A First Course on Kinetics and Reaction Engineering

Unit 28. Choosing a Reactor Type

Overview

Reaction engineering with each of the three types of ideal reactors was considered in the preceding sections of Part III of A First Course on Kinetics and Reaction Engineering. The advantages and disadvantages of each reactor type have been considered. However, in all of the reaction engineering tasks that have been considered, the type of reactor to be analyzed has always been specified. Suppose a different type of engineering task was assigned wherein a reaction was specified and the assignment was to design a reactor system for that reaction (or set of reactions). Unit 28 considers the situation where deciding which type of reactor to use is part of the engineering analysis.

Learning Objectives

Upon completion of this unit, you should be able to define, in words, the following terms:

- commodity chemical
- specialty chemical

Upon completion of this unit, you should be able to write the defining equation for the following quantities:

- instantaneous selectivity parameter

Upon completion of this unit, you should be able to perform the following specific tasks and be able to recognize when they are needed and apply them correctly in the course of a more complex analysis:

- list factors that should be considered when selecting the type of reactor to use for a given reaction system
- use qualitative analyses to determine the type of flow reactor that is most likely to give the best performance

Information

Perhaps the easiest choice to make is between a batch reactor and the continuous flow reactors. The operation of batch reactors is much more labor intensive which usually translates to a higher cost of operation. If the chemical to be produced is a commodity type chemical (one that is produced in very large amounts and sells for a comparatively low price), this higher cost of operation precludes use of a batch reactor, and one of the continuous flow types is preferred. Safety might be one possible exception to this rule of thumb: if continuous processing has a much higher level of risk with respect to health and safety issues, then batch reactors might be used despite the higher operating cost. If the chemical to be produced is a value-added chemical (sometimes called a specialty chemical) or pharmaceutical (one that is produced in smaller amounts and sells for a comparatively higher price) then the higher cost of batch processing is tolerable.

If a continuous flow system is deemed to be more appropriate for the reaction under consideration, it becomes necessary to choose between a CSTR and a PFR. Safety and practicality should be considered first. If one reactor type is inherently safer for the reaction system being investigated, the choice may be obvious. Similarly, if the reaction involves a solid catalyst and a gaseous fluid phase, then a PFR is likely to be the better choice because it’s much easier to perform that kind of processing in a PFR. It is also wise to examine the literature and any other information that is available for similar reactions. For example, if the reaction under consideration is the chlorination of a particular hydrocarbon, and if reactor systems are already in existence for the chlorination of a similar hydrocarbon, one should determine whether the same type of reactor system is appropriate.

If none of the preceding considerations lead to the selection of either a CSTR or a PFR, then a qualitative analysis like those considered in Units 18, 21 and 25 might prove insightful. It should be determined whether the reaction system is endothermic or exothermic. The rate expressions should be examined and used to determine the conditions that most favor a high rate and the desired selectivity. More specifically, it should be determined whether high rates and the desired selectivity are favored by (i) high or low reactant concentration, (ii) high or low product concentration and (iii) high or low temperature. The instantaneous selectivity parameter (see Unit 18), equation 28.1 can be useful in determining the conditions where the desired selectivity is favored.

$$S_{D/U} = \frac{r_D}{r_U} \tag{28.1}$$

Previous units have contrasted what happens to a fluid element during the time it spends inside a PFR to what happens during the time a fluid element is inside a CSTR. In a nutshell, the reagent concentrations and the temperature in a fluid element in a PFR progress continually from their inlet values to their outlet values over the time the fluid element spends in the reactor. In contrast, the reagent concentrations and the temperature are constant and equal to their outlet values for the entire time a fluid element is inside inside a CSTR. If the instantaneous rate or selectivity is more favorable at the final conditions than it is along the progression from initial to final conditions, then a CSTR is likely to be the preferred reactor. On this basis one can specify kinetics criteria for which operation at the final conditions would be preferred and so a CSTR would offer performance advantages:

- If the rate and/or the selectivity increases as the reactant concentration decreases
- If the rate and/or the selectivity increases as the product concentration increases
- If the reaction is exothermic and the rate and/or the selectivity increases as the temperature increases
- If the reaction is endothermic and the rate and/or selectivity increases as the temperature decreases

Kinetics criteria where a PFR would be preferred are effectively the opposite of those where a CSTR is preferred. Notice that some of the criteria above correspond to the classification of reactions and kinetics that was discussed in Unit 17. For example an auto-catalytic reaction is one where the rate increases as the product concentration increases. According to the second criterion listed above, a CSTR would be expected to offer a performance advantage over a PFR for an auto-catalytic reaction.

There could be a trade-off between conditions that favor high rates and conditions that favor high selectivity. In such cases, one will need additional information, probably in the form of economic data, in order to reach the optimum compromise between rate and selectivity. Once it has been determined what conditions are most favorable for the reaction system, the two reactor systems can be compared qualitatively. It's already been seen that in a CSTR, the reaction will take place exclusively at the final conditions. If the most favorable conditions for the reaction system correspond to high product concentrations, low reactant concentrations, and a temperature that is favored in adiabatic operation (i. e. higher temperature for exothermic systems and lower temperature for endothermic systems), then a CSTR would appear to be the clear choice. In contrast, for a single endothermic reaction with typical kinetics, a PFR would be favored because the reactant concentration and temperature will be higher, and hence the rate will be higher, than in a CSTR operating at the same conversion.

As noted, there may be trade-offs between rate and selectivity, or between thermal and concentration effects such that a clear decision on the reactor type can't be made. In any case, even when the choice of reactor type is obvious, the qualitative analysis is only used to create a starting point. The next step in the process will be to construct a quantitative model for the reactor system and optimize the parameters of that system. If there are a few reactor types that can't be differentiated in a qualitative analysis, then one would construct and optimize quantitative models for each of the candidate systems.

Finally, it is important to realize that some of the limitations of the ideal reactors can be offset by augmenting the ideal reactor with another piece of apparatus. Such augmented ideal reactors are the considered in the units following this one. Those units will show ways that certain characteristics of a CSTR can be partially imparted to PFRs, and vice versa. Therefore, if a no one type of ideal reactor appears to be completely appropriate for a particular reaction system, one should also consider using an augmented ideal reactor. In addition, there are reactors other than the three ideal types that have been designed for specific kinds of reacting systems. A few of these are mentioned in Unit 37.