A First Course on Kinetics and Reaction Engineering
Example 18.1

Problem Purpose

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

Problem Statement

Consider an irreversible auto-catalytic reaction taking place isothermally in a batch reactor. Sketch the reactant concentration versus time and the rate of reaction versus time. Describe why the curves are shaped as they are without using any equations.

Problem Analysis

This problem involves the qualitative analysis of an isothermal batch reactor where an auto-catalytic reaction takes place. We begin by considering how the concentrations will change during a brief interval at the start of the reaction. (We need not consider temperature changes because the reactor is isothermal.) We then consider whether concentration changes will be greater or smaller in a subsequent interval. If the trends revealed by this analysis will lead naturally to the equilibrium condition, the analysis is complete. If the trends will not lead naturally to the equilibrium condition, we infer what must change and why it must change so that the system asymptotically approaches equilibrium.

Problem Solution

We'll assume that initially there is no product present. During the first small increment of time, the concentration of reactant will decrease and the concentration of product will increase. The temperature will not change, since the system is isothermal. During the next short interval of time the rate will be greater than it was during the first increment. This is because, by definition, the rate of an auto-catalytic reaction increases as the concentration of the product increases. Therefore, the reactant concentration will decrease by a greater amount. This is the opposite of normal behavior: normally a plot of reactant concentration versus time is steepest initially and becomes less steep with increasing time, leading to a concave up shape; here the plot becomes steeper with increasing time, leading to a concave downward shape.

Clearly, this behavior can not continue indefinitely or the reactant concentration would become negative. At some point, effect of the reactant concentration becoming smaller has to predominate over the effect of the product concentration becoming larger. At that point, the rate will decrease with increasing time. Thus, the rate must pass through a maximum. Correspondingly, the reactant concentration will pass through an inflection point, beyond which the curve will be concave upward (become less steep as time increases). Eventually, the concentration will reach zero (since the reaction is irreversible) at which time the curve will become horizontal.

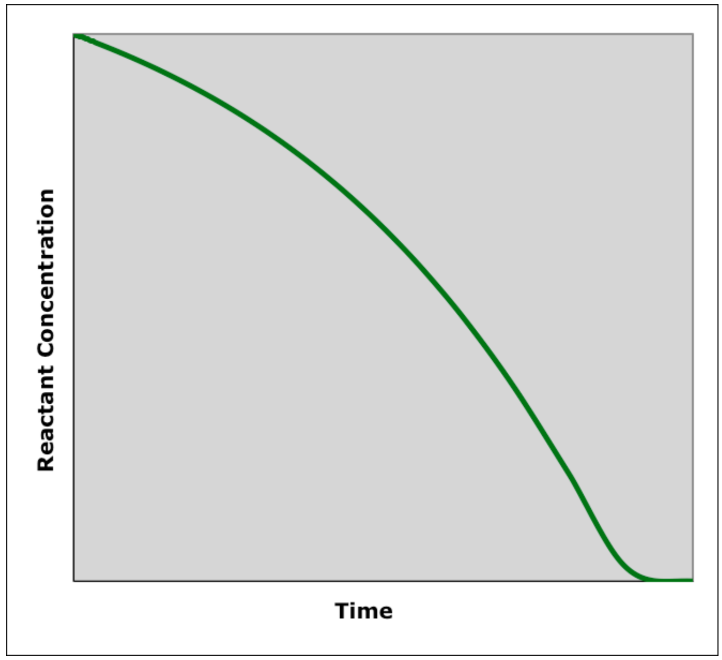

Figure 1. Typical reactant concentration as a function of isothermal batch reaction time for an auto-catalytic reaction.

The reactant concentration versus time is sketched in Figure 1. The critical features of the reactant concentration versus time curve are: it decreases monotonically, initially the slope becomes more negative with increasing time , it passes through an inflection point after which the slope becomes less negative with increasing time, and it eventually becomes horizontal at the same time the reactant concentration reaches zero.

The instantaneous rate versus time is sketched in Figure 2. The critical features of the rate versus time curve are that initially it increases with increasing time. It passes through a maximum, after which it decreases monotonically until reaching a value of zero. Once it reaches zero, it becomes horizontal (not shown). The specific shape will, of course, depend upon the particular rate expression for the reaction.

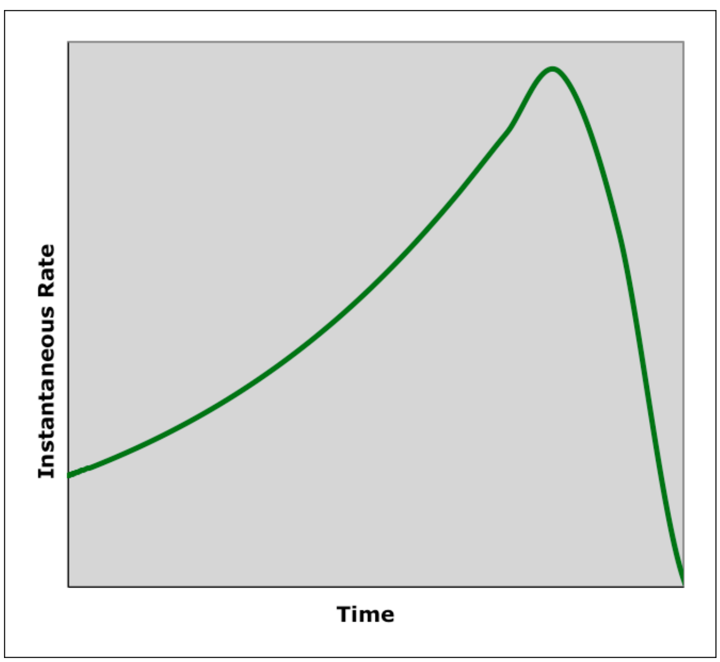

Figure 2. Typical reaction rate as a function of isothermal batch reaction time for an auto-catalytic reaction.