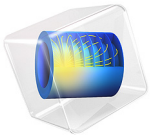

Optimal Cooling of a Tubular Reactor

This model is licensed under the COMSOL Software License Agreement 6.1.
All trademarks are the property of their respective owners. See www.comsol.com/trademarks.

Introduction

Maximizing product yield is a main task in chemical reaction engineering. This can be especially challenging if the desired product, once formed, can be consumed by further reactions. The following example investigates such a series reaction as it occurs in a tubular reactor. This starts by setting up the tightly coupled mass and energy balance equations describing the reactor applying predefined physics interfaces within the Chemical Reaction Engineering Module. This is followed by the addition of an Optimization Study node to compute the temperature conditions in the reactor that maximize the production of the intermediary product.

Note: This application requires the Optimization Module.

Model Definition

Two consecutive reactions take place in a tubular reactor. A heat exchanger jacket, run in cocurrent mode, is used to control the reaction rates and hence the product distribution in the reactor. The setup is shown in Figure 1.

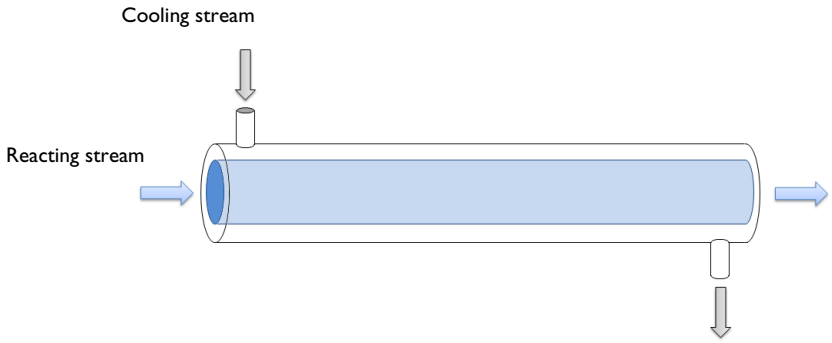

Figure 1: Reactions occur in a tubular reactor equipped with a heat exchanger jacket, run in cocurrent mode.

Temperature control in the reactor involves a delicate balance, where on the one hand, energy has to be supplied to the system to achieve acceptable reaction rates. On the other hand, the energy transfer to the reacting stream must be limited so that the desired intermediate product is not consumed by further reaction. The situation is further complicated by the fact that the temperature of the reacting stream is not only affected by

the heat transfer from the heat exchanger jacket, but also by the endothermic nature of the reactions. The idea for this challenge in reactor optimization is taken from a literature example (Ref. 1), although the present reactor model is considerably more detailed.

The model is set up in 1D, coupling mass and energy balances in the reactor tube with an energy balance for the heat exchanger jacket. Streams in both the tube and jacket are treated as plug flows.

CHEMISTRY

Two consecutive reaction occur in water (hydrolysis), where the desired product is species B:

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B}$$

$$\mathrm{B} \xrightarrow{k_2} \mathrm{C}$$

The following rate equations apply:

$$r_1 = k_1 c_A$$

$$r_2 = k_2 c_B$$

where the rate constants are temperature dependent according to the Arrhenius relation:

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T}\right)$$

The kinetic parameters are summarized in the table below:

J	AJ [1/S]	EJ [J/MOL]
1	1.6e8	75e3
2	1e15	125e3

MASS TRANSPORT

The mass transport is modeled by the convection-diffusion equation at steady-state using the Transport of Diluted Species interface:

$$\nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i$$

In this equation, c_i denotes the concentration (SI unit: mol/m^3) and D_i is the diffusivity (SI unit: m^2 /s). R_i is the rate expression for species i (SI unit: mol/(m^3·s)). The velocity $\mathbf{u}$ (SI unit: m/s) of the fluid in the reactor is represented by a constant profile:

$$\mathbf{u} = 0.0042 \text{ m/s}$$

At the inlet, the concentration of the reactant A is 700 mol/m^3. At the outlet, it is assumed that convective mass transport is dominant:

$$\nabla \cdot (-D_i \nabla c_i) = 0$$

ENERGY TRANSPORT - REACTOR

The energy transport in the reactor is modeled with the Heat Transfer in Fluids interface in which the following equation is solved:

$$\nabla \cdot (-k\nabla T) + \rho C_p \mathbf{u} \cdot \nabla T = Q_{\text{rxn}} + Q_j$$

Above, k is the thermal conductivity (SI unit: W/(m·K)) and T the temperature of the reacting stream (SI unit: K). ρ is the density (SI unit: kg/m_3) and C_p the heat capacity (SI unit: J/(kg·K)). The reacting species are diluted in water, and hence, the physical properties of the reacting mixture are assumed to be those of water.

