

# Optimal Cooling of a Tubular Reactor

## *Introduction*

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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. This example investigates such a series reaction as it occurs in a tubular reactor. You will start by setting up the tightly coupled mass and energy balance equations describing the reactor applying predefined physics interfaces of the Chemical Reaction Engineering Module. In a second step, you add an Optimization Study node to calculate the temperature conditions the reactor that maximize the production of the intermediary product.

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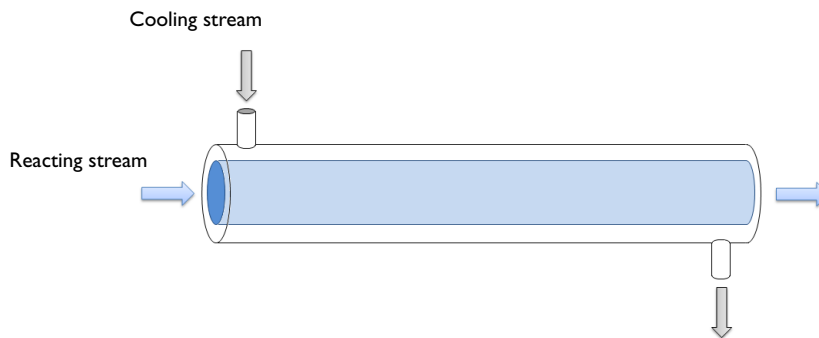
**Note:** This model requires the Optimization Module.

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## *Model Definition*

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Two consecutive reactions take place in a tubular reactor. A heat exchanger jacket, run in co-current mode, is used to control the reaction rates and hence the product distribution in the reactor.



*Figure 1: Reactions occur in a tubular reactor equipped with a heat exchanger jacket, run in co-current mode.*

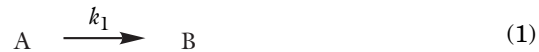
Temperature control in the reactor involves a delicate balance, where on the one hand, energy has to be supplied to the system to achieve acceptable reaction rates. On the

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, where the desired product is species B:



The following rate equations apply:

$$r_1 = k_1 c_A \quad (3)$$

$$r_2 = k_2 c_B \quad (4)$$

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

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T}\right) \quad (5)$$

The kinetic parameters are summarized in the table below:

J	A <sub>J</sub> [1/S]	E <sub>J</sub> [J/MOL]
1	1.6e8	75e3
2	1e15	125e3

### MASS TRANSPORT

The mass transport is modeled by the convection-diffusion equation at steady-state:

$$\nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \quad (6)$$

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

$$\mathbf{u} = 0.0042 \text{ m/s} \quad (7)$$

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

$$\nabla \cdot (-D_i \nabla c_i) = 0 \quad (8)$$

### ENERGY TRANSPORT - REACTOR

The energy transport in the reactor is described by:

$$\nabla \cdot (-k \nabla T) + \rho C_p \mathbf{u} \cdot \nabla T = Q_{rxn} + Q_j \quad (9)$$

Above,  $k$  is the thermal conductivity (W/(m·K)) and  $T$  the temperature of the reacting stream (K).  $\rho$  is the density (kg/m<sup>3</sup>) and  $C_p$  the heat capacity (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,  $Q_{rxn}$  (W/m<sup>3</sup>), is calculated from the reaction rates and the enthalpies of reaction:

$$Q_{rxn} = \sum_{j=1-2} -\Delta H_j r_j \quad (10)$$

Both of the reactions are endothermic, with  $\Delta H_1 = 200$  kJ/mol and  $\Delta H_2 = 100$  kJ/mol. Furthermore, the heat transferred from the reactor to the cooling jacket is given by:

$$Q_j = -UA(T - T_j) \quad (11)$$

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

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

$$\nabla \cdot (-k \nabla T) = 0 \quad (12)$$

**ENERGY TRANSPORT - COOLING JACKET**

Water serves as the cooling medium in the jacket, and the energy transport is given by

$$\nabla \cdot (-k \nabla T_j) + \rho C_p \mathbf{u}_j \cdot \nabla T = -\dot{Q}_j \quad (13)$$

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

$$\mathbf{u}_j = 0.001 \text{ m/s} \quad (14)$$

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 336 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  $355 \text{ mol/m}^3$ , to be compared to a concentration of  $159 \text{ mol/m}^3$  when the inlet temperature is 400 K.

