COMSOL ECRE

VERSION 3.1

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I

The COMSOL ECRE Version

Introduction

The technical staff at COMSOL has developed this special COMSOL ECRE Version (also referred to throughout this book simply as COMSOL ECRE) exclusively for H. Scott Fogler's book *Elements of Chemical Reaction Engineering*. As you will see in the following pages, COMSOL is an exceptionally powerful tool for performing PDE-based modeling and simulations in a broad number of disciplines, but here we focus on energy and mass balances. To help you better understand the underlying physics and principles, the COMSOL engine runs a number of ready-made models in which you can change key parameters and observe the results. Thus, the accompanying CD includes the COMSOL computational engine along with six complete models and full documentation. These illustrative models combine energy and mass balances in both isothermal and non-isothermal conditions using the appropriate application modes in COMSOL.

We have divided the examples into two section. The first section treats radial effects in tubular reactors induced by velocity distribution along the radius, and it examines the effects of external cooling at a reactor's outer wall. The second section deals with dispersion effects in tubular reactors, and it compares different assumptions for the inlet and outlet boundary conditions. It also compares 1-dimensional models with the solutions from axisymmetric models.

More specifically, the models we present are:

- Radial effects in tubular reactors
  - **a** Isothermal reactor
  - **b** Non-isothermal adiabatic reactor
  - **c** Non-isothermal reactor with isothermal cooling jacket
  - **d** Non-isothermal reactor with non-isothermal cooling jacket.
- Tubular reactors where the flow includes the effects of dispersion
  - **a** 1-dimensional model with Danckwerts boundary conditions
  - **b** 1-dimensional model with upstream and downstream sections

The two dispersion models in the second set investigate the Danckwerts boundary conditions by comparing them with results obtained from a reactor model that adds an inlet and outlet section.

In all of these models you can change input data—such as rate constants, flow rates, diffusivities, and conductivities—and have COMSOL again solve the model. It is also possible to visualize results through ready-made expressions or by entering arbitrary expressions of the solution variables into COMSOL.

The immediately following section provides a brief introduction to COMSOL and the Chemical Engineering Module, which together form the basis for the models just listed. If you are already familiar with COMSOL and would prefer to start with the exercises immediately, proceed to Chapter 2.

The Chemical Engineering Module

COMSOL Multiphysics is a modeling package that solves arbitrary systems of partial differential equations (PDEs). It allows you to solve these equations in two ways: First, in what we refer to as PDE modes, you enter the equations from scratch at the keyboard. Second, the software provides a far easier method of solving commonly encountered equations whereby you take advantage of ready-made application modes targeted at the problem areas the equations describe. For example, the Navier-Stokes application mode implements a predefined interface for the modeling of laminar flow as described by the Navier-Stokes equations.

The Chemical Engineering Module that comes as an add-on to COMSOL Multiphysics delivers a selection of these ready-made application modes for transport and reaction processes found in chemical engineering. That module was inspired by two classic chemical-engineering texts: Fogler's *Elements of Chemical Reaction Engineering* and Bird, Stewart, and Lightfoot's *Transport Phenomena*.

The Chemical Engineering Module is divided into three application mode menu trees:

- Momentum balances
- Energy balances
- Mass balances

All application modes in COMSOL Multiphysics are equation-based. This means that by selecting a ready-made application mode you can easily modify or extend the built-in equations. For example, you might elect to enter expressions for source and sink terms such as reaction terms.

The following sections offer a short presentation of the application modes in the Chemical Engineering Module.

Momentum Balances

The momentum balances application modes encompass the relevant equations for a large variety of fluid-flow applications.

Incompressible Navier-Stokes: This application mode defines and solves the Navier-Stokes equations where density is a constant, and it includes a range of possible boundary conditions. You can easily extend it to include driving forces from other phenomena such as electric fields in electrokinetic flow.

Figure 1-1 shows the flow profile at the junction of several micro-channels, where the inlet velocities at the star-like entrance vary in a sinusoidal fashion. You create these varying flow profiles by specifying a sinusoidal expression for the inlet pressures and introducing a phase shift among the different inlets.

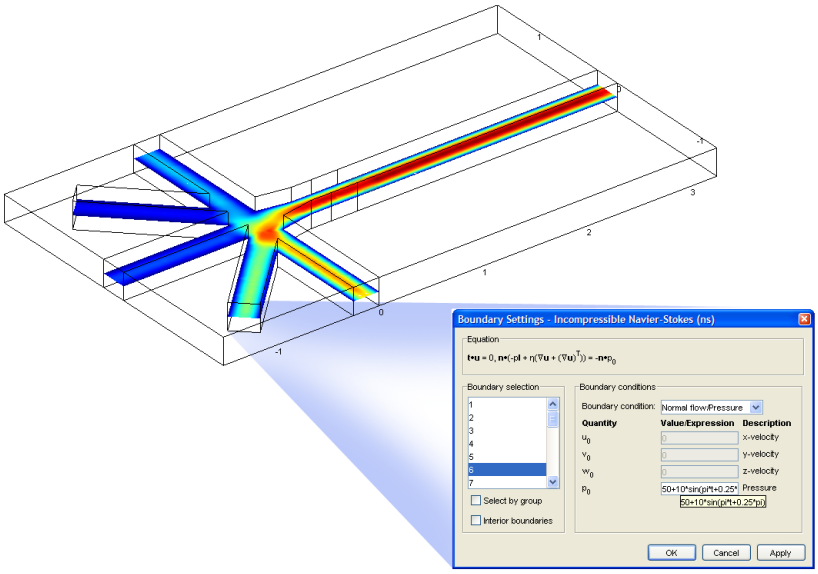


Figure 1-1: Flow velocity field in a star-like micro-channel structure. You enter the sinusoidal inlet pressure directly into the graphical user interface's dialog box for the boundary conditions.

Non-Newtonian Flow: This application mode includes two predefined models for non-Newtonian fluids—the Carreau model and the power law model, which together cover a large group of non-Newtonian fluids. The modeling interface and boundary conditions are similar to those for the general Navier-Stokes application mode.

Non-Isothermal Flow: This is also a version of the Navier-Stokes application mode but allows for density to include temperature dependencies.

k-ε Turbulence Model: This application mode solves the *k-ε* model equations for turbulent flow. It includes logarithmic wall laws and other boundary conditions needed for the simulation of turbulent flow with these equations.

Figure 1-2 illustrates results from a model of a baffled reactor solved with the *k-ε* Turbulence Model application mode. The graph shows the concentration distribution

ten seconds after injection at the inlet. The mixing improves with the number of baffles that follow the inlet.

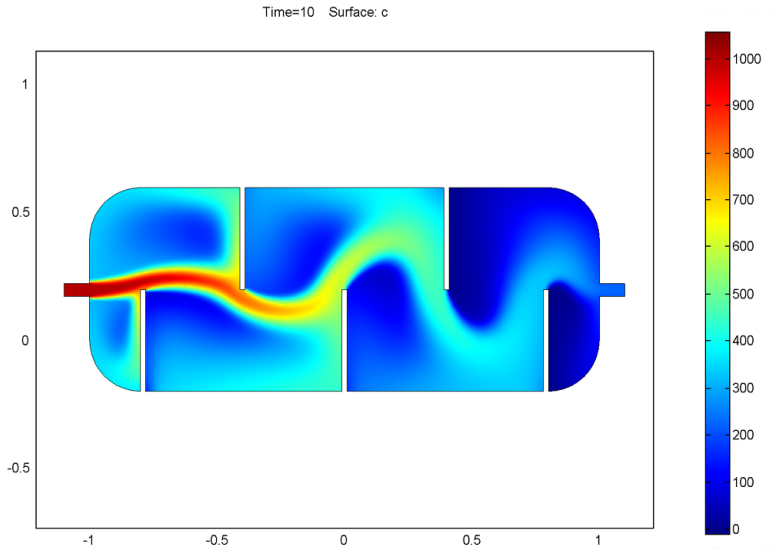


Figure 1-2: Concentration distribution in a baffled reactor solved with the k-ε Turbulence Model application mode. The extent of mixing increases with the number of baffles.

Darcy's Law: This application mode deals with porous media flow as described by Darcy's law in combination with the continuity equation.

Brinkman Equations: This extension of Darcy's law includes the influence of viscosity in porous media flow. With it you can treat highly porous structures or combinations of open channels and porous structures such as monolithic reactors.

Euler Flow: This application mode is suitable for the modeling of trans-sonic inviscid flow. It solves the momentum, mass, and energy balances needed to model compressible flow, handling the effects of work done by fluid compression and expansion.

Energy Balances

The energy balances application modes account for the transport of energy in fluids and solids as well as the generation of heat through chemical reactions.

Conduction: This application mode defines and solves heat-transfer problems where flux is dominated by conduction. It also includes arbitrary reaction terms where you can define heat generation from reactions.

Convection and Conduction: This application mode couples fluid flow with energy transport. It includes heat transport by conduction, convection, and species diffusion in a solution. In the source term it can incorporate arbitrary expressions for heat generation such as chemical reactions.

Figure 1-3 shows the temperature field in an enclosure where a heat source sits at its bottom and the vertical walls are being cooled. The model combines two application modes: Convection and Conduction, and Non-Isothermal Flow. The temperature and density variations induce buoyancy-driven flow in the cavity.

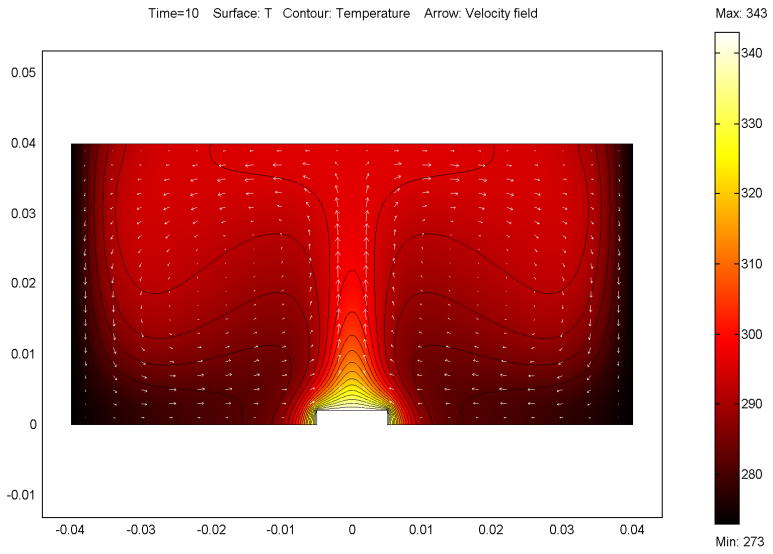


Figure 1-3: Temperature field in an enclosure where buoyancy drives the flow. The model combines the Conduction and Convection application mode with the Non-Isothermal Flow application mode.

Mass Balances

The mass balances application modes deal with a mass balance for each component in the system. They can handle arbitrary expressions for reaction kinetics or other source or sink terms such as phase transfer.

Diffusion: This application mode defines and solves Fick's law for diffusion in combination with the continuity equation for each species in a solution. You can also include reaction terms.

Diffusion and Convection: This application mode models the transport and reaction of species in dilute solutions. The diffusivity can be an arbitrary function of concentration or temperature, while the convective term can be easily coupled to fluid flow. Alternatively, you can enter independent expressions for convection.

Maxwell-Stefan: This application mode models concentrated solutions where the species in solution interact with each other as well as the solvent. It can also include reactions.

Figure 1-4 shows the oxygen iso-concentration surfaces in a gas-diffusion cathode for a fuel cell. The model couples the Maxwell-Stefan application mode to the Navier-Stokes application mode, which describes flow in the channels of the current collector.

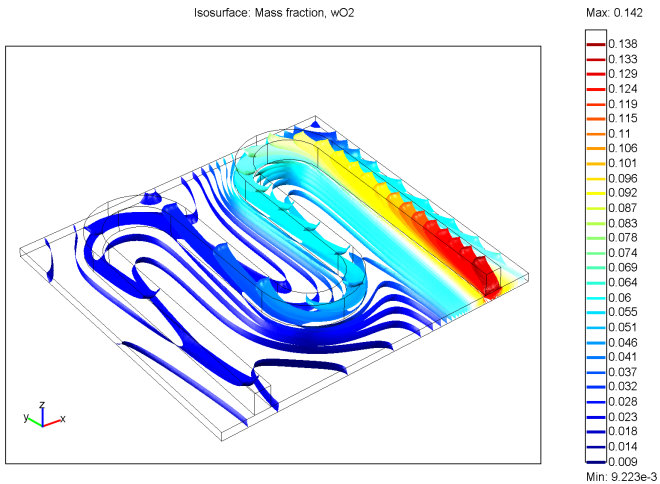


Figure 1-4: Oxygen concentration in a gas diffusion cathode. The concentration decreases from the inlet to the outlet in the serpentine-like structure of the gas channels.

Nernst-Planck: This application mode defines and solves mass balances where the model considers the transport of charged species in an electric field in addition to the diffusion and convective transport mechanisms. It serves to study electrokinetic transport in electrochemical cells and other devices where ions are subjected to electric fields.

Limitations in the COMSOL ECRE Version

The ECRE Version is a subset of the full version of COMSOL Multiphysics and the Chemical Engineering Module. We supply it with the full graphical user interface found in the standard COMSOL Multiphysics distribution including all the dialog boxes for data input plus the required solvers as defined by Professor Fogler. It also features all of the visualization and postprocessing functionality found in COMSOL Multiphysics.

Note, however, that the ECRE Version places a number of limitations on capabilities found in the standard package:

1. *CAD tool.* The ECRE Version does not include the drawing and geometry-creation functionality included in the full version. The models included in the ECRE Version therefore have predefined hard-wired geometries that you cannot modify.
2. *Mesh tool.* The models we supply in the ECRE Version include a mesh that gives good accuracy for a reasonable range of input parameters. You are not able to refine or otherwise manipulate the mesh as is possible in the full version.
3. *Problem definition.* COMSOL Multiphysics allows for the definition of arbitrary numbers of equations. The number of equations in the ECRE Version, however, cannot be changed. In other words, it is not possible to add or remove equations in the models included in this version.
4. *File storage.* The ECRE Version of COMSOL Multiphysics makes it possible to save images and graphs, but it does not allow someone to save a model so it can be opened and used at a later date.
5. *Model library.* COMSOL Multiphysics and the Chemical Engineering Module come with a library of solved models from various fields. The ECRE Version does not include this model library.

2

Radial Effects in Tubular Reactors

Model Description, Equations, and Input Data

This chapter uses the COMSOL ECRE Version to study an elementary, exothermic, 2nd-order reversible reaction

$$A + B \Leftrightarrow 2C$$

in a tubular reactor (liquid phase, laminar flow regime). To keep its temperature down, the reactor uses a cooling jacket with a variable coolant temperature. The following model setup proceeds in stages, gradually leading to the final configuration. The first version of the model deals with an isothermal tubular reactor with composition variations in both the radial and axial directions. The second stage extends the model to include the energy balance for the reactor. By this addition, the isothermal reactor is turned into an adiabatic reactor. The third stage introduces an isothermal cooling jacket, and finally the fourth stage models a non-isothermal cooling jacket.

The following section provides a general description for all of the above-mentioned models.

Model Description

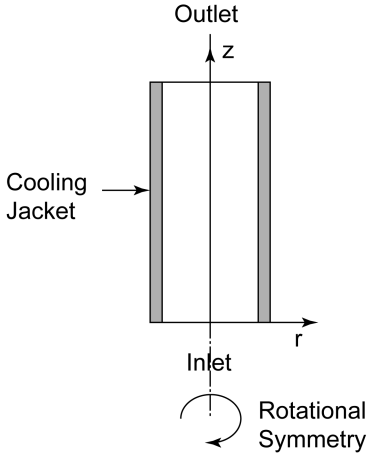


Figure 2-1: Model geometry for the 2-dimensional rotationally symmetric models.

Figure 2-1 illustrates the model geometry. We assume that the variations in angular direction around the central axis are negligible, and therefore the model can be axi-symmetric.

The system is described by a set of differential equations on a 2D surface that represents a cross section of the tubular reactor in the *z*-*r* plane. That 2D surface's borders represent the inlet, the outlet, the reactor wall, and the center line. Assuming that the diffusivity for the three species is of the same magnitude, you can model the reactor using three differential equations; one mass balance for one of the species (as noted in the next section, mass balances are not necessary for the other two species), one heat balance for the reactor core, and one heat balance for the heating jacket. Due to rotational symmetry, the software need only solve these equations for half of the domain shown in Figure 2-1.

Model Equations

You describe the mass balances and heat balances in the reactors with partial differential equations (PDEs), while one ordinary differential equation (ODE) is required for the heat balance in the cooling jacket. The equations are defined as follows.

MASS BALANCE, SPECIES A:

$$D_p \frac{1}{r}\frac{\partial C_A}{\partial r} + D_p \frac{\partial^2 C_A}{\partial r^2} + D_p \frac{\partial^2 C_A}{\partial z^2} - 2U\left(1 - \left(\frac{r}{R}\right)^2\right)\frac{\partial C_A}{\partial z} + r_A = 0$$

where D_p denotes the diffusion coefficient, C_A is the concentration of species A, U is the flow velocity, R gives the radius of the reactor, and r_A is the reaction rate. In this model we assume that the species A, B, and C have the same diffusivity, which implies that we must solve only one material balance; we know the other species' concentrations through stoichiometry.

BOUNDARY CONDITIONS FOR THE MASS BALANCE:

- Inlet ($z = 0$)

$$C_A(r, 0) = C_{A0}$$

- At the wall ($r = R$)

$$\frac{\partial C_A}{\partial r}(R, z) = 0$$

- Center (symmetry) line

$$\frac{\partial C_A}{\partial r}(0, z) = 0$$

The boundary condition selected for the outlet does not set any restrictions except that convection dominates transport out of the reactor. Thus this condition keeps the outlet boundary open and does not set any restrictions on the concentration.

