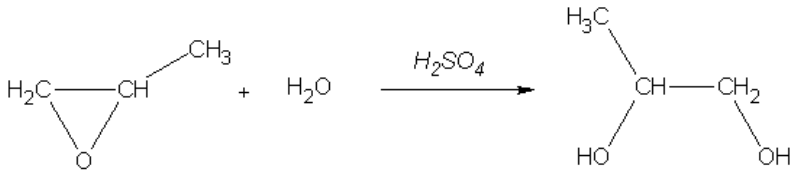
Web Example 12–8 Radial Effects in Tubular Reactor COMSOL T = f (r,z)

Web Modules

This example will highlight the radial effects in a tubular reactor, which up until now have been neglected to simplify the calculations. Now, however, the effects of parameters such as inlet temperature and flow rate will be studied using the software program COMSOL, www.comsol.com/ecre. Follow the step-by-step procedure in the Web Module.

We now discuss the reaction of propylene oxide (A) with water (B) to form propylene glycol (C). The hydrolysis of propylene oxide takes place readily at room temperature when catalyzed by sulfuric acid.

$$A + B \longrightarrow C$$



This exothermic reaction is approximated as a first-order reaction given that the reaction takes place in an excess of water.

The CSTR from Example 8-8 has been replaced by a tubular reactor 1.0 m in length and 0.2 m in diameter.

The feed to the reactor consists of two streams. One stream is an equivolumetric mixture of propylene oxide and methanol, and the other stream is water containing 0.1 wt % sulfuric acid. The water is fed at a volumetric rate 2.5 times larger than the propylene oxide–methanol feed. The molar flow rate of propylene oxide fed to the tubular reactor is 0.1 mol/s.

There is an immediate temperature rise upon mixing the two feed streams caused by the heat of mixing. In these calculations, this temperature rise is already accounted for, and the inlet temperature of both streams is set to 312 K.

The reaction rate law is

$$-r_A = kC_A$$

with

$$k = Ae^{-E/RT}$$

where E = 75362 J/mol and A = 16.96×10^{12} h^{-1}, which can also be put in the form

$$k(T) = k_0(T_0)\exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

with k_0 = 1.28 h^{-1} at 300 K. The thermal conductivity, k_e, of the reaction mixture and the diffusivity, D_e, are 0.599 W/m/K and 10^{-9} m^2/s, respectively, and are assumed to be constant throughout the reactor. In the case where there is a heat exchange between the reactor and its surroundings, the overall heat-transfer coefficient is 1300 W/m^2/K and the temperature of the cooling jacket is assumed to be constant and is set to 273 K. The other property data are shown in Table WE12-8.1.

TABLE WE12–8.1 PHYSICAL PROPERTY DATA

	Propylene Oxide	*Methanol*	*Water*	*Propylene Glycol*
Molar weight (g/mol)	58.095	32.042	18	76.095
Density (kg/m^3)	830	791.3	1000	1040
Heat capacity (J/mol • K)	146.54	81.095	75.36	192.59
Heat of formation (J/mol)	–154911.6		–286098	–525676

Solution

Mole Balances: Recalling Equation (12-44) and applying it to species A

A:
$$D_e\frac{\partial^2 C_A}{\partial r^2}+\frac{1}{r}D_e\frac{\partial C_A}{\partial r}+D_e\frac{\partial^2 C_A}{\partial z^2}-U_z\frac{\partial C_A}{\partial z}+r_A=0 \qquad \text{(WE12-8.1)}$$

Rate Law:

$$-r_A=k(T_1)\exp\left[\frac{E}{R}\left(\frac{1}{T_1}-\frac{1}{T}\right)\right]C_A \qquad \text{(WE12-8.2)}$$

Stoichiometry: The conversion along a streamline (r) at a distance z

$$X(r,z)=1-C_A(r,z)/C_{A0} \qquad \text{(WE12-8.3)}$$

The overall conversion is

$$\overline{X}(z)=1-\frac{2\pi\int_0^R C_A(r,z)U_z r\,dr}{F_{A0}} \qquad \text{(WE12-8.4)}$$

The mean concentration at any distance z

$$\overline{C_A}(z)=\frac{2\pi\int_0^R C_A(r,z)U_z r\,dr}{\pi R^2 U_0} \qquad \text{(WE12-8.5)}$$

For plug flow, the velocity profile is

$$U_z=U_0 \qquad \text{(WE12-8.6)}$$

The laminar-flow velocity profile is

$$U_z=2U_0\left[1-\left(\frac{r}{R}\right)^2\right] \qquad \text{(WE12-8.7)}$$

Recalling the Energy Balance

$$\boxed{k_e\frac{\partial^2 T}{\partial z^2}+\frac{k_e}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\Delta H^\circ_{Rx}r_A-U_zC_{P_m}\frac{\partial T}{\partial z}=0} \qquad \text{(12-55)}$$

Living Example Problem

Assumptions

1. U_r is zero.
2. Neglect axial diffusion/dispersion flux wrt convective flux when summing the heat capacity times their fluxes.
3. Steady state.

