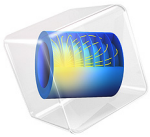

Multicomponent Tubular Reactor with Isothermal Cooling

Introduction

This example uses the Chemical Reaction Engineering Module to study an elementary, exothermic, irreversible reaction in a tubular reactor (liquid phase, laminar flow regime). The reactor uses a constant temperature cooling jacket to keep its temperature down. The steady-state behavior of the reactor is investigated. The reaction kinetics and physical properties of the species are modeled with the Chemistry interface, which is available in the Chemical Reaction Engineering Module.

The Model Definition section provides a general description of the complete reactor model, whereas the Modeling Instructions details how to set up and solve the model.

Model Definition

REACTION

The reaction is a reversible liquid phase conversion of propylene oxide and water into propylene glycol in the manner of

$$\text{poxide} + \text{H2O} \rightarrow \text{pglycol} \tag{1}$$

In the species named the prefix "p" stands for propylene. Water is in excess and is modeled as a solvent. The reaction kinetics is 1st order in regard to the concentration of propylene oxide:

$$r_{\text{poxide}} = k_1 c_{\text{poxide}} \tag{2}$$

GEOMETRY

Figure 1 illustrates the tubular reactor geometry.

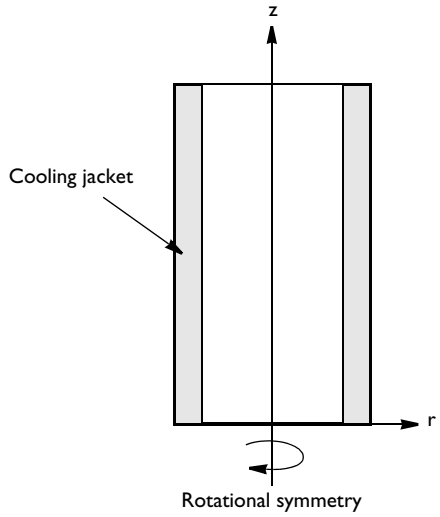

Figure 1: Model geometry for the 2-dimensional rotationally symmetric models.

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. That 2D surface's borders represent the inlet, the outlet, the reactor wall, and the centerline. The reactor model uses the following differential equations: mass balances for the species, a heat balance, combined with momentum and mass balance for the fluid flow. Due to rotational symmetry, the software need only to solve these equations for half of the domain as shown in Figure 1.

MODEL EQUATIONS

You describe the mass balances and heat balances in the reactors with partial differential equations (PDEs). The equations are defined as follows.

Mass Balance

$$\mathbf{u} \cdot \nabla C_i = \nabla \cdot (D_i \nabla C_i) + R_x \tag{3}$$

where D_i denotes the diffusion coefficient of species i, C_i is the concentration, $\mathbf{u}$ the flow velocity vector, and R_x is the reaction rate.

Using a two-dimensional axially symmetric geometry, and a constant diffusion coefficient, this equation corresponds to

$$u\frac{\partial C_i}{\partial r} + w\frac{\partial C_i}{\partial z} = D_i\frac{1}{r}\frac{\partial C_i}{\partial r} + D_i\frac{\partial C_i}{\partial r^2} + D_i\frac{\partial C_i}{\partial z} + R_x \tag{4}$$

where u and w denote the radial and axial velocity component respectively.

The mass balance equations are set up and solved for using the Transport of Diluted Species interface.

Mass Balance Boundary Conditions

- Inlet ($z = 0$)

$$C_i(r, 0) = C_{i0}$$

- At the wall ($r = R$)

$$\frac{\partial C_{\text{poxide}}}{\partial r}(R, z) = 0$$

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 ($z = L$)

$$\frac{\partial C_{\text{poxide}}}{\partial z}(r, L) = 0$$

  where L denotes the length of the reactor.

Energy Balance Inside the Reactor

$$\rho C_p \mathbf{u} \cdot \nabla T - \nabla \cdot (k\nabla T) = R_x(-\Delta H_{Rx}) \tag{5}$$

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

Using a two-dimensional axially symmetric geometry, and a constant thermal conductivity, this equation corresponds to

$$\rho C_p u\frac{\partial T}{\partial r} + \rho C_p w\frac{\partial T}{\partial z} - k\left(\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial T}{\partial r^2} + \frac{\partial T}{\partial z}\right) = R_x(-\Delta H_{Rx}) \tag{6}$$

The energy balance is solved for by the Heat Transfer in Fluids interface.