- Outlet ($z = L$)

$$\frac{\partial C_A}{\partial z}(r, L) = 0$$

where L denotes the length of the reactor.

ENERGY BALANCE INSIDE THE REACTOR:

$$k\frac{1}{r}\frac{\partial T}{\partial r} + k\frac{\partial^2 T}{\partial r^2} + k\frac{\partial^2 T}{\partial z^2} - 2U\left(1 - \left(\frac{r}{R}\right)^2\right)\rho C_p\frac{\partial T}{\partial z} - r_A(-\Delta H_{Rx}) = 0$$

where k denotes the thermal conductivity, T is temperature, ρ is density, C_p equals the heat capacity, and ΔH_{Rx} is the reaction enthalpy.

BOUNDARY CONDITIONS FOR THE ENERGY BALANCE:

- Inlet ($z = 0$)

$$T(r, 0) = T_0$$

- At the wall ($r = R$)

$$-\frac{\partial T}{\partial r}(R, z) = \frac{U_k}{k}(T - T_a)$$

where T_a denotes the temperature in the cooling jacket. For an adiabatic reactor, the right-hand side of the above equation is zero.

- Center (symmetry) line

$$-\frac{\partial T}{\partial r}(0, z) = 0$$

As for the mass balance, choose the boundary condition at the outlet for the energy balance such that it keeps the outlet boundary open. This condition sets only one restriction, that the heat transport out of the reactor be convective.

- Outlet ($z = L$)

$$-\frac{\partial T}{\partial z}(r, L) = 0$$

ENERGY BALANCE OF THE COOLANT IN THE COOLING JACKET:
Here we assume that only axial temperature variations are present in the cooling jacket. This assumption gives a single ODE for the heat balance:

$$\frac{\partial T_a}{\partial z} = \frac{2\pi R U_k (T - T_a)}{m_c C_{Pc}}$$

where m_c is the mass flow rate of the coolant, C_{Pc} represents its heat capacity, and U_k gives the heat-transfer coefficient between the reactor and the cooling jacket. You can neglect the contribution of heat conduction in the cooling jacket and thus assume that heat transport takes place only through convection.

BOUNDARY CONDITION FOR THE COOLING JACKET:
You can describe the cooling jacket with a 1D line. Therefore you need only an inlet boundary condition.

- Inlet ($z = 0$)

$$T_a(0) = T_{a0}$$

Model Parameters

We now list the model's input data. You define them either as constants or as logical expressions in COMSOL Multiphysics's **Option** menu. In defining each parameter in COMSOL Multiphysics, for the constant's **Name** use the left-hand side of the equality in the following list (in the first entry, for example, `Diff`), and use the value on the right-hand side of the equality (for instance, `1E-9`) for the **Expression** that defines it.

The constants in the model are:

- Diffusivity of all species, `Diff` = `1E-9` m^2/s
- Activation energy, `E` = `95238` J/mol

- Rate constant, `A = 1.1E8` $m^6/(mol \cdot kg \cdot s)$
- Gas constant, `R = 8.314` $J/mol \cdot K$ (do not confuse this constant with the geometrical extension of the radius)
- Inlet temperature, `T0 = 320` K
- Total flow rate, `v0 = 5` E-4 m^3/s
- Reactant concentrations in the feed, `CA0 = CB0 = 500` mol/m^3
- Reactor radius, `Ra = 0.1` m
- Catalyst density, ρ_{Cat}, `rhoCat = 1500` kg/m^3
- Heat of reaction, ΔH_{Rx}, `dHrx = -83680` J/mol
- Equilibrium constant at 303 degrees K, `Keq0 = 1000`
- Thermal conductivity of the reaction mixture, `ke = 0.559` $J/m \cdot s \cdot K$
- Average density of the reaction mixture, ρ, `rho = 1000` kg/m^3
- Heat capacity of the reaction mixture, `Cp = 4180` $J/kg \cdot K$
- Overall heat-transfer coefficient, `Uk = 1300` $J/m^2 \cdot s \cdot K$
- Inlet temperature of the coolant, `Ta0 = 298` K
- Heat capacity of the coolant, `CpJ = 4180` $J/kg \cdot K$
- Coolant flow rate, `mJ = 0.01` kg/s

Next, the following section lists the definitions for the expressions this model uses. Again, to put each expression in COMSOL Multiphysics form, use the left-hand side of the equality (for instance, `u0`) for the variable's **Name**, and use the right-hand side of the equality (for instance, `v0/(pi*Ra^2)`) for its **Expression**.

- The superficial flow rate is defined according to the analytical expression

$$u_0 = \frac{v_0}{\pi(Ra)^2}$$

which we define in COMSOL Multiphysics as `u0 = v0/(pi*Ra^2)`.

- The superficial, laminar flow rate

$$u_z = 2u_0\left(1 - \left(\frac{r}{Ra}\right)^2\right)$$

in COMSOL Multiphysics form becomes `uz = 2*u0*(1-(r/Ra).^2)`.

- The conversion of species A is given by

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

which in COMSOL Multiphysics form is `xA = (cA0-cA)/cA0`.

- The concentration of B is according to

$$C_B = C_{B0} - C_{A0} x_A$$

which in COMSOL Multiphysics form becomes `cB = cB0-cA0*xA`.

- The concentration of C is expressed as

$$C_c = 2C_{A0} x_A$$

which in COMSOL Multiphysics form becomes `cC = 2*cA0*xA`.

- The rate of reaction takes two forms:
  - Before adding the heat balance, the reaction looks like

$$r_A = -A \exp\left(-\frac{E}{RT_0}\right) \rho_{cat} \left(c_A c_B - \frac{c_c^2}{K_{eq}}\right),$$

which in COMSOL Multiphysics form is `rA = -A*exp(-E/R/T0)*rhoCat*(cA*cB-cC^2/Keq)`.

  - After you add the energy balance, the reaction expression becomes

$$r_A = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat} \left(c_A c_B - \frac{c_c^2}{K_{eq}}\right),$$

which in COMSOL Multiphysics form is `rA = -A*exp(-E/R/T)*rhoCat*(cA.*cB-cC^2/Keq)`.

- The temperature-dependent equilibrium constant is given by the following expressions:
  - For the isothermal case

$$K_{eq} = K_{eq0} \exp\left(\frac{\Delta H_{Rx}}{R}\left(\frac{1}{303} - \frac{1}{T_0}\right)\right)$$

which in COMSOL Multiphysics form is `Keq = Keq0*exp(dHrx/R*(1/303-1/T0))`.

- After adding the energy balance you obtain

$$K_{eq} = K_{eq0}\exp\left(\frac{\Delta H_{Rx}}{R}\left(\frac{1}{303}-\frac{1}{T}\right)\right)$$

which in COMSOL Multiphysics form is `Keq = Keq0*exp(dHrx/R*(1/303-1/T))`.

- The heat-production term becomes

$$Q = -r_a \Delta H_{Rx}$$

which in COMSOL Multiphysics form is `Q = -rA*dHrx`.

Isothermal Reactor

The first model with radial effects deals only with the material balances in a tubular reactor, so you can neglect temperature variations. The model equations can be found in the Mass Balance paragraph on page 13.

It is possible to define the model from scratch in the COMSOL Multiphysics Chemical Engineering Module. And while the COMSOL ECRE included with *Elements of Chemical Reaction Engineering* does not include the full program's drawing and meshing functionality, it does allow for changes of reaction kinetics and transport properties. It also implements all the postprocessing capabilities in the Chemical Engineering Module.

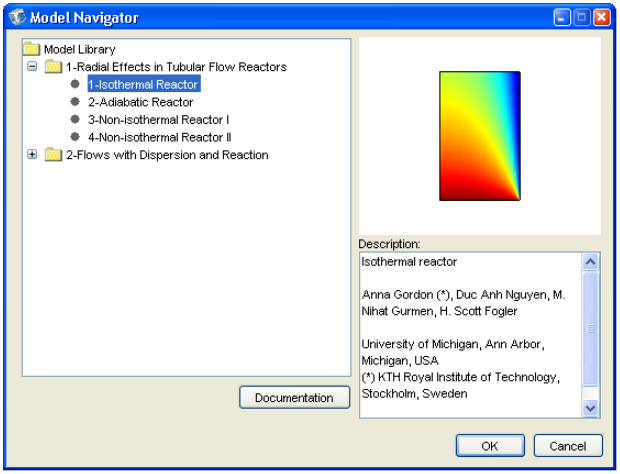
The following model setup is targeted at users of COMSOL ECRE, but note that it is possible to create the full implementation in the Chemical Engineering Module.

Reviewing the Model in the COMSOL ECRE Version

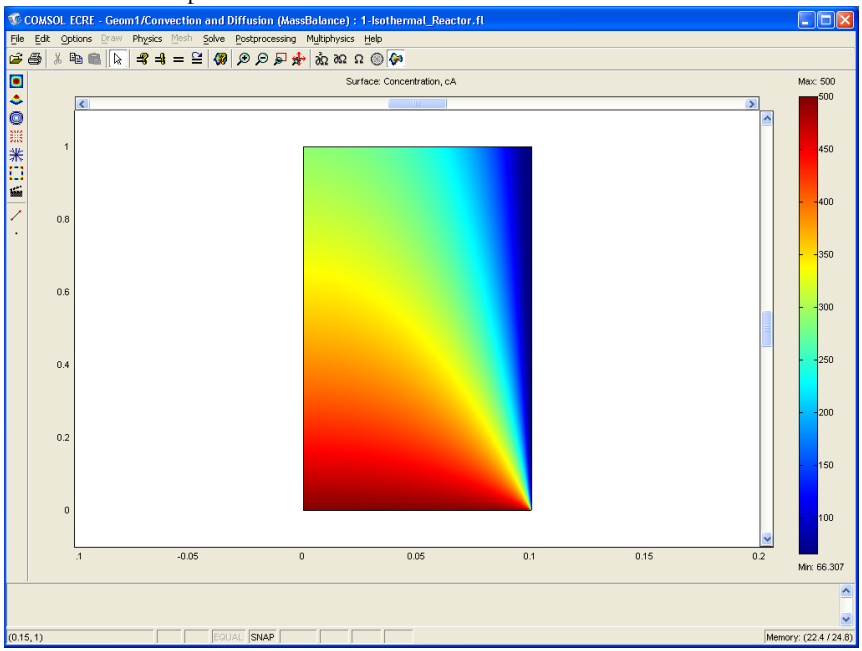
OPENING THE MODEL

1 Insert the COMSOL ECRE CD and select the platform on which you wish to run it. The **Model Navigator** window then appears on the screen.

2 In this window click the folder **1-Radial Effects in Tubular Flow Reactors**, and then select the model **1-Isothermal Reactor**. Click **OK**.



The model opens in Postprocessing mode, and the surface plot shows the concentration of species A in the reactor.



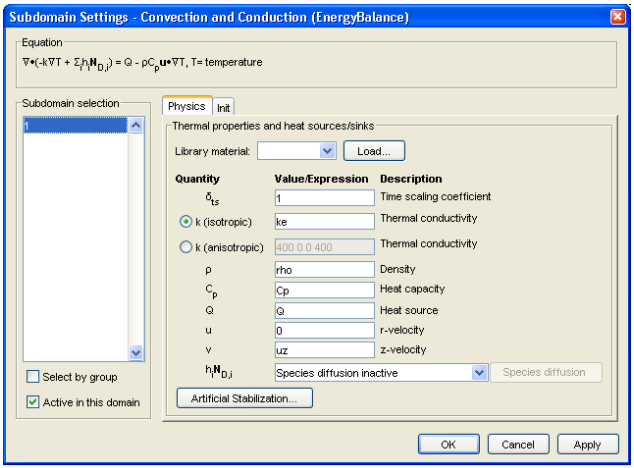
Note that the plot does not display the reactor's dimensions with equal axes in the *r*- and *z*-directions.

MODEL EQUATIONS AND INPUT DATA

In COMSOL ECRE you can review and change the model equations and input data, but you cannot add or remove the so-called application modes that implement the model. To review the application modes the model makes use of, do the following:

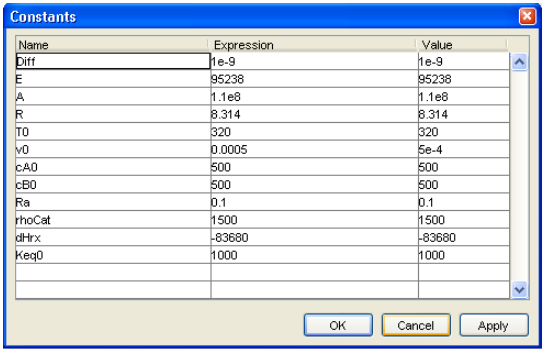
1. Click the **Multiphysics** menu. Doing so opens a drop-down list that contains any active application modes, in this case the **Convection and Diffusion (Mass Balance)** application mode.
2. Click on the **Multiphysics** menu again to close the list.
3. Go to the **Physics** menu and select **Subdomain Settings**, which opens up the corresponding dialog box. Select subdomain 1 in the **Subdomain Settings** list. This

dialog box displays the equation that forms the basis for this application mode, while the edit fields show the input data used in the equation.



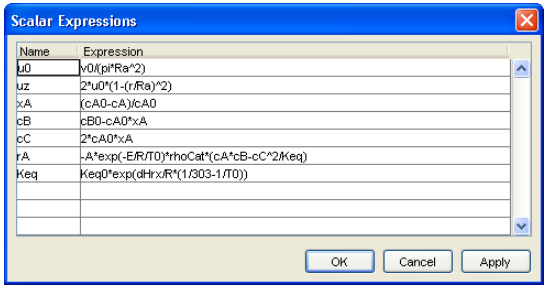
The edit fields correspond to the diffusion coefficient, reaction-rate expression, and velocity distribution in the reactor—all of which you can freely define. To review and change the definition of the input data, follow this procedure:

4 Go to the **Options** menu and select **Constants**. The resulting dialog box displays the names and definitions of all the constants used in the model.



You can freely define new constants and rename existing ones. In the dialog box in the preceding figure you can identify `Diff`, which is the diffusion coefficient entered in the **Diffusion coefficient** edit field in the **Subdomain Settings** dialog box. COMSOL ECRE also allows for the definition of expressions.

5 Go to the **Options** menu, then to the expandable menu item **Expressions**, and finally select **Scalar Expressions**.



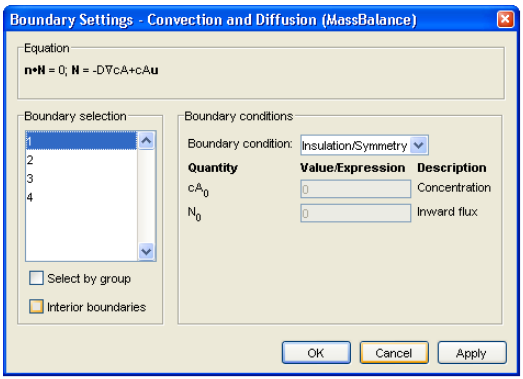
It is possible to move the **Scalar Expressions** dialog box in order to also display the **Constants** dialog box. Look closely at the definitions of the scalar expressions and recognize that they use constants from the **Constants** box. Note also that the constants and the scalar expressions are defined according to the list of Model Parameters in the preceding section. Examine the **Subdomain Settings** box and note that the scalar expression `rA` in the **Reaction rate** edit field defines that parameter, and the scalar expression `uz` in the **z-velocity** edit field defines the corresponding velocity component.

6 Click the **Cancel** button in both the **Scalar Expressions**, **Constants**, and **Subdomain Settings** dialog boxes.

Having reviewed the domain equations in the model, you can proceed to the boundary conditions.

7 Go to the **Physics** menu and select **Boundary Settings**.

8 Click on boundary number 1 in the **Boundary Selection** list. It corresponds to the reactor's central axis.



9 Select boundary number 2 to view the boundary condition at the reactor's inlet. In this case, the constant `cA0` defines the inlet concentration in the **Boundary Condition** of type **Concentration**. You can find the constant's value in the **Constants** dialog box under the **Options** menu.

10 Select boundary number 3 to review the outlet boundary condition, which in this case is a **Convective flux** condition. You can use this condition when it is safe to assume that the transport of mass perpendicular to the outlet is dominated by convection. The boundary condition sets the diffusion term in the mass-flux vector in the outlet direction to zero.

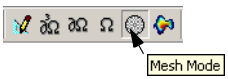
11 Select boundary number 4 to review the last condition, which corresponds to the reactor's outer wall and is therefore an insulating boundary for the mass balance.

12 Click the **Cancel** button to close the **Boundary Settings** dialog box.

You have now reviewed the input data, domain equations, and boundary conditions. To repeat, while you can change all these definitions, you cannot replace or expand the Convection Diffusion application mode when running COMSOL ECRE; you need the full COMSOL Multiphysics Chemical Engineering Module to extend the model to include, for example, additional mass balances.

VISUALIZING THE MESH

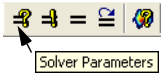
Further, while you cannot manipulate the mesh in COMSOL ECRE, it does allow you to visualize the mesh by pressing the **Mesh Mode** button.



Note in this case that the scales on the *r*- and *z*-axes are not equal, which gives a distorted view. If desired, you can select equal scale settings in the **Axis/Grid Settings** menu item under the **Options** menu. In order to return to the original unequal scale settings, once again go to the **Axes/Grid Settings** menu and clear the **Axis equal** check box. Enter `-0.1` in the **r min** edit field, `0.2` in the **r max** edit field and `-0.1` and `1.1` in the **z min** and **z max** edit fields, respectively.