The heat source due to reaction, Q_{rxn} (SI unit: W/m^3), is calculated from the reaction rates and the enthalpies of reaction:

$$Q_{rxn} = \sum_{j=1-2} -\Delta H_j r_j$$

Both reactions are endothermic, with ΔH_1 = 200 kJ/mol and ΔH_2 = 100 kJ/mol. Furthermore, the heat transferred from the reactor to the cooling jacket is given by:

$$Q_j = -UA(T - T_j)$$

Here, U is the overall heat transfer coefficient (SI unit: J/(K·m^2·s)), and A represents the heat exchange area per unit volume (SI unit: m^2/m^3).

The temperature of the reacting fluid at the inlet is 400 K. At the outlet, it is assumed that convective heat transport is dominant:

$$\nabla \cdot (-k\nabla T) = 0$$

ENERGY TRANSPORT - COOLING JACKET

Water serves as the cooling medium in the jacket, and the energy transport is given by the following equation, which is set up and solved with the Heat Transfer in Fluids interface:

$$\nabla \cdot (-k\nabla T_j) + \rho C_p \mathbf{u}_j \cdot \nabla T = -Q_j$$

The cooling stream is assumed to have plug flow character, and hence a constant velocity profile:

$$\mathbf{u}_j = 0.001 \text{ m/s}$$

The optimal temperature of the cooling fluid at the inlet is to be found such that the maximum concentration of species B is achieved at the outlet.

Results and Discussion

In a first simulation, the inlet temperatures of the jacket stream and the reacting stream are set to be equal, at 400 K. In a second simulation, an optimization calculation is performed to find the inlet temperature of the jacket stream that maximizes the concentration of the desired intermediary product (B) at the reactor outlet. Comparisons between the two cases follow below.

Figure 2 shows the concentration of reacting species as a function of the reactor length when the inlet temperature of the jacket stream is 400 K. Figure 3 shows concentration curves for the optimal inlet temperature of the jacket stream, found to be 335 K. Clearly, when the inlet temperature is 400 K the conversion of reactant A is high, but at the same time, the selectivity for the desired product B is unfavorable. Under the optimized conditions, the concentration of B at the reactor outlet is 352 mol/m^3, to be compared to a concentration of 153 mol/m^3 when the inlet temperature is 400 K.

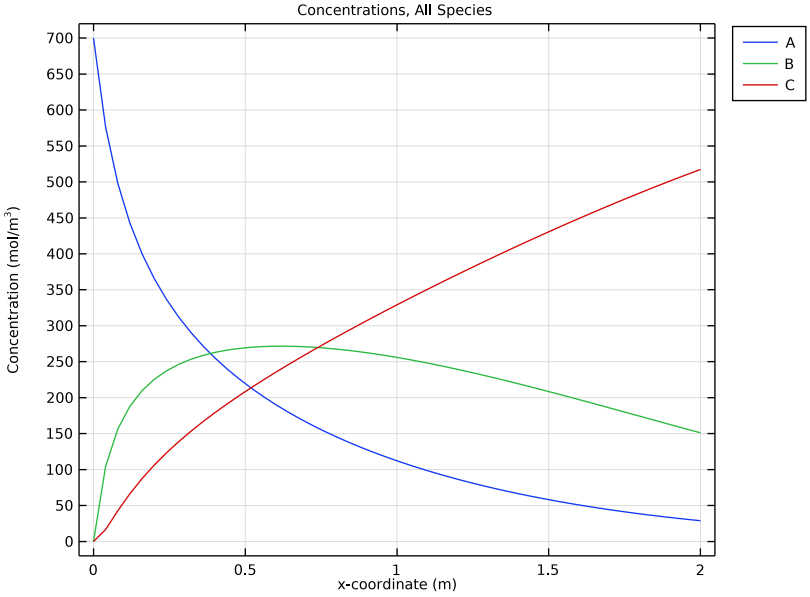

Figure 2: Species concentrations (blue c_A, green c_B, red c_C) as function of reactor position when the inlet temperature of the cooling fluid is 400 K.