Energy Balance Boundary Conditions

- Inlet ($z = 0$)

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

- At the wall ($r = R$)

$$-\frac{\partial T}{\partial r}(R, z) = U_{\mathrm{k}}(T - T_{\mathrm{a}})$$

  where T_{a} denotes the constant temperature in the cooling jacket, and U_{k} is an overall heat transfer coefficient.

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 is convective.

- Outlet ($z = L$)

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

Momentum Balance

The fluid flow is modeled with the Laminar flow interface that solves the Navier–Stokes equations computing the velocity and pressure. At the inlet, a fully developed laminar flow profile with an average flow velocity is prescribed. At the outlet, the pressure is prescribed.

MODEL PARAMETERS

Below is a list of the model's input data. You define them either as constants or as expressions involving other constants. In defining each parameter in COMSOL Multiphysics, for the constant's **Name**, use the left side of the equality in the following list and use the value on the right side of the equality for the **Expression** that defines it. Type the unit inside brackets, like this `[mol/m^3]`.

The constants in the model are:

- Activation energy, `E = 75362` J/mol
- Frequency factor, `A = 16.96E12` l/h
- Overall heat-transfer coefficient, `Uk = 1300` W/(m^2·K)
- Thermal conductivity of mixture, `ke = 0.559` W/(m·K)
- Inlet temperature, `T0 = 312` K
- Inlet temperature of the coolant, `Ta0 = 273` K
- Heat of reaction, ΔH_{Rx}, `dHrx = -84666` J/mol
- Total flow rate, `v0 = 0.1[mol/s]/cpoxide0`

- Average flow velocity, `u0 = v0/(pi*Ra^2)`
- Concentration of propylene oxide at inlet, `cpoxide0 = rho_poxide/M_poxide/9[1]`
- Concentration of water, `cwater0 = rho_H2O/M_H2O*(7/9)[1]`
- Molar heat capacity of water, `cpm_H2O = 74.5` J/(mol·K)
- Reactor radius, `Ra = 0.1` m
- Reactor length, `L = 1` m
- Molar weight of propylene oxide, `M_poxide = 58.095 g/mol`
- Molar weight of water, `M_H2O = 18 g/mol`
- Molar weight of propylene glycol, `M_pglycol = 76.095` g/mol
- Density of propylene oxide, `rho_poxide` = 830 kg/m^3
- Density of water, `rho_H2O` = 1000 kg/m^3
- Density of propylene glycol, `rho_pglycol` = 1040 kg/m^3
- Reference dynamic viscosity of water (at 293 K), `myref_H2O` = 1 mPa·s
- Molar heat capacity of water, `cpm_H2O = 75.36` J/mol/K
- The conversion of poxide is given by

$$x_{\text{poxide}} = \frac{C_{\text{poxide}0} - C_{\text{poxide}}}{C_{\text{poxide}0}}$$

All necessary reaction kinetics and mass transport properties are incorporated into the model with the Chemistry interface.

Results

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 since, 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 are shown in these figures as well.

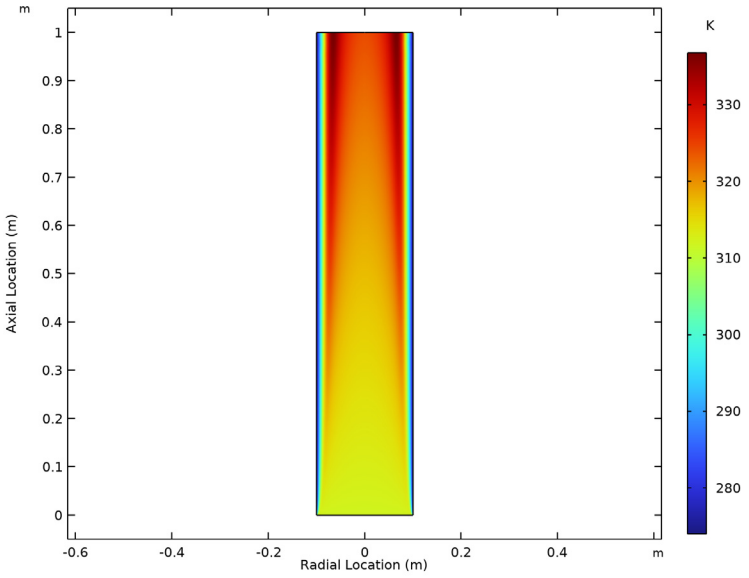

Figure 2: Temperature in the reactor.

