A First Course on Kinetics and Reaction Engineering

Unit 20. Optimization of Batch Reactor Processes

Overview

Unit 19 showed how to model a single processing step involving a perfectly mixed batch reactor. The commercial operation of a batch reactor typically involves a series of sequential processing steps. This unit examines the relationships between the component steps of an operational protocol both with respect to integration of the models for the individual steps and with respect to the optimization of the overall process

Learning Objectives

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

- net rate of (batch reactor) production

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

- net rate of (batch reactor) production

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 must be considered when specifying the batch processing time for a given chemical reaction taking place within a perfectly mixed batch reactor.
- Describe how the net productivity of a perfectly mixed batch reactor changes as the turnaround time increases and explain why it does so.
- Recommend a preferred operating protocol for a perfectly mixed batch reactor, given the reactions involved and appropriate economic data.

Information

The operational protocol for a batch reactor typically involves a sequence of steps, and each step is typically modeled separately. Previous units showed that the design equations for a batch reactor processing step are initial value ordinary differential equations. The dependent variables in the design equations are typically the number of moles of each reactant and product, the temperature and possibly the temperature of the heat transfer fluid. When one processing step ends, the next immediately begins. As such, the values of the dependent variables at the end of one processing step become the initial values of the dependent variables in the next processing step. There isn't time for any of them to change.

The thing that most typically does change from one processing step to the next is the heat input term. For example, the first step might involve heat input in order to raise the temperature of the reaction volume. Then as the temperature approaches some specified value, the heat input might either be turned off, allowing the reactor to continue operating adiabatically, or the heat input might be changed to cooling. The key points, from the perspective of solving the design equations are first, that the initial values of the dependent variables in the new step are equal to the final values of those variables at the end of the preceding step, and second, the design equations themselves will be different in each processing step.

The goal in operating a batch reactor process is to maximize the rate of profit associated with running that process. Optimizing the batch process involves defining some objective function, and then minimizing or maximizing that function with respect to process variables. In the later stages of a process design, the objective function might be a detailed economic calculation that takes a wide variety of factors into account. Those factors might include construction costs, maintenance costs, operating costs, return on investment, materials costs, revenue from sale of the product, waste disposal costs and others. In the earlier stages of a process design, simpler objective functions might be more appropriate. For instructional purposes, it is sufficient to use a simpler objective function.

The net rate of production determines how much product one can sell per unit time, early in the design process one might use the net rate of production as the objective function. The goal then would be to maximize the net rate of production with respect to various process variables. The net rate of production for a batch reactor is the moles of product generated per batch divided by the sum of the batch processing time and the turnaround time, equation (20.1). In that equation $r_{i,net}$ is the net rate of production of species i, n_i^f is the number of moles of species i at the end of the batch, n_i^0 is the number of moles of i at the start of the batch process, $t_{process}$ is the total duration of the operational protocol, and $t_{turnaround}$ is the turnaround time. The reactor design engineer must specify the operating protocol for the reactor, and this sets the batch processing time. Doing so often involves a “trade-off” that must be considered during the design of a batch reactor, and particularly during the specification of the operating protocol.

$$r_{i,net} = \frac{n_i^f - n_i^0}{t_{process} + t_{turnaround}} \tag{20.1}$$

To begin, let’s suppose that the turnaround time for the reactor is negligible and can be set equal to zero in equation (20.1). Since the reactor size is fixed, the amount of material processed will be the same in each batch. For illustration purposes, we’ll use the isothermal batch reactor behavior shown in Figure 20.1. It can be seen in that figure that if a batch is allowed to react for 10 minutes the conversion will be 63.3% whereas if it is allowed to react for 5 minutes the conversion will be 46.3%. Suppose the amount processed in a batch is 100 moles. If a single batch is allowed to run for 10 minutes, 63.3 moles of product will be produced. If those same 10 minutes instead

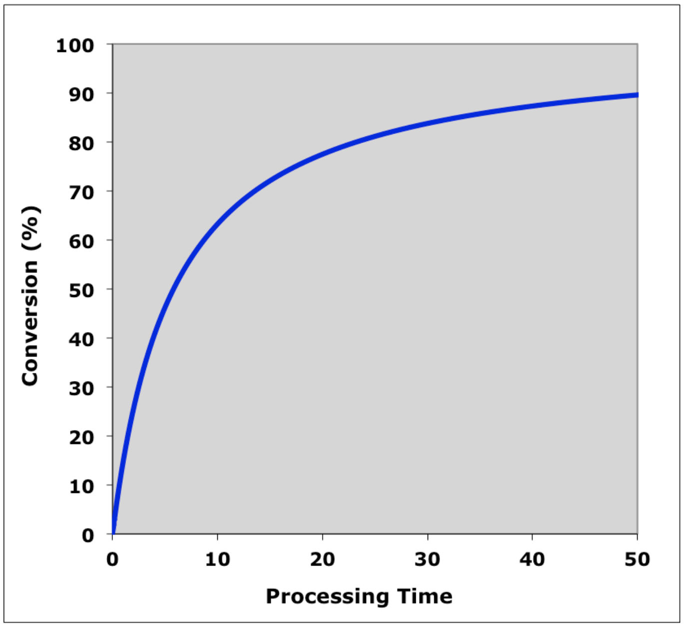

Figure 20.1 Conversion versus time for a typical batch reactor process.

are used to make two runs of 5 minutes each, a total of 92.6 moles of product will be produced. Thus one will make more product in 10 minutes time if one runs two 5 minute batches than if one runs a single 10 minute batch. The reason can be understood physically by noting that during the second half of the 10 minute run, the instantaneous rate of reaction within the reactor is lower than at the start of a new batch because the concentration of the reactant is smaller.

