A First Course on Kinetics and Reaction Engineering

Unit 34. 2-D and 3-D Tubular Reactor Models

Overview

Unit 34 describes two- and three-dimensional models for tubular reactors. One limitation of the ideal PFR model is that the temperature and composition cannot vary in the radial direction. This can be a serious shortcoming in some situations, such as those involving heat transfer through the reactor walls, that is, in the radial direction. It can also happen that variations in the angular direction are important, such as radiant heating configurations where the radiation only “sees” one side of the tube. In cases like these, a more rigorous model that allows for two- or three dimensional variation may be required in order to develop a reactor model that is quantitatively accurate.

Learning Objectives

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

- radial dispersion coefficients

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:

- Describe situations where it might be necessary to include radial and/or azimuthal variation of the temperature and composition when modeling a packed bed reactor.
- Describe the assumptions used in pseudo-homogeneous models for packed bed tubular reactors
- Write the appropriate steady state two-dimensional design equations for a psuedo-homogeneous packed bed tubular reactor along with the boundary conditions needed to solve them

Information

The plug flow reactor model used in the first three parts of this TExT can describe a large number of reacting systems with a high degree of accuracy. Still, there are situations where the ideal PFR model is not accurate. One example is a packed bed tubular reactor where a large amount of heat must be removed through the reactor wall due to the high exothermicity of the reactions taking place. In such cases the temperature near the wall of the reactor may be significantly lower than the temperature at the center of the tube. This temperature variation means that the reaction rate is larger at the center of the tube than it is near the wall, and consequently, the composition may also vary with radial position.

In other cases there may be variations in the angular direction, too. As an example, consider an endothermic reaction where the reactor must operate at high temperatures. One common way of operating such reactors is to build a furnace with reactor tubes passing horizontally above the flames of the furnace. In this configuration, the tubes right above the flames receive a very high radiant heat input, but only on the bottom half of the tube, as indicated in Figure 34.1. This can result in temperature variations around the tube, that is, in the azimuthal direction. As before, this can lead to *concentration* gradients in the azimuthal direction.

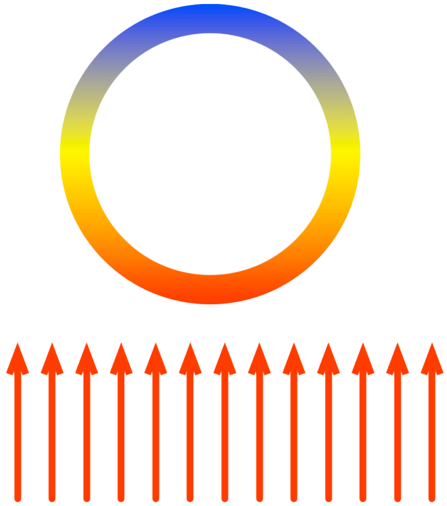

Figure 34.1. A radiant heat flux, represented as red arrows, from the bottom side of a tubular reactor can lead to temperature variations in the azimuthal direction. Here the shading of the tube wall represents the variation from higher temperatures (red) to lower temperatures (blue).

There are other scenarios where it is necessary to account for radial and/or azimuthal variation of the dependent variables in a tubular reactor. The molar flow rates of the chemicals present in the system are not appropriate as dependent variables in these cases. Specifically, the molar flow rate of a species is not a point quantity, it is an average or overall quantity that is representative of the flow in the tube as a whole. Consequently, 2-D and 3-D tubular reactor design equations *are not* written in terms of molar flow rates. Most commonly, the design equations are written in terms of linear velocities and concentrations, as was done in the axial dispersion model in Unit 33.

As was the case in Unit 33, here we will use the pseudo-homogeneous model for packed beds. That means that the equations are formulated as if there is no packing present and the entire tube cross section is filled with fluid. When this is done, additional factors, such as bed porosities, are added to account for the packed bed, leading to equations that look very similar to equations for a reactor containing a homogeneous fluid (hence the model is named “pseudo-homogeneous”). We will continue to use the assumption of plug flow. As a consequence the linear velocity of the fluid is assumed to be parallel to the tube axis; we do not include velocities in the r or θ directions., Furthermore, at any axial position, z, in the reactor, the velocity is the same for all r and θ (i. e. plug flow is assumed). This means that convection cannot be used to account for radial movement of heat or mass. Instead, these are incorporated as “effective” radial heat conduction and “effective” radial mass diffusion (or dispersion). It is also possible to include effective conduction and diffusion in the axial direction, as was done in Unit 33, but the models without axial conduction and diffusion are found to be quite accurate in most cases.

The radial conduction and diffusion are labeled as “effective” because it is assumed that they follow a straight radial path (as they would in a homogeneous fluid). In reality, the path may not be straight due to the presence of the solid, and for conduction, the heat will be conducted through both the fluid and the solid, not just a single homogeneous fluid. These effects are accounted for through the use of an “effective” radial thermal conductivity (or radial thermal dispersion coefficient) and an “effective” radial diffusivity (or radial dispersion coefficient). As was the case for axial dispersion, these “effective” transport properties are not properties of the materials involved; they depend upon the flow properties in the reactor. As such, they are often found using correlations involving dimensionless groups like the Reynolds, Peclet and Nusselt numbers. A good reference source or text on heat and mass transfer should be consulted to find appropriate correlations for the effective transport properties. One point to bear in mind when using these correlations is that some of the correlations use the superficial velocity in the calculation of the Reynolds number, etc. but other correlations use the interstitial velocity (the actual velocity in the spaces between the solid catalyst particles). These two are related to each other through the bed porosity, ε, and when using these correlations one should take care to use the proper velocity.

