Created in COMSOL Multiphysics 5.6

# Steam Reformer

## Introduction

This example illustrates the modeling of a steam reformer, serving a stationary fuel cell unit with hydrogen. The tightly coupled system of mass, energy, and momentum equations used to describe the system, is readily set up using the predefined physics interfaces of the Chemical Reaction Engineering Module.

## Model Definition

In fuel cell power generators, a steam reformer unit typically produces the hydrogen needed for the cell stack. Figure 1 shows the geometry of such a system. The reformation chemistry occurs in a porous catalytic bed where energy is supplied through heating tubes to drive the endothermic process. The reactor is enclosed in an insulating jacket.

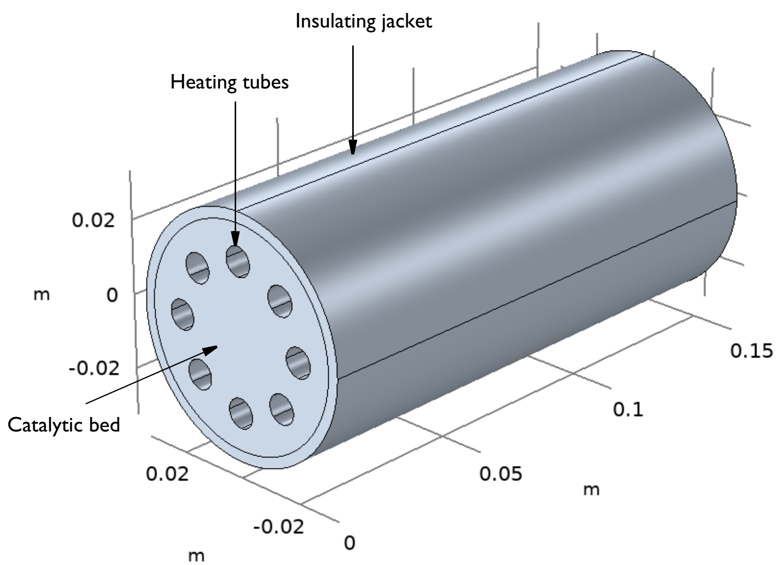


*Figure 1: Geometry of the steam reformer unit.*

In this example, propane and steam are mixed in stoichiometric amounts and enter through the inlet of the reactor. For heating purposes, hot gases from a burner are passed in the opposite direction, through a number of tubes perforating the reactor bed.

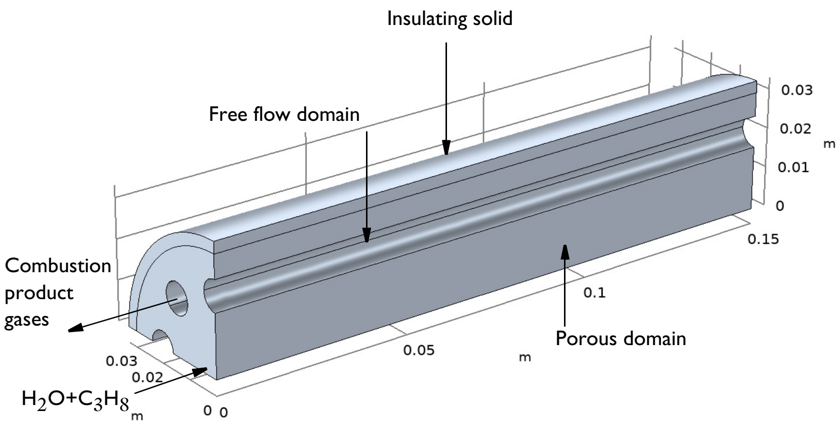


*Figure 2: Making use of symmetry, the modeling domain is reduced to a quarter of the full geometry.*

In the reformer, water and propane react to form hydrogen and carbon dioxide:

$$C_3H_8 + 6H_2O \xrightarrow{k} 10H_2 + 3CO_2$$

An overall kinetic model has been established from experiments (Ref. 1), where the reaction rate (SI unit: mol/(m$^3$·s)) has been found to be first order in the propane concentration:

$$r = kc_{\mathrm{C3H8}} \tag{1}$$

The rate constant follows Arrhenius equation, with the temperature dependence:

$$k = A\exp\left(-\frac{E_{\mathrm{a}}}{R_{\mathrm{g}}T}\right)$$

where the frequency factor $A$ is $7\cdot10^5$ s$^{-1}$ and the activation energy $E_{\mathrm{a}}$ is 83.14 kJ/mol.

### FLUID FLOW — REFORMER BED

The flow of gaseous species through the reformer bed is described by Darcy's law:

$$\nabla \cdot \left(\rho\left(-\frac{\kappa}{\eta}\nabla p_{sr}\right)\right) = 0$$

Here, ρ denotes the gas density (SI unit: $kg/m^3$), η the viscosity (SI unit: Pa·s), κ the permeability of the porous medium (SI unit: $m^2$), and $p_{sr}$ is the pressure in the reformer bed (SI unit: Pa). The Darcy's law equation is, in this example, solved with the **Darcy's law** interface.

The inlet and outlet boundary conditions describe a 50 Pa pressure drop across the bed. All other boundaries are impervious, corresponding to the condition:

$$-\frac{\kappa}{\eta}\nabla p_{sr} \cdot \mathbf{n} = 0$$

#### ENERGY TRANSPORT — REFORMER BED

A one-equation approach is used to describe the average temperature distribution in the porous bed:

$$(\rho C_p)_{eff}\frac{\partial T_{sr}}{\partial t} + \nabla \cdot (-k_{eff}\nabla T_{sr}) + (\rho C_p)_f\mathbf{u} \cdot \nabla T_{sr} = Q$$

The effective thermal conductivity of the bed, $k_{eff}$ (SI unit: W/(m·K)), is given by:

$$k_{eff} = \varepsilon k_f + (1-\varepsilon)k_{pm}$$

In the above equations, the indices "f" and "pm" denote fluid and porous matrix, respectively, and ε is the volume fraction of the fluid phase. The effective volumetric heat capacity of the bed is given by:

$$(\rho C_p)_{eff} = \varepsilon(\rho C_p)_f + (1-\varepsilon)(\rho C_p)_{pm}$$

Furthermore, $T_{sr}$ is the temperature (SI unit: K), $Q$ represents a heat source (SI unit: W/ $m^3$), and $\mathbf{u}$ the fluid velocity (SI unit: m/s). The equation is modeled using the **Heat Transfer in Porous Media** interface.

Assuming that the porous medium is homogeneous and isotropic, the steady-state equation becomes

$$\nabla \cdot (-k_{sr}\nabla T_{sr}) + (\rho C_p)_f\mathbf{u} \cdot \nabla T_{sr} = Q \qquad (2)$$

The heat source due to reaction is

$$Q = \Delta H_r \cdot r$$

where, $r$ is given by Equation 1. The steam reformation of propane is endothermic, with an enthalpy of reaction of $\Delta H_r = 410$ kJ/mol.