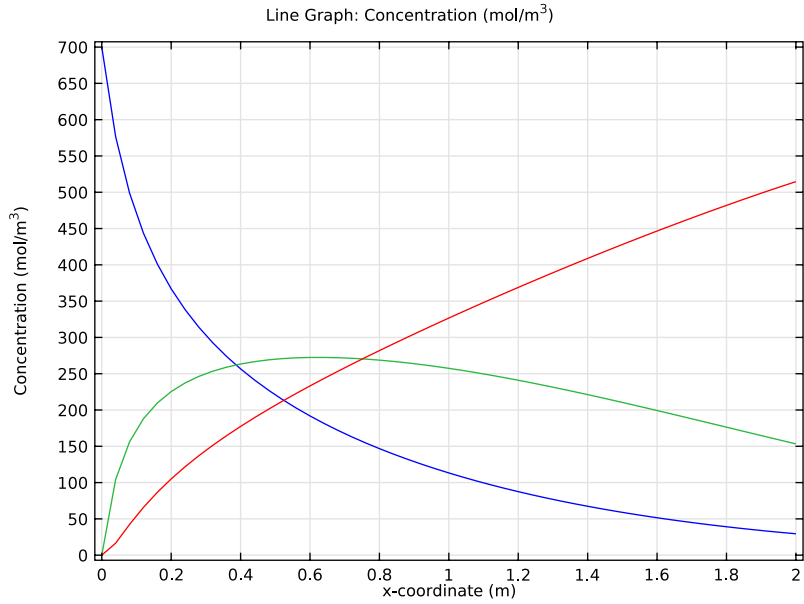


Figure 2: Species concentrations (blue  $c_A$ , green  $c_B$ , red  $c_C$ ) as function of reactor position when the inlet temperature of the cooling fluid is 400 K.

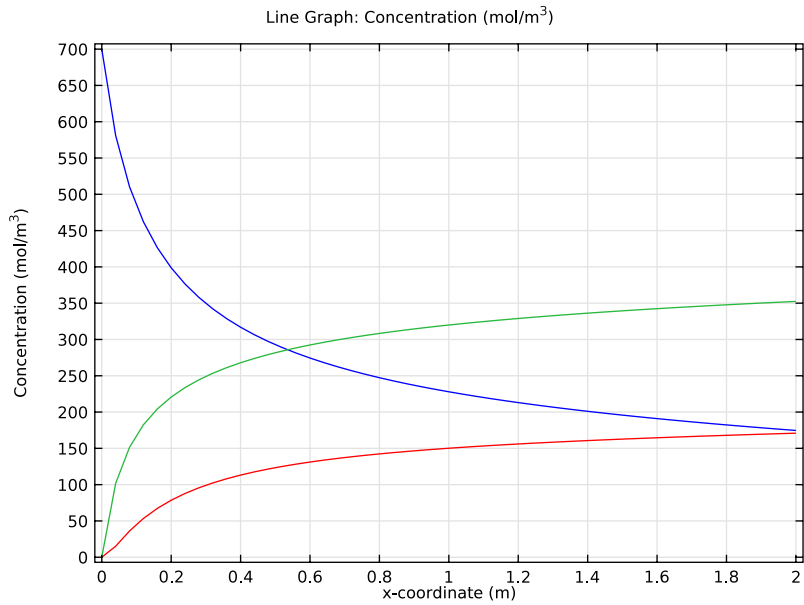


Figure 3: Species concentrations (blue  $c_A$ , green  $c_B$ , red  $c_C$ ) as function of reactor position when the inlet temperature of the cooling fluid is 336 K.

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.