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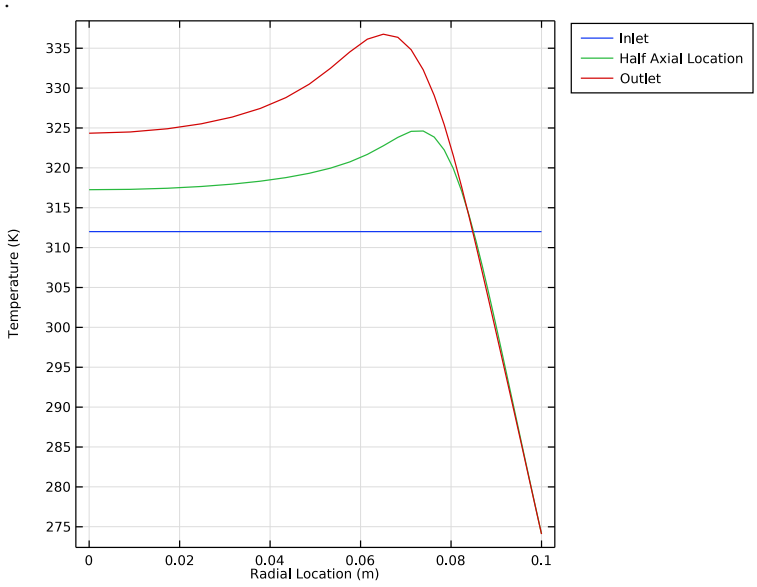


Figure 3: Radial temperature profiles.

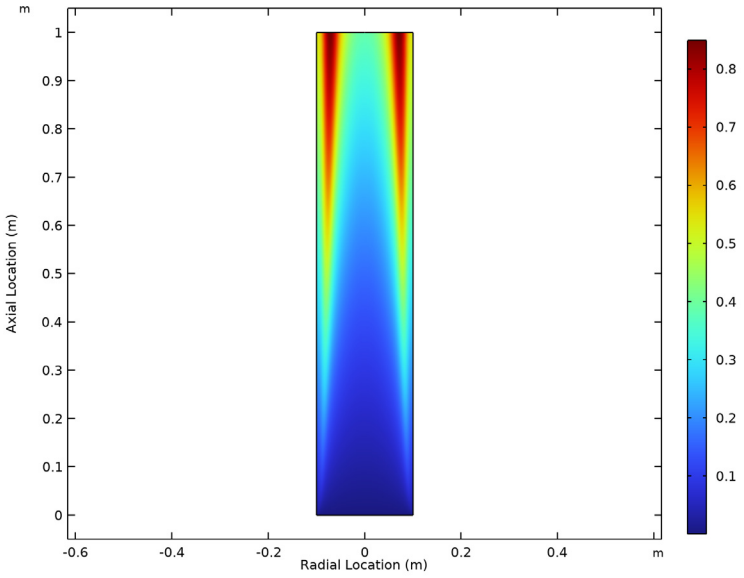


Figure 4: Conversion of propylene oxide in the reactor.

