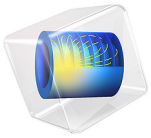


Model created in COMSOL Multiphysics 6.4

Tubular Reactor with Nonisothermal Cooling Jacket

Introduction

In this simple example, study an elementary, exothermic, and irreversible reaction in a tubular reactor (in a liquid phase and laminar flow regime). The reactor keeps its temperature down via a cooling jacket. In this model, you investigate the reactor's steady-state behavior.

The Model Definition section provides a general description of the complete reactor model, whereas the Modeling Instructions detail how to set up and solve a nonisothermal reactor model that accounts for the cooling jacket.

This model is based on the example in Ref. 1.

Model Definition

REACTION

The reaction is a conversion of species A, B, and C in liquid.

$$A + B \rightarrow C \tag{1}$$

A is the notation for propylene oxide, B is water, and C is propylene glycol. The reaction kinetics are first order in regard to the concentration of A.

GEOMETRY

Figure 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 axisymmetric.

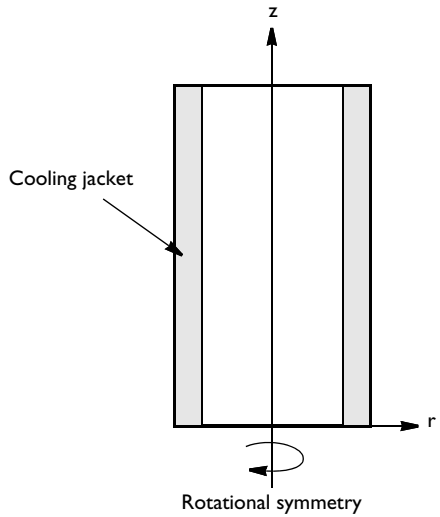


Figure 1: Geometry for the two-dimensional rotationally symmetric model.

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 *rz*-plane. The borders of the surface represent the inlet, outlet, reactor wall, and centerline. 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 only needs to solve these equations for half of the domain shown in Figure 1.

MODEL EQUATIONS

You describe the mass balances and heat balances in the reactors with partial differential equations (PDEs) as given in the Transport of Diluted Species and Heat Transfer in Fluids interfaces, while one ordinary differential equation (ODE) is required for the heat balance in the cooling jacket. The latter equation is set up with a Coefficient Form Boundary PDE. The equations are defined as follows.

Mass Balance for Species A

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

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 example, 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.

Mass Balance Boundary Conditions

- Inlet ($z = 0$)

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

- At the wall ($r = R$)

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

The boundary condition selected for the outlet states 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

$$k\frac{1}{r}\frac{\partial T}{\partial r} + k\frac{\partial^2 T}{\partial r^2} + k\frac{\partial^2 T}{\partial z^2} - 2U\left(1 - \left(\frac{r}{R}\right)^2\right)\rho C_P \frac{\partial T}{\partial z} - r_A(-\Delta H_{Rx}) = 0 \tag{3}$$

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.

Energy Balance Boundary Conditions

- 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 constant temperature in the cooling jacket.

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: the heat transport out of the reactor is purely convective.

- Outlet ($z = L$)

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

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:

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

where T_j is the coolant temperature, 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 ($z = 0$)

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

MODEL PARAMETERS

You can define the model's input data either as constants or as logical expressions. To define the constant's name, use the left-hand side of the equality in the following list (for example, `Diff`, for the diffusivity of all species). To define the expression, use the value on the right-hand side of the equality (for example, `1E-9`, for `Diff`).

