A First Course on Kinetics and Reaction Engineering

Example 28.1

Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit. It illustrates the use of a qualitative reactor analysis to choose between a CSTR and a PFR for a given reaction system.

Problem Statement

Suppose you have been asked to design a continuous flow reactor for a single reaction that is moderately exothermic and autocatalytic. Your options have been limited to using either a single PFR or a single CSTR. Qualitatively discuss the merits and shortcomings of each of the reactors, and on the basis of that comparison, identify the reactor you believe would be the most appropriate choice.

Problem Analysis

We do not have economic or cost data to use in this analysis. In lieu of that information, we'll assume that it is economically advantageous to (a) keep the reactor volume as small as possible and (b) use as little external heating and cooling as possible.

Problem Solution

For the auto-catalytic, exothermic reaction under consideration, there are three factors to consider with respect to the rate of the reaction. As the space time is increased, the reactant concentration will decrease, the product concentration will increase, and (assuming adiabatic operation) the temperature will increase. The decrease in reactant concentration will tend to decrease the rate while the increases in product concentration and temperature will tend to increase the reaction rate. At low space times, the latter effects are expected to predominate, and so, the rate will increase as the space time increases. Eventually the decrease in reactant concentration will come to predominate; at the corresponding space time the rate will reach its maximum value. As the space time increases further, the rate will steadily decrease. The rate versus space time for both reactors will display this behavior, but the maximum in the rate versus space time curves will not occur at equal space times. Specifically, the maximum rate will occur at a smaller space time in the CSTR than in the PFR. The next paragraph should help in understanding why this is so.

The difference between the PFR and the CSTR is that there is only one rate in the CSTR whereas the rate will vary along the length of the PFR. We do not know the final conversion (and therefore the space time) that is required for this particular problem, and so we will give a qualified answer. First, if the design specification for the reactor involves a space time that is less than or equal to the CSTR space time where the rate is at a maximum, then the CSTR will be the preferred reactor. The rate everywhere in the CSTR will equal the high rate corresponding to the final conversion, and if the rate is large everywhere, then the reactor volume will be smaller. In contrast, the rate at the inlet to the PFR will be smaller than that in the CSTR, and as one moves along the length of the PFR, it will only become equal to that in the PFR at the end of the reactor. Therefore, since the rate is smaller everywhere, the reactor will need to be larger. The opposite is true if the design specification calls for the reaction to proceed to a very high conversion, corresponding to a CSTR space time far greater than the space time where the rate is a maximum. In this case, the CSTR will have a low rate everywhere, while the rate in the PFR will first increase, pass through the maximum rate, and then decrease until it equals the CSTR rate just at its outlet. In the part of the PFR where the rate is high, more reaction is taking place per unit volume than in the CSTR, so the PFR is smaller. Finally, if the design specification calls for an intermediate conversion, corresponding to a CSTR space time beyond the one where the rate is a maximum, but before it becomes exceedingly small, then one can’t tell which of the two reactors will be preferred without doing a quantitative analysis.

The preceding discussion assumed that the reactors could be operated adiabatically. In the case of the PFR, this presumes that the rate will be sufficiently high at the feed temperature so that the reaction gets going, after which the heat of reaction will kick in and raise the temperature. If the feed is not sufficiently hot, then it will need to be pre-heated for the PFR. The CSTR, in contrast, might not need feed pre-heating because the feed gets mixed into the reactor contents which are at the higher, final temperature. This would be an advantage of the CSTR over the PFR. Units 30 and 31 will describe and consider ways to augment a PFR using either thermal back-mixing or recycle. These augmentations might offset some of the limitations of a PFR in the present design scenario.

In summary, the back-mixing in the CSTR means that the temperature and product concentration are greater than at the inlet to a PFR. At low to moderate conversions, this translates to a larger rate of reaction and a smaller reactor for the CSTR. At high conversions, the rate in the CSTR is low, and the PFR is favored. At intermediate conversions, a quantitative analysis would be required in order to determine the better reactor type. The performance of a PFR might be improved if recycle or thermal back-mixing is employed.