R5.1 Spherical Packed-Bed Reactors*

Another advantage of spherical reactors is that they are the most economical shape for high pressures. As a first approximation we will assume that the fluid moves down through the reactor in plug flow. Consequently, because of the increase in cross-sectional area, A_c, as the fluid enters the sphere, the superficial velocity, $G = \dot{m}/A_c$, will decrease. From the Ergun Equation [Equation (5-22)],

$$\frac{dP}{dz} = -\frac{G(1-\phi)}{\rho g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right] \tag{5-22}$$

we know that by decreasing G, the pressure drop will be reduced significantly, resulting in higher conversions.

Because the cross-sectional area of the reactor is small near the inlet and outlet, the presence of catalyst there would cause substantial pressure drop, thereby reducing the efficiency of the spherical reactor. To solve this problem, screens to hold the catalyst are placed near the reactor entrance and exit (Figures R5-1 and R5-2). Here L is the location of the screen from the center of the

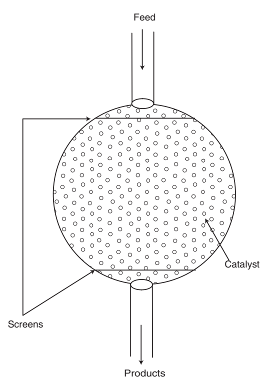

Figure R5-1 Schematic drawing of the inside of a spherical reactor.

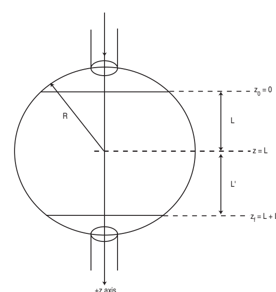

Figure R5-2 Coordinate system and variables used with a spherical reactor. The initial and final integration values are shown as z_0 and z_f

reactor. We can use elementary geometry and integral calculus to derive the following expressions for cross-sectional area and catalyst weight as a function of the variables defined in Figure R5-2:

$$A_c = \pi[R^2 - (z-L)^2] \tag{R5-1}$$

Spherical reactor catalyst weight

$$W = \rho_c(1-\phi)V = \rho_c(1-\phi)\pi\left[R^2 z - \frac{1}{3}(z-L)^3 - \frac{1}{3}L^3\right] \tag{R5-2}$$

*From 3rd edition of elements textbook

By using these formulas and the standard pressure drop algorithm, one can solve a variety of spherical reactor problems. Note that Equations (R5-1) and (R5-2) make use of L and not L'. Thus, one does not need to adjust these formulas to treat spherical reactors that have different amounts of empty space at the entrance and exit (i.e., $L \neq L'$). Only the upper limit of integration needs to be changed, $z_f = L + L'$.

Example R5–1 Dehydrogenation Reactions in a Spherical Reactor

Reforming reactors are used to increase the octane number of petroleum. In a reforming process, 20,000 barrels of petroleum are to be processed per day. The corresponding mass and molar feed rates are 44 kg/s and 440 mol/s, respectively. In the reformer, dehydrogenation reactions such as

$$\text{Paraffin} \rightarrow \text{Olefin} + \text{H}_2$$

occur. The reaction is first order in paraffin. Assume that pure paraffin enters the reactor at a pressure of 2000 kPa and a corresponding concentration of 0.32 mol/dm^3. Compare the pressure drop and conversion when this reaction is carried out in a tubular packed bed 2.4 m in diameter and 25 m in length with that of a spherical packed bed 6 m in diameter. The catalyst weight is the same in each reactor, 173,870 kg.

$$-r'_A = k' C_A$$
$$-r_A = \rho_B(-r'_A) = \rho_C(1-\phi)(-r'_A) = \rho_C(1-\phi)k' C_A$$

Additional information:

$$\rho_0 = 0.032 \text{ kg/dm}^3$$
$$D_P = 0.02 \text{ dm} \qquad \phi = 0.4$$
$$k' = 0.02 \text{ dm}^3\text{/kg cat} \cdot \text{s} \qquad \mu = 1.5 \times 10^{-6} \text{ kg/dm} \cdot \text{s}$$
$$L = L' = 27 \text{ dm} \qquad \rho_c = 2.6 \text{ kg/dm}^3$$

Solution

We begin by performing a mole balance over the cylindrical core of thickness Δz shown in Figure RE5-1.1.

Following the algorithm

1. **Mole balance**:

$$\text{In} - \text{Out} + \text{Generation} = 0$$
$$F_A\big|_z - F_A\big|_{z+\Delta z} + r_A A_c \Delta z = 0$$

Dividing by Δz and taking the limit as $\Delta z \longrightarrow 0$ yields

$$\frac{dF_A}{dz} = r_A A_c$$

In terms of conversion

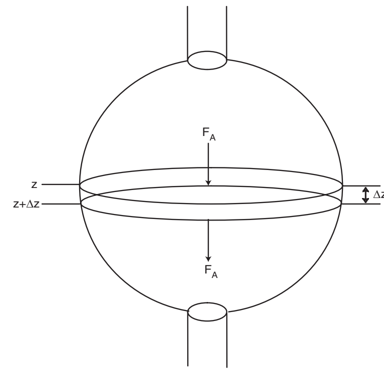

Figure RE5-1.1 Spherical reactor.

$$\boxed{\frac{dX}{dz} = \frac{-r_A A_c}{F_{A0}}} \tag{RE5-1.1}$$

2. **Rate law**:

$$\boxed{r_A = -kC_A = -k' C_A \rho_c (1-\phi)} \tag{RE5-1.2}$$

3. **Stoichiometry**. Gas, isothermal ($T = T_0$):

$$\boxed{C_A = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right) y} \tag{RE5-1.3}$$

$$\varepsilon = y_{A0}\delta = 1 \times (1+1-1) = 1 \tag{RE5-1.4}$$

where

$$y = \frac{P}{P_0} \tag{RE5-1.5}$$

Note that y_{A0} (y with a subscript) represents the mole fraction and y alone represents the pressure ratio, P/P_0.