CHECKING THE SOLVER SETTINGS

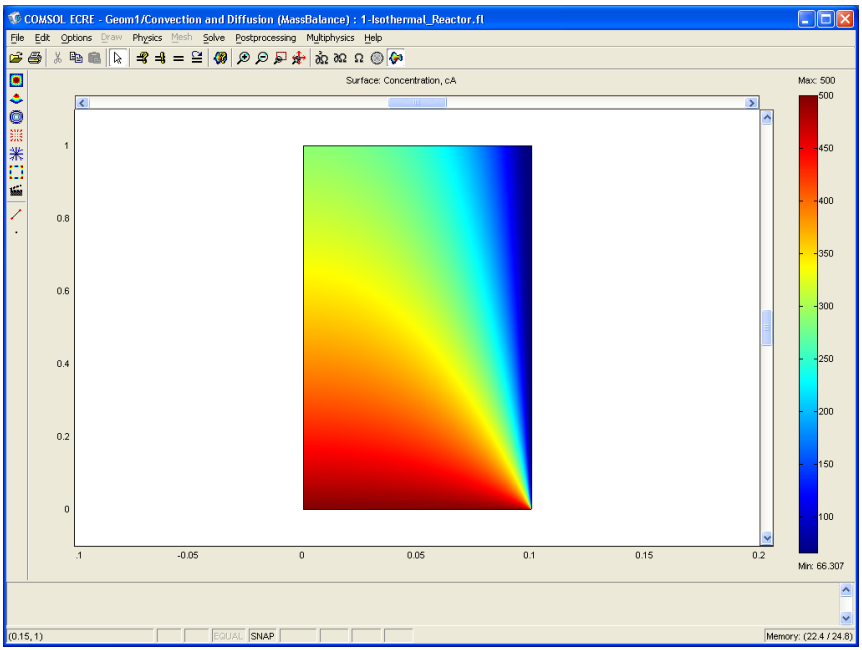
COMSOL ECRE allows you to change the equation parameters and reaction kinetics and then solve the problem again. The model in this exercise is nonlinear; thus press the **Solver Parameters** and verify that the **Stationary nonlinear** solver is selected.



POSTPROCESSING

COMSOL ECRE comes with the full set of COMSOL Multiphysics postprocessing capabilities. These include surface plots, cross-sectional plots, point plots, as well as boundary and subdomain integrations. Now is a good time to review some of the software's plotting and postprocessing capabilities.

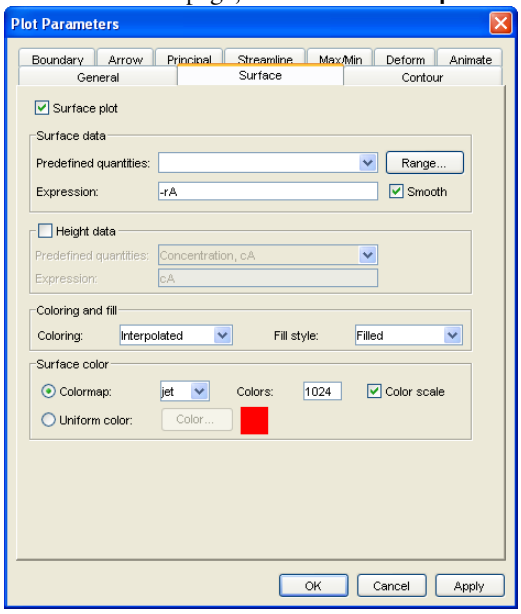
1 Click the **Postprocessing Mode** button. The default plot shows the concentration of species A in the reactor.



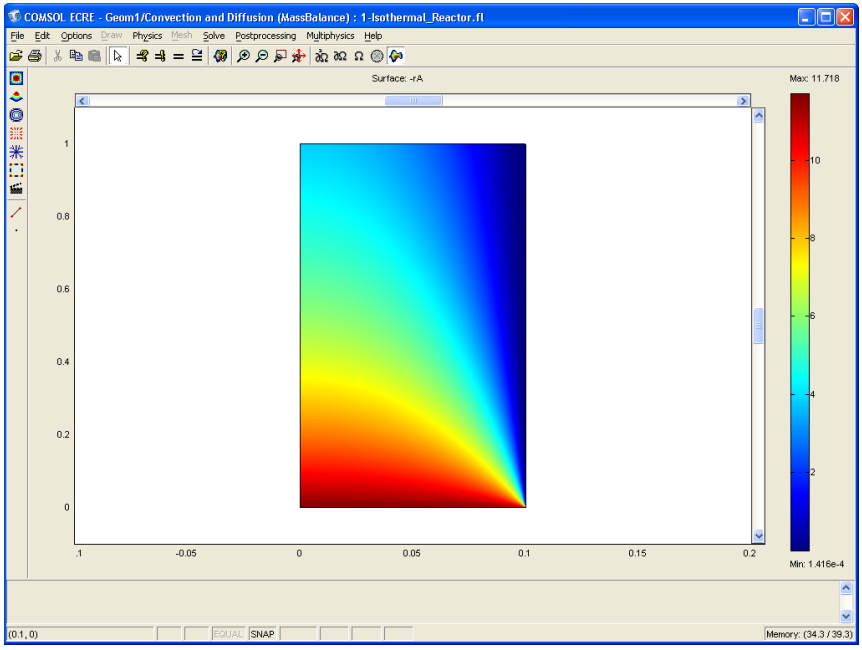
2 Click the **Plot Parameters** button.

3 Click on the **Surface** tab.

4 On the **Surface** page, enter `-rA` in the **Expression** edit field.

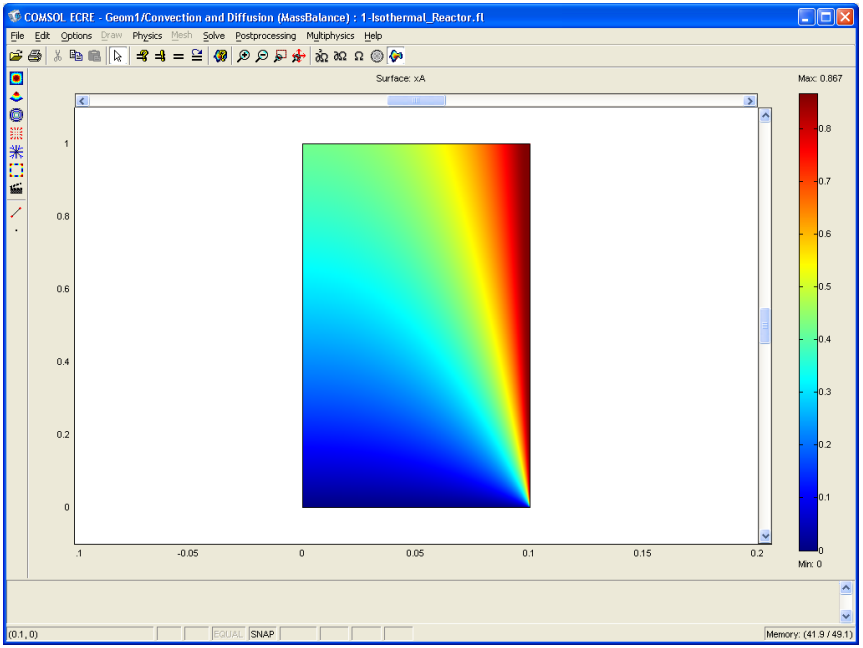


5 Click **Apply**.



6 To plot the conversion of species A, enter xA in the **Expression** edit field in the **Plot Parameters** dialog box.

7 Click **Apply**.



8 In order to define the location of the maximum and minimum conversion, click the **Max/Min** tab.

9 Enter xA in the **Expression** edit field in the **Subdomain max/min data** dialog box.

10 Click the **Max/min marker** check box and click **Apply**.

11 To visualize the local conversion in selected cross sections along the length of the reactor, first go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.

12 Click the **Line/Extrusion** tab.

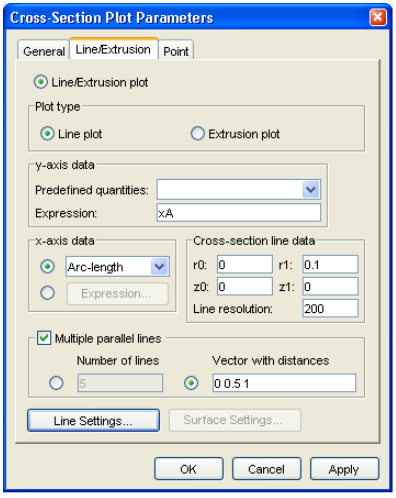
13 Enter xA in the **Expression** edit field.

14 Enter 0 in the **r0** edit field and 0.1 in the **r1** edit field.

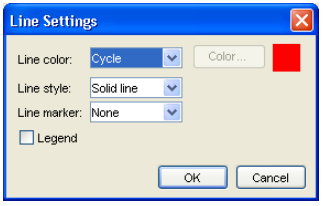
15 Enter 0 in both the **z0** and **z1** edit fields.

16 Check the **Multi parallel lines** box, then click the **Vector with distances** option.

I7 Enter `0 0.5 1` in the **Vector with distances** edit field to generate three cross-section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.



I8 Click the **Line Settings** button. In the dialog box that opens, select the **Cycle** option in the **Line color** drop-down list; select **Solid line** in the **Line style** drop-down list; and select **None** in the **Line marker** drop-down list.



19 Finally, to generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, and then in the **Cross-Section Plot Parameters** dialog box.

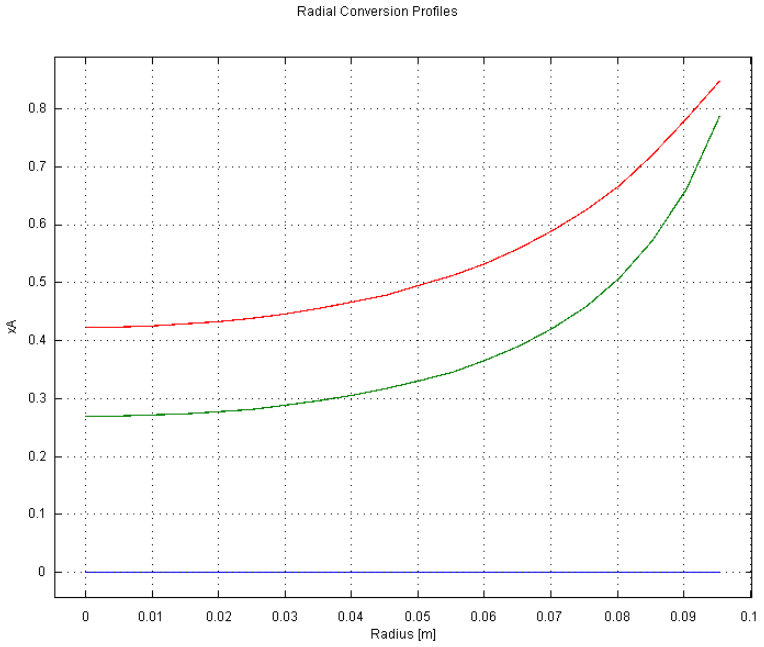


Figure 2-2: Radial conversion profiles at the inlet, outlet and halfway through an isothermal reactor.

COMSOL ECRE can also calculate integral expressions of the solution. One such entity is the mixing cup outlet concentration, which gives the average concentration in the liquid that exits the reactor. For species A, the average concentration is defined according to the equation

$$C_{A,av} = \frac{\int_{outlet} 2\pi r C_A u_z dr}{\int_{outlet} 2\pi r u_z dr}$$

along the outlet boundary. Start by calculating the integral of $C_A u_z$ over the outlet boundary.

20 Go to the **Postprocessing** menu and select **Boundary Integration**.

21 Select boundary 3 in the **Boundary selection** list.

22 Enter `2*pi*r*cA*uz` in the **Expression** edit field.

23 Click **Apply**.

The value of the integral appears in the status bar at the bottom and reads `0.115485`. You can now calculate the integral of u_z.

24 Enter `2*pi*r*uz` in the **Expression** edit field and click **Apply**.

The value of this integral is `5e-4`, which gives an average concentration of `0.115485/5e-4`, which is approximately `231` mole m^{-3}.

You have now completed a review of the model and are ready to run it with varying input parameters.

Questions and Exercises

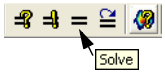
To answer the following questions you can either use the results in the model just described or you can solve it again with a new set of input data.

1 Why is the concentration of species A near the reactor wall lower than the concentration near the center?

2 Where in the reactor do you find the minimum and maximum reaction rates?

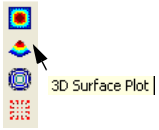
3 How much is the average conversion? (Hint: See the calculation of the average concentration using integrals in the previous section, page 29.)

4 This exercise requires that you change the activation energy for the reaction in the model. Do so by going to the **Options** menu and working with the **Constants** menu item (see item 5 in the section "Model Equations and Input Data" on page 21). We have already tabulated the notations in the section "Model Parameters" on page 15. After changing the input data, click the **Solve** button to solve the problem.



It is useful to take the graphs you obtain by changing the activation energy and examine them in both two and three dimensions. Once in the Postprocessing mode

you can toggle between a two- and three-dimensional plot by clicking the **2D Surface Plot** button or **3D Surface Plot** button.



a How do the conversion profiles and the average conversion change if you increase the activation energy by a factor of 1.5?

b How do these same entities change if you decrease the activation energy by multiplying the original value by a factor of 0.95?

The reaction rate is very sensitive to changes in activation energy. Altering the activation energy to a lower value increases the reaction rate. A high reaction rate in combination with the low flow rate close to the wall results in very large concentration gradients. In order to capture an accurate concentration profile, you must apply a dens mesh in the inlet area near the wall. This can be done in the full version of the Chemical Engineering Module but not in the COMSOL ECRE version.

You have now investigated the isothermal reactor example. Let's proceed by introducing the energy balance in the reactor.

Adiabatic Reactor

This second model with radial effects adds a heat balance to the material balance in the previous model. We assume the reactor is adiabatic, which means that its walls are insulated and do not exchange heat with the surroundings. The model equations are found in the Mass Balance paragraph on page 13, and in the Energy Balance paragraph on page 14.

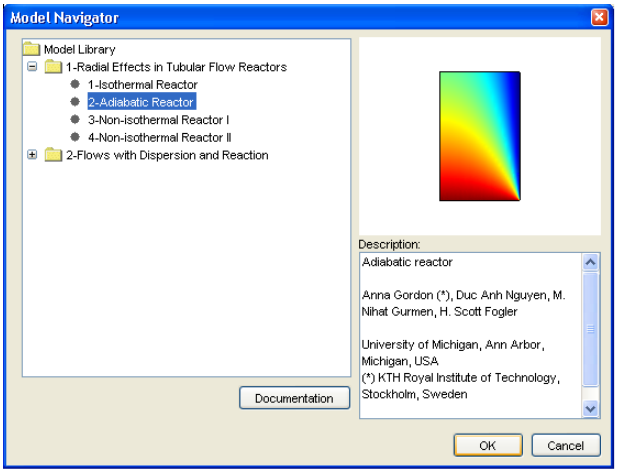
Those working with the COMSOL Multiphysics Chemical Engineering Module could generate this model by adding an additional application mode for energy balances to the mass balances already included in the previous model. However, COMSOL ECRE supplies this model predefined and ready to run. You can freely experiment with different input data and still use the full postprocessing capabilities in the Chemical Engineering Module.

Reviewing the Model in the COMSOL ECRE Version

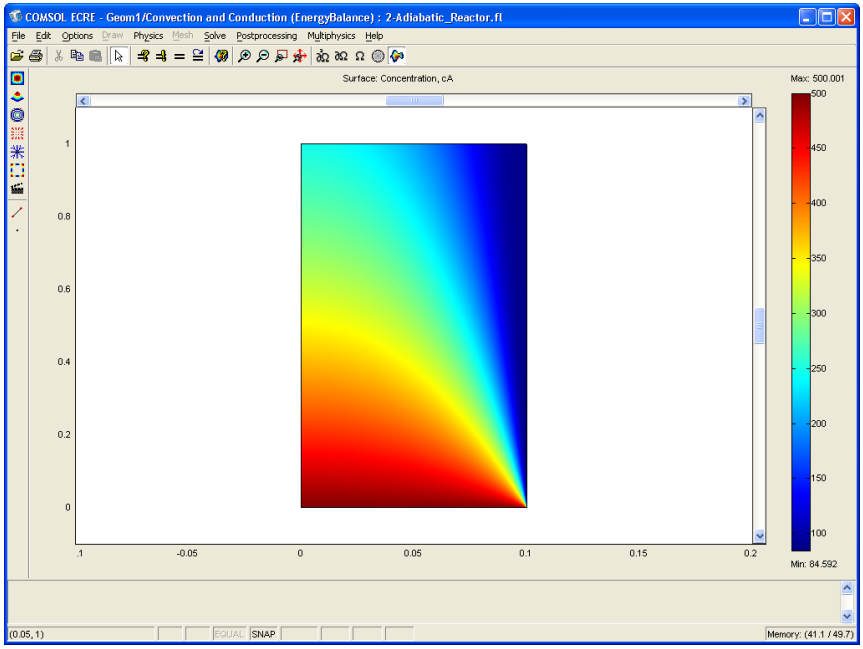
OPENING THE MODEL

1. If you have already installed COMSOL ECRE, double-click on its icon to open the **Model Navigator**. If not, go to step 1 in the preceding exercise to install the program. If you are already using COMSOL Multiphysics, go to the **File** menu and select **New** to open the **Model Navigator**.
2. In the **Model Navigator** click the folder **1-Radial Effects in Tubular Flow Reactors** and select the model **2-Adiabatic Reactor**.

3 Click **OK**.



The model opens in the Postprocessing mode, and the surface plot shows the concentration of species A in the reactor.