Equation 2 also accounts for the conductive heat transfer in the insulating jacket. As no reactions occur in this domain, the description reduces to:

$$\nabla \cdot (-k_\mathrm{i} \nabla T_\mathrm{sr}) = 0$$

where $k_\mathrm{i}$ is the thermal conductivity (W/(m·K)) of the insulating material.

The temperature of the gas is 700 K at the inlet. At the outlet, it is assumed that convective heat transport is dominant:

$$\mathbf{n} \cdot (-k_\mathrm{sr} \nabla T_\mathrm{sr}) = 0$$

The heat exchange between the bed and the tubes is described by:

$$q = h_\mathrm{ht}(T_\mathrm{sr} - T) \tag{3}$$

where $h_\mathrm{ht}$ is the heat transfer coefficient (SI unit: W/(m$^2$·K)) and $T$ is the temperature (K) of the heating tubes. A similar expression describes the heat flux from the insulating jacket to the surroundings:

$$q = -h_\mathrm{j}(T_\mathrm{sr} - T_\mathrm{amb})$$

where $h_\mathrm{j}$ is the heat transfer coefficient of the jacket (SI unit: W/(m$^2$·K)) and $T_\mathrm{amb}$ is the ambient temperature (K).

### MASS TRANSPORT — REFORMER BED

The **Transport of Concentrated Species** interface gives the equations for the mass transport. The mass-balance equations for the model are the Maxwell-Stefan diffusion and convection equations at steady state:

$$\nabla \cdot \left( \rho \omega_i \mathbf{u} - \rho \omega_i \sum_{k=1}^{n} \tilde{D}_{\mathrm{e},ik} \left( \nabla x_k + (x_k - \omega_k) \frac{\nabla p}{p} \right) - D^T_{\mathrm{e},i} \frac{\nabla T}{T} \right) = R_i$$

In the equations above, $\rho$ denotes the density (kg/m$^3$), $\omega_i$ is the mass fraction of species $i$, $x_k$ is the molar fraction of species $k$, $\tilde{D}_{\mathrm{e},ik}$ is the $ik$ component of the effective multicomponent Fick diffusivity (m$^2$/s). $D^T_{\mathrm{e},i}$ denotes the effective generalized thermal diffusion coefficient (kg/(m·s)), $T$ is the temperature (K), and $R_i$ the reaction rate (kg/(m$^3$·s)). The mass-balances are set up and solved with the Transport of Concentrated

Species interface. The effective parameters accounts for the impact of porosity on the diffusivity, this model uses the Millington and Quirk model:

$$D_{e,ik} = \varepsilon_p^{4/3} D_{ik}$$

$$D_{e,i}^T = \varepsilon_p^{4/3} D_i^T$$

The inlet weight fraction of propane is 0.28. At the outlet, the convective flux condition is used:

$$\mathbf{n} \cdot \left( \left( -\rho\omega_i \sum_{j=1}^{n} \tilde{D}_{ij} \left( \nabla x_j + (x_j - \omega_j) \frac{\nabla p}{p} \right) \right) - D^T \frac{\nabla T}{T} \right) = 0$$

All other boundaries use the insulating or symmetry condition.

#### FLUID FLOW — HEATING TUBES

The flow of heating gas in the tubes is described by the weakly compressible Navier-Stokes equations at steady-state:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - (2\mu/3)(\nabla \cdot \mathbf{u})\mathbf{I}]$$
$$\nabla \cdot (\rho\mathbf{u}) = 0$$

where $\rho$ denotes density (SI unit: $kg/m^3$), $\mathbf{u}$ represents the velocity (SI unit: m/s), $\mu$ denotes dynamic viscosity (SI unit: kg/(m· s)), and $p$ equals the pressure in the tubes (SI unit: Pa).

The boundary conditions are

$$\mathbf{u} \cdot \mathbf{n} = v_0 \qquad \text{inlet}$$
$$\mathbf{u} = \mathbf{0} \qquad \text{walls}$$
$$p = p_{\mathrm{ref}} \qquad \text{outlet}$$

At the outlet, viscous stresses are ignored and the pressure is set to 1 atmosphere.

The **Laminar Flow** interface sets up and solves the Navier-Stokes equations and is here used to model the gas flow in the tubes. Since the flow is nonisothermal, the **Heat Transfer in Fluids** interface is also used. These interfaces are coupled through the **Nonisothermal Flow** multiphysics coupling feature.

#### ENERGY TRANSPORT — HEATING TUBES

The energy transport in heating tubes is described by:

$$\nabla \cdot (-k_{\mathrm{ht}} \nabla T) + \rho C_p \mathbf{u} \cdot \nabla T = 0$$

where $k_{\mathrm{ht}}$ is the thermal conductivity (SI unit: W/(m·K)) of the heating gas. The temperature of the gas is 900 K at the inlet. Also this energy transport is modeled with the Heat Transfer in Fluids interface.

At the outlet, it is assumed that convective heat transport is dominant:

$$\mathbf{n} \cdot (-k_{\mathrm{ht}} \nabla T) = 0$$

The heat exchange between the bed and tubes is given by:

$$q = -h_{\mathrm{ht}}(T_{\mathrm{sr}} - T)$$

This is the same heat flux as given by Equation 3, but with reversed sign.

## *Results and Discussion*

Figure 3 shows the weight fraction of propane in the reformer bed. The inlet weight fraction is 0.28 while the fraction at the outlet is close to zero.

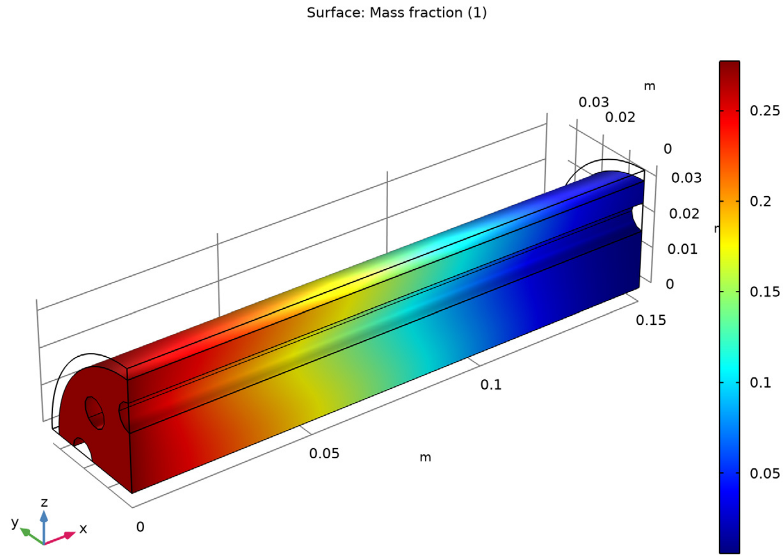


*Figure 3: Weight fraction distribution of propane in the reformer bed.*

A cross section plot through the center of the reformer reveals a concentration distribution in the bed. As the local reactivity is mainly controlled by the temperature, results indicate the heat supplied by the tubes is sufficient to efficiently make use of the entire catalytic bed.

