A First Course on Kinetics and Reaction Engineering
Unit 31. Back-Mixing in a PFR via Recycle

Overview

Unit 30 showed how augmenting a PFR with a heat exchanger can impart thermal back-mixing to the PFR, similar to that enjoyed naturally by a CSTR. Unit 31 extends the augmentation to include back-mixing of both heat and mass. This is accomplished by adding a recycle stream to an ideal PFR. The unit shows that by adjusting the amount of material that is back-mixed, the augmented PFR can span a range of performance characteristics from being a pure PRF to being a being essentially a pure CSTR.

Learning Objectives

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

- recycle

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

- recycle ratio

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:

- Sketch a recycle PFR system and identify the recycle stream
- Describe how the system's behavior changes as the PFR recycle ratio is varied
- Describe the advantages of a recycle PFR and explain the reason for those advantages on physical grounds
- Identify situations where use of a recycle PFR would offer performance advantages over the use of a PFR or a CSTR alone
- Quantitatively analyze the performance of a steady state recycle PFR
- Design a recycle PFR to meet process specifications

Information

Unit 30 showed that by adding a heat exchanger to a PFR, it was possible to introduce some CSTR-like thermal performance while retaining concentration behavior characteristic of a PFR. That proves to be useful for typical exothermic reactions being conducted adiabatically. Suppose, however, that the reaction system is such that high selectivity or activity is also favored by a high product concentration. One obvious choice would be to use a CSTR. In some situations, though, a PFR may offer practical advantages. A heterogeneous catalytic reaction utilizing a solid catalyst would be such a situation. The present unit examines a means of adding both thermal and compositional back-mixing to a PFR by adding a *recycle* stream, that is by splitting the reactor effluent stream and mixing part of it into the feed to the reactor.

Figure 31.1 depicts a PFR augmented with a recycle stream. The feed to the process, stream a, is mixed at the point labeled "1" with a recycle stream, stream r, that is split from the reactor effluent, stream c. The mixed stream, stream b, is then fed to the reactor. At the point labeled "2", the outlet stream from

the reactor, stream c, is split to form the recycle stream and the final stream leaving the process, stream d. The design equations for the PFR remain the same as for any other PFR, but it is often more difficult to solve them. The situation is much like the thermally back-mixed PFR considered in Unit 30 where the inlet temperature was unknown, requiring the simultaneous solution of the PFR design equations and the heat exchanger design equations. With a recycle PFR like that in Figure 31.1, the temperature and composition of stream a is often specified, in which case the composition and temperature of stream b, which are needed to solve the PFR design equations, are not known. As a consequence, the PFR design equations cannot be solved independently, instead, the PFR design equations and mass and energy balances on mixing point 1 must be solved simultaneously.
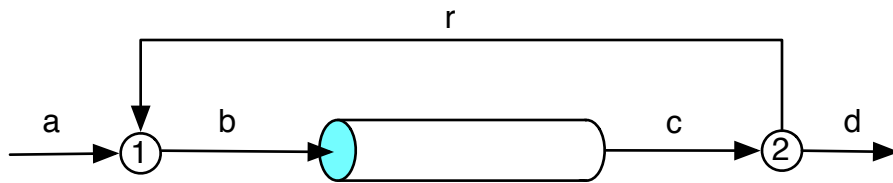

Figure 31.1 Plug flow reactor (gray rectangle) with a recycle stream.

Before writing mole and energy balances for mixing point 1, it is useful to note that since point 2 is a simple split, the composition (e. g. mole fractions or concentrations) and temperatures of streams c, d and r are equal. It is also useful to define a recycle ratio, R_R, as given in equation (31.1). Then, performing a mole balance at point 1 leads to equation (31.2). A mole balance can also be written for point 2, equation (31.3). Solving equation (31.3) for the molar flow rate of i in stream d, substituting into equation (31.2) and rearranging gives the mole balance on the mixing point 1 in terms of the reactor inlet and outlet streams, equation (31.5).

$$R_R = \frac{\dot{V}_r}{\dot{V}_d} = \frac{\dot{n}_{total,r}}{\dot{n}_{total,d}} = \frac{\dot{n}_{i,r}}{\dot{n}_{i,d}} \tag{31.1}$$

$$\dot{n}_{i,b} = \dot{n}_{i,a} + \dot{n}_{i,r} = \dot{n}_{i,a} + R_R \dot{n}_{i,d} \tag{31.2}$$

$$\dot{n}_{i,c} = \dot{n}_{i,d} + \dot{n}_{i,r} = \dot{n}_{i,d} + R_R \dot{n}_{i,d} = \left(1 + R_R\right)\dot{n}_{i,d} \tag{31.3}$$

$$\dot{n}_{i,d} = \frac{\dot{n}_{i,c}}{1 + R_R} \tag{31.4}$$

$$\dot{n}_{i,a} + \frac{R_R \dot{n}_{i,c}}{1 + R_R} - \dot{n}_{i,b} = 0 \tag{31.5}$$