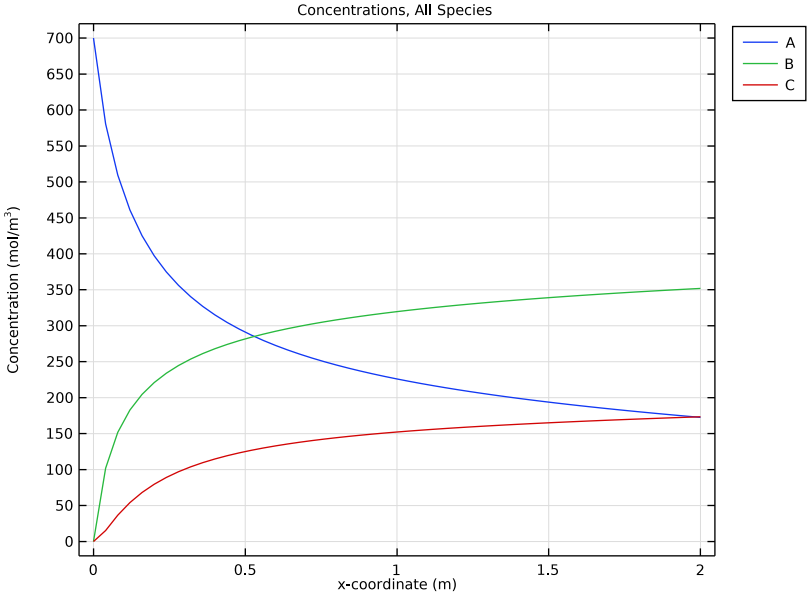

Figure 3: Species concentrations (blue c_A, green c_B, red c_C) as function of reactor position when the inlet temperature of the cooling fluid is 335 K.

Plots of reacting stream and jacket stream temperatures are shown in Figure 4 and Figure 5. The jacket stream heats up the reacting stream when its inlet temperature is kept at 400 K.

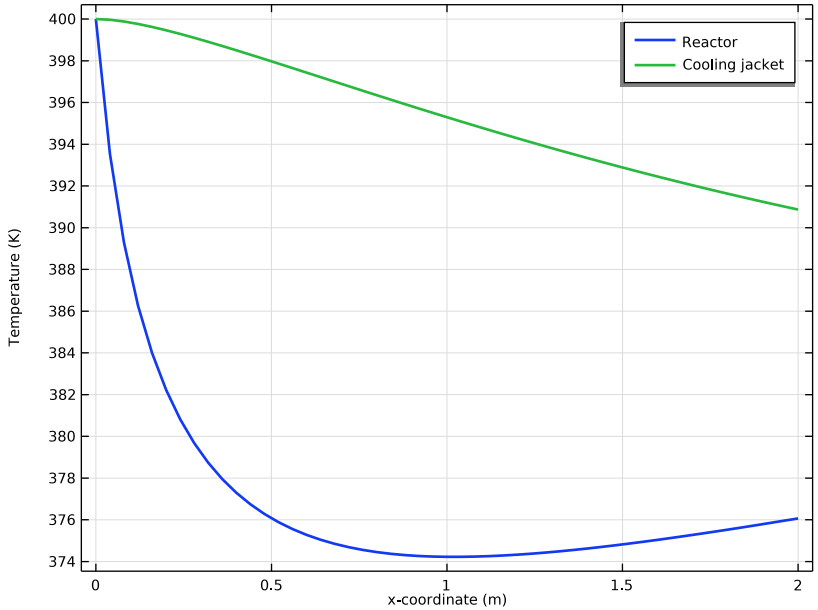

Figure 4: Temperature distribution for the reacting stream (blue) and jacket stream (green) when the inlet temperature of the jacket stream is 400 K.

In contrast, the jacket stream cools the reacting stream when its inlet temperature is 334 K.

