Web COMSOL

Web Example 18–3 Dispersion with Reaction

In Web Example 18-1 we used analytical solutions to solve for the conversion in nonideal reactors with first-order reactions. In this example we will use a software package, COMSOL, to resolve Example 18-1 and then extend to a second-order reaction taking place in a nonideal reactor with axial dispersion.

(a) First, use COMSOL to solve the dispersion part of Example 18-1 again. How does the COMSOL result compare with the solution to Example 18-1?

(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, $D_a = U_0 L/\text{Pe}_r$ = 1.05 m^2/min, and D_{AB} = 7.6E-5 m^2/min.

The different types of COMSOL boundary conditions are given in Problem P18-19$_c$.

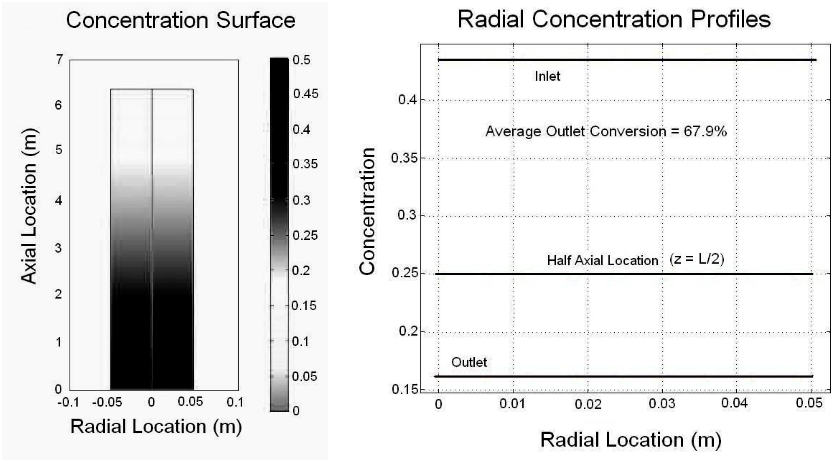
Note: For part (a), the two-dimensional model with no radial gradients (plug flow) becomes a one-dimensional model. The inlet boundary condition for part (a) and part (b) is a closed-closed vessel (flux[$z = 0^-$] = flux[$z = 0^+$] or $U_z \cdot C_{A0}$ = flux) at the inlet boundary. In COMSOL format,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

Solution

(a) Equation (18-52) 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 18-1. With the Aris-Taylor analysis, the two-dimensional profile becomes a one-dimensional plug-flow velocity profile. Figure WE18-2.1(a)



(a) (b)

Figure WE18-2.1 COMSOL results for a plug-flow reactor with first-order reaction (concentrations in mol/dm^3).

shows a uniform concentration surface and shows the plug-flow behavior of the reactor. Figure WE18-2.1(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

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

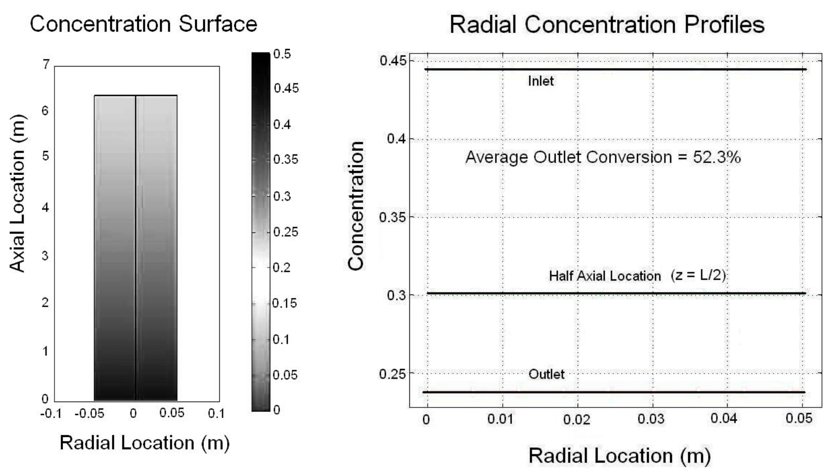
Be sure to view documentation on COMSOL on the CRE Web site to see a COMSOL tutorial with screen shots.

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

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

(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 $k = 0.5$ dm^3/mol·min and $C_{A0} = 0.5$ mol/dm^3. 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 WE18-2.2.

Living Example Problem



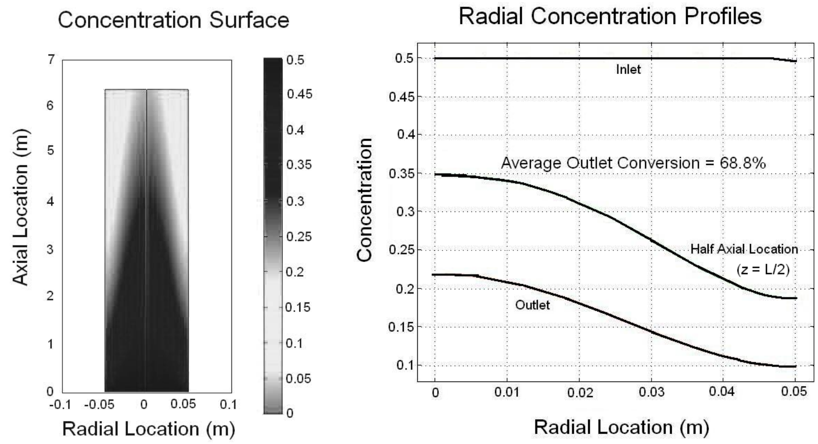
(a) (b)

Figure WE18-2.2 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 (18-51) for a first-order reaction.

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).



(a) (b)

Figure WE18-2.3 COMSOL output for laminar flow in the reactor (concentrations in mol/dm^3).

Analysis: In this example we used COMSOL to compare the outlet concentration for three experiments. The first one was for axial dispersion but no radial dispersion for a first-order reaction, which gave an average exit conversion of 67.9%. The conversion predicted by COMSOL is virtually the same as that predicted by the analytical solution in Example 14-2. For the second experiment, the reaction was second order and carried out again with axial dispersion but no radial dispersion; then, average exit conversion was 53.5%. In the third experiment, the same first order **(a)** was carried out in with both axial and radial dispersion.

Example 18-2. (1) Load the reaction and dispersion program from the CRE Web site. Vary the Damköhler number for a second-order reaction using the Aris-Taylor approximation (part (b) in Example 18-3). (2) Vary the Peclet and Damköhler numbers for a second-order reaction in laminar flow. What values of the Peclet number affect the conversion significantly?