

A First Course on Kinetics and Reaction Engineering

Unit 30. Thermal Back-Mixing in a PFR

Overview

One advantage offered by a CSTR when running an exothermic reaction is that the cool feed gets heated by mixing with the contents of the reactor. As a consequence the reaction takes place at the higher exit temperature where the rate coefficient will be large. Unit 30 shows how a PFR can be augmented by adding a heat exchanger that heats the feed using the product stream. By means of this augmentation, the PFR gains some of the thermal back-mixing benefits enjoyed by a CSTR.

Learning Objectives

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

- back-mixing
- hot or cold approach

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

- heat exchanger energy balance
- heat exchanger heat transfer equation
- cold approach

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 PFR-heat exchanger system that can be used to provide thermal back-mixing
- Describe the advantages of a PFR-heat exchanger system that provides thermal back-mixing and explain the reason for those advantages on physical grounds
- Quantitatively analyze the performance of a PFR-heat exchanger system that provides thermal back-mixing
- Design a PFR-heat exchanger system given feed conditions and desired outlet conditions

Information

When a typical exothermic reaction takes place in an adiabatic reactor, either a CSTR or a PFR, two competing effects are present. These have been discussed previously (see Unit 18) and are apparent from a qualitative analysis. Briefly, as the reaction proceeds, the temperature increases (a favorable effect, tending to increase the reaction rate) and the reactant concentration decreases (an unfavorable effect, tending to decrease the reaction rate). In many cases, the temperature effect predominates at lower conversions and the reactant concentration effect predominates at higher conversions. In a PFR, the reactant concentration decreases gradually (favorable behavior since it tends to keep the rate as high as possible), but the temperature also increases gradually (unfavorable behavior since the rate coefficient increases gradually). In a CSTR, the reactant concentration is low for the entire time the fluid reacts (unfavorable behavior since it tends to make the rate low), but the temperature is at its highest value

throughout the time the fluid reacts (favorable behavior since it tends to make the rate high). Thus, neither a single CSTR nor a single PFR is ideally suited to the reaction system.

In Unit 29, it was shown that using a cascade of CSTRs makes the CSTRs behave a little more like a PFR. Here, it will be seen that by augmenting a PFR with a heat exchanger, it is sometimes possible to impart CSTR-like thermal behavior to a PFR while retaining PFR-like behavior with respect to the composition. To see how this can be accomplished, examine Figure 30.1 which shows a heat exchanger connected to a PFR. There are two compartments in the heat exchanger; the feed flows through one compartment and the product stream from the PFR flows through the other. The two compartments are physically separated by a wall (red), so there is no mass exchanged between the streams. However, it is possible for heat to be conducted through the wall (red). In this way, as the feed flows through the lower compartment of the heat exchanger, heat is transferred to it from the PFR product stream flowing through the upper compartment. This is similar to what happens thermally in a CSTR where the complete *back-mixing* (mixing product into the feed) of the CSTR immediately heats the feed to the final outlet temperature. Due to the heat exchanger in Figure 30.1, the PFR inlet temperature is higher and consequently, the rate at the PFR inlet is larger than it would be without the heat exchanger.

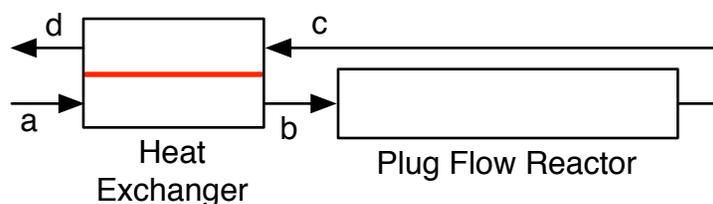


Figure 30.1 Addition of a heat exchanger to a PFR, thereby permitting thermal back-mixing without affecting composition.

Using an augmented PFR like that shown in Figure 30.1, it is sometimes possible for an exothermic reaction to occur auto-thermally. That is, with the heat exchanger the reaction can reach a high steady state conversion without the need to continually supply heat. In contrast, the steady state conversion could be much, much lower without the heat exchanger. In particular, consider a situation where the feed is supplied at a temperature where the rate of reaction is very small. If this feed is admitted directly to the reactor, without a heat exchanger, very little reaction will occur and consequently very little heat of reaction will be released. As a result, the temperature will not rise significantly, and so the rate will remain small through the entire reactor. If the same feed is used, but it first passes through a heat exchanger as in Figure 30.1, the feed will enter the reactor at a higher temperature where the rate is high enough to cause some reaction to occur. That, in turn will release more heat so that the rate is appreciable throughout the reactor. Of course, as the reactant is depleted, the rate will eventually decrease. Nonetheless, for a typical exothermic reaction taking place adiabatically, an augmented PFR like that shown in Figure 30.1 offers the best features of both a CSTR and a PFR: the feed is immediately heated, as in a CSTR, while the reactant concentration starts high and decreases gradually as the reaction progresses, as in a PFR.