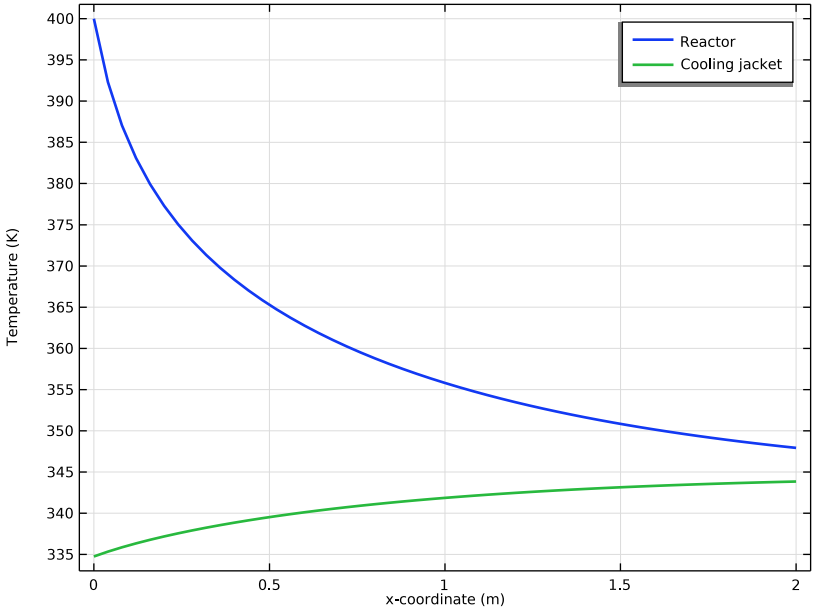

Figure 5: Temperature distribution for the reacting stream (blue) and jacket stream (green) when the inlet temperature of the jacket stream is 334 K.

The reaction rates are illustrated in Figure 6 and Figure 7. When the inlet temperature of the jacket stream is 400 K, the rate at which B is consumed (r_2) dominates over the production rate (r_1) from a point approximately 0.65 m down the reactor. This effect is

due to heat being transferred from the jacket stream, counteracting the cooling effect of the endothermic reactions.

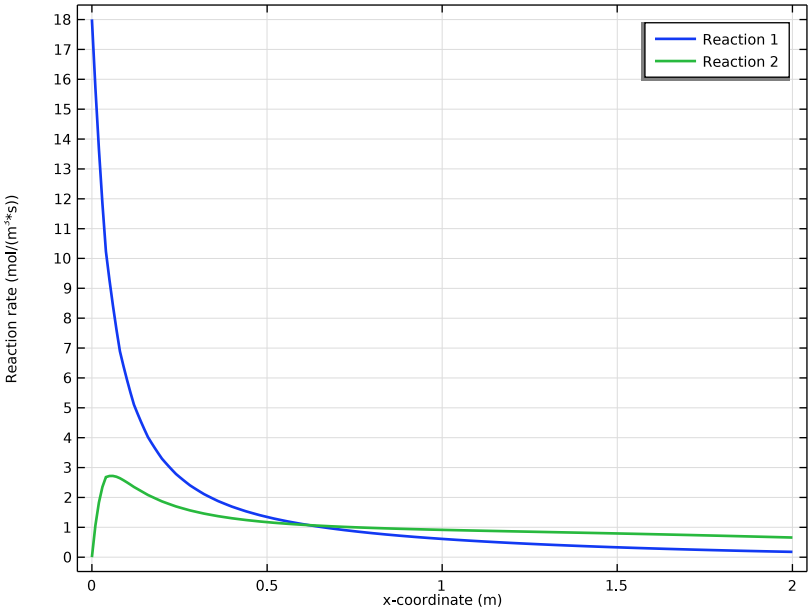

Figure 6: Rate of the production r_1 (blue) and rate consumption r_2 (green) of species B when the inlet temperature of the cooling fluid is 400 K.

At an inlet temperature of 334 K, the combined effect of cooling by the jacket stream and energy consumption due to reaction work together to quench the system, resulting in increased concentrations levels of B at the outlet.

