14.6 Numerical Solutions to Flows with Dispersion and Reaction

We now consider dispersion and reaction. We first write our mole balance on species A by recalling Equation (14-28) and including the rate of formation of A, r_A. At steady state we obtain

$$D_{AB}\left[\frac{1}{r}\frac{\partial\left(r\frac{\partial C_A}{\partial r}\right)}{\partial r}+\frac{\partial^2 C_A}{\partial z^2}\right]-U(r)\frac{\partial C_A}{\partial z}+r_A=0 \tag{14-51}$$

Analytical solutions to dispersion with reaction can only be obtained for isothermal zero- and first-order reactions. We are now going to use COMSOL to solve the flow with reaction and dispersion with reaction. A COMSOL CD-ROM is included with the text.

We are going to compare two solutions: one which uses the Aris–Taylor approach and one in which we numerically solve for both the axial and radial concentration using COMSOL.

Case A. Aris–Taylor Analysis for Laminar Flow

For the case of an nth-order reaction, Equation (14-15) is

$$\frac{D_a}{U}\frac{d^2 C_A}{dz^2}-\frac{dC_A}{dz}-\frac{kC_A^n}{U}=0 \tag{14-52}$$

If we use the Aris–Taylor analysis, we can use Equation (14-15) with a caveat that $\overline{\psi}=\overline{C}_A/C_{A0}$ where $\overline{C}_A$ is the average concentration from $r=0$ to $r=R$ as given by

$$\frac{1}{\mathrm{Pe}_r}\frac{d^2\overline{\psi}}{d\lambda^2}-\frac{d\overline{\psi}}{d\lambda}-\boldsymbol{Da}\,\overline{\psi}^n=0 \tag{14-53}$$

where

$$\mathrm{Pe}_r=\frac{UL}{D_a} \text{ and } \boldsymbol{Da}=\tau k C_{A0}^{n-1}$$

For the closed-closed boundary conditions we have

$$\text{At}\quad \lambda=0:\quad -\frac{1}{\mathrm{Pe}_r}\frac{d\overline{\psi}}{d\lambda}\bigg|_{0^+}=\overline{\psi}(0^+)=1 \tag{14-54}$$

Danckwerts boundary conditions

$$\text{At}\quad \lambda=1:\quad \frac{d\overline{\psi}}{d\lambda}=0$$

For the open-open boundary condition we have

$$\text{At} \quad \lambda = 0: \quad \bar{\psi}(0^-) - \frac{1}{\text{Pe}_r}\frac{d\bar{\psi}}{d\lambda}\bigg|_{0^-} = \bar{\psi}(0^+) - \frac{1}{\text{Pe}_r}\frac{d\bar{\psi}}{d\lambda}\bigg|_{0^+} \tag{14-55}$$

$$\text{At} \quad \lambda = 1: \quad \frac{d\bar{\psi}}{d\lambda} = 0$$

Equation (14-53) is a nonlinear second order ODE that is solved on the COMSOL CD-ROM.

Case B. Full Numerical Solution

To obtain axial and radial profile we now solve Equation (14-51)

$$D_{AB}\left[\frac{1}{r}\frac{\partial\left(r\dfrac{\partial C_A}{\partial r}\right)}{\partial r} + \frac{\partial^2 C_A}{\partial z^2}\right] - U(r)\frac{\partial C_A}{\partial z} + r_A = 0 \tag{14-51}$$

First we will put the equations in dimensionless form by letting $\psi = C_A/C_{A0}$, $\lambda = z/L$, and $\phi = r/R$. Following our earlier transformation of variables, Equation (14-51) becomes

$$\left(\frac{L}{R}\right)\frac{1}{\text{Pe}_r}\left[\frac{1}{\phi}\frac{\partial\left(r\dfrac{\partial\psi}{\partial\phi}\right)}{\partial\phi}\right] + \frac{1}{\text{Pe}_r}\frac{d^2\psi}{d\lambda^2} - 2(1-\phi^2)\frac{d\psi}{d\lambda} - \boldsymbol{Da}\psi^n = 0 \tag{14-56}$$

Example 14–3 Dispersion with Reaction

(a) First, use COMSOL to solve the dispersion part of Example 14-2 again. How does the COMSOL result compare with the solution to Example 14-2?

(b) Repeat (a) for a second-order reaction with k = 0.5 dm^3/mol • min.

(c) Repeat (a) but assume laminar flow and consider radial gradients in concentration. Use D_{AB} for both the radial and axial diffusion coefficients. Plot the axial and radial profiles. Compare your results with part (a).

Additional information:

C_{A0} = 0.5 mol/dm^3, $U_0 = L/\tau$ = 1.24 m/min, $D_a = U_0L/\text{Pe}_r$ = 1.05 m^2/min. D_{AB} = 7.6E-5 m^2/min.