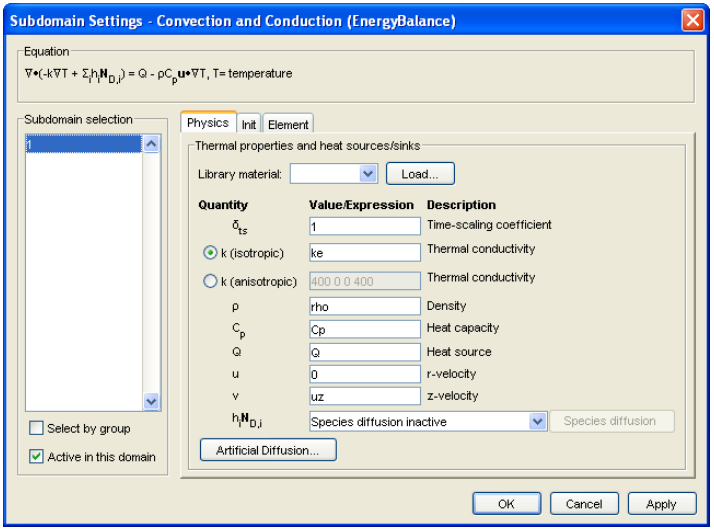


Note that the plot does not display the reactor's dimensions with equal axes in the *r*- and *z*-directions.

MODEL EQUATIONS AND INPUT DATA

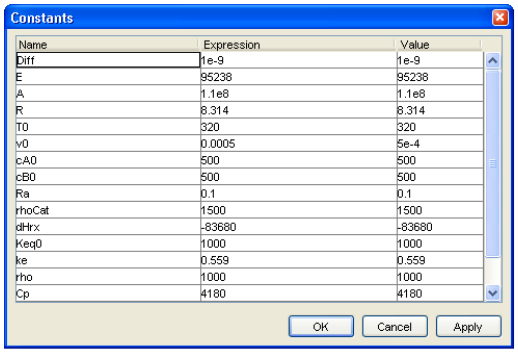
You can now review and change the model equations.

1. Click the **Multiphysics** menu. This opens a drop-down list that contains any active application modes, in this case both the **Convection and Diffusion (Mass Balance)** and the **Convection and Conduction (Energy Balance)** application modes. You can select among them by clicking on the desired application mode in the drop-down list.
2. Click on the **Convection and Conduction** application mode.
3. Go to the **Physics** menu and select **Subdomain Settings** to open the corresponding dialog box. Select subdomain 1 in the **Subdomain selection** list. This dialog box also displays the equation that forms the basis for the **Conduction and Convection** application mode, and the edit fields show the input data used in the energy balance.



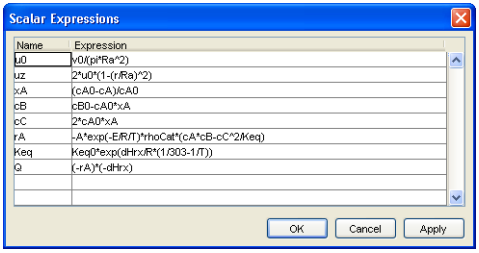
The edit fields correspond to the thermal conductivity, density, heat capacity, and velocity distribution in the reactor, all of which you can define freely. To review and change the definition of the input data, follow this procedure:

4 Go to the **Options** menu and select **Constants**. The resulting dialog box displays the names and definitions of all constants used in the model.



As already mentioned in the "Isothermal Reactor" example, you can freely define new constants and rename existing ones. In this case, focus on `ke`, the thermal conductivity. It is visible in the **Thermal conductivity** edit field in the **Subdomain Settings** dialog box in the above figure. Let's look at the definition of the expressions.

5 Go to the **Options** menu, then to the **Expressions** expandable menu item, and select **Scalar Expressions**.



The scalar expression denoted `Q` defines the heat generation in the **Heat source** edit field, and `uz` represents the **z-velocity** component visible in **Subdomain Settings**.

6 Click the **Cancel** button in the **Scalar Expressions**, **Constants**, and **Subdomain Settings** dialog boxes.

You have now reviewed the domain equations for the heat balance. You can later repeat this process for the mass balance by selecting it in the **Multiphysics** menu. Next proceed to the boundary conditions.

7 Go to the **Physics** menu and select **Boundary Settings**.

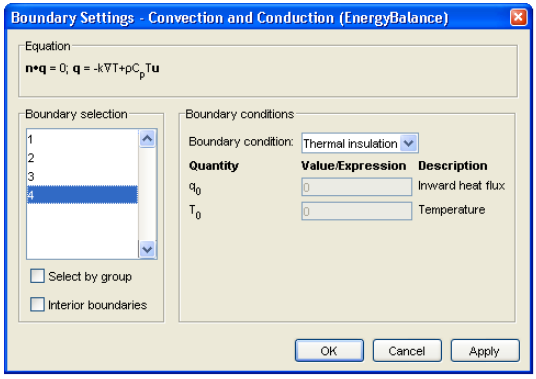
8 Click on boundary number 1 in the **Boundary Selection** list. This boundary corresponds to the reactor's central axis. You can click and drag the box aside to see

the selected boundary in the main graphical user interface. The selected boundary is marked in red.

9 Select boundary number 2 to view the boundary condition at the reactor inlet. In this case, the constant `T0` defines the inlet temperature in the **Boundary Condition** of type **Temperature**. You can find that constant's value by going to the **Options** menu and opening the **Constants** dialog box.

10 Select boundary number 3 to review the outlet boundary condition, which in this case is a **Convective flux** condition. You can use this condition when it is safe to assume that the transport of heat perpendicular to the outlet is dominated by convection. The boundary condition sets the conduction term in the heat-flux vector in the outlet direction to zero.

11 Select boundary number 4 to review the final condition, which corresponds to the reactor's outer wall and, because you are modeling an adiabatic reactor, it is therefore an insulating boundary.

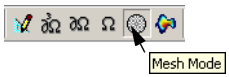


12 Click the **Cancel** button to close the **Boundary Settings** dialog box.

You have now reviewed the input data, domain equations, and boundary conditions for the energy balance. You can run the corresponding procedure for the mass balance by selecting it in the **Multiphysics** menu.

VISUALIZING THE MESH

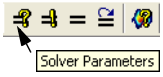
To visualize the mesh click the **Mesh Mode** button.



Note that the scales on the *r*- and *z*-axes are not equal, which results in a distorted view. If desired, you can select equal scale settings by going to the **Options** menu and checking the **Axis equal** box in the **Axis/Grid Settings** menu item. In order to return to the original unequal scale settings, once again go to the **Axes/Grid Settings** menu and clear the **Axis equal** check box. Enter `-0.1` in the **r min** edit field, `0.2` in the **r max** edit field and `-0.1` and `1.1` in the **z min** and **z max** edit fields, respectively.

CHECKING THE SOLVER SETTINGS

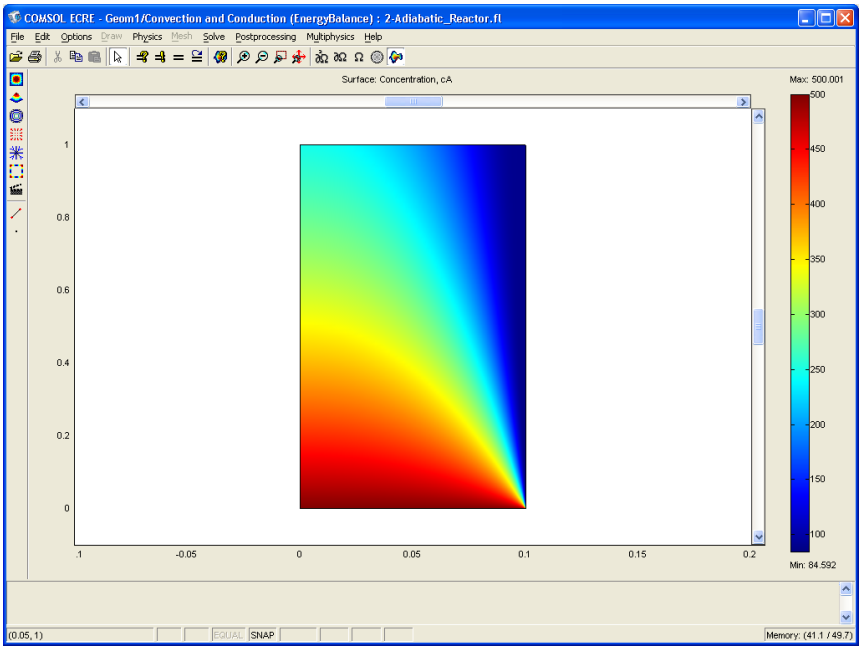
The model we solve in this exercise is nonlinear. To verify the solver settings, click the **Solver Parameters** button and make certain that the **Stationary nonlinear** solver is selected.



POSTPROCESSING

Let's examine the new results now that we have introduced the energy balance, and let's compare them to those from the "Isothermal Reactor" exercise.

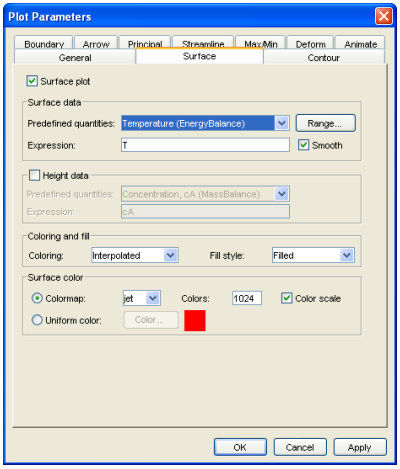
1 Click the **Postprocessing Mode button**. The default plot shows the concentration of species A in the reactor.



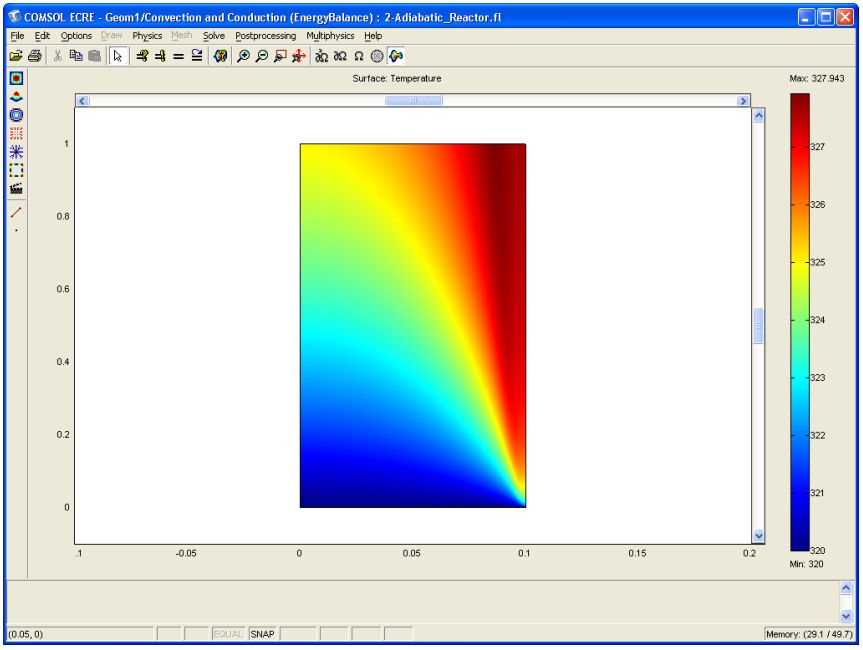
2 Click the **Plot Parameters** button.

3 Click the **Surface** tab.

4 On the **Surface** page, go to the **Predefined quantities** drop-down list and select **Temperature**.

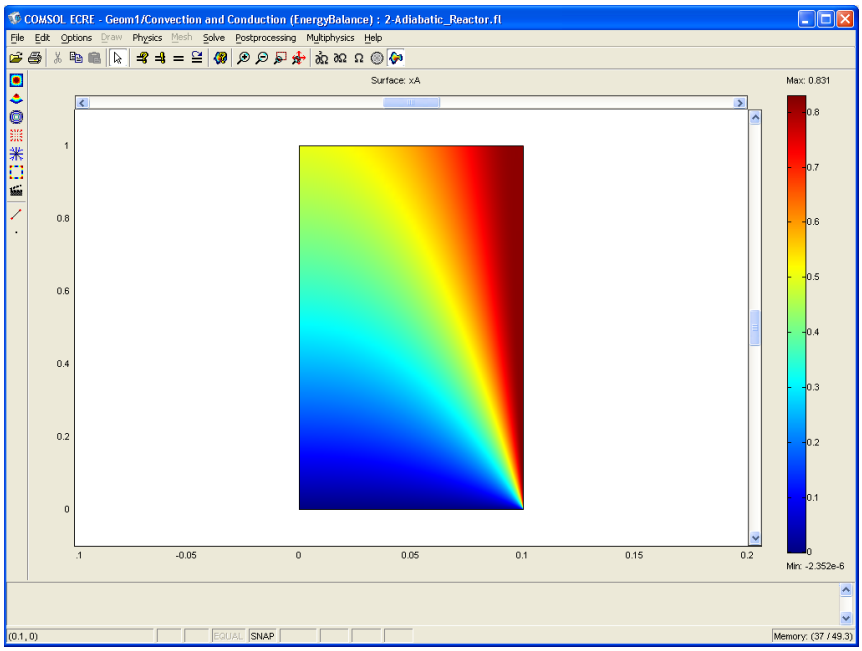


5 Click **Apply**.



6 To plot the conversion of A, enter `xA` in the **Expression** edit field in the **Surface** page.

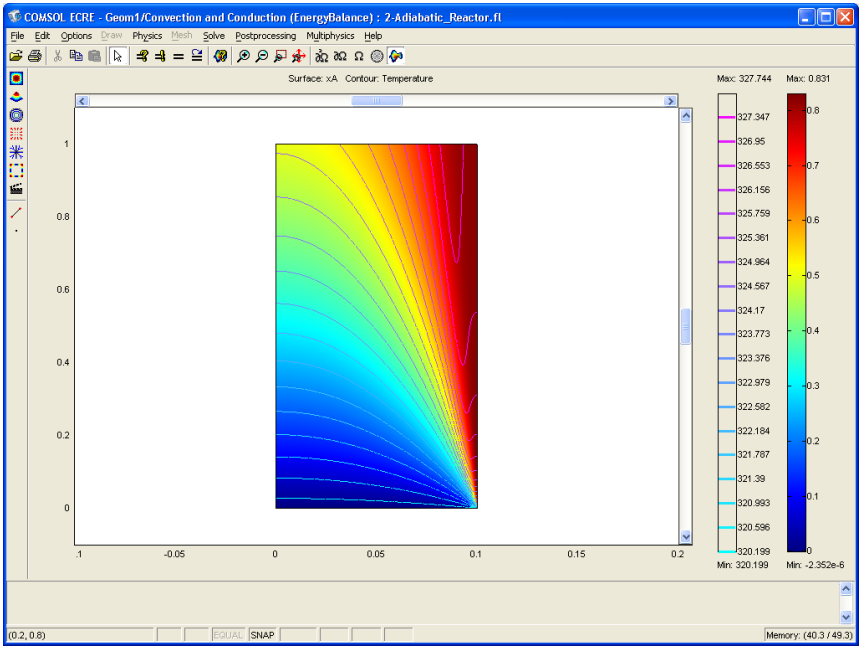
7 Click **Apply**.



8 To visualize the relation between temperature and conversion, first click the **Contour** tab.

9 Select `Temperature (EnergyBalance)` in the **Predefined quantities** drop-down list.

10 Click the **Contour plot** check box and click OK.



11 To visualize the local conversion in selected cross sections along the length of the reactor, go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.

12 Click the **Line/Extrusion** tab.

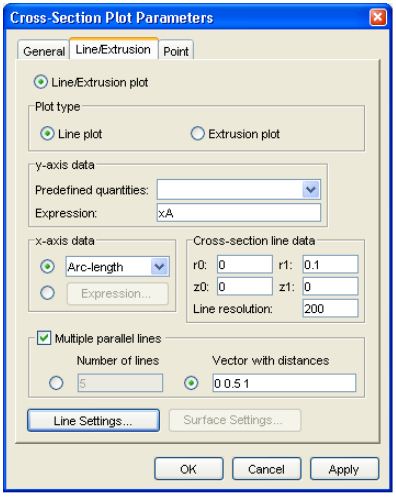
13 Enter `xA` in the **Expression** edit field.

14 Enter `0` in the **r0** edit field and `0.1` in the **r1** edit field.

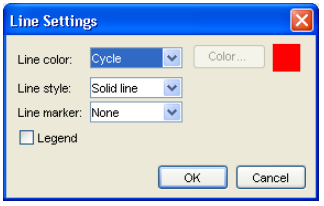
15 Enter `0` in both the **z0** and **z1** edit fields.

16 Check the **Multi parallel lines** box and click the **Vector with distances** option.

I7 Enter `0 0.5 1` in the **Vector with distances** edit field to generate three cross-section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.



I8 Click the **Line Settings** button. In the dialog box that opens, select the **Cycle** option in the **Line color** drop-down list; select **Solid line** in the **Line style** drop-down list; and select **None** in the **Line marker** drop-down list.



19 To generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, then again in the **Cross-Section Plot Parameters** dialog box.

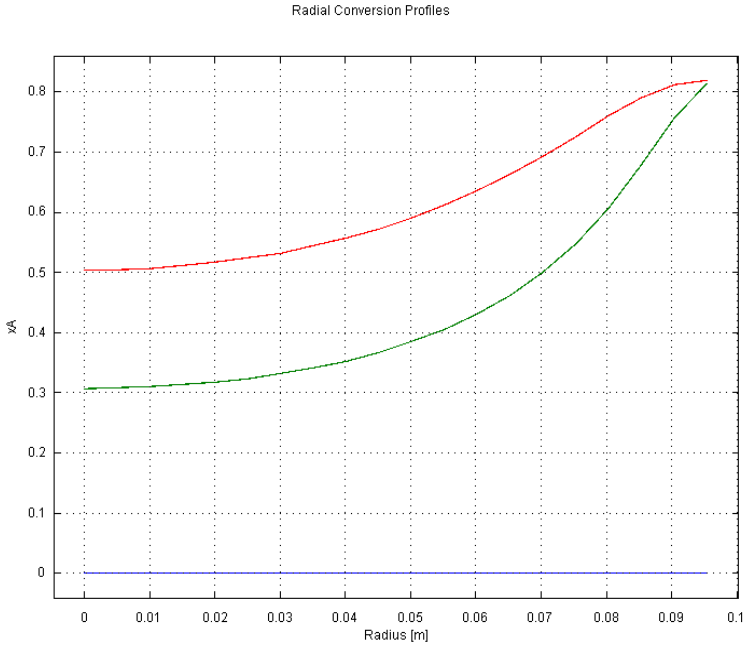


Figure 2-3: Radial conversion profiles at the inlet, outlet and halfway through an adiabatic reactor.