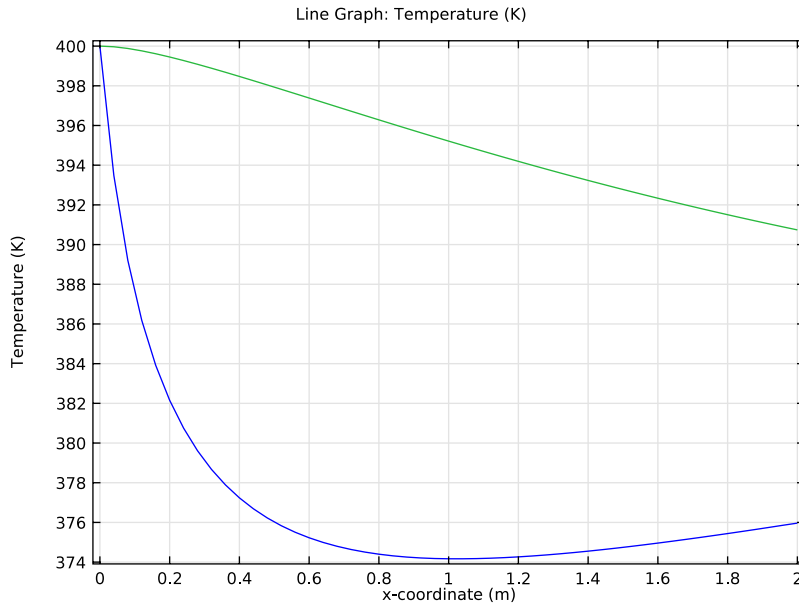


Figure 4: Temperature distribution for the reacting stream (blue) and jacket stream (green) when the inlet temperature of the jacket stream is 400 K.

In contrast, the jacket stream cools the reacting stream when its inlet temperature is 336 K.

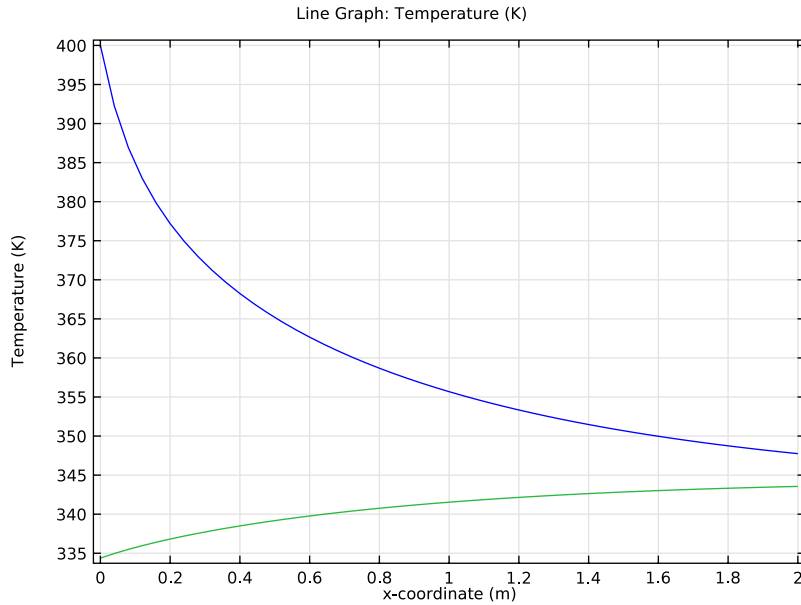


Figure 5: Temperature distribution for the reacting stream (blue) and jacket stream (green) when the inlet temperature of the jacket stream is 336 K.

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 endothermal reactions.