The variation in the dimensionless pressure, y, is given by incorporating the variable y in Equation (5-24):

$$\boxed{\frac{dy}{dz} = -\frac{\beta_0}{P_0 y}(1+\varepsilon X)} \tag{RE5-1.6}$$

The units of β_0 for this problem are kPa/dm^3.

The equations in boxes are the key equations used in the ODE solver program

$$\beta_0 = \frac{G(1-\phi)}{\rho_0 g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right] \tag{RE5-1.7}$$

$$G = \frac{\dot{m}}{A_c} \tag{RE5-1.8}$$

For a spherical reactor

$$\boxed{A_c = \pi[R^2 - (z-L)^2]} \tag{RE5-1.9}$$

$$\boxed{W = \rho_c(1-\phi)\pi\left[R^2 z - \frac{1}{3}(z-L)^3 - \frac{1}{3}L^3\right]} \tag{RE5-1.10}$$

Parameter evaluation:
Recall that $g_c = 1$ for metric units.

$$\beta_0 = \left[\frac{G(1-0.4)}{(0.032\ \text{kg/dm}^3)(0.02\ \text{dm})(0.4)^3}\right] \times \left[\frac{150(1-0.4)(1.5\times 10^{-6}\ \text{kg/dm}\cdot\text{s})}{0.02\ \text{dm}} + 1.75G\right] \tag{RE5-1.11}$$

$$\boxed{\beta_0 = [(98.87\ \text{s}^{-1})G + (25{,}630\ \text{dm}^2/\text{kg})G^2] \times \left(0.01\ \frac{\text{kPa/dm}}{\text{kg/dm}^2\cdot\text{s}^2}\right)} \tag{RE5-1.12}$$

The last term in brackets converts (kg/dm$^2\cdot$s) to (kPa/dm). Recalling other parameters, $\dot{m}$ = 44 kg/s, L = 27 dm, R = 30 dm, and ρ_{cat} = 2.6 kg/dm^3.

Table RE5-1.1 shows the POLYMATH input used to solve the above equations. The MATLAB program is given as a living example problem on the CD-ROM.

Living Example Problem

TABLE R5-1.1 POLYMATH PROGRAM

Equations	*Initial Values*
d(X)/d(z)=–ra*Ac/Fao	0
d(y)/d(z)=–beta/Po/y*(1+X)	1
Fao=440	
Po=2000	
CaO=0.32	
R=30	
phi=0.4	
kprime-0..02	
L=27	
rhocat=2.6	
m=44	
Ca=CaO*(1–X)*y/(1+X)	
Ac=3.1416*(R^2–(z–L)^2)	
V=3.1416*(z*R^2–1/3*(z–L)^3–1/3*L^3)	
S=m/Ac	
ra=–kprime*Ca*rhocat*(1–phi)	

TABLE R4-1.1 POLYMATH PROGRAM (CONTINUED)

beta=(98.87*G+25630*G^2)*0.01
W=rhocat*(1–phi)*V
$z_0 = 0, \quad z_f = 54$

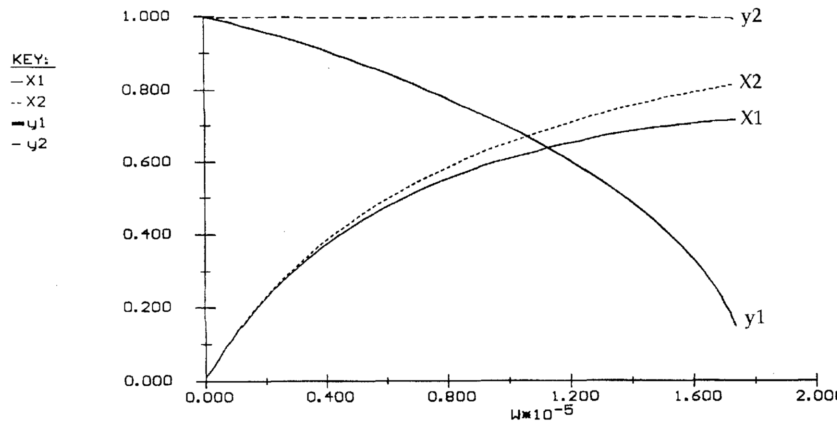

Figure RE5-1.2 Pressure and conversion for: 1, tubular PBR; 2, spherical PBR.

A comparison between reactors

For the spherical reactor, the conversion and the pressure at the exit are

$$X = 0.81 \qquad P = 1980 \text{ kPa}$$

If similar calculations are performed for the tubular PBR, one finds that for the same catalyst weight the conversion and pressure at the exit are

$$X = 0.71 \qquad P = 308 \text{ kPa}$$

Figure RE5-1.2 shows how conversion, X, and dimensionless pressure, y, vary with catalyst weight in each reactor. Here X_1 and y_1 represent the tubular reactor and X_2 and y_2 represent the spherical reactor. In addition to the higher conversion, the spherical reactor has the economic benefit of reducing the pumping and compression cost because of higher pressure at the exit.

Because the pressure drop in the spherical reactor is very small, one could increase the reactant flow rate significantly and still maintain adequate pressure at the exit. In fact, Amoco uses a reactor with similar specifications to process 60,000 barrels of petroleum naphtha per day.