reaction that has suddenly become of interest again. Two reports were written but in one the reaction is said to be exothermic while in the other it is said to be endothermic. Both reports agree that the reaction is irreversible. A figure similar to Figure 1 appeared in both reports. The figure shows the conversion versus time in an adiabatic batch experiment. Assuming this to be a "normal" reaction, is it endothermic or exothermic and how do you know?



Figure 1. Conversion versus time for a reaction taking place in an adiabatic batch reactor.

Problem Analysis

No quantitative data are provided in this problem. The shape of a conversion versus time plot for an adiabatic exothermic reaction will differ from that for an endothermic reaction. Therefore, a qualitative analysis should reveal whether the reaction is exothermic or endothermic.

Problem Solution

The figure, and particularly the slight inflection point somewhere between one and two minutes, suggests that the reaction is exothermic. This can be seen by observing the change in slope of the conversion versus time plot. Looking at small values of time, the slope can be seen to be increasing as time increases. That is, if you placed a ruler or straightedge at the origin and aligned it so it was tangent to the red line at the origin, you would see that the red line curves up away from the ruler. The slope of the curve is proportional to the rate of reaction. If the reaction was irreversible and endothermic, and if the reaction was being run adiabatically then as the time increased, both the temperature and the reactant concentration would decrease. Both of these phenomena would cause the rate of a normal reaction to decrease and so the slope would continually decrease as the time increases. In contrast, if the reaction is exothermic, then as the time increase the rate (and hence the slope) while the latter would tend to decrease the rate (and hence the slope). Since the temperature appears in an exponential while the reactant concentration appears raised to a power typically around 1 to 2, it would be expected that initially the temperature term would predominate and the rate would increase.