A First Course on Kinetics and Reaction Engineering

Example 28.3

Problem Purpose
This problem will help you determine whether you have mastered the learning objectives for this unit. It illustrates the use of the instantaneous selectivity factor and a qualitative analysis in the selection of the best reactor for a particular reacting system.

Problem Statement
Suppose that you have been asked to perform the preliminary design for a reactor to produce the desired product, D from the reactant A. The rate expression is \( r = k_D C_A^2 \). Reactant A also reacts to produce an undesired co-product, U, with a rate that is given by \( r = k_U C_A \). The reactions take place in a solvent, and the heats of the reactions are small, so that the reactor will be nearly isothermal. Discuss the merits and shortcomings of the three ideal reactor types for this application, and indicate which one or ones you would consider first.

Problem Analysis
In the absence of economic data, we will assume that the preferred reactor will provide high selectivity at a small volume. A qualitative analysis will be used to compare the three ideal reactor types.

Problem Solution
The instantaneous selectivity parameter, \( S_{D/U} \), is the ratio of the desired to undesired reaction rates, as given in equation (1). Equation (1) shows that the selectivity for the desired product increases as the concentration of the reactant, A, increases. With this information, it becomes apparent that a CSTR is not well-suited to this application. In a CSTR, the reaction takes place only at the final conditions where the concentration of A will be its lowest. That translates to a small rate of reaction (requiring a large reactor), and in this case it also translates to a lower selectivity because of the low concentration of A.

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S_{D/U} = \frac{r_D}{r_U} = \frac{k_D C_A^2}{k_U C_A} = \frac{k_D}{k_U} C_A
\]

In both a PFR and a batch reactor, the concentration of A will initially be high (leading to a high rate and favorable selectivity), and will decrease as the reaction progresses (i.e. with processing time in a batch reactor or with length of reactor in a PFR). These reactors are better suited to this particular application. The choice of which to use would depend upon the volume of reactant A to be processed, and whether these reactions are an integral part of a larger process or not. If the quantities are small and these reactions are not part of a larger continuous process, then a batch reactor might be a good choice. If the amount to be processed is high and the profit margin small, then a PFR would likely be a better choice.