- Activation energy, `E` = `75362` J/mol
- Frequency factor, `A` = `16.96E12` 1/h

- Diffusivity of all species, `Diff` = `1E-9` m^2/s
- Thermal conductivity of the reaction mixture, `ke` = `0.559` $W/(m \cdot K)$
- Overall heat transfer coefficient, `Uk` = `1300` $W/(m^2 \cdot K)$
- Inlet temperature, `T0` = `312` K
- Inlet temperature of the coolant, `Ta0` = `277` K
- Heat of reaction, ΔH_{Rx}, `dHrx` = `-84666` J/mol
- Total flow rate, `v0` = `0.1` m^3/s
- Mass flow rate of coolant, `mc` = `0.1` kg/s
- Concentration A at inlet, `cA0` = `1587` mol/m^3
- Concentration B at inlet, `cB0` = `43210` mol/m^3
- Concentration methanol at inlet, `cMe0` = `1587` mol/m^3
- Heat capacity at inlet, `Cp0` = `(146.54*cA0_po+75.36*cB0+81.095*cMe0)/rho0` J/(kg·K) (here, the numerical factors are the molar specific heat values in the unit J/(mol·K))
- Heat capacity per mass of coolant, `Cpc` = `4180` J/(kg·K)
- Density at inlet, `rho0` = `cA0_po*M_po+cB0_po*M_w+cMe0_po*M_po` kg/m^3
- Reactor radius, `Ra` = `0.1` m
- Reactor length, `L` = `1` m
- Density, propylene oxide, `rho_po_p` = `830` kg/m^3
- Density, methanol, `rho_m_p` = `791.3` kg/m^3
- Density, water, `rho_w_p` = `1000` kg/m^3

The following section lists the definitions for the model expressions. 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**. 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

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

  which you define in COMSOL Multiphysics as `u0` = `v0/(pi*Ra^2)`.
- The superficial, laminar flow rate

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

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 species 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 species C is expressed as

$$C_C = C_{A0}x_A$$

which becomes `cC = cA0*xA`.

- The rate of reaction takes the following form:

$$r_A = -A\exp\left(-\frac{E}{RT}\right)C_A$$

which in COMSOL Multiphysics form is `rA = -A*exp(-E/R_const/T)*cA`.

- The heat production term becomes

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

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

Results

The following figures collect the results as shown in Ref. 1.

Surface plots for the surface temperature and conversion are shown in Figure 2 and Figure 4. These show that where the temperature is low, little conversion takes place and vice versa. This is because the rate of the reaction is temperature dependent. The low temperature closest to the wall is due to the coolant.

Figure 3 and Figure 5 show the temperature and conversion surface profiles at three locations along the length of the reactor. The further along the reactor the reactants travel,

the more reaction takes place and the higher the temperature becomes. The impact of the coolant is shown in these figures as well.

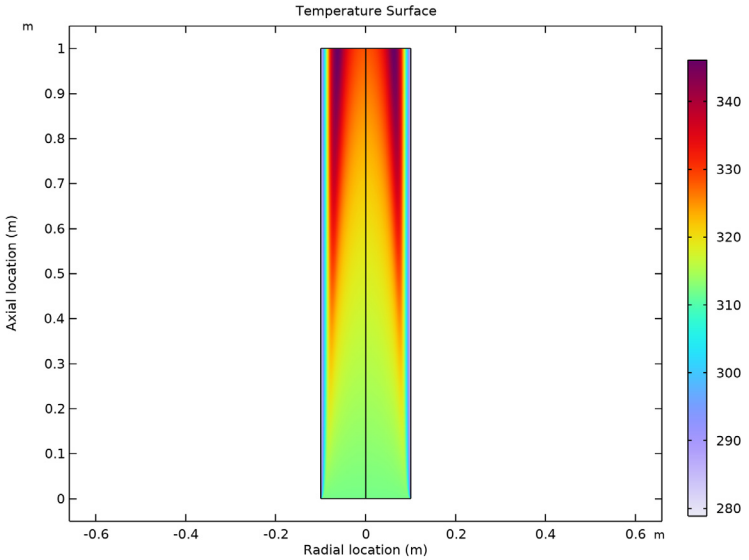


Figure 2: Temperature surface.