Using the assumptions just described, the mole, energy and momentum balances for a steady state, psuedo-homogeneous, plug flow, packed bed reactor with radial temperature and concentration gradients are given in equations (34.1) through (34.3). The diffusion coefficient and thermal conductivity appearing in these equations are effective diffusivities and conductivities as just described; there is one effective radial diffusion coefficient for all species present. The subscript e denotes “effective,” r denotes “radial direction” and s denotes that u_s is a superficial velocity. The heat capacity, $\tilde{C}_{p,fluid}$, is the mass-specific heat capacity for the fluid as a whole and ρ_{fluid} is similarly the density of the fluid as a whole. The f appearing in the momentum balance is a friction factor, and the momentum balance, as written, assumes it is defined in terms of the effective diameter of the catalyst particles, d_p. It accounts for the pressure drop caused by flow through the reactor in the same way that the Ergun equation did in the ideal PFR design equations we used previously. It should be noted that in this form the design equations assume that the fluid viscosity does not vary with radial position. That could happen if the viscosity was a strong function of temperature, so here we are assuming that the viscosity is constant.

$$D_{er}\left(\frac{\partial^2 C_i}{\partial r^2}+\frac{1}{r}\frac{\partial C_i}{\partial r}\right)-\frac{\partial}{\partial z}\left(u_s C_i\right)=\sum_{\substack{j=all\\reactions}}\nu_{i,j}r_j \tag{34.1}$$

$$\lambda_{er}\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}\right)-u_s\rho_{fluid}\tilde{C}_{p,fluid}\frac{\partial T}{\partial z}=\sum_{\substack{j=all\\reactions}}r_j\Delta H \tag{34.2}$$

$$-\frac{dP}{dz}=f\,\frac{\rho_{fluid}u_s^2}{d_p} \tag{34.3}$$

In order to solve the design equations (34.1) through (34.3), boundary conditions are needed. Most typically, the inlet (i. e. at z = 0) concentration, C_i^0, temperature, T^0, and pressure, P^0, are known, equations (34.4) through (34.6). The radial concentration boundary conditions assume that the concentration gradient goes to zero at the wall and at the centerline of the reactor tube, equations (34.7) and (34.8). Similarly, the temperature gradient is assumed to go to zero at the centerline, equation (34.9). Assuming that heat transfer with the surroundings will be taking place through the wall, the other radial temperature boundary condition is given by equation (34.10), where α_w is the heat transfer coefficient at the wall and T_w is the wall temperature. The value of the heat transfer coefficient at the wall is often found from correlations; again, see a good reference on heat transfer.

$$C_i\left(r,0\right)=C_{i,feed} \tag{34.4}$$

$$T\left(r,0\right)=T_{feed} \tag{34.5}$$

$$P\left(0\right)=P_{feed} \tag{34.6}$$

$$\left.\frac{\partial C_i}{\partial r}\right|_{r=0}=0 \tag{34.7}$$

$$\left.\frac{\partial C_i}{\partial r}\right|_{r=R}=0 \tag{34.8}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=0}=0 \tag{34.9}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=R}=\frac{\alpha_w}{\lambda_{er}}\left(T\left(R,z\right)-T_w\right) \tag{34.10}$$

Notice that the derivative of the product, u_sC_i, appears in the mole balance, equation (34.1). For a gas phase system, the superficial velocity will vary along the length of the reactor due to thermal expansion/contraction as well as any change in the total molar concentration due to the reaction. It is fairly common to neglect this variation in superficial velocity. This is equivalent to assuming constant density. With this assumption, u_s can be taken outside the derivative, and the solution of the design equations is relatively straightforward.

If one wishes to formally account for the variation in the superficial velocity along the length of the reactor, one mole balance must be replaced by an equation of state. For example, if ideal gas behavior is assumed, the superficial velocity can be related to the fluid density as in equation (34.11), where G represents the so-called mass velocity as defined in equation (34.12). In a steady state reactor, G will be a constant since mass is neither consumed nor generated by chemical reactions. It is then necessary to express the fluid density in terms of all of the concentrations except one (as noted, mole balances are written for all but one species). If the index j is used to denote the species for which a mole balance is *not* written, the density can be related to the concentrations through the species' molecular weights as in equation (34.13). The concentration of species j can be found from the total concentration and the concentrations of the other species, equation (34.14), and the total concentration can be expressed using the equation of state (here, the ideal gas law), equation (34.15). Combining equations (34.11) and (34.13) through (34.15) gives an expression for the superficial velocity, equation (34.16). This expression can then be substituted into the mole balance, equation (34.1). The chain rule for derivatives can then be used to generate a set of equations where the product, u_sC_i, no longer appears in any derivatives. The mathematics needed to solve the resulting equations is significantly more complicated than the constant density case where u_s is simply taken outside of the derivative.

$$u_s\rho_{fluid} = G \quad \Rightarrow \quad u_s = \frac{G}{\rho_{fluid}} \tag{34.11}$$

$$G = \frac{\dot{m}}{A} \tag{34.12}$$

$$\rho_{fluid} = C_jM_j + \sum_{i\neq j} C_iM_i \tag{34.13}$$

$$C_j = C_{total} - \sum_{i\neq j} C_i \tag{34.14}$$

$$C_{total} = \frac{P}{RT} \tag{34.15}$$

$$u_s = \frac{G}{\left(\frac{P}{RT} - \sum\limits_{i\neq j} C_i\right)M_j + \sum\limits_{i\neq j} C_iM_i} \tag{34.16}$$

There are other formulations of two- and three-dimensional tubular packed bed reactor models besides the pseudo-homogeneous model given here. They vary in the way they handle the presence of two phases in the reactor, whether they account for the porous nature of the catalyst and other factors. The interested student is encouraged to consult more advanced textbooks on reaction engineering or take a more advanced course on the topic.