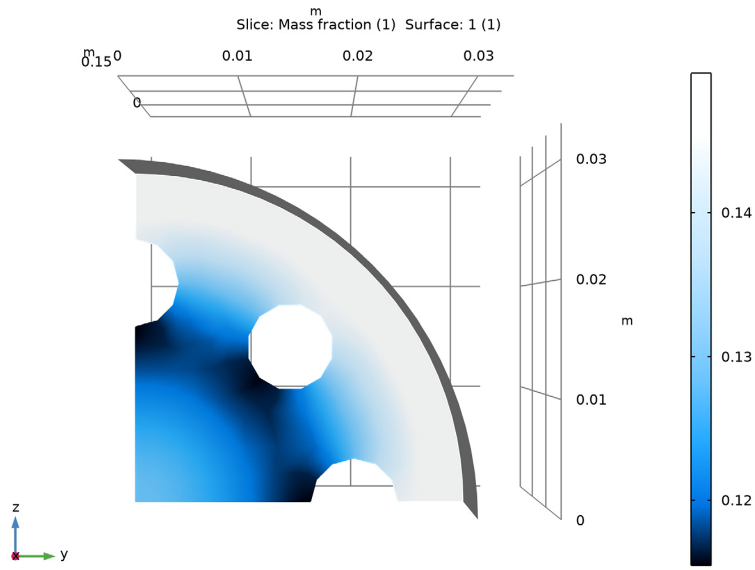


*Figure 4: Weight fraction distribution of propane in a cross section through the middle of the reformer bed.*

[Figure 5](#) shows the weight fractions of all reacting species in the bed, evaluated along the reactor centerline. The plot shows that the entire bed length is active in converting propane.

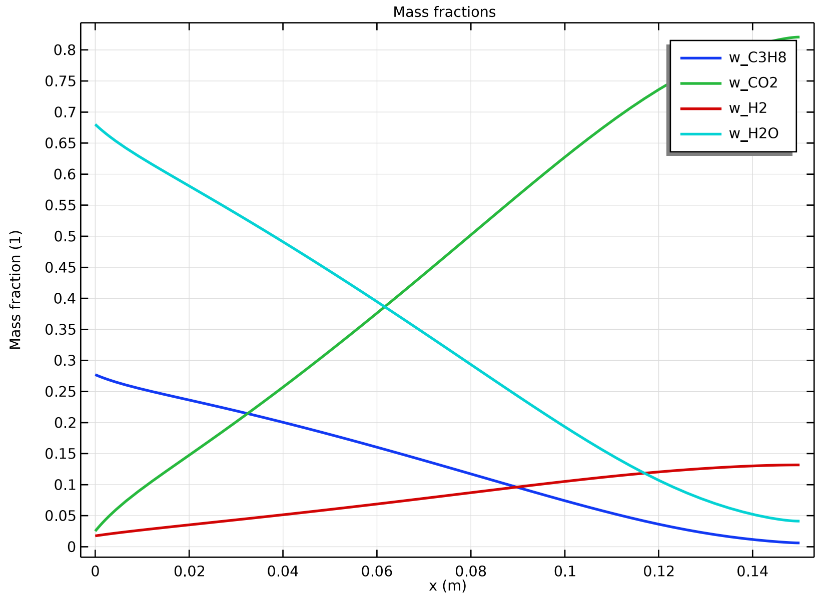


*Figure 5: Weight fraction of reacting species as function of reactor position, plotted along the reactor centerline.*

The energy exchange between the heating tubes and reformer bed is clearly illustrated in Figure 6. The gas of the heating tubes enters at 900 K and exits at approximately 716 K.

The gas temperature in the reformer bed is 700 K at the inlet, goes through a minimum, and finally exits with an average temperature of 843 K.

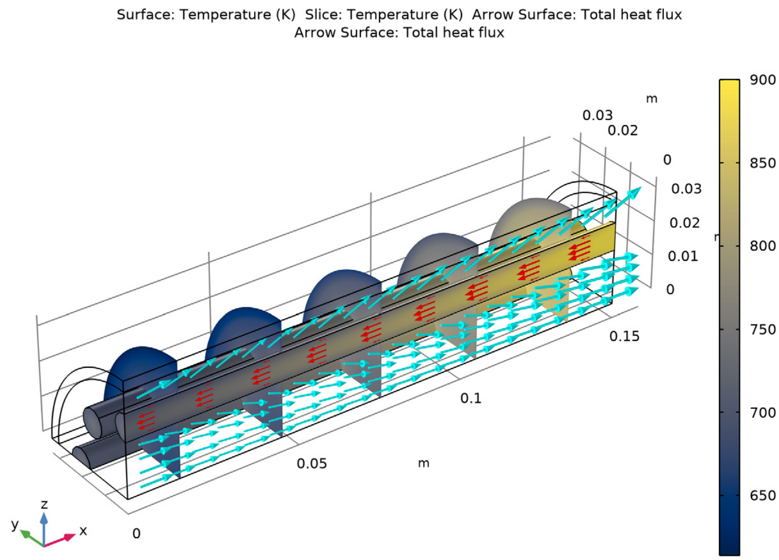


*Figure 6: Temperature distributions in the reformer system, including the reformer bed, heating tubes and insulating wall.*

A line plot through the center of the reactor shows how the temperature initially decreases due to the endothermic reformation reactions. When the reaction rate is reduced as a function of lower temperature and propane content, the energy supplied by the heating tubes dictates the temperature evolution.

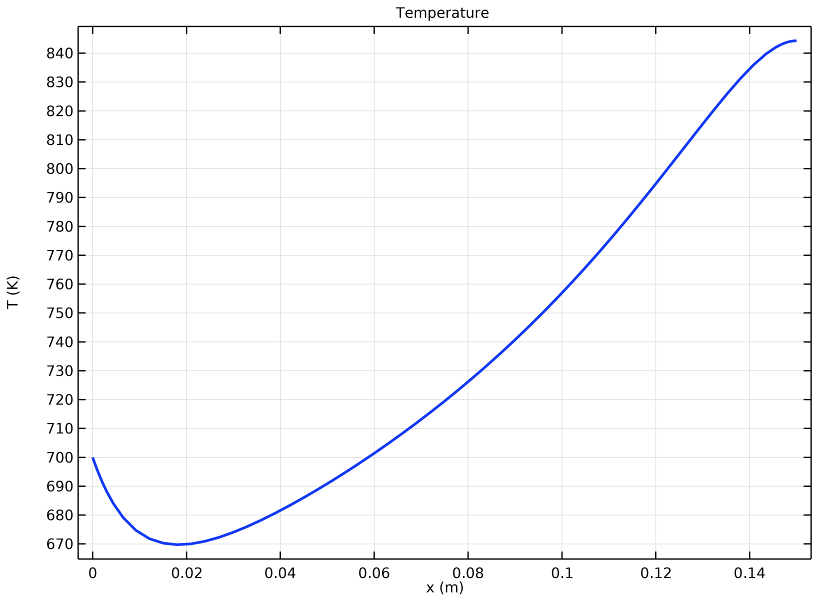


*Figure 7: Bed temperature as a function of position, plotted along the reactor centerline.*

Figure 8 shows the velocity fields of both the heating gas in the tubes and the reacting gas in the bed. The flow in the heating tubes is laminar and the parabolic velocity distribution is clearly seen. The gas velocity in the porous bed increases significantly through the reactor, and, at the outlet, the gas velocity is approximately than twice that at the inlet.