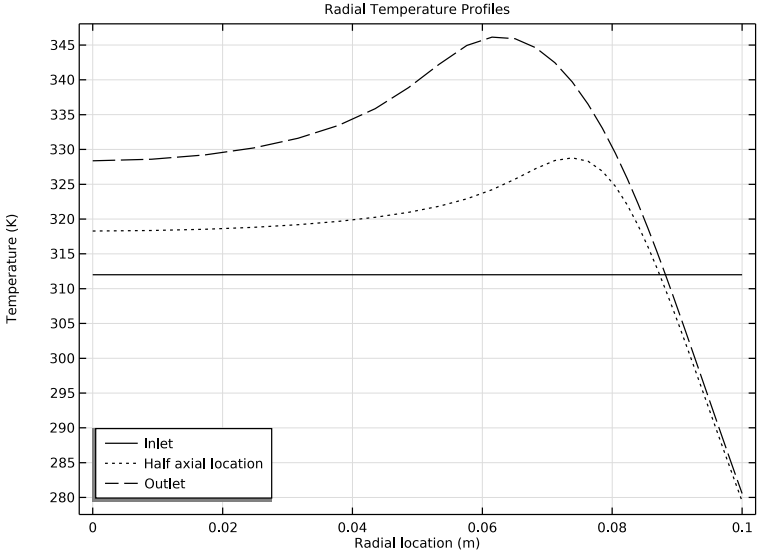


Figure 3: Radial temperature surface profiles.

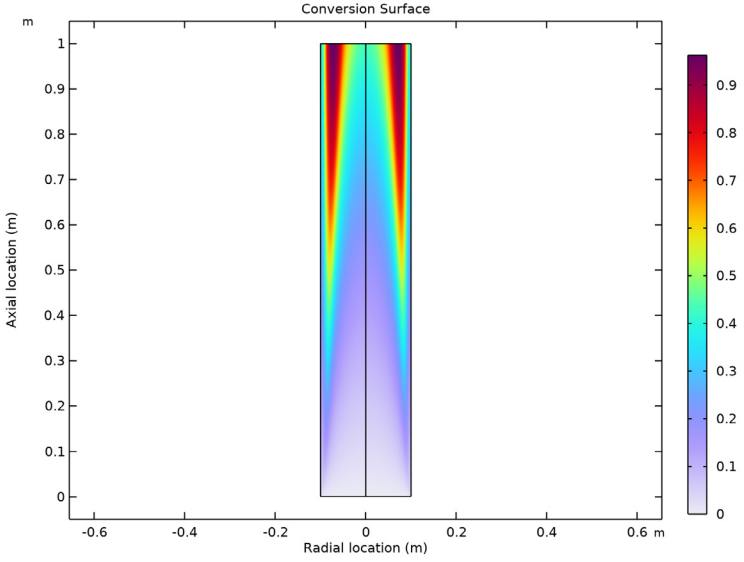


Figure 4: Conversion surface.

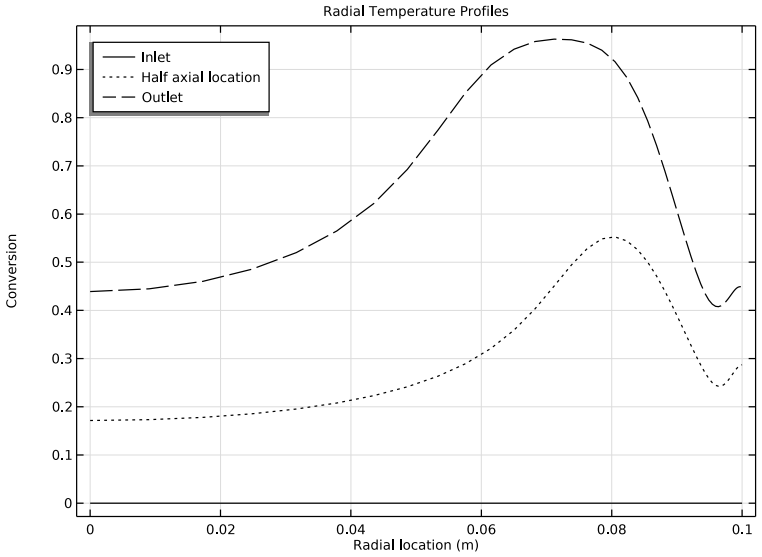


Figure 5: Radial conversion surface profiles.