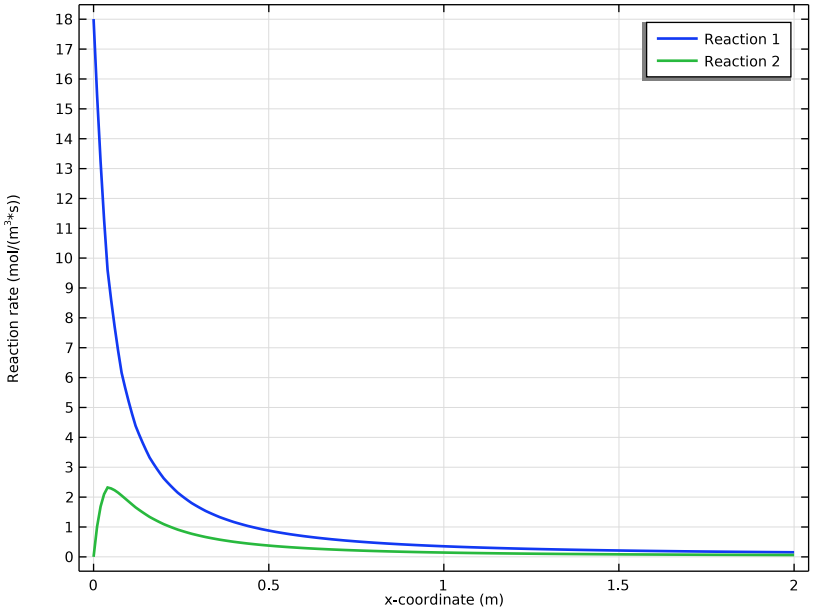

Figure 7: Rate of the production r_1 (blue) and rate consumption r_2 (green) of species B when the inlet temperature of the cooling fluid is 335 K.

Reference

1. T.F. Edgar and D.M. Himmelblau, *Optimization of Chemical Processes*, McGraw-Hill, 1988.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/optimal_cooling`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Chemical Species Transport>Chemistry (chem)**.

3 Click **Add**.

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

5 Click **Add**.

6 In the **Number of species** text field, type 3.

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

cA
cB
cC

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

9 Click **Add**.

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

11 Click **Add**.

12 In the **Temperature** text field, type `Tj`.

13 Click **Study**.

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

15 Click **Done**.

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 `optimal_cooling_parameters.txt`.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
L_r

4 Click **Build Selected**.

DEFINITIONS

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 2 only.

Variables 1

1 In the **Definitions** toolbar, click **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
cB_out	intop1(cB)	mol/m³	Outlet concentration

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Liquids and Gases>Liquids>Water**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

CHEMISTRY (CHEM)

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 Click to expand the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

Reaction 1

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

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

3 In the **Formula** text field, type `A=>B`.

4 Click **Apply**.

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

6 In the A^{f} text field, type `A1`.

7 In the E^{f} text field, type `E1`.

8 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

9 In the H text field, type `H1`.

Reaction 2

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

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

3 In the **Formula** text field, type `B=>C`.

4 Click **Apply**.

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

6 In the A^{f} text field, type `A2`.

7 In the E^{f} text field, type `E2`.

8 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

9 In the H text field, type `H2`.

Species: C

As for B, species C does not correspond to carbon and it is therefore necessary to clear the box in **Enable formula**

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

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

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

4 In the M text field, type `Mn_C`.

Species 1

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

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

3 In the text field, type `H2O`.

4 Click **Apply**.

5 Locate the **Type** section. From the list, choose **Solvent**.

6 Locate the **Chemical Formula** section. In the M text field, type `Mn_H2O`.

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

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

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

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

Species	Type	Molar concentration	Value (mol/m^3)
A	Variable	cA	Solved for
B	Variable	cB	Solved for
C	Variable	cC	Solved for
H2O	Solvent	User defined	`c_solv`

TRANSPORT OF DILUTED SPECIES (TDS)

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 **Convection** section.

3 Set the x-component of $\mathbf{u}$ to `u`.

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

5 In the D_{cB} text field, type `D`.

6 In the D_{cC} text field, type `D`.

Inflow 1

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

2 Select Boundary 1 only.

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

4 In the $c_{0,cA}$ text field, type `cA_in`.

Outflow 1

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

2 Select Boundary 2 only.

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 From the R_{cA} list, choose **Reaction rate for species A (chem)**.

5 From the R_{cB} list, choose **Reaction rate for species B (chem)**.

6 From the R_{cC} list, choose **Reaction rate for species C (chem)**.

HEAT TRANSFER IN FLUIDS - REACTOR

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

2 In the **Settings** window for **Heat Transfer in Fluids**, type `Heat Transfer in Fluids - Reactor` in the **Label** text field.

Fluid 1

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

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

3 Set the x-component of $\mathbf{u}$ to `u`.

Temperature 1

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

2 Select Boundary 1 only.

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

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

Outflow 1

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

2 Select Boundary 2 only.

Heat Source 1

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

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 `-UA*(T-Tj)+chem.Qtot`.

HEAT TRANSFER IN FLUIDS - COOLING JACKET

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Fluids 2 (ht2)**.

2 In the **Settings** window for **Heat Transfer in Fluids**, type `Heat Transfer in Fluids - Cooling jacket` in the **Label** text field.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids - Cooling jacket (ht2)** click **Fluid 1**.