You can now calculate the mixing cup outlet concentration (see the previous example for its definition). Start by calculating the integral of the outlet flux over the outlet boundary.

20 Go to the **Postprocessing** menu and select **Boundary Integration**.

21 Select boundary 3 in the **Boundary selection** list.

22 Enter `2*pi*r*cA*uz` in the **Expression** edit field.

23 Click **Apply**.

The value of the integral appears in the status bar at the bottom of the user interface and reads `0.093323`. You can now calculate the integral of u_z.

24 Enter `2*pi*r*uz` in the **Expression** edit field and click **Apply**.

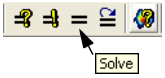
The value of this integral is `5e-4`, which gives an average concentration of `0.093323/5e-4`, which is approximately `187` mole m^{-3}.

You have now completed a review of the model and are ready to run it with varying input parameters.

Questions and Exercises

To answer the following questions and perform the exercises, you can either use the results in the model just presented, or you can solve it again with new input data.

1. How do you explain the difference in outlet conversion between the isothermal and non-isothermal adiabatic reactor? (For a clue, examine the temperature plot.)
2. This section deals with the model of an adiabatic reactor. What is special about the solution's surface plot of the temperature? Explain the resulting radial temperature distribution.
3. Increase the thermal conductivity, `ke`, by a factor of 10 and explain how this affects the temperature profiles. At what radial position do you find the highest conversion? You can change the thermal conductivity by going to the **Options** menu and then the **Constants** item. Click the **Solve** button to solve the problem with the new thermal conductivity.



Non-Isothermal Reactor with Isothermal Cooling Jacket

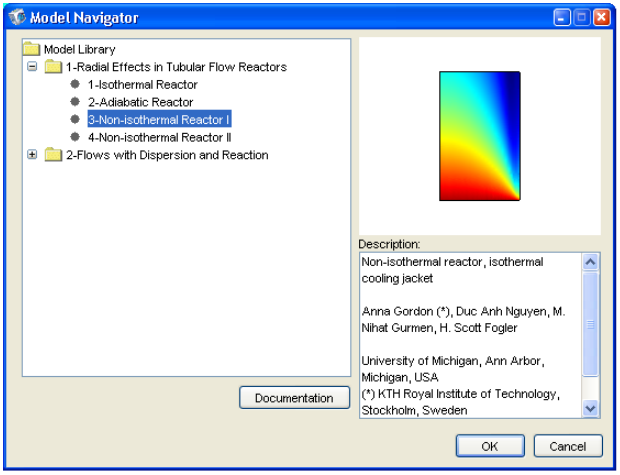
The "Adiabatic Reactor" in the preceding exercise is valid under the assumption that the reactor cannot interchange heat in the radial direction with the surrounding media. This implies that the boundary condition for the energy balance at the radial boundary is thermally insulating. Thus, in this next exercise we introduce a cooling jacket around the reactor; it has virtually unlimited cooling power because we set its temperature to a constant. You can implement this enhancement to the model in the COMSOL Multiphysics Chemical Engineering Module by changing the insulating boundary condition to a flux boundary condition, where the flux is proportional to the temperature difference at the inner wall of the reactor and the cooling jacket. COMSOL ECRE already makes this change, and you need only review the new constants introduced to express this new boundary condition and the boundary condition itself. The model equations are found in the Mass Balance paragraph on page 13, and in the Energy Balance paragraph on page 14.

Reviewing the Model in the COMSOL ECRE Version

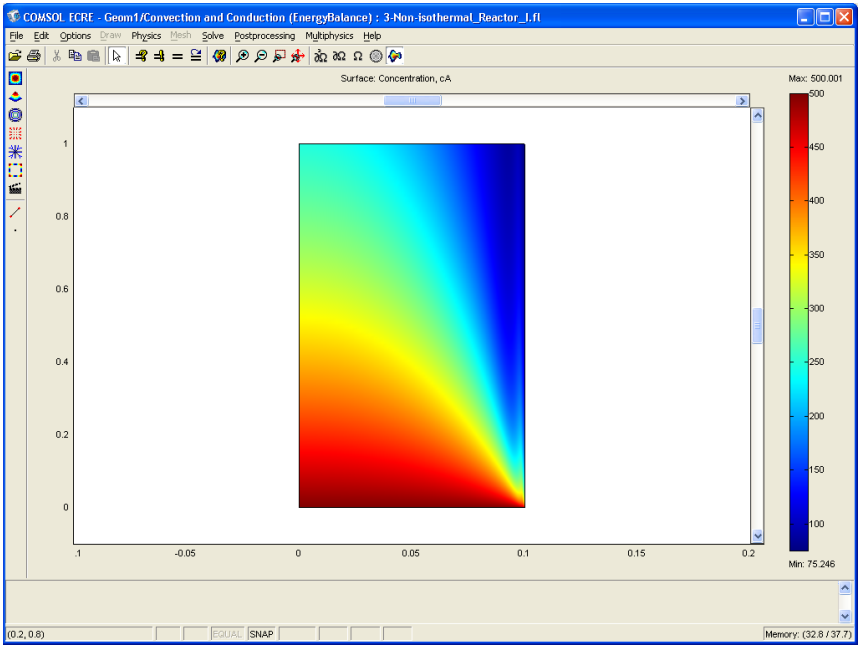
OPENING THE MODEL

1 Double click on the COMSOL ECRE icon to open the **Model Navigator**. If you are already using COMSOLCOMSOLcomsol, go to the **File** menu and select **New** to open the **Model Navigator**.

2 Click the folder **1-Radial Effects in Tubular Flow Reactors** and select the model **3-Non-isothermal Reactor I**. Click **OK**.



The model opens in the Postprocessing mode, and the surface plot illustrates the concentration of species A in the reactor.

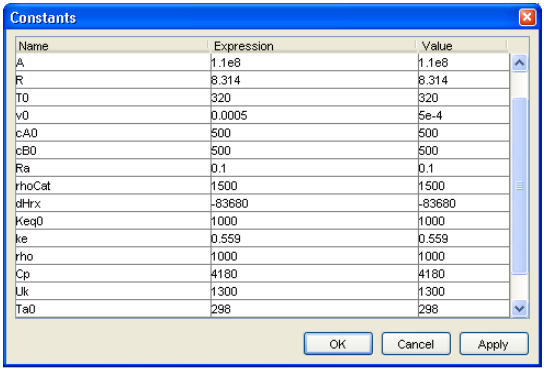


Note that the plot does not display the reactor's dimensions with equal axes in the *r*- and *z*-directions.

MODEL EQUATIONS AND INPUT DATA

Next it is a good idea to review the model equations and the input data. The model equations are almost identical to those for the "Adiabatic Reactor" in the preceding exercise. The only differences appear in the list of constants, where this model introduces two new constants, and in the radial boundary conditions. Let's review these changes.

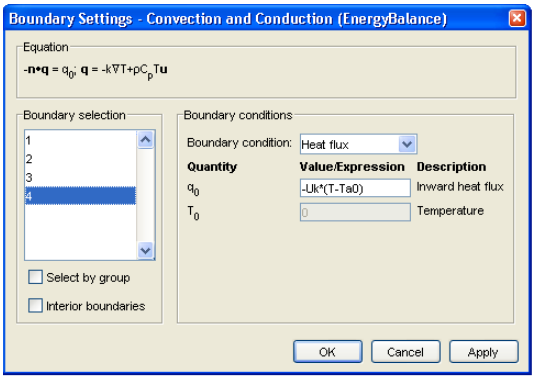
1. Click the **Multiphysics** menu. This opens a drop-down list that contains any active application modes, in this case the **Convection and Diffusion (Mass Balance)** and the **Convection and Conduction (Energy Balance)** application modes.
2. Click on the **Convection and Conduction** application mode.
3. Go to the **Options** menu and select the menu item **Constants**. The resulting dialog box displays the name and definition of all the constants this model uses. Scroll down to examine the new constants `Uk` and `Ta0`.



   You can freely define any additional constants and rename existing ones. For this exercise, however, leave them as they are.

4. Click the **Cancel** button to close the dialog box.
5. Go to the **Physics** menu and select **Boundary Settings**.
6. Click on boundary number 4 in the **Boundary Selection** list. It corresponds to the reactor wall. Here you can see the new **Heat flux** boundary condition. The heat flux is proportional to the difference between the temperature at the reactor's inner wall

(T) and that of the cooling jacket (Ta0). The heat-transfer coefficient, denoted Uk, is visible in the **Constants** item under the **Options** menu.



7 Click the **Cancel** button to close the dialog box.

You have now reviewed the changes in input data and boundary conditions for the energy balance compared to the "Adiabatic Reactor" example.

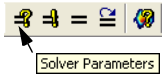
VISUALIZING THE MESH

To visualize the mesh, click the **Mesh Mode** button.

Note that the scales on the *r*- and *z*-axes are not equal, resulting in a distorted view. If desired, you can select equal scale settings by going to the **Options** menu and checking the **Axis equal** box in the **Axis/Grid Settings** menu. In order to return to the original unequal scale settings, once again go to the **Axes/Grid Settings** menu and clear the **Axis equal** check box. Enter -0.1 in the **r min** edit field, 0.2 in the **r max** edit field and -0.1 and 1.1 in the **z min** and **z max** edit fields, respectively.

CHECKING THE SOLVER SETTINGS

The model in this exercise is nonlinear. Verify that the **Stationary nonlinear** solver is selected for this problem by pressing the **Solver Parameters** button.



POSTPROCESSING

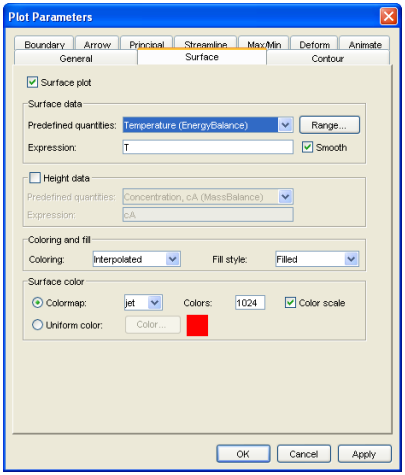
Now examine the temperature profile with the new boundary condition.

1 Click the **Postprocessing Mode** button. The default plot shows the concentration of species A in the reactor.

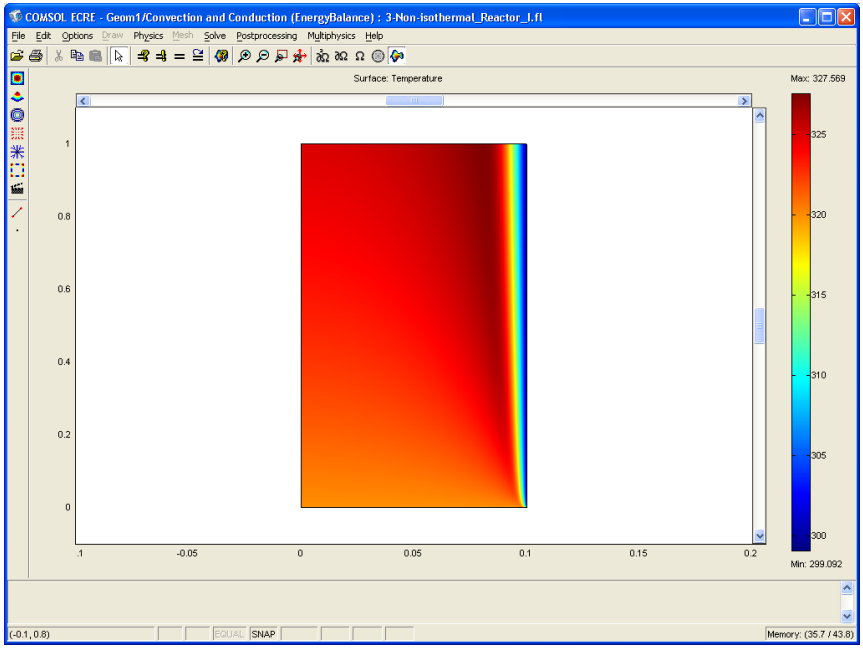
2 Click the **Plot Parameters** button.

3 Click the **Surface** tab.

4 Select **Temperature** in the **Predefined quantities** drop-down list on the **Surface** page.



5 Click **OK**.



6 To visualize the local temperature in selected cross sections along the length of the reactor, go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.

7 Click the **Line/Extrusion** tab.

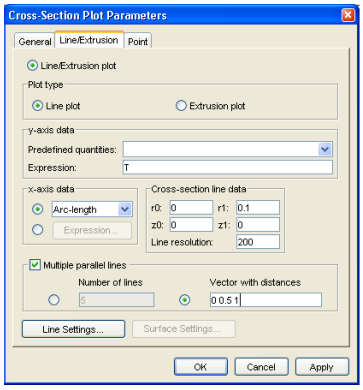
8 Enter `T` in the **Expression** edit field.

9 Enter `0` in the **r0** edit field and `0.1` in the **r1** edit field.

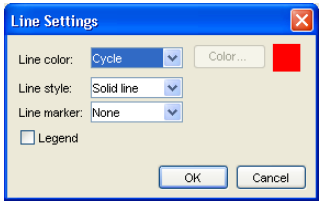
10 Enter `0` in both the **z0** and **z1** edit fields.

11 Check the **Multi parallel lines** box, then click the **Vector with distances** option.

I2 Enter `0 0.5 1` in the **Vector with distances** edit field to generate three cross section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.



I3 Click the **Line Settings** button. In the dialog box that opens, select the **Cycle** option in the **Line color** drop-down list; select **Solid line** in the **Line style** drop-down list; and select **None** in the **Line marker** drop-down list.



I4 Finally, to generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, and then again in the **Cross-Section Plot Parameters** dialog box.

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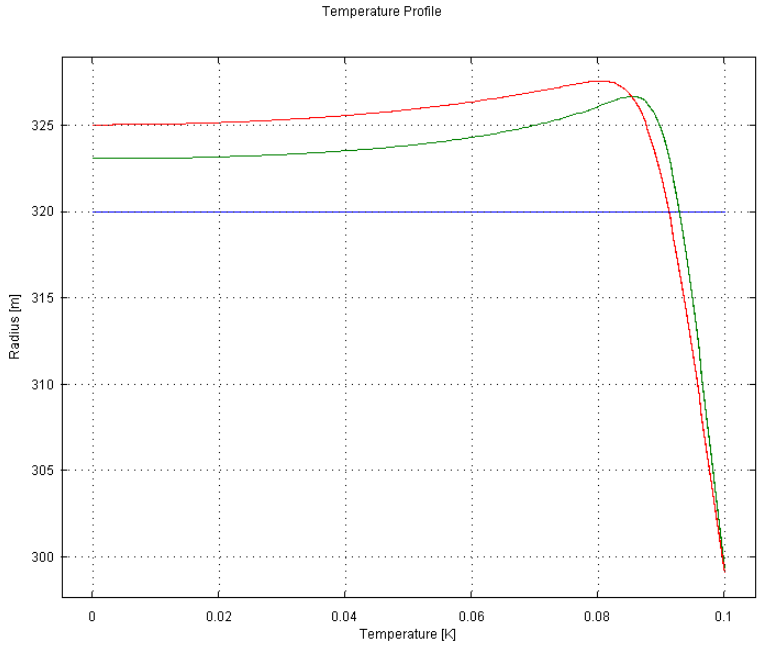


Figure 2-4: Radial temperature profiles at the inlet, outlet and halfway through a non-isothermal reactor with an isothermal cooling jacket.

You have now completed a review of the model and are ready to run it with varying input parameters.

Questions and Exercises

Now that we have added a cooling jacket, let's see how it affects the results. Remember that we assumed that the coolant flow is high enough to ensure a constant coolant temperature.

1. How does the outlet conversion change compared to the adiabatic reactor model? (Hint: See the calculation of the average concentration using integrals in the section treating **Boundary integration** on page 29 and use the same procedure to calculate the total conversion.)
2. How does the temperature profile change, and why does it change in this way? Where is the maximum temperature now located?

3 How does the conversion profile change? At which radial position do you find the highest conversion? Compare it with that from the adiabatic reactor model in the previous exercise.

Non-Isothermal Reactor with Non-Isothermal Cooling Jacket

This model is an extension of the previous one, which has an isothermal cooling jacket, and the cooling power is more or less unlimited because the cooling media's temperature is constant along the reactor's length. In contrast, this exercise limits the cooling power by introducing a heat balance for the cooling jacket. Thus the cooling power decreases as the temperature of the fluid in the jacket increases. The model equations are found in the Mass Balance paragraph on page 13, and in the Energy Balance paragraph on page 14.

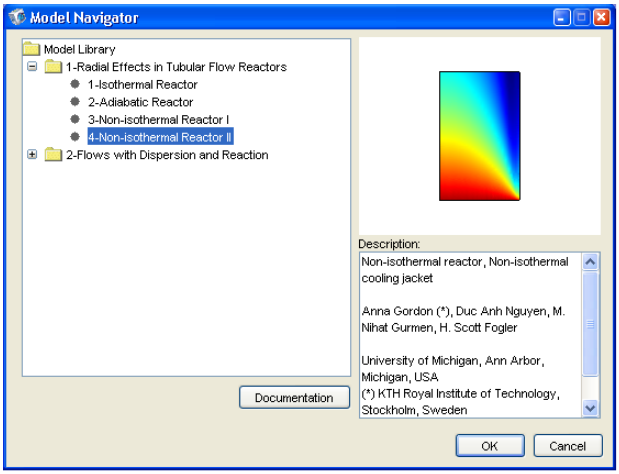
Before starting with this exercise, we can review the model as before with the previous models. Then we are ready to change the model parameters to investigate different operating conditions for the reactor.