Exercises

Try these example exercises with the model to better understand the system:

1. How does the thermal conductivity of the mixture affect the temperature distribution?
2. How does the coolant temperature decrease the mixture temperature at the outlet?
3. Expand the model. Is the convection in the radial direction important?

Reference

1. S. Fogler, *Elements of Chemical Reaction Engineering 4th ed.*, p. 557, *Example 8–12 Radial Effects in Tubular Reactor*, Prentice Hall, 2005.

Application Library path: `COMSOL_Multiphysics/Chemical_Engineering/tubular_reactor`

Modeling Instructions

When you start COMSOL Multiphysics, you are greeted by the **Model Wizard**. Here, you choose the dimension of your model geometry as well as the physics interfaces required. You can return to the **Model Wizard** later in the modeling process if you want to expand your model to include additional physics interfaces.

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Chemical Species Transport** > **Transport of Diluted Species (tds)**.

This sets up the required mass balance equation for species A.

3 Click **Add**.

4 In the **Concentration (mol/m³)** text field, type `cA`.

`cA` is the dependent variable name.

5 In the **Select Physics** tree, select **Heat Transfer** > **Heat Transfer in Fluids (ht)**.

6 Click **Add**.

Selecting this physics interface adds an energy balance to the model.

Finally, select the **Coefficient Form Boundary PDE** to model the cooling jacket. `Tc` is the temperature of the coolant.

7 In the **Select Physics** tree, select **Mathematics** > **PDE Interfaces** > **Lower Dimensions** > **Coefficient Form Boundary PDE (cb)**.

8 Click **Add**.

9 In the **Dependent variables (1)** table, enter the following settings:

`Tj`

10 Click **Select Dependent Variable Quantity**.

11 In the **Physical Quantity** dialog, type `temperature` in the text field.

12 In the tree, select **General** > **Temperature (K)**.

13 Click **OK**.

14 In the **Model Wizard** window, In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	W/m

15 click **Study**.

16 In the **Select Study** tree, select **General Studies** > **Stationary**.

The **Stationary** analysis type lets you investigate the steady-state behavior of the reactor.

17 Click **Done**.

GEOMETRY 1

Start by defining the reactor geometry. In 2D axisymmetry, the representation of the tubular reactor is reduced to a simple rectangle.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

The geometry is automatically drawn as you leave the **Geometry** node. You can also click the **Build All** button in the **Settings** toolbar.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `0.1`.

4 Click **Build All Objects**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

ROOT

Now, move on to define model-specific constants and expressions. You can type in constant names and their values in the **Parameters** section. Note that you can enter units enclosed in brackets after the constant values. This can be very useful, as the software is able to keep track of unit consistency throughout the model setup procedure.

In this case, the model parameters are available in a text file that is imported.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `tubular_reactor_parameters.txt`.

Just as with the model constants, you will find it convenient to group user-defined expressions in a list. You can type in expressions that contain constants from the **Parameters** list as well as dependent variables that you solve for; for example, `cA`.

DEFINITIONS

In this case, the model variables are available in a text file that is imported.

Variables 1

1 In the **Definitions** toolbar, click a= **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `tubular_reactor_variables.txt`.

TRANSPORT OF DILUTED SPECIES (TDS)

In the next step of the model setup, you will specify the parameters and source terms needed for the mass balance equation defined for species A. As you click the **Transport of Diluted Species** node, the **Equations** section of the **Settings** window will tell you which equations are being solved for. The **Domains** section shows a list of the geometry domains to which the equations apply. Note that you can change the mass transport mechanisms included in the mass balance equation through selections in the **Transport Mechanism** section. This can be done at any time in the modeling process.

Moving on to the **Fluid** node, you are expected to provide input defining the velocity field of the reacting mixture as well as the diffusivity of species A. In this model the velocity field is given by an expression describing a parabolic laminar flow profile. The variable names you type in have previously been defined in the **Variables** section and the **Parameters** section. The velocity field could also be calculated by COMSOL Multiphysics using a **Fluid Flow** interface.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport of Diluted Species (tds)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Convection** section.

3 Specify the **u** vector as

0	r
uz	z

4 Locate the **Diffusion** section. In the D_{cA} text field, type `Diff`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *cA* text field, type `cA0`.