However, there is a trade-off. In the single 10 minute batch, the product has a higher purity (there's only 36.7% of the reactant left at the end of the single batch) than in the 5 minute batches (where there's 53.7% of the reactant left at the end of each of the batches). Figure 20.2 shows this trade-off by plotting (as the blue line) the net rate of production against the conversion (the higher the conversion in this case, the higher the product purity). The figure shows that *<u>if the turnaround time is negligible</u>*, the higher the purity (i. e. the higher the conversion per batch), the lower the net production rate. Hence, in the case of negligible turnaround time, there is a trade-off between high conversion and high purity.

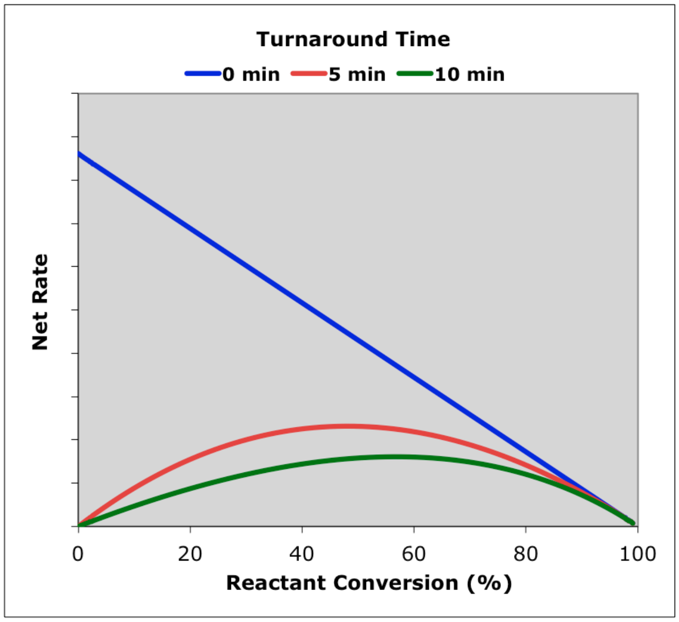

Figure 20.2 Net rate of reaction versus reactant conversion in a batch reactor for three different turnaround times.

In a more realistic situation, the required product purity would have been set in advance, based upon market demands and selling prices. In that case, the cost of any additional purification of the product from the reactor to meet the final specification would be added to the objective function. This cost would likely vary depending how close to the final specification the product from the reactor came. Here, however, we'll continue with our simplistic objective function that ignores product purity. With that simple objective function, and with zero turnaround time, Figure 20.2 clearly shows that the batch processing time should be as short as possible to keep the net rate of production high.

Including the turnaround time in the analysis makes a significant difference. This is especially true when the duration of the run is comparable to or smaller than the turnaround time. Continuing with the same example, let's assume that the turnaround time is 10 minutes, and consider 60 minutes of operation. If a ten minute batch processing time is utilized, it will be possible to make three complete batch runs in 60 minutes of operation because each batch requires 10 minutes of processing and 10 minutes of turnaround. If, as before, 100 moles of reactant are processed per batch, the net production of product will be 189.9 moles (three batches at 63.3% conversion per batch). If five minute batches are used instead, it will be possible to make 4 complete batch runs in 60 minutes of operation because each batch requires 5 minutes of processing and 10 minutes of turnaround. In this case the net production of product will be 185.2 moles (four batches at 46.3% conversion per batch). Thus, in this case, the net rate is greater if 10 minute batches are used.

Generalizing this analysis, in the regime where the batch processing time is smaller than the turnaround time, the net rate increases with conversion. Eventually, as the conversion becomes greater, the batch processing time and the turnaround time will become comparable, and the net rate will pass through a maximum. Beyond this point, the batch processing time becomes the predominant term in the denominator of equation (20.1) and the net rate decreases with increasing conversion. This general behavior is seen in Figure 20.2 (red and green lines) where it can be seen that the net rate reaches its maximum value when the turnaround time and the processing time are comparable (for the 5 min. turnaround time the maximum is near 46.3% conversion which corresponds to a 5 min. processing time and for the 10 min turnaround time the maximum net rate occurs near 63.3% conversion which corresponds to 10 minutes of processing). Of course, the exact shape of curves like these will depend upon the actual rate expression.

This was a simple case where it was assumed that no heating or cooling was required. Suppose that the reaction rate was negligible at ambient temperature, so that after the reactor was charged, it had to be heated, and then at the end of the process the contents had to be cooled back to ambient temperature. This would introduce several additional variables into the optimization process. These might include the duration of the heating stage, the temperature of the steam used for heating, the duration of the reaction stage, the use of heating or cooling during the reaction stage and the associated temperature of the steam or cooling water used, the temperature of the cooling water used in the cooling stage, the cost of steam as a function of temperature, the cost of cooling water as a function of temperature, etc. One can see that the optimization of the overall batch process can be a challenging task. Ultimately, when specifying the reactor operating protocol, the engineer (or more likely a team that includes the engineer along with accountants, marketing representatives, a plant manager, and others) chooses a protocol that factors in all the important economic aspects, along with safety, environmental compliance, operability, etc., and optimizes that protocol.