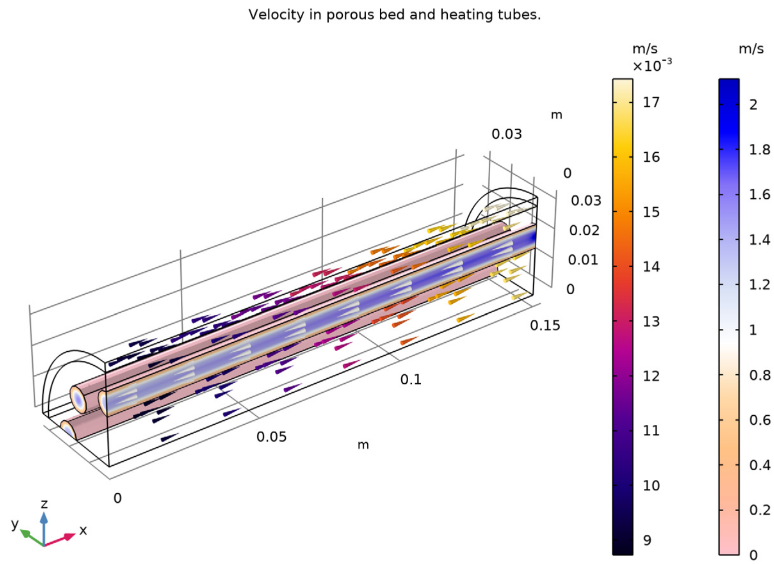


*Figure 8: Velocity fields of the heating tubes and the reformer bed.*

The increased velocity is mainly due to gas expansion caused by chemical reaction and, to a lesser extent, by temperature increase. Figure 9 illustrates the associated density variations in the reformer bed, accounting for both composition and temperature effects.

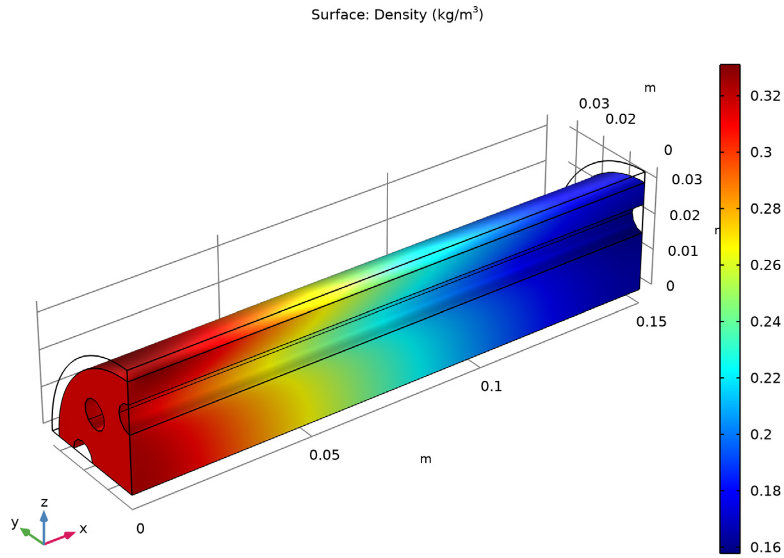


*Figure 9: Overall gas density in the reformer bed.*

In summary, this example illustrates the simulation of a reactor described by fully coupled mass, energy and flow equations.

## Reference


1. P.Gateau, *Design of Reactors and Heat Exchange Systems to Optimize a Fuel Cell Reformer*, Proceedings of the COMSOL User's Conference Grenoble, 2007.


**Application Library path:** `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/steam_reformer`

# *Modeling Instructions*

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

### NEW

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

### GLOBAL DEFINITIONS

In the **Model Builder** window, right-click **Global Definitions** and choose **Thermodynamics> Thermodynamic System**.

### SELECT SYSTEM

1 Go to the **Select System** window.

2 Click **Next** in the window toolbar.

### SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list, select **propane (74-98-6, C3H8)**.

3 Click **Add Selected**.

4 In the **Species** list, select **water (7732-18-5, H2O)**.

5 Click **Add Selected**.

6 In the **Species** list, select **hydrogen (1333-74-0, H2)**.

7 Click **Add Selected**.

8 In the **Species** list, select **carbon dioxide (124-38-9, CO2)**.

9 Click **Add Selected**.

10 Click **Next** in the window toolbar.

### SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.

2 Click **Finish** in the window toolbar.

### GLOBAL DEFINITIONS

#### *Gas System 1 (pp1)*

In the **Model Builder** window, under **Global Definitions>Thermodynamics** right-click **Gas System 1 (pp1)** and choose **Generate Chemistry**.

### SELECT SPECIES

1. Go to the **Select Species** window.
2. Click **Add All**.
3. Click **Next** in the window toolbar.

### CHEMISTRY SETTINGS

1. Go to the **Chemistry Settings** window.
2. From the **Mass transfer** list, choose **Concentrated species**.
3. Click **Finish** in the window toolbar.

### GEOMETRY 1

Now create the geometry. To simplify this step, insert a prepared geometry sequence:

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
2. In the **Geometry** toolbar, point to **Import/Export** and choose **Insert Sequence**.
3. Browse to the model's Application Libraries folder and double-click the file `steam_reformer.mph`.
4. Click **Build All** in the **Geometry** toolbar.

### DEFINITIONS

*Catalytic Bed*

1. In the **Definitions** toolbar, click **Explicit**.
2. In the **Settings** window for **Explicit**, type `Catalytic Bed` in the **Label** text field.
3. Select Domain 1 only.

*Remaining explicit definitions*

Analogous to the explicit definition for the Catalytic Bed, proceed to create the following explicit definitions:

| Label | Geometric entity level | Numbers |
|---|---|---|
| Catalytic Bed | Domain | 1 |
| Heating Tubes | Domain | 2, 4, 5 |
| Jacket | Domain | 3 |
| Bed Inlet | Boundary | 1 |
| Bed Outlet | Boundary | 24 |
| Tubes Inlet | Boundary | 25, 27, 28 |

| Label | Geometric entity level | Numbers |
|---|---|---|
| Tubes Outlet | Boundary | 4, 13, 17 |
| Tubes/Bed | Boundary | 6, 8, 14-16, 18, 20, 21 |
| Bed/Jacket | Boundary | 11 |
| Jacket/Ambient | Boundary | 12 |
| Bed Symmetry | Boundary | 2, 3, 7, 22 |
| Tubes Symmetry | Boundary | 5, 19 |
| Jacket Symmetry | Boundary | 10, 23 |

Also create a union selection containing all inlet and outlet boundaries. This will be used to refine the mesh in these areas.

### *Inlets and Outlets*

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Inlets and Outlets` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Under **Selections to add**, click **+ Add**.

5 In the **Add** dialog box, in the **Selections to add** list, choose **Bed Inlet**, **Bed Outlet**, **Tubes Inlet**, and **Tubes Outlet**.