At this point, right-click the **Transport of Diluted Species** node, select a **Reactions** feature and associate it with the reactor domain. Click the reactor domain to highlight it in red. Right-clicking the same domain changes the color to blue, meaning the domain is selected. The number of selected domains appears in the **Selection** list of the **Reactions** node. This adds a sink term to the mass balance equations that takes the depletion of species A through chemical reaction into account.

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 Select Domain 1 only.

3 In the **Settings** window for **Reactions**, locate the **Reaction Rates** section.

4 In the R_{cA} text field, type `rA`.

Now that the domain equations have been defined for the model, it is time to set the boundary conditions. First, you will select a concentration inflow condition at the inlet boundary.

Concentration 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species cA** checkbox.

5 In the $c_{0,cA}$ text field, type `cA0`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 3 only.

Assigning the **Outflow** condition to the outlet boundary imposes $-\mathbf{n}\cdot D\nabla c = 0$, that is, the transport of mass across the boundary is dominated by convection. Note that the mathematical representation of the boundary conditions is displayed in the **Equations** section of the **Settings** window. The boundary conditions for the axis of symmetry as well as the no flux condition for the reactor wall are set by default.

This concludes the definition of the mass balance for species A. Next, set up the **Heat Transfer** interface.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Heat Transfer in Fluids (ht)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Heat Convection** section.

3 Specify the $\mathbf{u}$ vector as

0	r
uz	z

In addition to the velocity field, the **Heat Transfer in Fluids** feature asks for the thermal conductivity, density, and heat capacity of the fluid.

4 Locate the **Heat Conduction, Fluid** section. From the k list, choose **User defined**. In the associated text field, type `ke`.

5 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.

6 From the ρ list, choose **User defined**. In the associated text field, type `rho0`.

7 From the C_p list, choose **User defined**. In the associated text field, type `cpm`.

8 From the γ list, choose **User defined**.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `T0`.

Heat Source 1

1 In the **Physics** toolbar, click **Domains** and choose **Heat Source**.

Add a **Heat Source** feature to include the effect of the exothermic reactions to the heat balance.

2 Select Domain 1 only.

3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.

4 In the Q_0 text field, type `Q`.

Next, add the boundary conditions specifying a temperature at the inlet, the heat flux between the reactor and cooling jacket, and an outflow condition at the outlet.

Temperature 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Temperature**, locate the **Temperature** section.

4 In the T_0 text field, type `T0`.

Heat Flux 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Heat Flux**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.

4 In the q_0 text field, type `-Uk*(T-Tj)`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 3 only.

Finally, add an energy balance describing the temperature distribution in the cooling jacket.

COEFFICIENT FORM BOUNDARY PDE (CB)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Coefficient Form Boundary PDE (cb)**.

2 In the **Settings** window for **Coefficient Form Boundary PDE**, locate the **Boundary Selection** section.

3 In the list, choose **1**, **2**, and **3**.

4 Click **Remove from Selection**.

5 Select Boundary 4 only.

Coefficient Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Coefficient Form Boundary PDE (cb)** click **Coefficient Form PDE 1**.

2 In the **Settings** window for **Coefficient Form PDE**, locate the **Diffusion Coefficient** section.

3 In the *c* text field, type `0`.

4 Locate the **Source Term** section. In the *f* text field, type `2*pi*Ra*Uk*(T-Tj)`.

5 Click to expand the **Convection Coefficient** section. Specify the β vector as

`0`	`r`
`Cpc*mc`	`z`

Dirichlet Boundary Condition 1

1 In the **Physics** toolbar, click **Points** and choose **Dirichlet Boundary Condition**.

The only required boundary condition is the temperature at the inlet of the jacket, `Ta0`.

2 Select Point 3 only.

3 In the **Settings** window for **Dirichlet Boundary Condition**, locate the **Dirichlet Boundary Condition** section.

4 In the *r* text field, type `Ta0`.

This completes the setup of the physics interfaces. The next step of the modeling process involves meshing.