Reviewing the Model in COMSOL ECRE Version

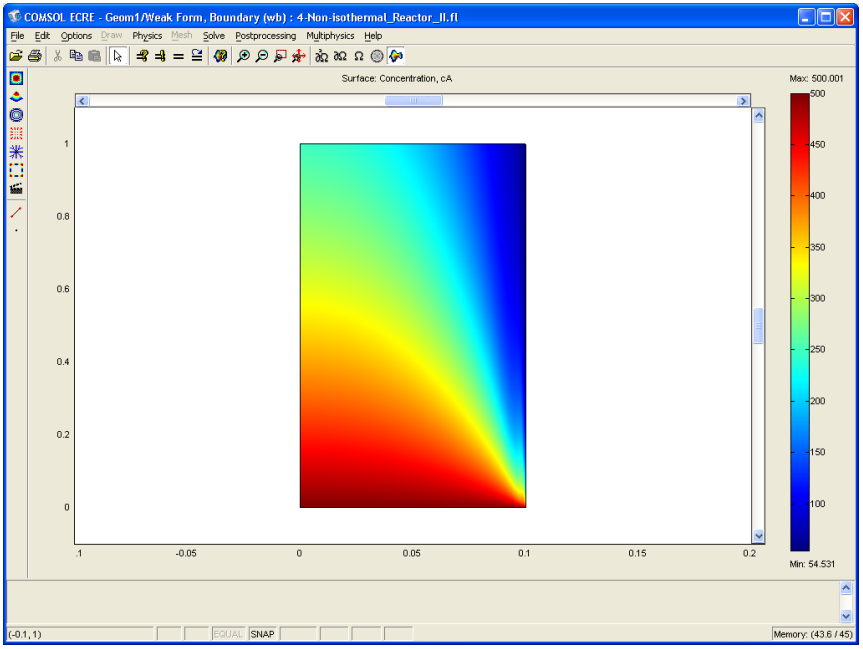
OPENING THE MODEL

1 Double click on the COMSOL ECRE icon to open the **Model Navigator**. If you are already using COMSOL Multiphysics, go to the **File** menu and select **New** to open the **Model Navigator**.

2 In this dialog, click the folder **1-Radial Effects in Tubular Flow Reactors** and select the model **4-Non-isothermal Reactor II**. Click **OK**.



The model opens in the Postprocessing Mode and the surface plot shows the concentration of species A in the reactor.

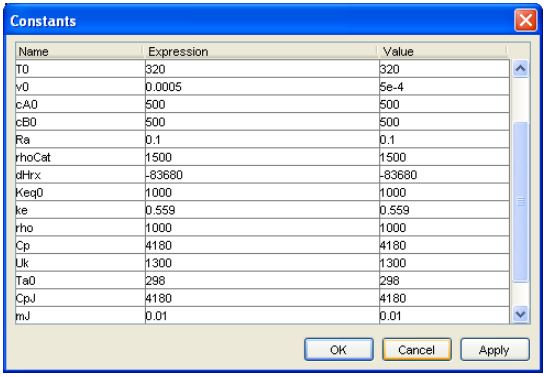


Note that the dimensions of the reactor are not displayed with equal axes in the *r*- and *z*-directions.

MODEL EQUATIONS AND INPUT DATA

The model equations in the reactor are almost identical to those for the "Reactor with Isothermal Cooling Jacket" in the preceding exercise. To account for the jacket temperature we must introduce two new entries in the list of constants and also change the radial boundary condition. In addition, we introduce a new application mode for the heat balance in the cooling jacket. Let's review these changes.

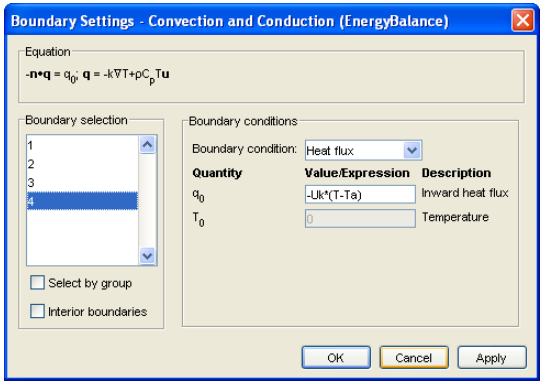
1. Click the **Multiphysics** menu. Doing so opens a drop-down list that contains any active application modes, in this case the **Convection and Diffusion (Mass Balance)**, the **Convection and Conduction (Energy Balance)** and **Weak Form, Boundary (wb)** application modes.
2. Click on the **Convection and Conduction** application mode.
3. Go to the **Options** menu and select the menu item **Constants**. The resulting dialog box displays the names and definitions of all the constants the model uses. Scroll down to examine the new constants `CpJ` and `mJ`.



   You can freely define any additional constants and rename existing ones. For this exercise, however, leave them as they are.

4. Click the **Cancel** button to close the dialog box.
5. Go to the **Physics** menu and select **Boundary Settings**.
6. Click on boundary number 4 in the **Boundary Selection** list. It corresponds to the reactor wall. Here you can see the new **Heat flux** boundary condition. As in the previous example, the heat flux is proportional to the difference between the temperature at the reactor's inner wall (`T`) and that of the cooling jacket (`Ta`).

However, in this case `Ta` is not a constant and instead is the dependent variable for the temperature in the cooling jacket.

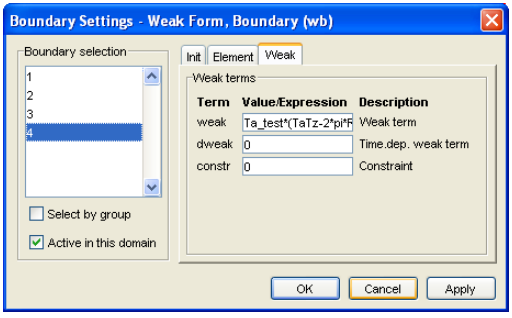


7 Click the **Cancel** button to close the dialog box.

8 Click the **Multiphysics** menu and select the **Weak Form, Boundary (wb)** application mode.

9 Go to the **Physics** menu and select **Boundary Settings**.

10 Click on the **Weak** tab and select boundary number 4 in the **Boundary Selection** list. In the **Weak Value/Expression** edit field you can see the energy balance expression for the non-isothermal cooling jacket.



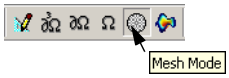
The model uses the Weak Form, Boundary application mode to define a partial differential equation in one dimension, along the boundary, to represent the heat balance in the cooling jacket. You can identify the expression within the brackets as the heat balance of the coolant in the cooling jacket as described in the introduction. This heat balance is written in a so-called weak form, which is the form used internally in COMSOL Multiphysics. The weak term represents the left-hand side of an equation that equals zero. `Ta_test` is a base function used to define `Ta` along the boundary and is an internal COMSOL Multiphysics syntax.

11 Click the **Cancel** button to close the dialog box.

You have now reviewed the changes in input data and boundary conditions for the energy balance compared to the "Isothermal Jacket" example.

VISUALIZING THE MESH

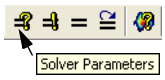
To visualize the mesh click the **Mesh Mode** button.



Note that the scales on the *r*- and *z*- axes are not equal, resulting in a distorted view. If desired, you can select equal scale settings by going to the **Options** menu and checking the **Axis equal** box in the **Axis/Grid Settings** menu. In order to return to the original unequal scale settings, go to the **Axes/Grid Settings** menu once again and clear the **Axis equal** check box. Enter `-0.1` in the **r min** edit field, `0.2` in the **r max** edit field, and `-0.1` and `1.1` in the **z min** and **z max** edit fields, respectively.

CHECKING THE SOLVER SETTINGS

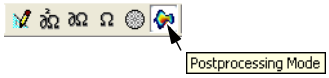
The model in this exercise is nonlinear. You can verify that the **Stationary nonlinear** solver is selected for this problem by pressing the **Solver Parameters** button.



POSTPROCESSING

Let's look at the temperature profile with the new boundary condition and the non-isothermal cooling jacket.

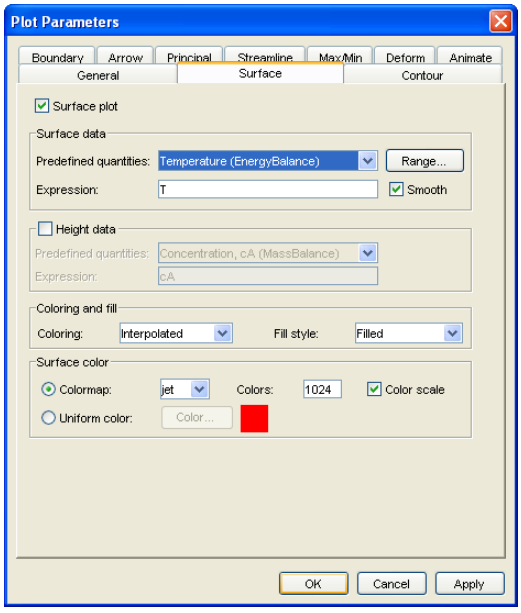
1 Click the **Postprocessing Mode** button. The default plot shows the concentration of species A in the reactor.



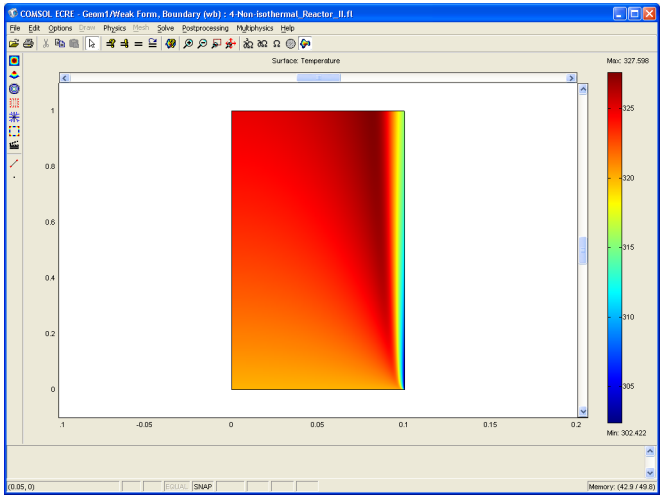
2 Click the **Plot Parameters** button.

3 Click the **Surface** tab.

4 Select **Temperature** in the **Predefined quantities** drop-down list on the **Surface** page.



5 Click **OK**.



6 To visualize the local temperature in selected cross sections along the length of the reactor, go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.

7 Click the **Display cross-section in main** axes check box to clear it.

8 Click the **Line/Extrusion** tab.

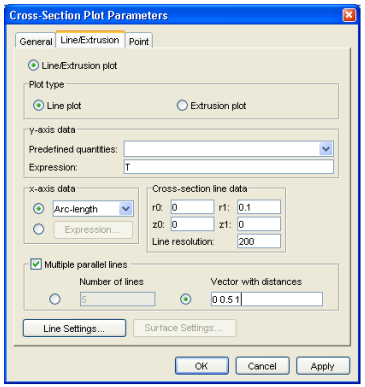
9 Enter `T` in the **Expression** edit field.

10 Enter `0` in the **r0** edit field and `0.1` in the **r1** edit field.

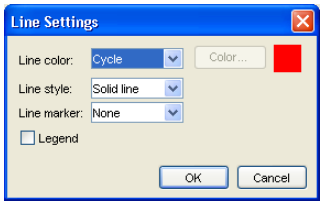
11 Enter `0` in both the **z0** and **z1** edit fields.

12 Check the **Multi parallel lines** box, then click the **Vector with distances** option.

13 Enter `0 0.5 1` in the **Vector with distances** edit field to generate three cross-section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.



14 Click the **Line Settings** button. In the resulting dialog box, select the **Cycle** option in the **Line color** drop-down list; select **Solid line** in the **Line style** drop-down list; and select **None** in the **Line marker** drop-down list.



15 Finally, to generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, and then again in the **Cross-Section Plot Parameters** dialog box.

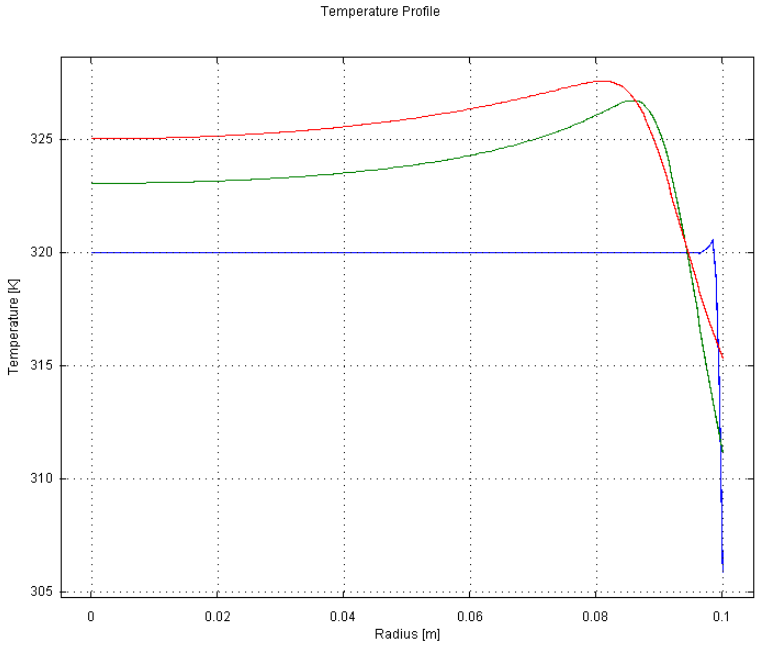


Figure 2-5: Radial temperature profiles at the inlet, outlet and halfway through a non-isothermal reactor with a non-isothermal cooling jacket.

16 To visualize the temperature in the cooling jacket first go to the **Domain Plot Parameters** in the **Postprocessing menu**.

17 Click the **Line/Extrusion** tab.

18 Select boundary number 4 in the **Boundary Selection** list and **z** from the **x-axis data** drop-down list.

19 Enter `Ta` in the **Expressions** edit field and click **OK**.

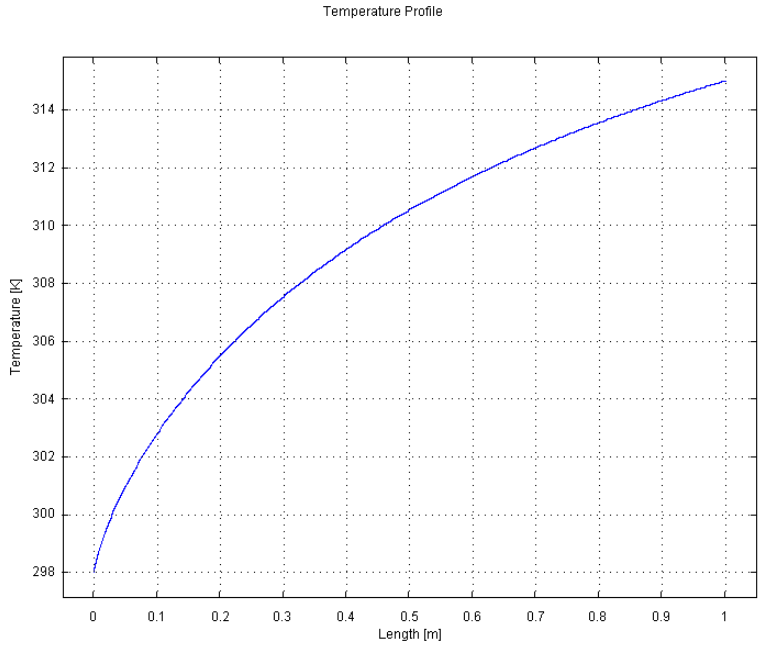


Figure 2-6: The cooling jacket's temperature profile along the length of the reactor.

You have now completed a review of the model and are ready to run it with varying input parameters.

Questions and Exercises

1. How does the temperature profile of the coolant in the cooling jacket change? How does it affect the temperature and concentration profiles in the reactor?
2. Increase the coolant flow rate by a factor of 10. How does the conversion change? (Hint: See the calculation of the average concentration using integrals in the section treating **Boundary integration** on page 29 and use the same procedure to calculate the total conversion.)
3. What would you do to increase the average outlet conversion?
4. Write two paragraphs describing what you found when you varied the parameters for the different types of reactors studied in this chapter.

3

Flows with Dispersion and Reaction

Model Description, Equations, and Input Data

This chapter uses COMSOL ECRE to study the effects of open and closed boundary conditions in the modeling of tubular reactors. The following two models also exemplify two ways to treat the different types of boundary conditions. The first model achieves open or closed boundary conditions using the predefined boundary conditions in COMSOL Multiphysics' Chemical Engineering Module. The second model adds an upstream and downstream section to the reactor. It then achieves open and closed boundary conditions by varying the Peclet number in these sections.

These exercises model an arbitrary reaction with undefined reaction order, while a dimensionless mass balance, expressed in terms of the Peclet and Damkohler numbers, defines the model. The first model studies the effects of reaction order as well as the Peclet and Damkohler number.