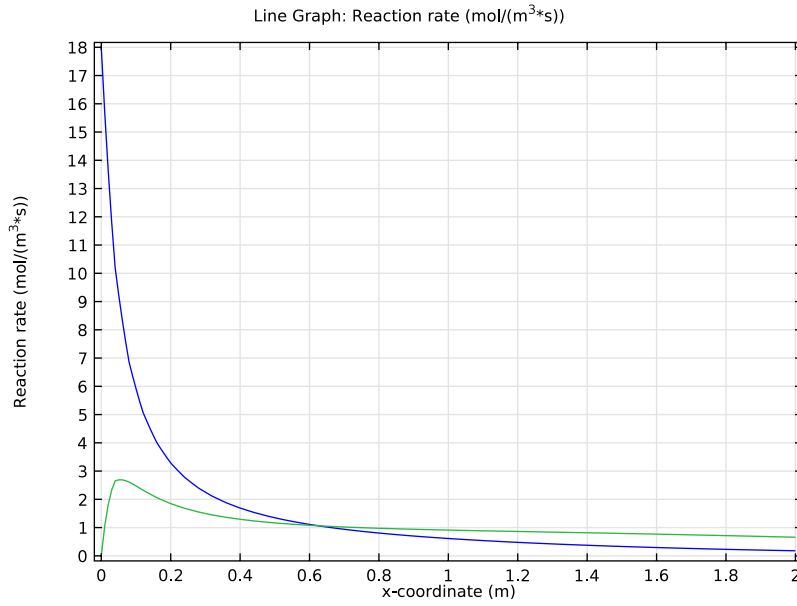


Figure 6: Rate of the production  $r_1$  (blue) and rate consumption  $r_2$  (green) of species B when the inlet temperature of the cooling fluid is 400 K.



At an inlet temperature of 336 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.

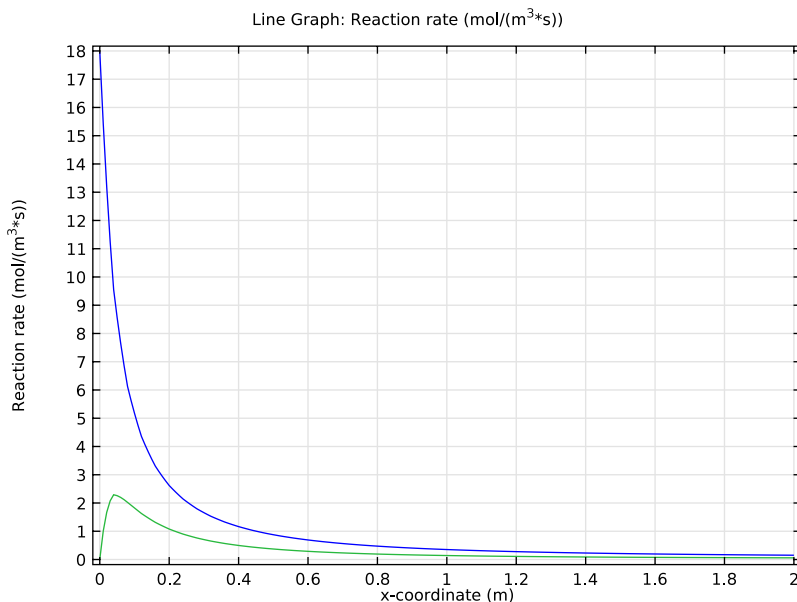


Figure 7: Rate of the production  $r_1$  (blue) and rate consumption  $r_2$  (green) of species B when the inlet temperature of the cooling fluid is 336 K.

### Reference

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

**Model Library path:** Chemical\_Reaction\_Engineering\_Module/  
Optimization/optimal\_cooling

### Modeling Instructions

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

**NEW**

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

**MODEL WIZARD**

1 In the **Model Wizard** window, click the **ID** button.

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

3 Click the **Add** button.

4 In the **Number of species** edit field, type 3.

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

c_A
c_B
c_C

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

7 Click the **Add** button.

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

9 Click the **Add** button.

10 In the **Temperature** edit field, type  $T_j$ .

11 Click the **Study** button.

12 In the tree, select **Preset Studies for Selected Physics>Stationary**.

13 Click the **Done** button.

**GEOMETRY I***Interval I*

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

2 In the **Interval** settings window, locate the **Interval** section.

3 In the **Right endpoint** edit field, type 2.

4 Click the **Build Selected** button.

**GLOBAL DEFINITIONS***Parameters*

1 On the **Home** toolbar, click **Parameters**.

- 2 In the **Parameters** settings window, locate the **Parameters** section.
- 3 Click **Load from File**.
- 4 Browse to the model's Model Library folder and double-click the file `optimal_cooling_parameters.txt`.

#### *Variables 1*

- 1 In the **Model Builder** window, right-click **Global Definitions** and choose **Variables**.
- 2 In the **Variables** settings window, locate the **Variables** section.
- 3 Click **Load from File**.
- 4 Browse to the model's Model Library folder and double-click the file `optimal_cooling_variables.txt`.

### **DEFINITIONS**

#### *Integration 1*

- 1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.
- 2 In the **Integration** settings window, locate the **Source Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 2 only.