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

3 Set the x-component of $\mathbf{u}$ to `uj`.

Temperature 1

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

2 Select Boundary 1 only.

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

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

Outflow 1

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

2 Select Boundary 2 only.

Heat Source 1

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

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 `UA*(T-Tj)`.

MESH 1

Edge 1

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

Size

1 In the **Model Builder** window, click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

4 Click **Build All**.

STUDY 1

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

RESULTS

Concentrations, All Species (tds)

Go through the steps below to save a copy of the solution where the coolant temperature is 400 K at the inlet.

STUDY 1

Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.

2 Right-click **Solution 1 (sol1)** and choose **Solution>Copy**.

Tj_in=400K

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Solution 1 - Copy 1 (sol2)**.

2 In the **Settings** window for **Solution**, type `Tj_in=400K` in the **Label** text field.

RESULTS

Concentrations for Tj_in=400K

1 In the **Model Builder** window, under **Results** click **Concentrations, All Species (tds)**.

2 In the **Settings** window for **1D Plot Group**, type `Concentrations for Tj_in=400K` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Tj_in=400K (sol2)**.

4 Locate the **Plot Settings** section.

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

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

7 In the **Concentrations for Tj_in=400K** toolbar, click **Plot**.

Temperature for Tj_in=400K

1 In the **Model Builder** window, under **Results** click **Temperature (ht)**.

2 In the **Settings** window for **1D Plot Group**, type `Temperature for Tj_in=400K` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Tj_in=400K (sol2)**.

Reactor

1 In the **Model Builder** window, expand the **Temperature for Tj_in=400K** node, then click **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Reactor` in the **Label** text field.

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

4 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

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
Reactor

Cooling jacket

1 Right-click **Reactor** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Cooling jacket` in the **Label** text field.

3 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 - Cooling jacket> Temperature>Tj - Temperature - K**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Cooling jacket

5 In the **Temperature for Tj_in=400K** toolbar, click **Plot**.

Production Rates for Tj_in=400K

1 In the **Model Builder** window, under **Results** click **Temperature (ht2)**.

2 In the **Settings** window for **1D Plot Group**, type `Production Rates for Tj_in=400K` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Tj_in=400K (sol2)**.

Reaction 1

1 In the **Model Builder** window, expand the **Production Rates for Tj_in=400K** node, then click **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Reaction 1` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Chemistry>chem.r_1 - Reaction rate - mol/(m³·s)**.

5 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

6 Locate the **Legends** section. Select the **Show legends** check box.

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

8 In the table, enter the following settings:

Legends
Reaction 1

Reaction 2

1 Right-click **Reaction 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Reaction 2` in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Chemistry>chem.r_2 - Reaction rate - mol/(m³·s)**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Reaction 2

5 In the **Production Rates for Tj_in=400K** toolbar, click **Plot**.

Now, solve the optimization problem.

STUDY 1

Optimization

1 In the **Study** toolbar, click **Optimization** and choose **Optimization**.

2 In the **Settings** window for **Optimization**, locate the **Optimization Solver** section.

3 From the **Method** list, choose **BOBYQA**.

4 Locate the **Objective Function** section. In the table, enter the following settings:

Expression	Description	Evaluate for
`comp1.cB_out`	`Outlet concentration`	Stationary

5 From the **Type** list, choose **Maximization**.

6 Locate the **Control Variables and Parameters** section. Click **Add**.

7 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
Tj_in (Inlet temperature, jacket)	`400[K]`	`400[K]`		

Prescribing scales for the estimation parameters increases the efficiency of the optimization procedure. A good starting point is to use scales of the same order as the initial values.

8 In the **Model Builder** window, click **Study 1**.

9 In the **Settings** window for **Study**, locate the **Study Settings** section.

10 Clear the **Generate default plots** check box.

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

RESULTS

Concentrations for Optimized Tj_in

1 In the **Model Builder** window, right-click **Concentrations for Tj_in=400K** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 In the **Concentrations for Optimized Tj_in** toolbar, click **Plot**.

Temperature Tj_in for Optimized Tj_in

1 In the **Model Builder** window, right-click **Temperature for Tj_in=400K** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 In the **Temperature Tj_in for Optimized Tj_in** toolbar, click **Plot**.

Production Rates for Optimized Tj_in

1 In the **Model Builder** window, right-click **Production Rates for Tj_in=400K** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Production Rates for Optimized Tj_in` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 In the **Production Rates for Optimized Tj_in** toolbar, click **Plot**.

RESULTS

Objective Table 2

Scroll down the table to find the resulting values of the inlet temperature.