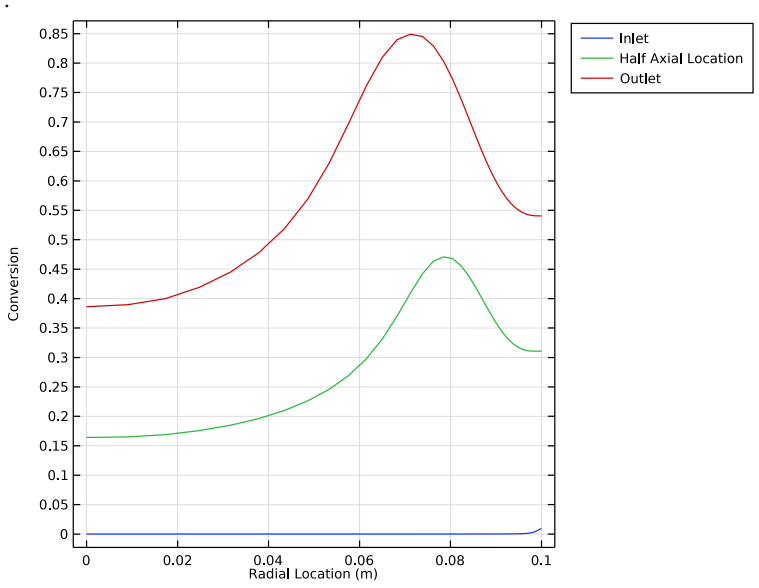


Figure 5: Radial conversion profiles for propylene oxide.

Exercises

Some example exercises below can easily be performed with the model to understand the system better.

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. Add more reacting components, for example, a side reaction to the Chemistry interface. How will this affect the results?
4. Use more complicated reaction kinetics. The reaction can be shifted to a second order reversible reaction.

References

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: `Chemical_Reaction_Engineering_Module/Tutorials/multicomponent_tubular_reactor`

Modeling Instructions

Starting **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 should 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>Chemistry (chem)**.

   This interface can be used to calculate reaction kinetics and thermal- and mass transport properties.

3 Click **Add**.

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

This sets up the required mass balance equation for propylene oxide and propylene glycol. Water is a solvent and is not accounted for here.

5 Click **Add**.

6 In the **Number of species** text field, type 2.

7 In the **Concentrations** table, enter the following settings:

cpoxide
cpglycol

`cpoxide` and `cpglycol` are the dependent variable names, where p stands for propylene.

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

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

9 Click **Add**.

Also, set up the **Laminar Flow** interface to describe the fluid flow in the reactor.

1 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

2 Click **Add**.

3 Click **Study**.

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

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

5 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Start by adding the **Parameters**. You can type in constant names and their values in the **Parameters** dialog. 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.

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 `multicomponent_tubular_reactor_parameters.txt`.

GEOMETRY 1

Now, move on to define the reactor geometry. In **2D axisymmetry**, the representation of the tubular reactor is reduced to a simple rectangle.

Rectangle 1 (r1)

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.

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

2 In the **Width** text field, type `Ra`.

3 In the **Height** text field, type `L`.

4 Click **Build All Objects**.

Add a variable computing the conversion of propylene oxide.

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`Xpoxide`	`(cpoxide0-cpoxide)/cpoxide0`		`Conversion of propylene oxide`

Select the mixture type and enable transport mixture properties to be computed.

CHEMISTRY (CHEM)

First the reaction kinetics and mixture properties will be set up, this is done in the **Chemistry** interface.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Model Input** section.

3 From the T list, choose **Temperature (ht)**.

4 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

5 Click to expand the **Calculate Transport Properties** section.

Reaction 1

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

The reaction is irreversible and contains three species: propylene oxide (poxide), water and propylene glycol (pglycol).

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `poxide+H2O=>pglycol`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the r_j text field, type `chem.kf_1*chem.c_poxide`.

7 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

Define the reaction expression and use the in-built Arrhenius expression for calculation of the reaction rate constant.

8 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

9 In the A^{f} text field, type `A`.

10 In the E^{f} text field, type `E`.

11 Locate the **Reaction Thermodynamic Properties** section. From the **Heat source of reaction** list, choose **User defined**.

12 In the Q text field, type `-chem.r_1*dHrx`.

Under each species, their respective chemical formulas can be entered. Entering a chemical formula gives the species' molar mass and enables balancing the reaction.

Species: poxide

1 In the **Model Builder** window, click **Species: poxide**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Select the **Enable formula** check box.

4 In the text field, type `C3H6O`.

5 In the ρ text field, type `rho_poxide`.

Species: H2O

Since the species' name (H2O) is a chemical formula, the chemical formula field is already filled in. As a result, so is the molar mass.

1 In the **Model Builder** window, click **Species: H2O**.

2 In the **Settings** window for **Species**, locate the **Type** section.

3 From the list, choose **Solvent**.

4 Locate the **Chemical Formula** section. In the ρ text field, type `rho_H2O`.

5 Click to expand the **Transport Expressions** section. In the k text field, type `ke`.

6 Click to expand the **Thermodynamic Expressions** section. From the list, choose **User defined**.

7 In the C_p text field, type `cpm_H2O`.

Species: pglycol

1 In the **Model Builder** window, click **Species: pglycol**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Select the **Enable formula** check box.