The different types of COMSOL Boundary Conditions are given in Problem P14-19$_c$

Note: For part (a), the two-dimensional model with no radial gradients (plug flow) becomes a one-dimensional model. The inlet boundary condition for part (a) and part (b) is a closed-closed vessel (flux[$z = 0^-$] = flux[$z = 0^+$] or $U_z \cdot C_{A0}$ = flux) at the inlet boundary. In COMSOL format it is: $-N_i \cdot n$ = U0*CA0. The boundary condition for laminar flow in COMSOL format for part (c) is: $-N_i \cdot n$ = 2*U0*(1–(r/Ra)$_2$)*CA0.

Solution

(a) Equation (14-52) was used in the COMSOL program along with the rate law

$$r_A = -kC_A = -kC_{A0}\,\psi$$

We see that we get the same results as the analytical solution in Example 14-2. With the Aris–Taylor analysis the two-dimensional profile becomes one-dimensional plug flow velocity profile. Figure E14-3.1(a) shows a uniform concentration surface and shows the plug flow behavior of the reactor. Figure E14-3.1(b) shows the corresponding cross-section plots at the inlet, half axial location, and outlet. The average outlet conversion is 67.9%.

The average outlet concentration at an axial distance z is found by integrating across the radius as shown below

$$C_A(z) = \int_0^R \frac{2\pi r C_A(r,z)dr}{\pi R^2}$$

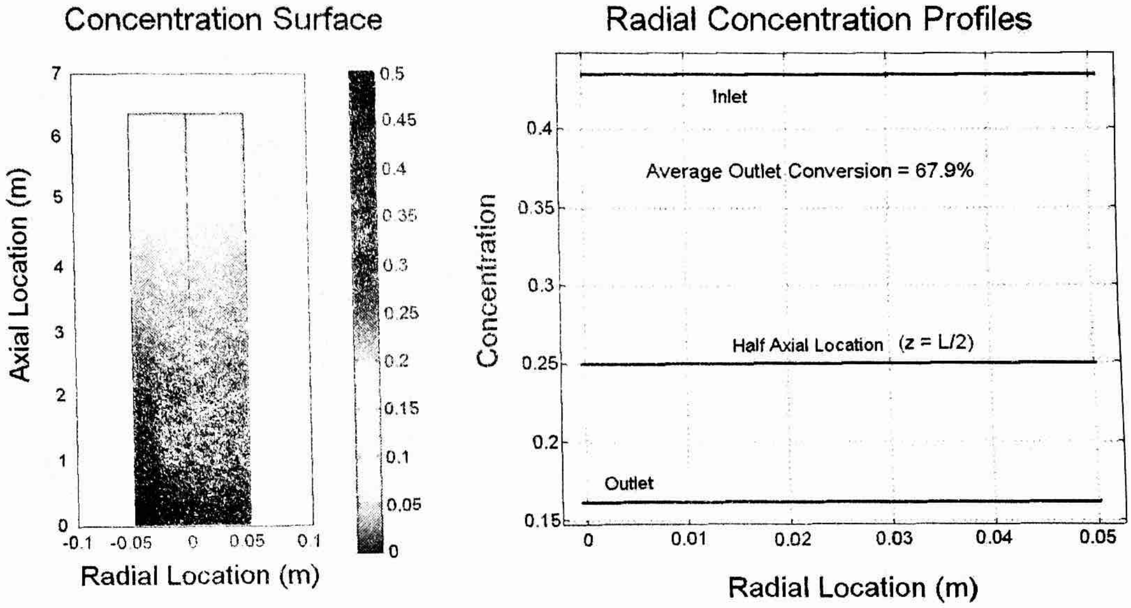
Be sure to view documentation on COMSOL CD-ROM to see COMSOL tutorial with screen shots

From the average concentrations at the inlet and outlet we can calculate the average conversion as