6 Click **OK**.

### *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 1 only.

## GLOBAL DEFINITIONS

A set of parameters useful when building the model are available in a text file.

### *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 `steam_reformer_parameters.txt`.

### ADD PHYSICS

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

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

3 In the tree, select **Chemical Species Transport>Transport of Concentrated Species (tcs)**.

4 Click **Add to Component 1** in the window toolbar.

### TRANSPORT OF CONCENTRATED SPECIES (TCS)

1 In the **Settings** window for **Transport of Concentrated Species**, locate the **Transport Mechanisms** section.

2 Select the **Mass transfer in porous media** check box.

3 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type 4.

4 In the **Mass fractions** table, enter the following settings:

| |
|---|
| w_H2O |
| w_C3H8 |
| w_H2 |
| w_CO2 |

### ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.

3 Click **Add to Component 1** in the window toolbar.

### DARCY'S LAW (DL)

1 In the **Settings** window for **Darcy's Law**, locate the **Physical Model** section.

2 In the $p_{ref}$ text field, type p_ref.

3 Click to expand the **Dependent Variables** section. In the **Pressure** text field, type p_sr.

### ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the tree, select **Heat Transfer>Heat Transfer in Porous Media (ht)**.

3 Click **Add to Component 1** in the window toolbar.

### HEAT TRANSFER IN POROUS MEDIA (HT)

1 In the **Settings** window for **Heat Transfer in Porous Media**, click to expand the **Dependent Variables** section.

2 In the **Temperature** text field, type T_sr.

### ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the tree, select **Fluid Flow>Nonisothermal Flow>Laminar Flow**.

3 Click **Add to Component 1** in the window toolbar.

4 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

### LAMINAR FLOW (SPF)

1 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

2 In the $p_{ref}$ text field, type p_ref.

3 Click to expand the **Dependent Variables** section. In the **Pressure** text field, type p_tubes.

### HEAT TRANSFER IN FLUIDS 2 (HT2)

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**, click to expand the **Dependent Variables** section.

3 In the **Temperature** text field, type T_tubes.

### CHEMISTRY (CHEM)

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

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

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

| Species | Species mass fraction type | Mass fraction (1) | From Thermodynamics |
|---|---|---|---|
| C3H8 | Free species | w_C3H8 | C3H8 |
| CO2 | Free species | w_CO2 | CO2 |
| H2 | Free species | w_H2 | H2 |
| H2O | Free species | w_H2O | H2O |

**4** Click to expand the **Calculate Transport Properties** section. Click to collapse the **Calculate Transport Properties** section.

*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 `C3H8 + H2O => H2 + CO2`.

**4** Click **Balance** in the upper-right corner of the **Reaction Formula** section.

**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_C3H8`.

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

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

**9** In the $A^{\mathrm{f}}$ text field, type `A`.

**10** In the $E^{\mathrm{f}}$ text field, type `Ea`.

## TRANSPORT OF CONCENTRATED SPECIES IN BED

**1** In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Concentrated Species (tcs)**.

**2** In the **Settings** window for **Transport of Concentrated Species**, type `Transport of Concentrated Species in Bed` in the **Label** text field.

**3** Locate the **Domain Selection** section. From the **Selection** list, choose **Catalytic Bed**.

**4** Locate the **Transport Mechanisms** section. From the **Diffusion model** list, choose **Maxwell-Stefan**.

*Initial Values 1*

**1** In the **Model Builder** window, under **Component 1 (comp1)> Transport of Concentrated Species in Bed (tcs)** click **Initial Values 1**.

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

**3** In the $\omega_{0,\mathrm{wC3H8}}$ text field, type `w_C3H8_in`.

**4** In the $\omega_{0,\mathrm{wH2}}$ text field, type `w_H2_in`.

**5** In the $\omega_{0,\mathrm{wCO2}}$ text field, type `w_CO2_in`.

*Porous Media Transport Properties 1*

**1** In the **Physics** toolbar, click **Domains** and choose **Porous Media Transport Properties**.

**2** In the **Settings** window for **Porous Media Transport Properties**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Catalytic Bed**.

4 Locate the **Matrix Properties** section. In the $\varepsilon_p$ text field, type `porosity`.

5 Locate the **Density** section. From the $M_{\mathrm{wH2O}}$ list, choose **Molar mass (chem/H2O)**.

6 From the $M_{\mathrm{wC3H8}}$ list, choose **Molar mass (chem/C3H8)**.

7 From the $M_{\mathrm{wH2}}$ list, choose **Molar mass (chem/H2)**.

8 From the $M_{\mathrm{wCO2}}$ list, choose **Molar mass (chem/CO2)**.

9 Locate the **Convection** section. From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl)**.

10 Locate the **Diffusion** section. In the table, enter the following settings:

| Species 1 | Species 2 | Diffusivity | Diffusion coefficient (m^2/s) |
|---|---|---|---|
| w_H2O | w_C3H8 | Maxwell-Stefan diffusivity , C3H8-H2O (chem) | comp1.chem.D_C3H8_H2O |
| w_H2O | w_H2 | Maxwell-Stefan diffusivity , H2-H2O (chem) | comp1.chem.D_H2_H2O |
| w_H2O | w_CO2 | Maxwell-Stefan diffusivity , CO2-H2O (chem) | comp1.chem.D_CO2_H2O |
| w_C3H8 | w_H2 | Maxwell-Stefan diffusivity , C3H8-H2 (chem) | comp1.chem.D_C3H8_H2 |
| w_C3H8 | w_CO2 | Maxwell-Stefan diffusivity , C3H8-CO2 (chem) | comp1.chem.D_C3H8_CO2 |
| w_H2 | w_CO2 | Maxwell-Stefan diffusivity , CO2-H2 (chem) | comp1.chem.D_CO2_H2 |

### *Reaction Sources 1*

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

2 In the **Settings** window for **Reaction Sources**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Catalytic Bed**.

4 Locate the **Reactions** section. From the $R_{\mathrm{wC3H8}}$ list, choose **Reaction rate for species C3H8 (chem)**.

5 From the $R_{\mathrm{wH2}}$ list, choose **Reaction rate for species H2 (chem)**.

6 From the $R_{\mathrm{wCO2}}$ list, choose **Reaction rate for species CO2 (chem)**.

7 Locate the **Reacting Volume** section. From the **Reacting volume** list, choose **Pore volume**.

### *Inflow 1*

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

## 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 |
|---|---|---|---|
| J_in_C3H8 | intop1(tcs.rho*dl.U*w_C3H8_in) | kg/s | Mass flow rate, C3H8 |
| J_in_H2 | intop1(tcs.rho*dl.U*w_H2_in) | kg/s | Mass flow rate, H2 |
| J_in_CO2 | intop1(tcs.rho*dl.U*w_CO2_in) | kg/s | Mass flow rate, CO2 |

## TRANSPORT OF CONCENTRATED SPECIES IN BED (TCS)

*Inflow 1*

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Concentrated Species in Bed (tcs)** click **Inflow 1**.

2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Bed Inlet**.