Cooling jacket

$$\dot{m}C_{P_i}\frac{\partial T_a}{\partial z} = 2\pi R U_{\text{ht}}(T(\text{R},z) - T_a) \tag{12-56}$$

Boundary conditions

$$\text{At } r = 0, \text{ then } \frac{\partial C_i}{\partial r} = 0 \text{ and } \frac{\partial T}{\partial r} = 0 \tag{WE12-8.8}$$

$$\text{At } r = R, \text{ then } \frac{\partial C_i}{\partial r} = 0 \text{ and } -k_e\frac{\partial T}{\partial r} = U_{\text{ht}}(T(\text{R},z) - T_a) \tag{WE12-8.9}$$

$$\text{At } z = 0, \text{ then } C_i = C_{i0} \text{ and } T = T_0 \tag{WE12-8.10}$$

These equations were solved using COMSOL for a number of cases including adiabatic and non-adiabatic plug flow and laminar flow; they were also solved with and without axial and radial dispersion. A detailed accounting on how to change the parameter values in the COMSOL program can be found in the COMSOL Instructions section on the Web in screen shots similar to Figure E12-8.1. Figure E12-8.1 gives the data set in SI units used for the COMSOL example on the CRE Web site.

Note: There is a step-by-step COMSOL tutorial using screen shots for this example on the CRE Web site.

Case 2: Constant cooling jacket temperature and water volumetric flow rate 2.5 times that of the propytene oxide and methanol mixture

Settings

Parameters

Parameters

Name	Expression	Value	Description
E	75362[J/mol]	75362 J/mol	Activation energy
A	16.96e12[1/h]	4.7111E9 1/s	Frequency factor
Diff	1e-9[m^2/s]	1.0000E-9 m²/s	Diffusion coefficient
ke	0.559[W/m/K]	0.55900 W/(m·K)	Thermal conductivity
Uk	1300[W/m^2/K]	1300.0 W/(m²·K)	Overall heat-transfer coefficient
T0	312[K]	312.00 K	Inlet temperature
Ta0	273[K]	273.00 K	Inlet temperature of the coolant
dHrx	-84666[J/mol]	-84666 J/mol	Heat of reaction
v0	0.1[mol/s]/cA0	6.2995E-5 m³/s	Total flow rate
cA0	rho_po_p/M_po/9[1]	1587.4 mol/m³	Propylene oxide concentration, inlet
cB0	rho_w_p/M_w*(7/9)[1]	43210 mol/m³	Water concentration, inlet
cMe0	rho_m_p/M_m/9[1]	2744.0 mol/m³	Methanol concentration, inlet
Cp0	(146.54[J/mol/K]*cA0+81.095[J/mol/K]*cMe0+75.36[J/mol/K]*cB0)/rho0	3874.5 J/(kg·K)	Heat capacity at inlet
rho0	(cA0*M_po+cB0*M_w+cMe0*M_m)	957.92 kg/m³	Density at inlet
Ra	0.1[m]	0.10000 m	Reactor radius
L	1[m]	1.0000 m	Reactor length
M_po	58.095[g/mol]	0.058095 kg/mol	Molar weight, propylene oxide
M_m	32.042[g/mol]	0.032042 kg/mol	Molar weight, methanol
M_w	18[g/mol]	0.018000 kg/mol	Molar weight, water
rho_po_p	830[kg/m^3]	830.00 kg/m³	Density, propylene oxide
rho_m_p	791.3[kg/m^3]	791.30 kg/m³	Density, methanol
rho_w_p	1000[kg/m^3]	1000.0 kg/m³	Density, water

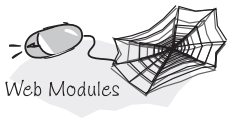
Web Figure E12-8.1 COMSOL screenshot of the parameters used for the *Radial effects in tubular reactor* exercises.

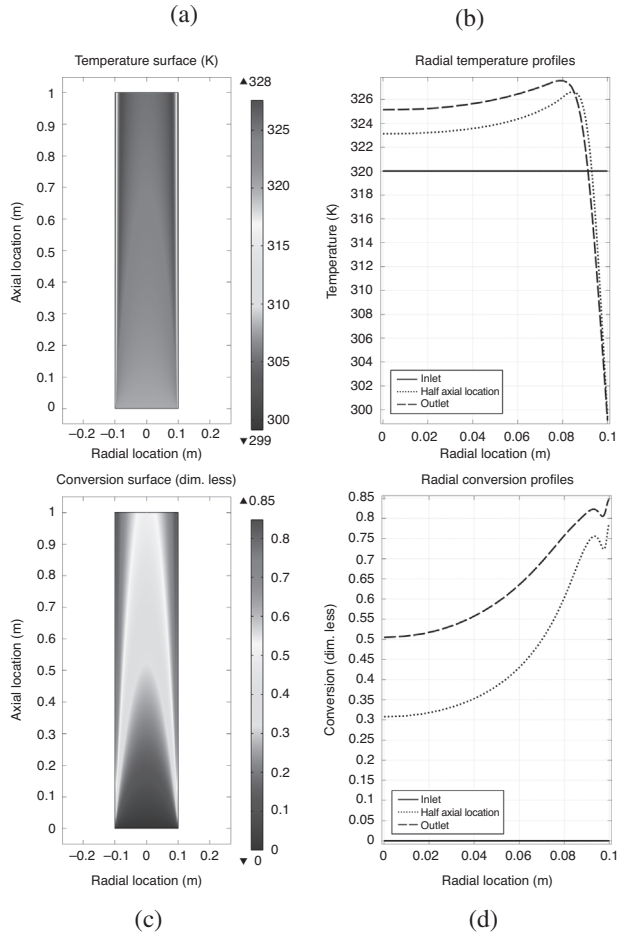
Color surfaces are used to show the concentration, conversion, and temperature profiles, similar to the black-and-white figures shown in Figure E12-8.2. Use the COMSOL app on the COMSOL Web site (*www.comsol.com/ecre*) to develop temperature concentration profiles similar to the ones shown here. Read through the COMSOL Web Module entitled "Radial and Axial Temperature Gradients" before running the simulations.