$$X = \frac{C_{A0} - C_A}{C_{A0}}$$

Load enclosed COMSOL CD

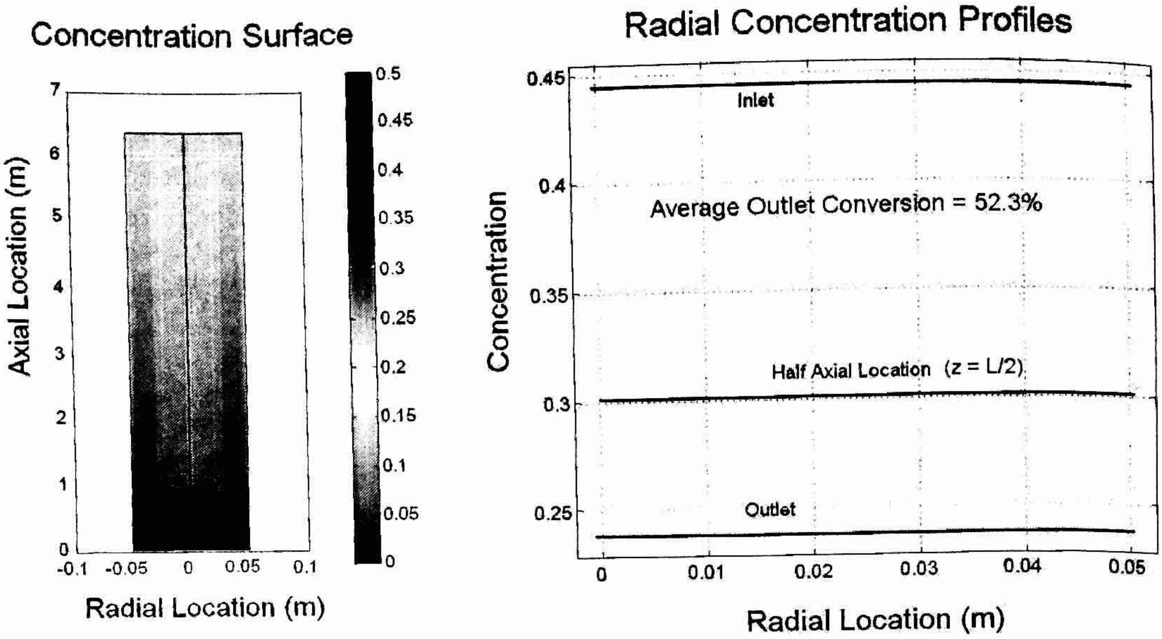
Living Example Problem



(a) (b)

Figure E14-3.1 COMSOL results for a plug flow reactor with first-order reaction. (Concentrations in mol/dm³.)

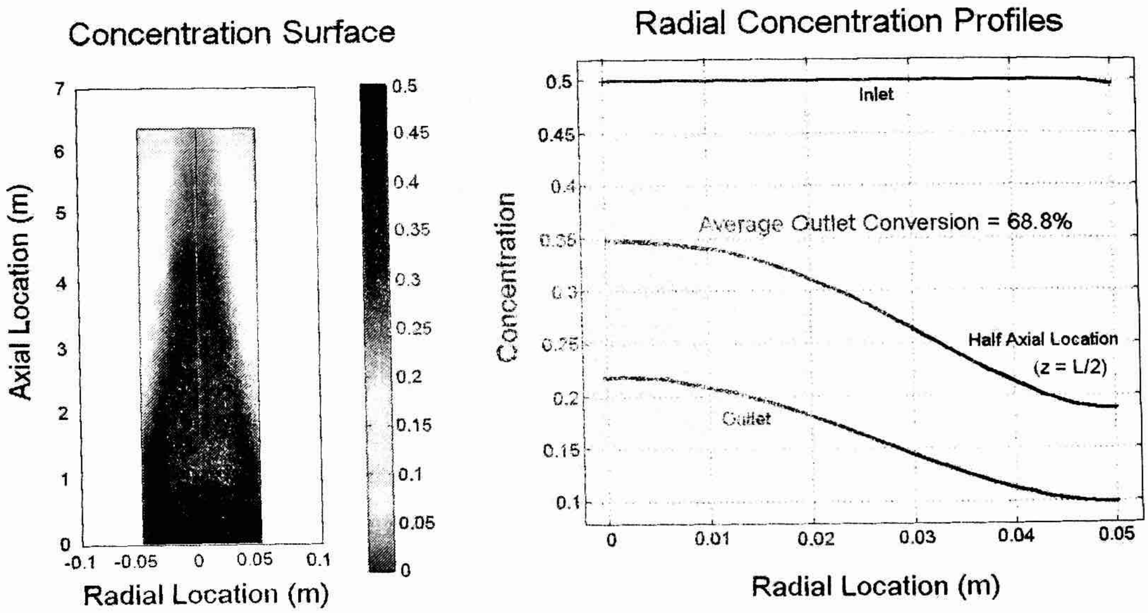
(b) Now we expand our results to consider the case when the reaction is second order ($-r_A = kC_A^2 = kC_{A0}^2\psi^2$) with $k = 0.5$ dm³/mol·min and $C_{A0} = 0.5$ mol/dm³. Let's assume the radial dispersion coefficient is equal to the molecular diffusivity. Keeping everything else constant, the average outlet conversion is 52.3%. However, because the flow inside the reactor is modeled as plug flow the concentration profiles are still flat, as shown in Figure E14-3.2.



(a) (b)

Figure E14-3.2 COMSOL results for a plug flow reactor with second-order reaction. (Concentrations in mol/dm^3.)

(c) Now, we will change the flow assumption from plug flow to laminar flow and solve Equation (14-51) for a first-order reaction.



(a) (b)

Figure E14-3.3 COMSOL output for laminar flow in the reactor. (Concentrations in mol/dm^3.)

The average outlet conversion becomes 68.8%, not much different from the one in part (a) in agreement with the Aris–Taylor analysis. However, due to the laminar flow assumption in the reactor, the radial concentration profiles are very different throughout the reactor.

(d) As a homework exercise, repeat part (c) for the second-order reaction given in part (b).