4 In the text field, type `C3H8O2`.

5 In the ρ text field, type `rho_pglycol`.

1: poxide+H2O=>pglycol

1 In the **Model Builder** window, under **Component 1 (comp1)>Chemistry (chem)** click **1: poxide+H2O=>pglycol**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 Click **Balance** in the upper-right corner of the section.

As can be seen, no coefficients appeared in front of any of the species when balancing the reaction, which means that 1 mole of propylene oxide and water is needed to form 1 mole of propylene glycol.

4 In the **Model Builder** window, click **Chemistry (chem)**.

5 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

6 From the **Species solved for** list, choose **Transport of Diluted Species**.

7 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)
H2O	Solvent	User defined	cH2O0
pglycol	Variable	cpglycol	Solved for
poxide	Variable	cpoxide	Solved for

8 Locate the **Calculate Transport Properties** section. In the μ_{ref} text field, type `myref_H2O`.

9 In the T_{ref} text field, type `Tref_my`.

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 propylene oxide and propylene glycol. As you click the **Transport of Diluted Species** node the **Equation** section of the **Settings** window will tell you which equations that are being solved for. The **Domain Selection** 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 Mechanisms** section. This can be done at any time in the modeling process.

Moving on to the **Transport Properties** node, you are expected to provide diffusivity of propylene oxide and propylene glycol. The variable names you type in have previously been defined in the **Variables** and **Parameters** lists. Here, it is also possible to couple the interface to other interfaces. In this example, you instead use the **Multiphysics** node to do this.

Transport Properties 1

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

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 In the D_{cpoxide} text field, type `chem.D_poxide`.

4 In the D_{cpglycol} text field, type `chem.D_pglycol`.

Reactions 1

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

The reaction rates are selected from the **Chemistry** interface.

1 Select Domain 1 only.

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

3 From the R_{cpoxide} list, choose **Reaction rate for species poxide (chem)**.

4 From the R_{cpglycol} list, choose **Reaction rate for species pglycol (chem)**.

Inflow 1

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

2 Select Boundary 2 only.

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

4 In the $c_{0,\text{cpoxide}}$ text field, type `cpoxide0`.

Selecting the Danckwerts boundary condition is a manner to speed up the computation and improve the solution.

5 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

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 $-n*Dgrad(c)=0$, that is, the transport of mass across the boundary is dominated by convection. Note that the mathematical representation of the boundary conditions are displayed in the **Equation** 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 propylene oxide and propylene glycol. Now, move on to set up the **Heat Transfer in Fluids** interface.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

The **Heat Transfer in Fluids** feature asks for the thermal conductivity, density, and heat capacity of the fluid mixture. These are taken from the **Chemistry** interface.

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 Conduction, Fluid** section.

3 From the k list, choose **Thermal conductivity (chem)**.

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

5 From the ρ list, choose **Density (chem)**.

6 From the C_p list, choose **Heat capacity at constant pressure (chem)**.

7 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 as defined in the **Chemistry** interface to the heat balance.

2 Select Domain 1 only.

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

4 From the Q_0 list, choose **Heat source of reactions (chem)**.

Next, add the boundary conditions specifying a temperature at the inlet, the heat flux between 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 From the **Flux type** list, choose **Convective heat flux**.

5 In the h text field, type `Uk`.

6 In the T_{ext} text field, type `Ta0`.

Outflow 1

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

2 Select Boundary 3 only.

Now, move on to the **Laminar Flow** interface.

LAMINAR FLOW (SPF)

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties 1**.

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

3 From the ρ list, choose **Density (chem)**.

4 From the μ list, choose **Dynamic viscosity (chem)**.

Assume that the flow has a **Laminar Flow** pattern as it enters the reactor.

Inlet 1

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

2 Select Boundary 2 only.

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

4 From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type u0.

Outlet 1

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

2 Select Boundary 3 only.

Last, couple the interfaces with the **Multiphysics** node.

MULTIPHYSICS

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain> Nonisothermal Flow**.

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

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 partial 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 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** check box.

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`.