4 Locate the **Inflow** section. From the **Mixture specification** list, choose **Mass flow rates**.

5 In the $J_{\mathrm{in,wC3H8}}$ text field, type J_in_C3H8.

6 In the $J_{\mathrm{in,wH2}}$ text field, type J_in_H2.

7 In the $J_{\mathrm{in,wCO2}}$ text field, type J_in_CO2.

*Outflow 1*

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

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Bed Outlet**.

## DARCY'S LAW IN BED

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Darcy's Law (dl)**.

2 In the **Settings** window for **Darcy's Law**, type Darcy's Law in Bed in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Remove from Selection**.

4 From the **Selection** list, choose **Catalytic Bed**.

### *Fluid and Matrix Properties 1*

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law in Bed (dl)** click **Fluid and Matrix Properties 1**.

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

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

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

5 Locate the **Matrix Properties** section. From the $\varepsilon_p$ list, choose **User defined**. In the associated text field, type `porosity`.

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

### *Inlet 1*

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

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

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

4 Locate the **Pressure** section. In the $p_0$ text field, type `p_in_sr`.

5 Locate the **Boundary Selection** section. From the **Selection** list, choose **Bed Inlet**.

### *Outlet 1*

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

2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Bed Outlet**.

4 Locate the **Boundary Condition** section. From the list, choose **Pressure**.

### *Symmetry 1*

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

2 In the **Settings** window for **Symmetry**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Bed Symmetry**.

## HEAT TRANSFER IN POROUS MEDIA IN BED

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

2 In the **Settings** window for **Heat Transfer in Porous Media**, type `Heat Transfer in Porous Media in Bed` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Catalytic Bed**.

4 Select Domains 1 and 3 only.

*Fluid 1*

1 In the **Model Builder** window, expand the **Component 1 (comp1)> Heat Transfer in Porous Media in Bed (ht)>Porous Medium 1** node, then click **Fluid 1**.

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

3 From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl)**.

4 Locate the **Heat Conduction, Fluid** section. From the $k_{\mathrm{f}}$ list, choose **Thermal conductivity (chem)**.

5 Locate the **Thermodynamics, Fluid** section. From the $\rho_{\mathrm{f}}$ list, choose **Density (tcs)**.

6 From the $C_{p,\mathrm{f}}$ list, choose **Heat capacity at constant pressure (chem)**.

7 From the $\gamma$ list, choose **Ratio of specific heats (chem)**.

*Porous Matrix 1*

1 In the **Model Builder** window, click **Porous Matrix 1**.

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

3 From the $\varepsilon_{\mathrm{p}}$ list, choose **User defined**. In the associated text field, type `porosity`.

4 From the **Define** list, choose **Solid phase properties**.

5 Locate the **Heat Conduction, Porous Matrix** section. From the $k_{\mathrm{s}}$ list, choose **User defined**. In the associated text field, type `k_pm`.

6 Locate the **Thermodynamics, Porous Matrix** section. From the $\rho_{\mathrm{s}}$ list, choose **User defined**. In the associated text field, type `dens_pm`.

7 From the $C_{\mathrm{p,s}}$ list, choose **User defined**. In the associated text field, type `Cp_pm`.

*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 $T_{\mathrm{sr}}$ text field, type `T_in_sr`.

*Solid 1*

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

2 In the **Settings** window for **Solid**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Jacket**.

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

5 Locate the **Thermodynamics, Solid** section. From the $\rho$ list, choose **User defined**. In the associated text field, type `dens_foam`.

**6** From the $C_p$ list, choose **User defined**. In the associated text field, type `Cp_foam`.

### *Temperature 1*

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

**2** In the **Settings** window for **Temperature**, locate the **Boundary Selection** section.

**3** From the **Selection** list, choose **Bed Inlet**.

**4** Locate the **Temperature** section. In the $T_0$ text field, type `T_in_sr`.

### *Outflow 1*

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

**2** In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

**3** From the **Selection** list, choose **Bed Outlet**.

### *Heat Flux 1*

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

**2** In the **Settings** window for **Heat Flux**, locate the **Boundary Selection** section.

**3** From the **Selection** list, choose **Tubes/Bed**.

**4** Locate the **Heat Flux** section. Click the **Convective heat flux** button.

**5** In the $h$ text field, type `h_tubes`.

**6** In the $T_{ext}$ text field, type `T_tubes`.

### *Heat Flux 2*

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

**2** In the **Settings** window for **Heat Flux**, locate the **Boundary Selection** section.

**3** From the **Selection** list, choose **Jacket/Ambient**.

**4** Locate the **Heat Flux** section. Click the **Convective heat flux** button.

**5** In the $h$ text field, type `h_j`.

**6** In the $T_{ext}$ text field, type `T_amb`.

### *Heat Source 1*

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

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

**3** In the $Q_0$ text field, type `porosity*chem.Qtot`.

**4** Locate the **Domain Selection** section. From the **Selection** list, choose **Catalytic Bed**.

## 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 **Search** text field, type `air`.

4 Click **Search**.

5 In the tree, select **Liquids and Gases>Gases>Air**.

6 Click **Add to Component 1 (comp1)**.

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

## MATERIALS

### *Air (mat1)*

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Heating Tubes**.

## LAMINAR FLOW IN HEATING TUBES

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

2 In the **Settings** window for **Laminar Flow**, type `Laminar Flow in Heating Tubes` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Heating Tubes**.

### *Inlet 1*

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

2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Tubes Inlet**.

4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

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

### *Outlet 1*

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

2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Tubes Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** check box.

### *Symmetry 1*

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

2 In the **Settings** window for **Symmetry**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Tubes Symmetry**.

### HEAT TRANSFER IN HEATING TUBES

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 Heating Tubes` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Heating Tubes**.

*Initial Values 1*

1 In the **Model Builder** window, under **Component 1 (comp1)> Heat Transfer in Heating Tubes (ht2)** click **Initial Values 1**.

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

3 In the $T_{\text{tubes}}$ text field, type `T_in_tubes`.

*Temperature at Inlet*

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

2 In the **Settings** window for **Temperature**, type `Temperature at Inlet` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Tubes Inlet**.

4 Locate the **Temperature** section. In the $T_0$ text field, type `T_in_tubes`.

*Outflow 1*

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

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Tubes Outlet**.

*Heat Flux to bed*

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

2 In the **Settings** window for **Heat Flux**, type `Heat Flux to bed` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Tubes/Bed**.

4 Locate the **Heat Flux** section. Click the **Convective heat flux** button.

5 In the $h$ text field, type `h_tubes`.

6 In the $T_{\text{ext}}$ text field, type `T_sr`.

### MESH 1

*Free Triangular 1*

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

2 Select Boundaries 4, 9, 13, and 17 only.

### *Free Quad 1*

1. In the **Mesh** toolbar, click **Boundary** and choose **Free Quad**.
2. In the **Settings** window for **Free Quad**, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **Bed Inlet**.

### *Boundary Layers 1*

1. In the **Mesh** toolbar, click **Boundary Layers**.
2. In the **Settings** window for **Boundary Layers**, locate the **Geometric Entity Selection** section.
3. From the **Geometric entity level** list, choose **Boundary**.
4. Select Boundaries 1, 4, 13, and 17 only.