MESH 1

Following the steps below, you will discretize the geometry with a mesh. The software uses the mesh when applying the finite element method to numerically solve the differential equations. In this particular model, you will create a mapped mesh. This meshing technique is often a good choice for simple geometries as it allows detailed control over the mesh distribution. The mesh is dense near the reactor inlet and reactor outer wall. This is needed to resolve the sharp concentration and temperature gradients expected when the reactor is run under nonisothermal conditions.

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

First set up 50 vertical mesh lines by selecting the inlet and outlet boundaries and using predefined distribution settings. Then, in the same fashion, set up the horizontal lines to complete the mapped mesh.

2 Select Boundaries 2 and 3 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type `50`.

6 In the **Element ratio** text field, type `0.01`.

7 From the **Growth rate** list, choose **Exponential**.

8 Select the **Reverse direction** checkbox.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 4 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type `200`.

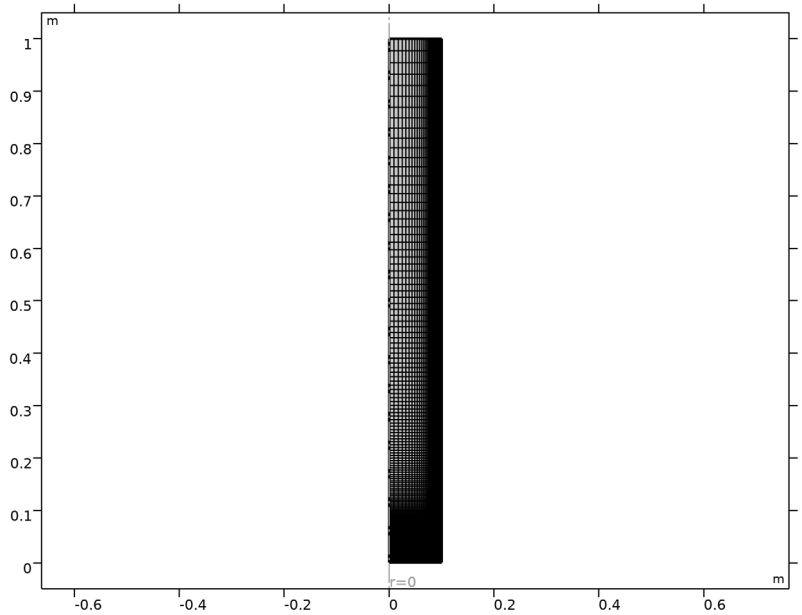
6 In the **Element ratio** text field, type `0.01`.

7 From the **Growth rate** list, choose **Exponential**.

8 Select the **Reverse direction** checkbox.

9 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

The figure below shows the created mesh, containing 10,000 elements.



STUDY 1

The model will be solved using two study steps. First, the software solves for the mass balance with the temperature kept constant. The computed solution is then used as an initial guess when solving the coupled mass and energy balance equations. This step-wise approach is often useful for tightly coupled equation systems, as a good initial guess helps to improve numerical convergence. It is straightforward to set up the mentioned solver sequence by defining two separate study steps under the **Study 1** node.

The **Study 1** node has a single **Stationary** step set up as a subnode. This study was generated as a consequence of selections in the **Model Wizard**, initiating the model building process. To set up a two-step solution process, add a second **Stationary** step to the **Study 1** node.

Step 2: Stationary 2

1 In the **Study** toolbar, click **Stationary**.

Keep the default settings for this study step, which implies solving for all dependent variables; the automatically generated solver settings are defined so as to solve for all dependent variables in each step.

To solve only for the concentration of A in the first step, follow the instructions below.

Step 1: Stationary

1 In the **Model Builder** window, click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Heat Transfer in Fluids (ht)**.

4 In the **Study** toolbar, click **Compute**.

The following instructions produce Figure 1 through Figure 4.

The default plot does not show the results as in Ref. 1. These plots instead require setting up two kinds of datasets: **Cut Line 2D** and **Mirror 2D** datasets.

RESULTS

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.