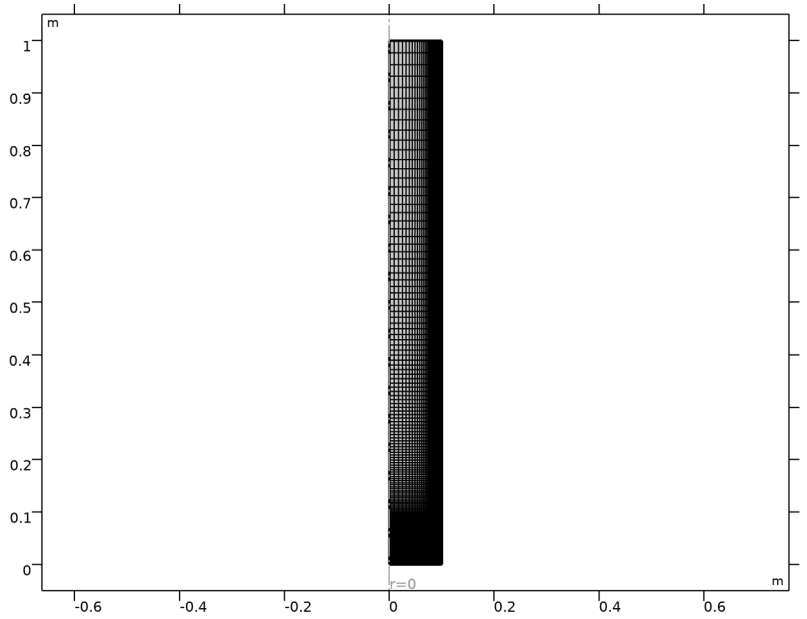
6 In the **Element ratio** text field, type `0.01`.

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

8 Select the **Reverse direction** check box.

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

The figure below shows the created mesh.



STUDY 1

Solve the model.

1 In the **Home** toolbar, click **Compute**.

The following instructions produce Figure 2 through Figure 5.

Two of these 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** check box.

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

Mirror 2D 1

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

2 In the **Settings** window for **Mirror 2D**, click to expand the **Advanced** section.

3 Select the **Remove elements on the symmetry axis** check box.

This setting removes the symmetry axis in the figure and makes the resulting plots look cleaner.

4 Click **Plot**.

Start with the **Mirror 2D** plots. Proceed as follows to create a mirrored temperature 2D plot (Figure 2).

Temperature, surface (mirrored)

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

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

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

4 In the **Label** text field, type `Temperature, surface (mirrored)`.

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Color Legend** section. Select the **Show units** check box.

7 Locate the **Plot Settings** section.

8 Select the **x-axis label** check box. In the associated text field, type `Radial Location (m)`.

9 Select the **y-axis label** check box. In the associated text field, type `Axial Location (m)`.

Surface 1

1 Right-click **Temperature, surface (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, surface (mirrored)** toolbar, click **Plot**.

Duplicate the **Temperature, surface** Mirror 2D plot to make the Conversion, surface Mirror 2D plot, Figure 4.

Conversion, surface (mirrored)

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

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

Surface 1

1 In the **Model Builder** window, expand the **Conversion, surface (mirrored)** 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>Xpoxide - Conversion of propylene oxide**.

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

4 In the **Conversion, surface (mirrored)** toolbar, click  **Plot**.

Temperature, profiles

In the **Home** toolbar, click  **Add Plot Group** and choose **1D Plot Group**.

Continue with the **Cut Line 2D** plots. First create the temperature plot with a **1D Plot Group** with a **Line Graph**, Figure 3.

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

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

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** check box. In the associated text field, type `Radial Location (m)`.

6 Select the **y-axis label** check box. In the associated text field, type `Temperature (K)`.

7 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Line Graph 1

1 Right-click **Temperature, profiles** 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 **Solid**.

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

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

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

7 In the table, enter the following settings:

Legends
Inlet
Half Axial Location
Outlet

8 In the **Temperature, profiles** toolbar, click **Plot**.

Duplicate the **Temperature, profile** Cut Line 2D plot to create a `Conversion, profile Cut Line 2D plot`, Figure 5.

Conversion, profiles

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

2 In the **Settings** window for **1D Plot Group**, type `Conversion, profiles` 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, profiles** 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>Xpoxide - Conversion of propylene oxide**.

3 In the **Conversion, profiles** toolbar, click **Plot**.