Model Description

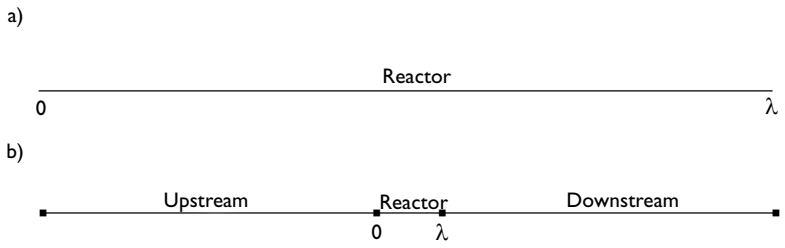


Figure 3-1: Model geometry for the 1-dimensional models, first using predefined COMSOL Multiphysics boundary settings (a), and then using long upstream and downstream sections to simulate different boundary conditions (b).

Figure 3-1 depicts the model geometries. The models assume fully developed turbulent flow, which reduces the problem to a one-dimensional model, graphically represented with a line. The line edges represent the reactor's inlet and outlet (Figure 3-1a) or the inlet and outlet of the upstream and downstream sections (Figure 3-1b).

Model Equations

The mass balance for the reactor is described by a dimensionless ordinary differential equation:

MASS BALANCE

$$-\frac{1}{Pe_r}\frac{d^2\Psi}{d\lambda^2}+\frac{d\Psi}{d\lambda}=-Da\cdot\Psi^n$$

where Ψ denotes the dimensionless concentration, λ the dimensionless length of the reactor, and Pe_r and Da are the dimensionless Peclet and Damkohler numbers, respectively.

We can also use this mass balance when adding sections upstream and downstream to the reactor in the second step of the modeling process. However, in these sections we set the reaction term–the right-hand side of the mass balance–to zero.

BOUNDARY CONDITIONS

As mentioned in the introduction, the first part of this exercise uses the predefined subdomain settings in the Chemical Engineering Module to apply open or closed boundary conditions. In the second step, we apply an open boundary condition for the upstream section. We then create an open or closed boundary condition for the reactor by varying the Peclet number.

The closed-closed boundary conditions for the mass balance are:

- Inlet $\lambda = 0$

$$-\frac{1}{Pe_r}\frac{d\Psi}{d\lambda}+\Psi=1$$

- Outlet $\lambda = 1$

$$\frac{d\Psi}{d\lambda}=0$$

At steady state, the open boundary condition for the outlet is identical to the closed boundary condition. For the inlet, however, the open boundary condition is the following:

- Inlet $\lambda = 0 \quad \Psi = 1$.

Model Parameters

Now examine the model's input data. You define them either as constants or as logical expressions in COMSOL Multiphysics' **Option** menu. In defining each parameter in COMSOL Multiphysics, use the left-hand side of the equality in the following list (for example, `Per`) for the constant's **Name**, and use the value on the right-hand side of the equality (for instance, `7.5`) for the **Expression** that defines it.

The constants used in the model are the following:

- Peclet number in the reactor, `Per = 7.5`
- Damkohler number, `Da = 1.29`
- Reaction order, `n = 1`
- Peclet number in the upstream section, `Per_up = 1`
- Peclet number in the downstream section, `Per_down = 1`

Only one expressions is defined for this model.

- The conversion of reactant A is defined according to the analytical expression,

$$x_A = 1 - \Psi$$

which is defined in COMSOL Multiphysics as: `xA = 1-psi`.

Dispersion Reactor Model

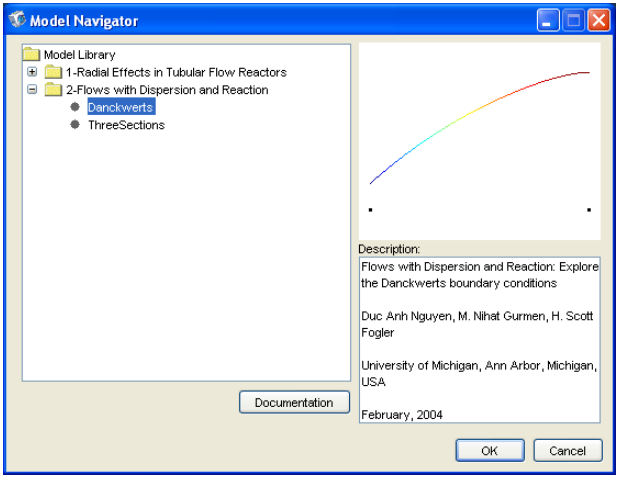
The first model uses the predefined boundary settings in COMSOL Multiphysics' Chemical Engineering Module to apply open or closed boundary conditions. Initially, the model is set up with closed-closed boundary conditions.

A user of the COMSOL Multiphysics Chemical Engineering Module can define the model from scratch. However, the COMSOL ECRE Version included in *Elements of Chemical Reaction Engineering* does not include the draw and mesh functionality in COMSOL Multiphysics. Nonetheless, COMSOL ECRE does allow for the change of reaction kinetics and transport properties, and it also implements all the postprocessing capabilities in the Chemical Engineering Module.

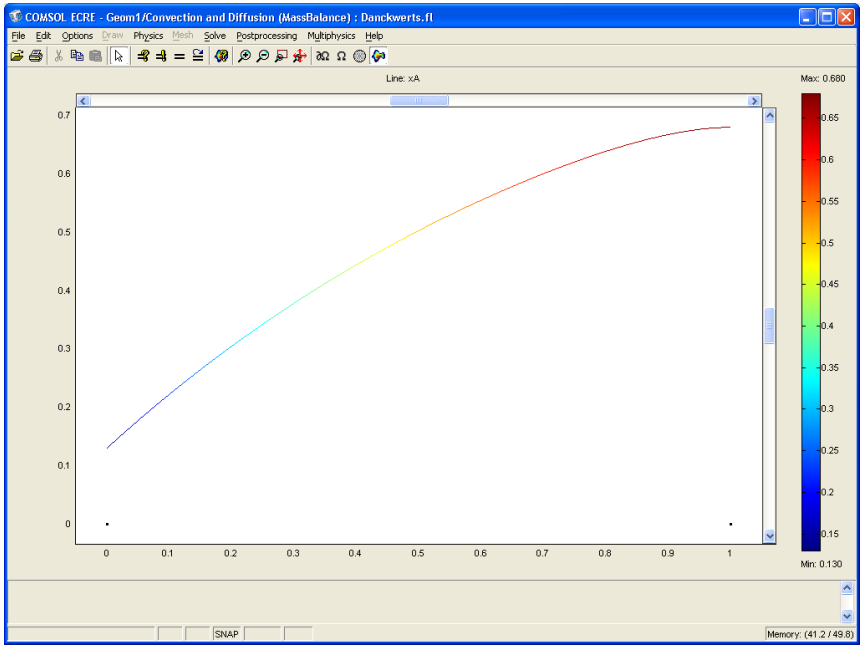
Reviewing the Model in the COMSOL ECRE Version

OPENING THE MODEL

1. Insert the COMSOL ECRE CD and select the platform on which you wish to run it. You then see the **Model Navigator** dialog on the screen.
2. In this dialog box click the folder **2-Flows with Dispersion and Reaction** and then select the **Danckwerts** model. Click **OK**.



The model opens in the Postprocessing mode and automatically shows the conversion profile.

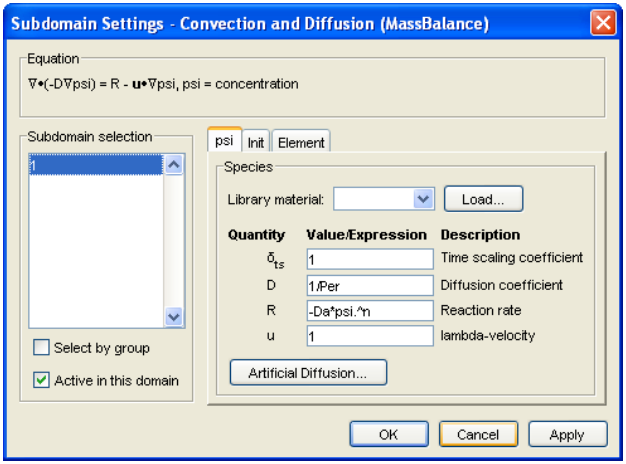


MODEL EQUATIONS AND INPUT DATA

In COMSOL ECRE you can review and change model equations and input data, but you cannot add or remove the application modes that make up the model. To review the application modes the model makes use of, do the following:

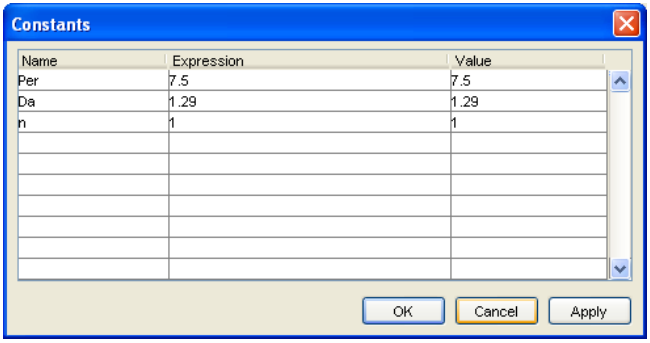
1. Click the **Multiphysics** menu. Doing so opens a drop-down list that contains any active application modes, in this case the **Convection and Diffusion (Mass Balance)** application mode.
2. Click again on the **Multiphysics** menu to close the list.
3. Go to the **Physics** menu and select **Subdomain Settings**, which opens up the corresponding dialog box. Select subdomain 1 in the **Subdomain Settings** list. The

resulting dialog box displays the equation that forms the basis for this application mode, while the edit fields show the input data used in the equation.



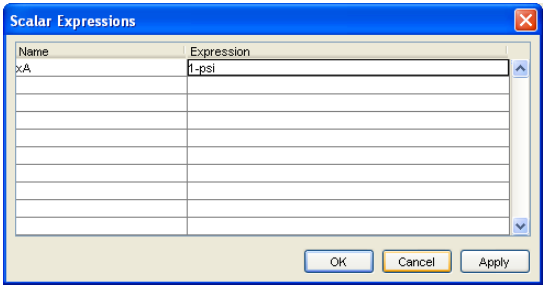
The edit fields correspond to the diffusion coefficient, reaction-rate expression, and λ-velocity in the reactor—all of which you can freely define. To review and change the definition of the input data, follow this procedure:

4 Go to the **Options** menu and select **Constants**. The resulting dialog box displays the names and definitions of all the constants the model uses.



You can freely define new constants and rename existing ones. In the dialog box in the preceding figure you can identify `Per`, which represents the inverted diffusion coefficient entered in the **Diffusion coefficient** edit field in the **Subdomain Settings** dialog box. COMSOL ECRE also allows for the definition of expressions.

5 Go to the **Options** menu, then to the expandable menu item **Expressions**, and finally select **Scalar Expressions**.



It is possible to move the **Scalar Expressions** dialog box in order to also display the **Constants** dialog box. Note that the constants and the scalar expressions are defined according to the list of Model Parameters in the preceding section. Examine the **Subdomain Settings** box and note that the constants are used to define the **Diffusion coefficient** parameters.

6 Click the **Cancel** button both in the **Scalar Expressions** and **Constants** dialog boxes.

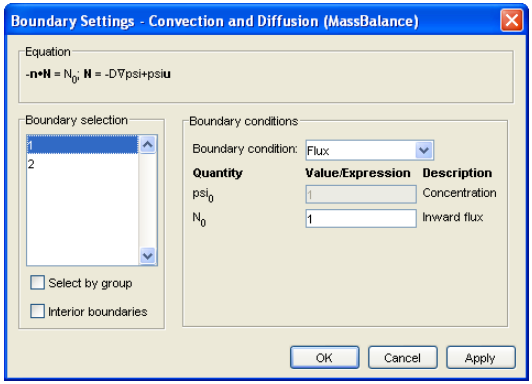
7 Click the **Init** tab in the **Subdomain Settings** dialog box. Here you could enter an initial guess for Ψ that the non-linear solver could use. In this case, because the reaction order is set to 1, the problem is linear and you need no initial guess. However, if you later want to change the reaction order to higher values, you will need to supply an initial guess.

8 Click the **Cancel** button to exit the **Subdomain Settings** dialog box.

Having reviewed the domain equations in the model, you can proceed to the boundary conditions.

9 Go to the **Physics** menu and select **Boundary Settings**.

10 Click on boundary number 1 in the **Boundary Selection** list. It corresponds to the reactor's inlet.



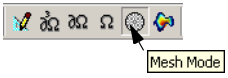
11 Select boundary number 2 to view the boundary condition at the reactor's outlet.

12 Click the **Cancel** button to close the **Boundary Settings** dialog box.

You have now reviewed the input data, domain equations, and boundary conditions.

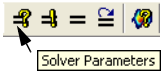
VISUALIZING THE MESH

Although you cannot manipulate the mesh in COMSOL ECRE, this version does allow you to visualize the mesh by pressing the **Mesh Mode** button. In this case the mesh consists only of points on the line representing the tubular reactor.



CHECKING THE SOLVER SETTINGS

COMSOL ECRE allows you to change the equation parameters and reaction kinetics and then solve the problem again. The model in this first exercise is nonlinear for reaction orders higher than 1. In order to solve the model for higher reaction orders, click the **Solver Parameters** button and verify that the **Stationary nonlinear** solver is selected.

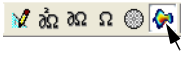


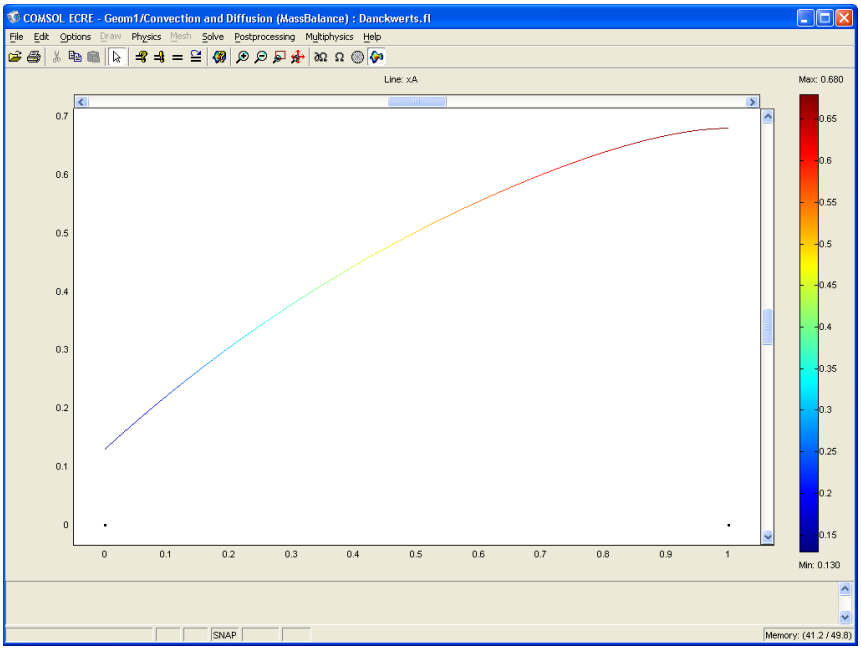
POSTPROCESSING

COMSOL ECRE comes with the full set of COMSOL Multiphysics postprocessing capabilities. These include surface plots, cross-sectional plots, point plots, as well as

boundary and subdomain integrations. Now is a good time to review some of the software's plotting and postprocessing capabilities.

1 Click the **Postprocessing Mode** button. The default plot shows the conversion in the reactor.

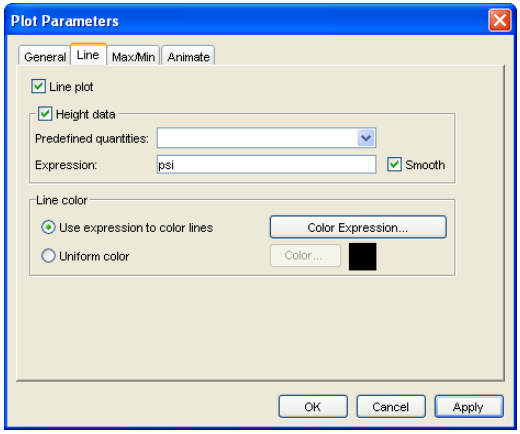




2 To plot the concentration, click the **Plot Parameters** button.

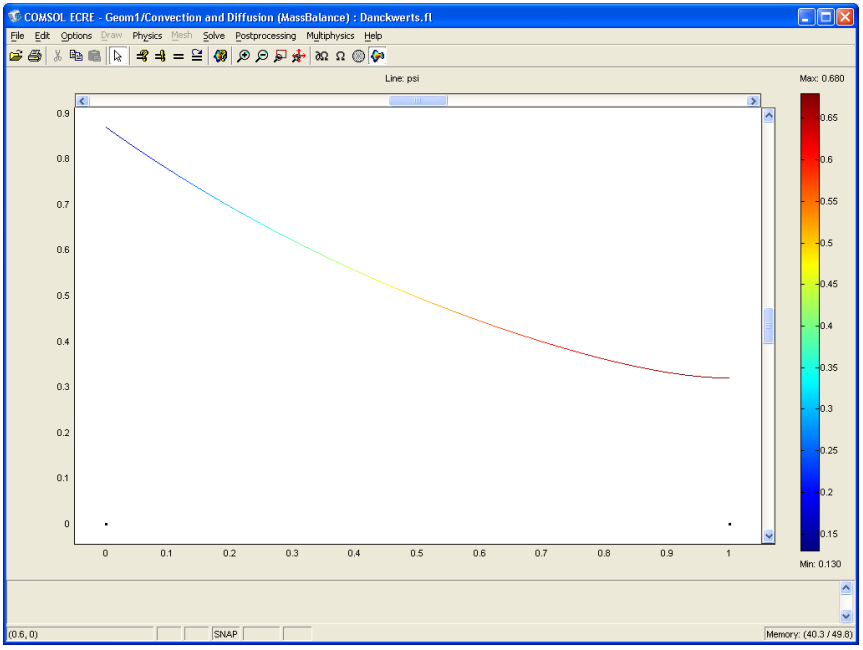
3 Click on the **Line** tab.