### *Boundary Layer Properties*

1. In the **Model Builder** window, click **Boundary Layer Properties**.
2. Select Edges 5, 8, 16, 17, 19, 21, 24, and 27 only.
3. In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Layer Properties** section.
4. In the **Number of boundary layers** text field, type `3`.
5. From the **Thickness of first layer** list, choose **Manual**.
6. In the **Thickness** text field, type `3e-4`.

### *Swept 1*

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

### *Distribution 1*

1. Right-click **Swept 1** and choose **Distribution**.
2. In the **Settings** window for **Distribution**, locate the **Distribution** section.
3. In the **Number of elements** text field, type `50`.

### *Size*

1. In the **Model Builder** window, click **Size**.
2. In the **Settings** window for **Size**, locate the **Element Size** section.
3. Click the **Custom** button.
4. Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `2e-3`.
5. In the **Minimum element size** text field, type `1e-3`.

*Boundary Layers 2*

1 In the **Mesh** toolbar, click **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, click to expand the **Transition** section.

3 Clear the **Smooth transition to interior mesh** check box.

*Boundary Layer Properties*

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Geometric Entity Selection** section.

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

4 From the **Selection** list, choose **Inlets and Outlets**.

5 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type `6`.

6 From the **Thickness of first layer** list, choose **Manual**.

7 In the **Thickness** text field, type `0.0003`.

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

## ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study**.

## STUDY 1

*Solution 1 (sol1)*

In the **Study** toolbar, click **Show Default Solver**.

*Stationary 2*

In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

*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 table, clear the **Solve for** check boxes for **Transport of Concentrated Species in Bed (tcs)**, **Heat Transfer in Porous Media in Bed (ht)**, and **Heat Transfer in Heating Tubes (ht2)**.

*Solution 1 (sol1)*

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1>Solver Configurations> Solution 1 (sol1)>Stationary Solver 2** node.

4 Right-click **Stationary Solver 2** and choose **Fully Coupled**.

5 In the **Settings** window for **Stationary Solver**, locate the **General** section.

6 In the **Relative tolerance** text field, type `0.1`.

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

## RESULTS

In the first part of the results processing, create the default plots giving Figure 3, Figure 4 and Figure 8.

*Velocity (dl)*

1 In the **Model Builder** window, expand the **Results>Velocity (dl)** node, then click **Velocity (dl)**.

2 In the **Settings** window for **3D Plot Group**, click to expand the **Title** section.

*Streamline 1*

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

2 In the **Settings** window for **Streamline**, click to expand the **Quality** section.

*Color Expression 1*

1 In the **Model Builder** window, expand the **Streamline 1** node, then click **Color Expression 1**.

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

3 From the **Color table** list, choose **HeatCamera**.

*Streamline 1*

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

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 In the **Points** text field, type `6`.

*Volume 1*

1 In the **Model Builder** window, right-click **Velocity (dl)** and choose **Volume**.

**2** In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Laminar Flow in Heating Tubes>Velocity and pressure>spf.U - Velocity magnitude - m/s**.

*Selection 1*

**1** Right-click **Volume 1** and choose **Selection**.

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

**3** From the **Selection** list, choose **Heating Tubes**.

*Streamline 1*

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

**2** In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

**3** In the **Points** text field, type `20`.

**4** From the **Positioning** list, choose **Uniform density**.

**5** In the **Separating distance** text field, type `.05`.

*Volume 1*

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

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

**3** From the **Color table** list, choose **Twilight**.

*Streamline 1*

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

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

**3** Find the **Point style** subsection. From the **Arrow type** list, choose **Cone**.

**4** Find the **Line style** subsection. From the **Type** list, choose **None**.

*Arrow Surface 1*

**1** In the **Model Builder** window, right-click **Velocity (dl)** and choose **Arrow Surface**.

**2** In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Laminar Flow in Heating Tubes>Velocity and pressure>u,v,w - Velocity field**.

*Selection 1*

**1** Right-click **Arrow Surface 1** and choose **Selection**.

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

**3** From the **Selection** list, choose **Tubes Symmetry**.

*Arrow Surface 1*

1 In the **Model Builder** window, click **Arrow Surface 1**.
2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.
3 From the **Arrow type** list, choose **Cone**.
4 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type `40`.
5 From the **Placement** list, choose **Uniform anisotropic**.
6 In the **x weight** text field, type `.4`.
7 In the **z weight** text field, type `4`.
8 Locate the **Coloring and Style** section. From the **Color** list, choose **White**.

*Velocity*

1 In the **Model Builder** window, under **Results** click **Velocity (dl)**.
2 In the **Settings** window for **3D Plot Group**, type `Velocity` in the **Label** text field.
3 Locate the **Title** section. From the **Title type** list, choose **Manual**.
4 In the **Title** text area, type `Velocity in porous bed and heating tubes.`.
5 Locate the **Color Legend** section. Select the **Show units** check box.
6 In the **Velocity** toolbar, click **Plot**.
   This is Figure 8.

The 3D plot group showing the velocity field in the tubes can be deleted, since this was visualized in the previous plot.

*Velocity (spf)*

In the **Model Builder** window, right-click **Velocity (spf)** and choose **Delete**.

*Mass fraction propane midreactor*

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.
2 In the **Settings** window for **3D Plot Group**, type `Mass fraction propane midreactor` in the **Label** text field.
3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

*Slice 1*

1 Right-click **Mass fraction propane midreactor** and choose **Slice**.
2 In the **Settings** window for **Slice**, locate the **Expression** section.
3 In the **Expression** text field, type `w_C3H8`.
4 Locate the **Plane Data** section. In the **Planes** text field, type `1`.

**5** Locate the **Coloring and Style** section. From the **Color table** list, choose **JupiterAuroraBorealis**.

**6** Locate the **Plane Data** section. In the **Planes** text field, type 3.

**7** In the **Mass fraction propane midreactor** toolbar, click **Plot**.

**8** In the **Planes** text field, type 1.

**9** In the **Mass fraction propane midreactor** toolbar, click **Plot**.

*Surface 1*

In the **Model Builder** window, right-click **Mass fraction propane midreactor** and choose **Surface**.

*Selection 1*

**1** In the **Model Builder** window, right-click **Surface 1** and choose **Selection**.

**2** Select Boundary 12 only.

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

**4** Click **Remove from Selection**.

**5** In the list, select **12**.

**6** Click **Remove from Selection**.

**7** Select Boundary 11 only.

**8** In the list, select **11**.

*Surface 1*

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

**2** In the **Settings** window for **Surface**, locate the **Expression** section.

**3** In the **Expression** text field, type 1.

**4** Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

**5** From the **Color** list, choose **Gray**.

**6** In the **Mass fraction propane midreactor** toolbar, click **Plot**.

**7** Click the **Go to YZ View** button in the **Graphics** toolbar.

**8** In the **Mass fraction propane midreactor** toolbar, click **Plot**.

This is Figure 4.