3 In row **Point 2**, set **R** to `Ra`.

4 Select the **Additional parallel lines** checkbox.

5 In the **Distances** text field, type `0.5*L 1*L`.

Mirror 2D 1

In the **Results** toolbar, click **More Datasets** and choose **Mirror 2D**.

Start by making the **Mirror 2D** plots. Start with the **Temperature Mirror 2D** plot, Figure 1.

Temperature (Mirrored)

1 In the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Temperature (Mirrored)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 2D 1**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Temperature Surface`.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** checkbox. In the associated text field, type `Radial location (m)`.

8 Select the **y-axis label** checkbox. In the associated text field, type `Axial location (m)`.

Surface 1

1 Right-click **Temperature (Mirrored)** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Heat Transfer in Fluids** > **Temperature** > **T - Temperature - K**.

3 Click the  **Zoom Extents** button in the **Graphics** toolbar.

4 In the **Temperature (Mirrored)** toolbar, click  **Plot**.

Duplicate the **Temperature Mirror 2D** plot to make the **Conversion Mirror 2D** plot, Figure 3.

Conversion

1 In the **Model Builder** window, right-click **Temperature (Mirrored)** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Conversion` in the **Label** text field.

3 Locate the **Title** section. In the **Title** text area, type `Conversion Surface`.

Surface 1

1 In the **Model Builder** window, expand the **Conversion** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **xA - Conversion species A - 1**.

3 Click the  **Zoom Extents** button in the **Graphics** toolbar.

4 In the **Conversion** toolbar, click  **Plot**.

Continue with the **2D Cut Line** plots. First, create the Temperature plot with a **1D Plot Group** with a **Line Graph**, Figure 2.

Temperature, 1D

1 In the **Results** toolbar, click  **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Temperature, 1D` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Radial Temperature Profiles`.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** checkbox. In the associated text field, type `Radial location (m)`.

8 Select the **y-axis label** checkbox. In the associated text field, type `Temperature (K)`.

Line Graph 1

1 Right-click **Temperature, 1D** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Heat Transfer in Fluids** > **Temperature** > **T - Temperature - K**.

3 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

4 From the **Color** list, choose **Black**.

5 Click to expand the **Legends** section. Select the **Show legends** checkbox.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
Inlet
Half axial location
Outlet

Temperature, 1D

1 In the **Model Builder** window, click **Temperature, 1D**.

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Position** list, choose **Lower left**.

4 In the **Temperature, 1D** toolbar, click **Plot**.

Duplicate the **Temperature 2D Cut Line** plot to make a **Conversion 2D Cut Line** plot, Figure 4.

Conversion, 1D

1 Right-click **Temperature, 1D** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Conversion, 1D` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Conversion`.

Line Graph 1

1 In the **Model Builder** window, expand the **Conversion, 1D** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **xA - Conversion species A - 1**.

Conversion, 1D

1 In the **Model Builder** window, click **Conversion, 1D**.

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Position** list, choose **Upper left**.

4 In the **Conversion, 1D** toolbar, click **Plot**.

Fix the naming of Plot Group 5, which shows the temperature in the cooling jacket.

Temperature Cooling Jacket

1 In the **Model Builder** window, under **Results** click **Coefficient Form Boundary PDE**.

2 In the **Settings** window for **2D Plot Group**, type `Temperature Cooling Jacket` in the **Label** text field.

Line 1

1 In the **Model Builder** window, expand the **Temperature Cooling Jacket** node, then click **Line 1**.

2 In the **Settings** window for **Line**, locate the **Coloring and Style** section.

3 From the **Line type** list, choose **Tube**.

4 In the **Tube radius expression** text field, type `3`.

5 In the **Temperature Cooling Jacket** toolbar, click **Plot**.

Last, you can select a model thumbnail by following these steps.

Concentration, 3D (tds)

1 In the **Model Builder** window, under **Results** click **Concentration, 3D (tds)**.

2 In the **Concentration, 3D (tds)** toolbar, click **Plot**.

ROOT

1 In the **Model Builder** window, click the root node.

2 In the root node's **Settings** window, locate the **Presentation** section.

3 Find the **Thumbnail** subsection. Click **Set from Graphics Window**.