Color surfaces are used to show the concentration and temperature profiles, similar to the black-and-white figures shown in Figure E12-8.2. Use the COMSOL program on the COMSOL Web site (*www.comsol.com*) to develop temperature concentration profiles similar to the ones shown here. Read through the COMSOL Web Module entitled "Radial and Axial Temperature Gradients" before running the simulations.

Results

Results of the COMSOL simulation





Web Figure E12-8.2 (a) Temperature surface, (b) temperature surface profiles, (c) conversion surface, and (d) radial conversion profile.

The volumetric flow rate of water is 3.5 times propylene oxide in the methanol volumetric flow rate.

Analysis: One notes from the temperature surface plot, the temperature at the entrance (0 – 0.2 m) does not vary much radially and stays around 280 K. One also notes in Figure E12-8.2 that the conversion is lower near the wall because of the cooler fluid temperature. These same profiles can be found in color on the CRE Web site in the Web Modules. Be sure to note the predicted maximum and minimum in the temperature and concentration profiles. Near the wall, the temperature of the mixture is lower because of the cold wall temperature. Consequently, the rate will be lower, and thus the conversion will be lower. However, right next to the wall, the velocity through the reactor is almost zero so the reactants spend a long time in the reactor; therefore, a greater conversion is achieved as noted by the upturn right next to the wall.

Web Example 12-8. *COMSOL LEP Instructions:* Make sure that you have COMSOL Multiphysics 5 installed on your computer. Double-click the COMSOL Multiphysics icon on your desktop. Select "Model Libraries" from the File menu in the COMSOL Multiphysics user interface to open the Model Libraries page. On the Model Libraries page, navigate to the catalogue, Chemical Reaction Engineering Module > Tutorial Models. Select the model "4-Non-Isothermal Reactor II," and press "Open Model and PDF." Browse the model documentation in the PDF document and review the model equations. Find the step-by-step instructions and read them to familiarize yourself with the model set-up.

(1) Why is the concentration of A near the wall lower than the concentration near the center? (2) Where in the reactor do you find the maximum and minimum reaction rates? Why? *Instructions:* In the Model Builder window, navigate to Results > Reaction Rate > Surface, select the "Surface" node, and press "Plot" in the toolbar of the Settings window for Surface. This plot shows the reaction rate for the consumption of species A in the reactor. (3) Increase the activation energy of the reaction by 5%. How do the concentration profiles change? Decrease. *Instructions:* In the Model Builder, navigate to Global > Definitions > Parameters and select the "Parameters" node. In the Settings window, select the parameter "E" for the activation energy and multiply this parameter by 1.05 (just type in "*1.05" behind the existing value in the Expression cell for "E" or in the corresponding edit field below the parameter table; type "*0.95" to decrease). In the "Mode" tab (toolbar on Mac and Linux), press "Compute" ("=" icon) found in the Study section. In the Model Builder, select the "Results > Reaction Rate > Surface" node to update the plot. Repeat this procedure for the lower activation energy value. (4) Change the activation energy back to its original expression by removing "*0.95" in the corresponding cell in the Parameters table. (5) Increase the thermal conductivity, k_e, by a factor of 10 and explain how this change affects the temperature profiles. At what radial position do you find the highest conversion? *Instructions:* In the Parameters list, select the parameter "ke" for the thermal conductivity and multiply the expression for this parameter by 10 (type "*10" behind the existing value in the corresponding Expression cell). Press "Compute" in the Model tab. Select "Results > Conversion, 1D > Line Graph" to update the conversion profile plot. (6) Increase the coolant flow rate by a factor of 10 and explain how this change affects conversion. (7) In two or three sentences, describe your finding when you varied the parameters (for all parts). (8) What would be your recommendation to maximize the average outlet conversion? (9) Review Figure E12-8.2 and explain why the temperature profile goes through a maximum and why the conversion profile goes through a maximum *and* a minimum. (10) See other problems in the web module.