4 Enter `psi` in the **Expression** edit field.



5 Click the **Color Expression** button and enter `psi` in the **Expression** edit field.

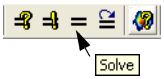
6 Click **OK** in the **Line Color Expression** frame and again in the **Plot Parameters** window.



Questions and Exercises

To answer the following questions and perform the exercises, you can either use the results in the model just described or you can solve it again with a new set of input data.

1. Describe how the outlet conversion changes when you alter the following parameters:
   - Change the Peclet number to 0.1 (to do so, go to the **Options** menu, select **Constants**, enter `0.1` in the **Expression** edit field, and finally click **Apply**). Click the **Solve** button to obtain a new solution.)

     Make sure to reset the Peclet number to the default value (7.5) before moving on to the next exercise.
   - Change the Damkohler number to 100. Make sure to reset it to the default value (1.29) before moving on to the next exercise.
   - Change the reaction order to 2. Make sure to reset it to the default value (1) before moving on to the next exercise.
2. How does an open or closed boundary condition affected the outlet conversion? Change the inlet boundary condition to open with this procedure:
   - Go to the **Physics** menu and select **Boundary Settings**.
   - Select boundary number 1 from the **Boundary Selection** list.
   - Select **Concentration** from the **Boundary condition** drop-down list.
   - Enter 1 in the **Concentration** edit field and click **OK**.
   - Click the **Solve** button to obtain the new solution.
   - To switch back to the closed boundary condition, select **Flux** from the **Boundary condition** drop-down list and enter 1 in the **Inward flux** edit field.

Model With Long Inlet and Outlet Sections Added to the Reactor

In this second model we introduce two new sections to the existing reactor, one part upstream and the other downstream relative the reactor. The reaction, however, is still limited to the original reactor section; in other words, the Damkohler number for the new sections equals zero. The inlet boundary condition for the upstream section and the outlet boundary for the downstream section are open. We simulate open or closed boundary conditions for the original reactor by altering the Peclet number in the new sections.

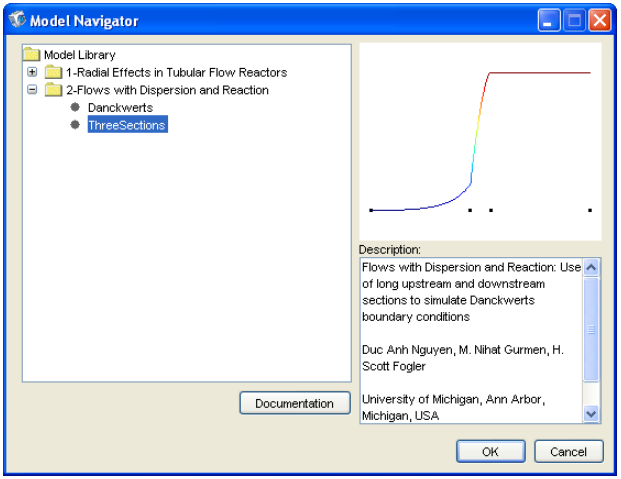
Those working with the COMSOL Multiphysics Chemical Engineering Module could generate this model from scratch by adding the new sections to the geometry in the previous model. COMSOL ECRE, however, supplies this model predefined and ready to run. You can freely experiment with different input data and still access the full postprocessing capabilities in the Chemical Engineering Module.

Reviewing the Model in the COMSOL ECRE Version

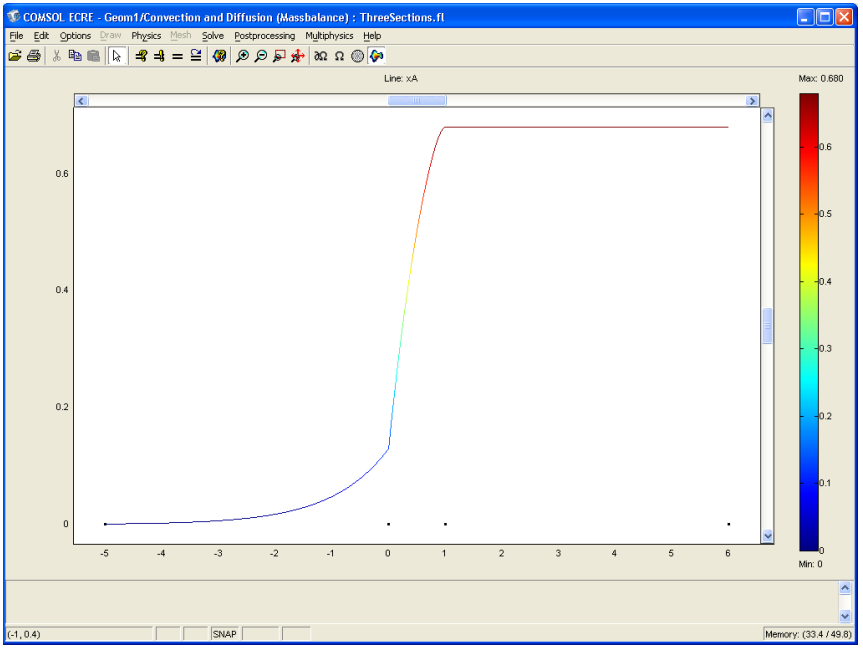
OPENING THE MODEL

1 If you have already installed COMSOL ECRE, double-click on its icon to open the **Model Navigator**. If not, go to step 1 in the preceding exercise to install the program. If you are already using COMSOL Multiphysics, go to the **File** menu and select **New** to open the **Model Navigator**.

2 In the resulting dialog box click the folder **2-Flows with Dispersion and Reaction** and select the model **Three Sections**. Click **OK**.



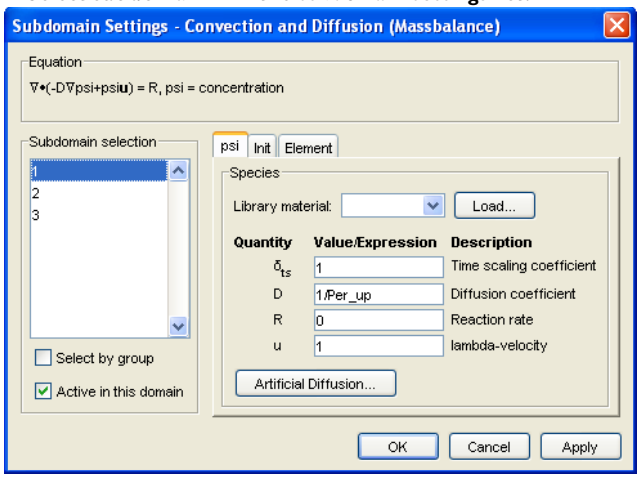
The model opens in the Postprocessing mode and automatically shows the conversion profile.



MODEL EQUATIONS AND INPUT DATA

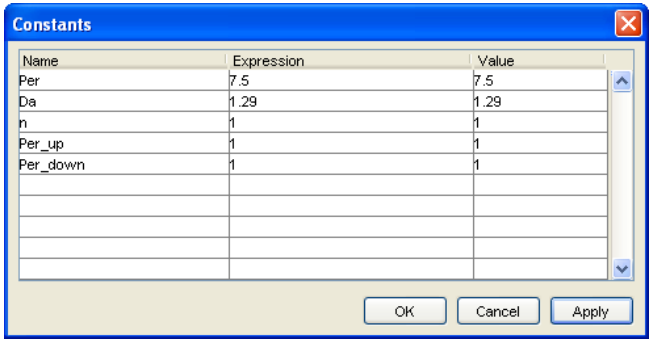
In COMSOL ECRE you can review and change model equations and input data but you cannot add or remove the application modes that make up the model. To review the application modes this model consists of, do the following:

1. Click the **Multiphysics** menu. Doing so opens a drop-down list that contains any active application modes, in this case the **Convection and Diffusion (Mass Balance)** application mode.
2. Click on the **Multiphysics** menu again to close the list.
3. Go to the **Physics** menu and select **Subdomain Settings**, which opens up the corresponding dialog box. You can now see two new subdomains, corresponding to the two new sections. This dialog box displays the equation that forms the basis for this application mode, while the edit fields show the input data used in the equation. Select subdomain 1 in the **Subdomain Settings** list.



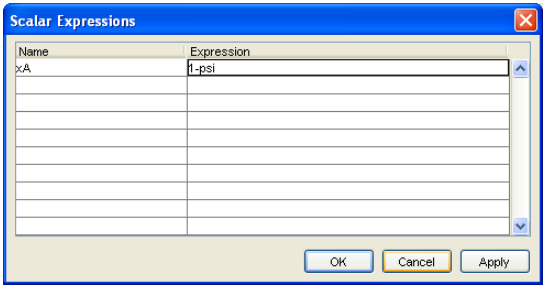
Subdomain number 1 corresponds to the upstream section. The edit fields correspond to the diffusion coefficient, reaction-rate expression, and λ-velocity in the reactor—all of which you can freely define. In this case, note that the **Reaction rate** is set to zero. To review and change the definition of the input data, follow this procedure:

4 Go to the **Options** menu and select **Constants**. The resulting dialog box displays the names and definitions of all the constants the model uses.



You can freely define new constants and rename existing ones. In the dialog box in the preceding figure you can identify `Per`, which represents the inverted diffusion coefficient entered in the **Diffusion coefficient** edit field in the **Subdomain Settings** dialog box. COMSOL ECRE also allows for the definition of expressions.

5 Go to the **Options** menu, then to the expandable menu item **Expressions**, and finally select **Scalar Expressions**.



It is possible to move the **Scalar Expressions** dialog box to also display the **Constants** dialog box. Note that the constants and the scalar expressions are defined according to the list in of Model Parameters in the preceding section. Examine the **Subdomain Settings** box and note that the constants are used to define the **Diffusion coefficient** and **Reaction rate** parameters.

6 Select subdomain 2 in the **Subdomain Selection** list to review the reactors subdomain settings, which are identical to those in the previous exercise.

7 Select subdomain 3 in the **Subdomain Selection** list to review the subdomain settings for the downstream section. As for subdomain 1, the reaction rate is set to zero.

8 Click the **Cancel** button in the **Scalar Expressions** and **Constants** dialog boxes.

9 Click the **Init** tab in the **Subdomain Settings** dialog box. Here you could enter an initial guess for Ψ that the nonlinear solver could use. In this case, because the reaction order is set to 1, the problem is linear and no initial guess is needed. However, if you later want to change the reaction order to higher values you need to define an initial guess.

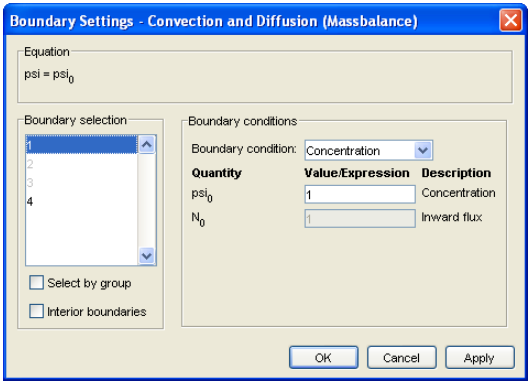
10 Different initial values are defined in the various subdomains. View the initial guesses by switching among the subdomains in the **Subdomain Selection** list.

11 Click the **Cancel** button to exit the **Subdomain Settings** dialog box.

Having reviewed the model's domain equations, you can proceed to the boundary conditions.

12 Go to the **Physics** menu and select **Boundary Settings**.

13 Click on boundary number 1 in the **Boundary Selection** list. It corresponds to the upstream section's inlet.



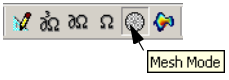
14 Select boundary number 4 to view the boundary condition at the outlet of the downstream section.

15 Click the **Cancel** button to close the **Boundary Settings** dialog box.

You have now reviewed the input data, domain equations, and boundary conditions.

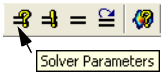
VISUALIZING THE MESH

Although you cannot manipulate the mesh in COMSOL ECRE, this version does allow you to visualize the mesh by pressing the **Mesh Mode** button. In this case the mesh consists only of points on the line representing the tubular reactor.



CHECKING THE SOLVER SETTINGS

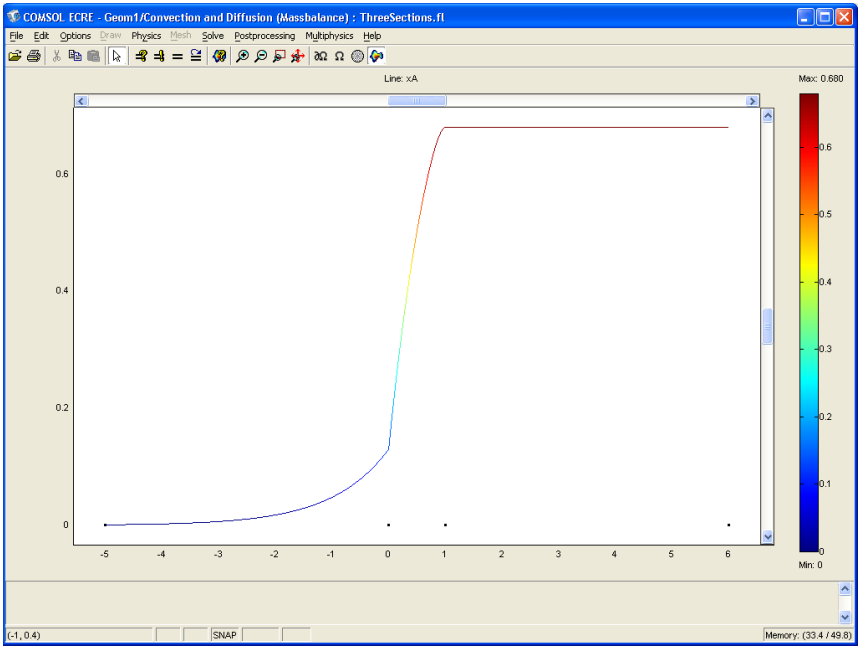
COMSOL ECRE allows you to change equation parameters and reaction kinetics and solve the problem again. For reaction orders equal to 1 this model is linear. However, to solve the model for higher reaction orders you must use a nonlinear solver; thus click the **Solver Parameters** button and verify that the **Stationary nonlinear** solver is selected.



POSTPROCESSING

COMSOL ECRE comes with the full set of COMSOL Multiphysics postprocessing capabilities. Now is a good time to review some of the software's plotting and postprocessing functionality.

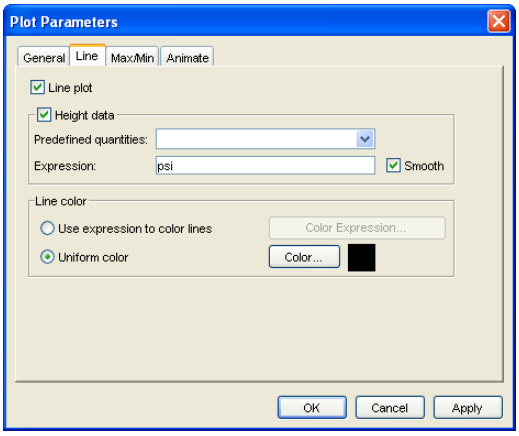
1 Click the **Postprocessing Mode** button. The default plot shows the conversion in the reactor.



2 To plot the dimensionless concentration, click the **Plot Parameters** button.

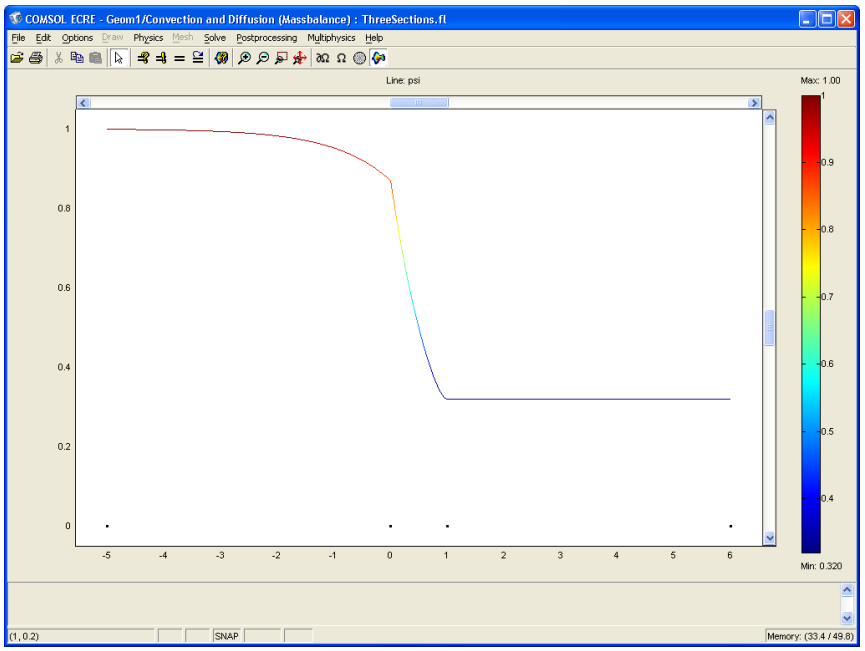
3 Click on the **Line** tab.

4 Enter `psi` in the **Expression** edit field.



5 Click the **Color Expression** button and enter `psi` in the **Expression** edit field.

6 Click **OK** in the **Line Color Expression** frame and again in the **Plot Parameters** window.

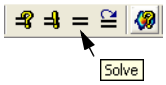


Questions and Exercises

To perform the following exercise, solve the model again with a new set of input data.

1 Describe how the outlet conversion changes when you alter the Peclet number in the new sections to simulate open-open and closed-closed boundary conditions. Small values of the Peclet number indicate negligible dispersion and simulate a closed boundary condition. Values of the Peclet number in the new sections comparable to the those in the reactor section indicate substantial dispersion and simulate an open condition.

   Go to the **Options** menu, then to **Constants**, then change the upstream and downstream Peclet numbers. Click the **Solve** button to obtain a new solution.



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