Assuming no phase changes occur anywhere in the system and assuming the mixing and split points to be perfectly insulated, an energy balance at mixing point 1 takes the form of equation (31.6),

where it has been noted that the temperatures of streams c, d and r are all the same. Equations (31.6) is written in terms of the species' individual molar specific heats; a similar expression could be written in terms of the overall volume-specific or mass-specific heat capacity of the fluid as a whole. In that case, the molar flow rate would be replaced by the volumetric or mass flow rate and there would be no summation.

$$\sum_{\substack{i=all \\ species}} \dot{n}_{i,a} \int_{T_a}^{T_b} \hat{C}_{p,i}\, dT + \sum_{\substack{i=all \\ species}} \dot{n}_{i,r} \int_{T_c(=T_r)}^{T_b} \hat{C}_{p,i}\, dT = 0 \tag{31.6}$$

A few additional points need to be remembered when analyzing a recycle PFR like that in Figure 31.1. First, there are at least two ways to define the conversion in a system like this. One is the per-pass conversion given in equation (31.7) and the other is the overall conversion given in equation (31.7). A problem specification might use either of these.

$$f_{i,pass} = \frac{\dot{n}_{i,b} - \dot{n}_{i,c}}{\dot{n}_{i,b}} \tag{31.7}$$

$$f_{i,overall} = \frac{\dot{n}_{i,a} - \dot{n}_{i,d}}{\dot{n}_{i,a}} \tag{31.8}$$

The other point to remember is that the volumetric flow rate within the reactor is greater than the volumetric flow rate entering the process. This becomes important if the rate expression contains concentrations that must be calculated from given values of the molar flow rates. The definition of concentration, equation (31.9), is used as usual. For a gas phase system, the volumetric flow rate in the denominator is re-written using the ideal gas law (or whatever equation of state is appropriate) just as is done in a PFR without recycle. However, when the fluid is a liquid of constant density, the volumetric flow rate within the reactor must be used as in equation (31.10). In generating the last equality of equation (31.10) it was noted that for steady state operation with a constant density fluid, the volumetric flow rate of stream a equals the volumetric flow rate of stream d.

$$C_i = \frac{\dot{n}_i}{\dot{V}} \tag{31.9}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}_b} = \frac{\dot{n}_i}{\dot{V}_a + \dot{V}_r} = \frac{\dot{n}_i}{\dot{V}_a + R_R \dot{V}_d} = \frac{\dot{n}_i}{\dot{V}_a (1 + R_R)} \tag{31.10}$$

The numerical analysis of a recycle PFR is very similar to the numerical analysis of an integrated heat exchanger and PFR. The following approach, sometimes with slight modification, will often permit the solution of the design equations for the PFR and the mixing point:

1. Formulate the design equations for the PFR and write the code needed to solve them numerically
   a. If the PFR design equations can be solved at this point, do so

  b. otherwise, write the code for solving them in the form of a function that is passed the molar flow rates and temperature of stream b as arguments and that returns the molar flow rates and temperature of stream c

2. Formulate the design equations for the mixing point using equation (31.5) and equation (31.6)

  a. Choose the molar flow rates of the species and the temperature of stream b as the unknowns to be found by solving the mixing point design equations

  b. Since the code that will be written to solve the equations will be given values for the unknowns, it can use those values to solve the PFR design equations and thereby obtain the corresponding values for stream c

3. Use the results of solving the design equations to answer the questions posed in the problem.

Before concluding, it is interesting and useful to briefly consider the qualitative behavior of a recycle PFR like that shown in Figure 31.1. Clearly, if the recycle ratio equals zero, then the reactor is a PFR. However, if the recycle ratio is very, very high, the reactor will behave as if it is a CSTR. This was discussed in the context of laboratory reactors in Unit 11. Thus, a recycle reactor can be thought of as a kind of hybrid between a PFR and a CSTR. By varying the recycle ratio, the recycle PFR can be adjusted to be more like one than the other. Under appropriate kinetic conditions, this versatility can offer substantial performance improvements over either of the ideal reactors alone. If the reaction system involves the use of a solid catalyst, a recycle PFR can offer the practicality of handling the solids as a packed bed along with the contacting and thermal behavior of a CSTR. Finally, it should be noted that back-mixing introduces the possibility of multiple steady states, just as were found for CSTRs.