#### *Variables 2*

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Variables** settings window, locate the **Variables** section.
- 3 In the table, enter the following settings:

<b>Name</b>	<b>Expression</b>	<b>Unit</b>	<b>Description</b>
<code>c_B_out</code>	<code>intop1(c_B)</code>	<code>mol/m<sup>3</sup></code>	Outlet concentration

### **MATERIALS**

On the **Home** toolbar, click **Add Material**.

#### **ADD MATERIAL**

- 1 Go to the **Add Material** window.
- 2 In the tree, select **Liquids and Gases>Liquids>Water**.
- 3 In the **Add material** window, click **Add to Component**.

## TRANSPORT OF DILUTED SPECIES

### *Convection and Diffusion 1*

- 1 In the **Model Builder** window, expand the **Component 1**>**Transport of Diluted Species** node, then click **Convection and Diffusion 1**.
- 2 In the **Convection and Diffusion** settings window, locate the **Model Inputs** section.
- 3 Specify the **u** vector as

<b>u</b>	<b>x</b>
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- 4 Locate the **Diffusion** section. In the  $D_{cA}$  edit field, type D.
- 5 In the  $D_{cB}$  edit field, type D.
- 6 In the  $D_{cC}$  edit field, type D.

### *Inflow 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
- 2 Select Boundary 1 only.
- 3 In the **Inflow** settings window, locate the **Concentration** section.
- 4 In the  $c_{0,cA}$  edit field, type 700.

### *Outflow 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
- 2 Select Boundary 2 only.

### *Reactions 1*

- 1 On the **Physics** toolbar, click **Domains** and choose **Reactions**.
- 2 Select Domain 1 only.
- 3 In the **Reactions** settings window, locate the **Reactions** section.
- 4 In the  $R_{cA}$  edit field, type -r1.
- 5 In the  $R_{cB}$  edit field, type r1 - r2.
- 6 In the  $R_{cC}$  edit field, type r2.

## HEAT TRANSFER IN FLUIDS

### *Heat Transfer in Fluids 1*

- 1 In the **Model Builder** window, expand the **Component 1**>**Heat Transfer in Fluids** node, then click **Heat Transfer in Fluids 1**.
- 2 In the **Heat Transfer in Fluids** settings window, locate the **Model Inputs** section.

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

$$\mathbf{u} = x$$

*Temperature 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.
- 2 Select Boundary 1 only.
- 3 In the **Temperature** settings window, locate the **Temperature** section.
- 4 In the  $T_0$  edit field, type  $T_{in}$ .

*Outflow 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
- 2 Select Boundary 2 only.

*Heat Source 1*

- 1 On the **Physics** toolbar, click **Domains** and choose **Heat Source**.
- 2 Select Domain 1 only.
- 3 In the **Heat Source** settings window, locate the **Heat Source** section.
- 4 In the  $Q$  edit field, type  $-UA*(T-T_j)+Q_{rxn}$ .

## HEAT TRANSFER IN FLUIDS 2

*Heat Transfer in Fluids 1*

- 1 In the **Model Builder** window, expand the **Component 1 > Heat Transfer in Fluids 2** node, then click **Heat Transfer in Fluids 1**.
- 2 In the **Heat Transfer in Fluids** settings window, locate the **Model Inputs** section.
- 3 Specify the  $\mathbf{u}$  vector as

$$\mathbf{u}_j = x$$

*Temperature 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.
- 2 Select Boundary 1 only.
- 3 In the **Temperature** settings window, locate the **Temperature** section.
- 4 In the  $T_0$  edit field, type  $T_{j\_in}$ .

*Outflow 1*

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

- 2 Select Boundary 2 only.