*Mass fraction propane midreactor*

**1** In the **Model Builder** window, click **Mass fraction propane midreactor**.

**2** In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Select the **Plot dataset edges** check box.

4 In the **Mass fraction propane midreactor** toolbar, click **Plot**.

*Mass fraction propane*

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Mass fraction propane` in the **Label** text field.

*Surface 1*

1 Right-click **Mass fraction propane** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `w_C3H8`.

4 Click the **Go to Default View** button in the **Graphics** toolbar.

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

6 In the **Mass fraction propane** toolbar, click **Plot**.

This is Figure 3.

7 Locate the **Coloring and Style** section. From the **Color table** list, choose **JupiterAuroraBorealis**.

*Contour 1*

1 In the **Model Builder** window, right-click **Mass fraction propane** and choose **Contour**.

2 In the **Settings** window for **Contour**, locate the **Expression** section.

3 From the menu, choose **Chemistry>chem.r_1 - Reaction rate - mol/(m³·s)**.

4 In the **Expression** text field, type `chem.r_1`.

*Selection 1*

1 Right-click **Contour 1** and choose **Selection**.

2 Select Boundaries 2 and 7 only.

3 In the **Mass fraction propane** toolbar, click **Plot**.

*Reaction Rate Contour*

1 In the **Model Builder** window, under **Results>Mass fraction propane** click **Contour 1**.

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

3 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

4 Clear the **Color legend** check box.

Next, create new plot groups to process results for the mass fractions and temperature distribution in the reactor (Figures 5, 6, 7, and 9).

### *Mass fractions along centerline*

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Mass fractions along centerline` in the **Label** text field.
3. Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type `Mass fractions`.
5. Locate the **Plot Settings** section. Select the **x-axis label** check box.
6. In the associated text field, type `x (m)`.

### *C3H8*

1. Right-click **Mass fractions along centerline** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. Click **Paste Selection**.
4. In the **Paste Selection** dialog box, type `3` in the **Selection** text field.
5. Click **OK**.
6. In the **Settings** window for **Line Graph**, type `C3H8` in the **Label** text field.
7. Locate the **y-Axis Data** section. In the **Expression** text field, type `w_C3H8`.
8. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
9. In the **Expression** text field, type `x`.
10. Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.
11. Click to expand the **Legends** section. Select the **Show legends** check box.
12. From the **Legends** list, choose **Manual**.
13. In the table, enter the following settings:

| **Legends** |
|---|
| w_C3H8 |

### *CO2*

1. Right-click **C3H8** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `CO2` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `w_CO2`.

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

| **Legends** |
| --- |
| w_CO2 |

*H2*

**1** Right-click **CO2** and choose **Duplicate**.

**2** In the **Settings** window for **Line Graph**, type H2 in the **Label** text field.

**3** Locate the **y-Axis Data** section. In the **Expression** text field, type w_H2.

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

| **Legends** |
| --- |
| w_H2 |

*H2O*

**1** Right-click **H2** and choose **Duplicate**.

**2** In the **Settings** window for **Line Graph**, type H2O in the **Label** text field.

**3** Locate the **y-Axis Data** section. In the **Expression** text field, type w_H2O.

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

| **Legends** |
| --- |
| w_H2O |

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

**6** In the **Mass fractions along centerline** toolbar, click **Plot**.

This is Figure 5.

*Mass fractions along centerline*

**1** In the **Model Builder** window, click **Mass fractions along centerline**.

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

**3** From the **Position** list, choose **Middle right**.

*Temperature*

**1** In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

**2** In the **Settings** window for **3D Plot Group**, type Temperature in the **Label** text field.

*Surface 1*

**1** Right-click **Temperature** and choose **Surface**.

**2** In the **Settings** window for **Surface**, locate the **Expression** section.

**3** In the **Expression** text field, type `T_tubes`.

**4** Locate the **Coloring and Style** section. From the **Color table** list, choose **Cividis**.

*Slice 1*

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

**2** In the **Settings** window for **Slice**, locate the **Expression** section.

**3** In the **Expression** text field, type `T_sr`.

**4** Locate the **Coloring and Style** section. From the **Color table** list, choose **Thermal**.

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

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

**7** Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

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

*Arrow Surface 1*

Right-click **Temperature** and choose **Arrow Surface**.

*Selection 1*

**1** In the **Model Builder** window, right-click **Arrow Surface 1** and choose **Selection**.

**2** Select Boundaries 2 and 7 only.

*Arrow Surface 1*

**1** In the **Model Builder** window, click **Arrow Surface 1**.

**2** In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Heat Transfer in Porous Media in Bed>Domain fluxes>ht.tfluxx,...,ht.tfluxz - Total heat flux**.

**3** Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type `100`.

**4** From the **Placement** list, choose **Uniform anisotropic**.

**5** In the **x weight** text field, type `.3`.

**6** In the **z weight** text field, type `.5`.

**7** Locate the **Coloring and Style** section. Select the **Scale factor** check box.

**8** From the **Color** list, choose **Cyan**.

**9** In the **Scale factor** text field, type `5e-6`.

**10** In the **Temperature** toolbar, click **Plot**.

### Arrow Surface 2

1 In the **Model Builder** window, right-click **Temperature** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Heat Transfer in Heating Tubes>Domain fluxes>ht2.tfluxx,...,ht2.tfluxz - Total heat flux**.

### Selection 1

1 Right-click **Arrow Surface 2** and choose **Selection**.

2 Select Boundary 5 only.

### Arrow Surface 2

1 In the **Model Builder** window, click **Arrow Surface 2**.

2 In the **Settings** window for **Arrow Surface**, locate the **Arrow Positioning** section.

3 In the **Number of arrows** text field, type `40`.

4 From the **Placement** list, choose **Uniform anisotropic**.

5 In the **x weight** text field, type `0.3`.

6 In the **z weight** text field, type `3`.

7 Locate the **Coloring and Style** section. Select the **Scale factor** check box.

8 In the associated text field, type `3E-8`.

9 In the **Temperature** toolbar, click **Plot**.

This is Figure 6.

### Temperature along centerline

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

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

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Temperature`.

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `x (m)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `T (K)`.

### Line Graph 1

1 Right-click **Temperature along centerline** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 3 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

7 In the **Expression** text field, type T_sr.

8 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

9 In the **Expression** text field, type x.

10 Locate the **Coloring and Style** section. In the **Width** text field, type 2.

11 In the **Temperature along centerline** toolbar, click **Plot**.

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

This is Figure 7.

*Gas density reformer bed*

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type Gas density reformer bed in the **Label** text field.

*Surface 1*

1 Right-click **Gas density reformer bed** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type dl.rho.

4 In the **Gas density reformer bed** toolbar, click **Plot**.

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

This is Figure 9.

Finally, calculate the average outlet temperatures for the gas in the heating tubes and in the reformer bed.

*Average temperature in bed outflow*

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type Average temperature in bed outflow in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| ht.ofl1.Tave | K | Weighted average temperature |

4 Click **Evaluate**.

*Average temperature in heat tube outflow*

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Average temperature in heat tube outflow` in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `ht2.ofl1.Tave` | K | `Weighted average temperature` |

4 Click **Evaluate**.