

# A First Course on Kinetics and Reaction Engineering

## Example 21.1

### Problem Purpose

This example illustrates the use of a qualitative analysis to assess and compare different operational modes of a CSTR.

### Problem Statement

Suppose reaction (1) and reaction (2) are typical irreversible reactions and further assume that they have exactly the same rate expression (same reaction orders, same pre-exponential factor and same activation energy). In fact, the only difference between them is that reaction (1) is exothermic and reaction (2) is endothermic. Make a single graph showing conversion of A versus space time, and on that graph sketch what the plot would look like (a) for reaction (1) taking place in an adiabatic CSTR, (b) for reaction (1) taking place in an isothermal CSTR, (c) reaction (2) taking place in an adiabatic CSTR and (d) reaction (2) taking place in an isothermal CSTR. For each plot explain why it has the shape it does, and then explain why the plots differ from each other in the ways they do.

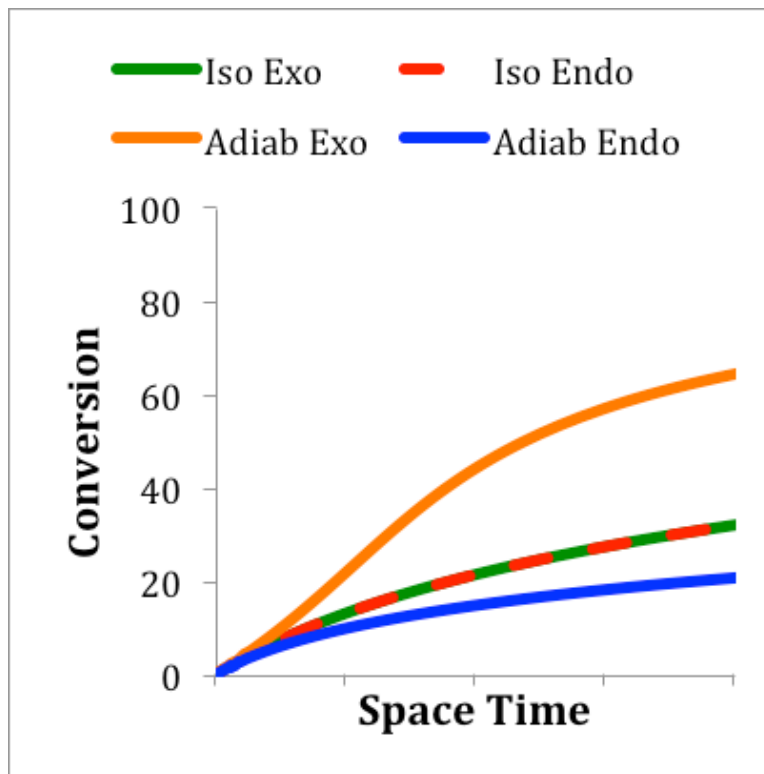
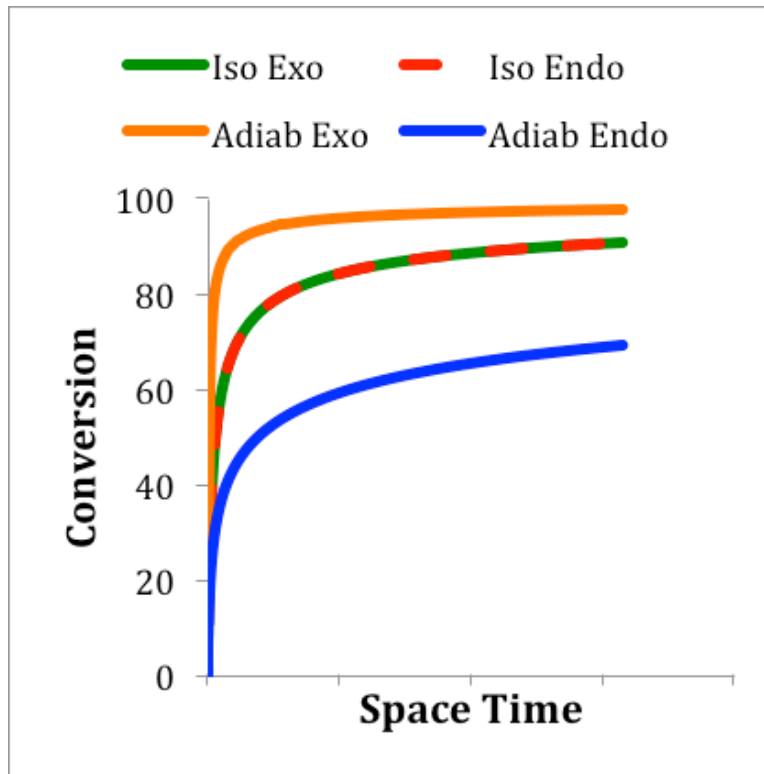


### Problem Analysis

This problem does not ask for any quantitative information, so it can be solved through a qualitative analysis. The reactions involved are stated to be typical irreversible reactions. This means that the rate is expected to decrease as the reactant concentration decreases, to increase as the temperature increases, and to be negligibly affected by changes in the product concentrations. It also means that the reactions will eventually go to 100% conversion.

### Problem Solution

The behavior of the four systems is sketched on the following page. The upper figure shows the behavior over a wide range of space times, while the lower figure only shows the performance at small space times.



The first thing to notice is that the two isothermal systems will be identical since the problem states that the rate expressions are identical. The plots start at zero conversion with a positive slope that continually decreases so that by the time the space time approaches infinity, the slope approaches zero and the conversion approaches 100%, since the reaction is irreversible. As the space time increases, the fluid has more time to react. Consequently, as the space time increases, the reactant concentration decreases. As a result, the rate decreases, and this results in the continually decreasing slope in the isothermal systems. In the adiabatic, endothermic system, in addition to the decreasing reactant concentration, the temperature also decreases with increasing space time. Hence the rate decreases faster in the endothermic system, and consequently, the conversion versus space time profile lies below the isothermal systems. It, too has a continually decreasing slope, leading to a concave downward shape.

In the adiabatic exothermic system, two opposing factors are at play. As with the other systems, the concentration of reactant will decrease continually, and by itself, this would cause the rate to decrease as already seen. However, as the space time increases, the temperature in the exothermic system increases, and by itself, this would cause the rate to increase. At very low space times, the temperature effect is expected to predominate, while at larger space times, the reactant concentration effect is expected to predominate. Hence, the rate is expected to increase initially before passing through a maximum and then decreasing continually. As a consequence, the conversion profile is expected to initially display a slope that is increasing. Then, at the space time where the rate reaches a maximum, it will pass through an inflection point, beyond which the slope will decrease continually. Looking at the lower figure on the preceding page, where only small space times are plotted, the increasing, then decreasing slope can be seen. The profile for the exothermic system lies above the other systems because the rate initially increases in the exothermic system.