*Heat Source 1*

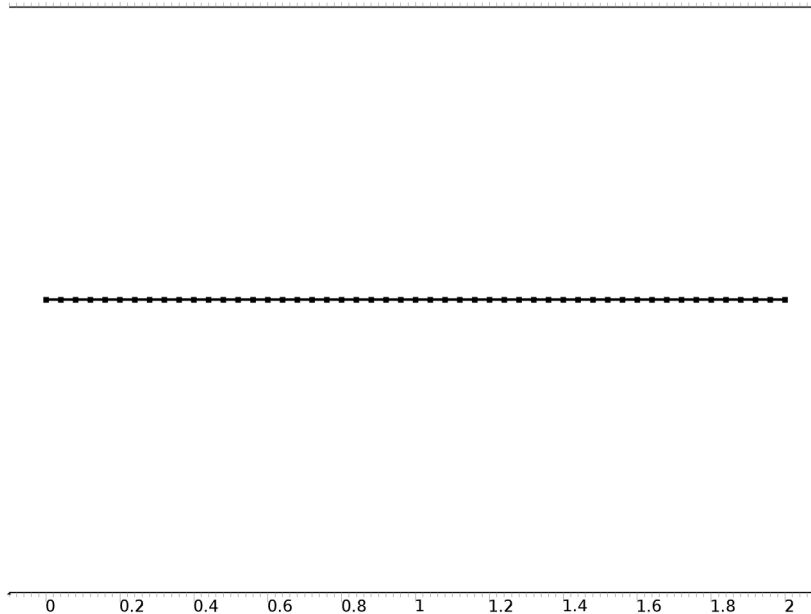
- 1 On the **Physics** toolbar, click **Domains** and choose **Heat Source**.
- 2 Select Domain 1 only.
- 3 In the **Heat Source** settings window, locate the **Heat Source** section.
- 4 In the  $Q$  edit field, type  $UA*(T-T_j)$ .

**MESH 1**

*Size*

- 1 In the **Model Builder** window, under **Component 1** right-click **Mesh 1** and choose **Edge**.
- 2 In the **Size** settings window, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Extra fine**.
- 4 Click the **Build All** button.
- 5 Click the **Zoom Extents** button on the Graphics toolbar.

The mesh should look as below.



**STUDY 1**

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

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

*Copy 2*

- 1 In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Solver 1** and choose **Solution>Copy**.
- 2 Right-click **Copy 2** and choose **Rename**.
- 3 Go to the **Rename Solver** dialog box and type Tj\_in 400K in the **New name** edit field.
- 4 Click **OK**.

**RESULTS***Concentration (chds)*

- 1 In the **Model Builder** window, expand the **Results>Concentration (chds)** node.
- 2 Right-click **Line Graph 1** and choose **Duplicate**.
- 3 In the **Line Graph** settings window, locate the **y-axis data** section.
- 4 Click **Concentration (c\_B)** in the upper-right corner of the section. Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 5 Right-click **Results>Concentration (chds)>Line Graph 2** and choose **Duplicate**.
- 6 In the **Line Graph** settings window, locate the **y-axis data** section.
- 7 Click **Concentration (c\_C)** in the upper-right corner of the section. On the **ID plot group** toolbar, click **Plot**.

*Temperature (ht)*

- 1 In the **Model Builder** window, under **Results>Temperature (ht)** right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Line Graph** settings window, locate the **y-axis data** section.
- 3 Click **Temperature (Tj)** in the upper-right corner of the section. Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 On the **ID plot group** toolbar, click **Plot**.

*Temperature (ht2)*

- 1 In the **Model Builder** window, expand the **Results>Temperature (ht2)** node, then click **Line Graph 1**.
- 2 In the **Line Graph** settings window, locate the **y-axis data** section.

- 3 Click **Reaction rate (r1)** in the upper-right corner of the section. Right-click **Results>Temperature (ht2)>Line Graph 1** and choose **Duplicate**.
- 4 In the **Line Graph** settings window, locate the **y-axis data** section.
- 5 Click **Reaction rate (r2)** in the upper-right corner of the section. Locate the **Title** section. From the **Title type** list, choose **None**.
- 6 On the **ID plot group** toolbar, click **Plot**.

## STUDY 1

Now, solve the optimization problem.

### Optimization

- 1 On the **Study** toolbar, click **Optimization**.
- 2 In the **Optimization** settings window, locate the **Optimization Solver** section.
- 3 From the **Method** list, choose **BOBYQA**.
- 4 In the table, enter the following settings:

Expression	Description
comp1.c_B_out	Outlet concentration

- 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 names	Initial value	Lower bound	Upper bound
Tj_in	400 [K]		

- 8 On the **Home** toolbar, click **Compute**.

## RESULTS

The plots you set up earlier now show the optimized solution.

### Temperature (ht2)

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