Before considering the analysis of a system like that shown in Figure 30.1, it may be useful to briefly consider how a heat exchanger works, the limitations upon its performance and the design equations needed in order to model it. Entire books and courses are devoted to heat transfer processes, and there are numerous variations in the design of heat exchangers. Here we will limit the discussion to a cursory consideration of a counter-current flow geometry like that shown in the figure. We will further assume that there are no heat losses from the heat exchanger to the surroundings, that no phase changes occur in either of the fluid streams and that no mechanical work is performed by the heat exchanger. An energy balance then dictates that the sensible heat lost by the upper stream must appear as a sensible heat gain by the lower stream, as expressed, for example, in equation (30.1). An equivalent expression could be written in terms of the total volumetric flow rates of the streams using overall volumetric heat capacities or in terms of the mass flow rates of the streams with heat capacities per unit mass.

$$\sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_{i,c} \int_{T_c}^{T_d} \hat{C}_{p,i} dT + \sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_{i,a} \int_{T_a}^{T_b} \hat{C}_{p,i} dT = 0 \quad (30.1)$$

The molar flow rates of the species in one of the two streams in equation (30.1) will be known as will at least one of the four temperatures. (It should be noted that thermodynamics requires that if $T_a < T_d$, then T_b must be less than T_c , and vice versa.) The physical design and dimensions of the heat exchanger and the properties of the fluids determine how much heat is transferred from stream c to stream a . A common way to express this mathematically is in the form of heat transfer equations like equations (30.2) or (30.3) where U_{LMTD} and U_{AMTD} represent the appropriate heat transfer coefficients, A is the heat transfer area, ΔT_{LM} is the log-mean temperature difference defined in equation (30.4) and ΔT_{AM} is the arithmetic-mean temperature difference defined in equation (30.5).

$$\sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_{i,c} \int_{T_c}^{T_d} \hat{C}_{p,i} dT + U_{LM} A \Delta T_{LM} = 0 \quad (30.2)$$

$$\sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_{i,c} \int_{T_c}^{T_d} \hat{C}_{p,i} dT + U_{AM} A \Delta T_{AM} = 0 \quad (30.3)$$

$$\Delta T_{LM} = \left(\frac{(T_d - T_a) - (T_c - T_b)}{\ln \left\{ \frac{(T_d - T_a)}{(T_c - T_d)} \right\}} \right) \quad (30.4)$$

$$\Delta T_{AM} = \frac{T_c + T_d}{2} - \frac{T_a + T_b}{2} \quad (30.5)$$

Notice also that no mass is transferred between the two streams, only heat. as a consequence, the molar flow rate of each species in stream a is equal to the molar flow rate of that species in stream b , equation (30.6). Similarly, the molar flow rate of each species in stream c is equal to the molar flow rate of that species in stream d , equation (30.7).

$$\dot{n}_{i,a} = \dot{n}_{i,b} \quad (\text{for each species, } i) \quad (30.6)$$

$$\dot{n}_{i,c} = \dot{n}_{i,d} \quad (\text{for each species, } i) \quad (30.7)$$

Most commonly with a system like that shown in Figure 30.1, the composition of stream a is known, and consequently, the composition of stream b is also known. One of the four temperatures will also be known. To analyze the system, first construct a model for the PFR. If sufficient information is known to solve the PFR design equations, do so. At that point, the composition of all four streams will be known as will T_b and T_c . The heat exchanger design equations (equation (30.1) and either equation (30.2) or equation (30.3)) can then be solved to find the other two temperatures. In some problems the *cold approach*, equation (30.8), may be specified instead of the heat transfer coefficient and area. In that case equation (30.8) replaces the heat transfer equation (equation (30.2) or equation (30.3)). The cold approach is the temperature difference between the two streams at the point where the warmer stream exits the heat exchanger.

$$\Delta T_{cold} = T_d - T_a \quad (30.8)$$

In many cases, it won't be possible to solve the PFR design equations independently because T_b will not be known. In that situation, numerical code can be written where T_b is passed to the code as an argument, and using that value, the design equations are solved and the outlet molar flows and temperature are returned. Then write the design equations for the heat exchanger. As before, they will consist of two non-linear equations (equation (30.1) and either equation (30.2), equation (30.3) or equation (30.8)) which contain three unknown temperatures (most commonly T_b , T_c and T_d) and a set of unknown molar flow rates (most commonly for stream c).

Since there are only two heat exchanger design equations, they can only be solved to obtain the values of two unknowns. The key to solving the equations is that T_b should be chosen as one of the unknowns and T_c should not be chosen as the other unknown. Recall, that in order to solve nonlinear equations numerically you need to (a) identify a set of unknowns, equal in number to the number of equations, (b) provide a guess for the value of each unknown and (c) provide code that is given values for the unknowns as input and uses them to evaluate the equations being solved. We just identified the equations and unknowns, making sure that T_c was not one of them. We can certainly guess values for the unknowns. The code we must provide to solve the heat exchanger design equations numerically will be given a value for T_b , and the other unknown. Since it is given a value for T_b , it can call the code that was written earlier to model the PFR. When the PFR code is called, it will return the species' molar flow rates

and the temperature of stream c . Having those values and the values of the unknowns, the heat exchanger design equations can be evaluated. In this way, the heat exchanger design equations can be solved numerically for the two unknown temperatures. Then, knowing the value of T_b , the code that models the PFR can be called one last time to find the value of T_c and the molar flow rates of all the species in stream c .

The approach described here may need to be modified depending on the manner in which the problem is specified, but this should be possible in most situations. The key steps are as follows:

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 T_b as an argument and that returns T_c and molar flow rates of the species in stream c
2. Formulate the design equations for the heat exchanger using equation (30.1) and either equation (30.2), equation (30.3) or equation (30.8) and identify all unknown quantities
 - a. If there are only two unknown temperatures, solve the equations to find their values
 - b. If there are more than two unknown quantities, choose T_b as one of the two unknowns for the heat exchanger design equations and either T_a or T_d as the other
 - i. The code to evaluate the heat exchanger design equations during their numerical solution will be given a value for T_b
 1. using that value, the PFR design equations can be solved to find $\dot{n}_{i,c}$ for all i and T_c
 - ii. Using those values and the value of the other unknown, code can be written for the numerical solution of the heat exchanger design equations.

The examples that accompany this unit follow the above approach to analyze integrated heat exchangers and PFRs.