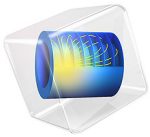

# Charging of a Metal Hydride Tank

## *Introduction*

Metal hydride tanks offer high volumetric energy density storage of hydrogen, compared to compressed gas tanks and liquid hydrogen (Ref. 1). This is a result of hydrogen being absorbed into the matrix of a metal alloy. The metal hydride resulting from such absorption is a solid-state storage system. These systems are relatively safe since there is a low risk of gas leaks due to the chemically bound hydrogen.

The operation principle for metal hydride tanks is simple: let hydrogen gas absorb into a porous metal alloy at increased pressure. This results in a metal hydride. The absorption process releases heat that should be removed to increase the charging rate and storage capacity. When the gas is needed, the hydrogen is released from the solid matrix by decreasing the pressure while heating the tank.

The capacity of metal alloys is usually expressed as the number of hydrogen atoms (H) that can be absorbed into the matrix per metal site (M). The metal alloy used in this model is based on $LaNi_5$ and has a theoretical H/M ratio of 6 (Ref. 2).

Figure 1 illustrates the tank studied in this model. The tank is cylindrical and equipped with a water filled cooling jacket. The porous metal alloy is placed in cartridges that can

be reached by the gas from a central distribution channel. The gas, in this case hydrogen with low amounts of nitrogen, enters the reactor from the top.

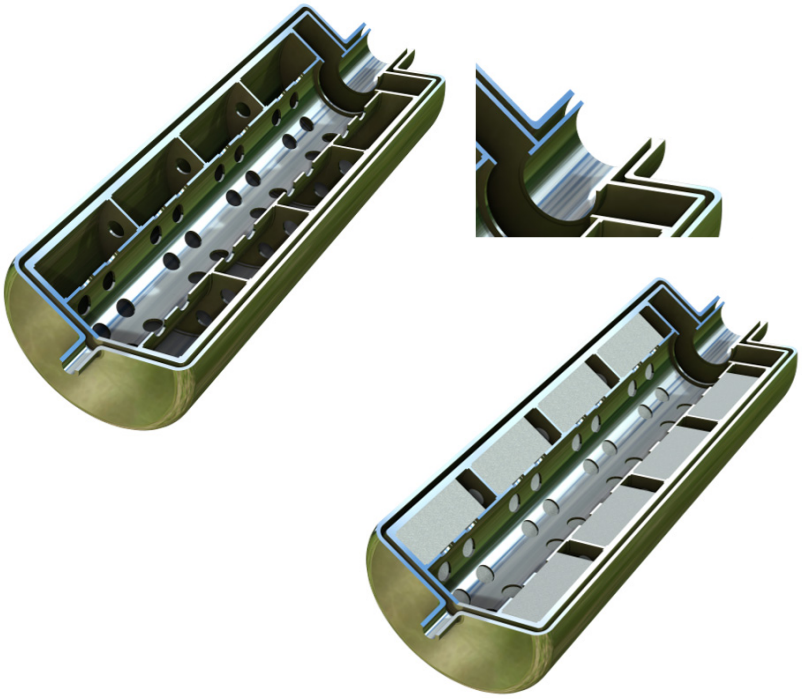

*Figure 1: Tank reactor design used in this example.*

This model describes the coupled reaction kinetics, fluid, heat, and mass transfer during the charging process. Models like this can be used to design storage systems, and to optimize operation conditions (gas composition, pressure, and temperature). Examples of system design parameters are metal composition, porosity, and geometric dimensions.

## *Model Definition*

Figure 2 shows the modeled domain which consists of 1/8 of the tank geometry. This simplification can be made due to the geometric symmetry of the cartridges. To further

simplify the geometry, and to save computational memory, the porous metal is modeled as a porous medium. This means that the pore structure is not resolved.

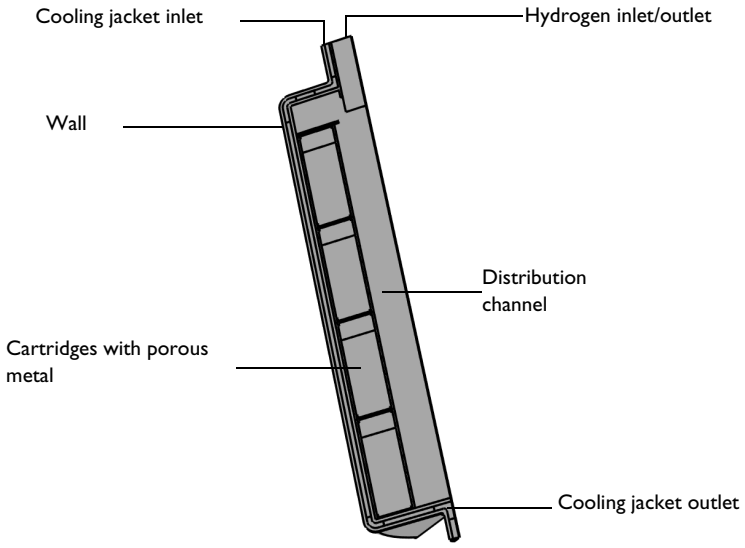


*Figure 2: Model geometry including the domain and boundary labels.*

The model is based on the following assumptions:

- The gas phase is modeled as an ideal gas
- The porosity and volume of the porous metal alloy does not change due to absorption
- Local thermal equilibrium exists in the porous bed
- Gravity effects are negligible

### ABSORPTION OF HYDROGEN

During charging, hydrogen atoms absorb into the solid metal matrix to form metal hydride. This can be described with the following chemical equation for the gas phase

$$0{,}5\mathrm{H}_2(\mathrm{g}) \rightarrow 0\mathrm{H}_2(\mathrm{g}). \tag{1}$$

The absorption rate of hydrogen atoms $\delta XH/\delta t$ $(1/\mathrm{s})$ has been defined as (Ref. 2, Ref. 3)

$$\frac{\partial}{\partial t}XH = C_{\mathrm{a}} \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right) \ln\left(\frac{p_{\mathrm{H2}}}{p_{\mathrm{eq}}}\right)(\mathrm{XH}_{\mathrm{max}} - XH), \tag{2}$$

where $XH$ (mol/mol) is the number of absorbed hydrogen atoms per metal atom site

$$XH = \frac{n_{\mathrm{H}}}{n_{\mathrm{M}}}.$$

$XH_{\max}$ is the maximum number of hydrogen atoms that can be absorbed per metal site, $C_{\mathrm{a}}$ is a pre-exponential factor, $E_{\mathrm{a}}$ is the activation energy, $p_{\mathrm{H2}}$ is the partial pressure of hydrogen, and $p_{\mathrm{eq}}$ is the equilibrium hydrogen pressure. The equilibrium pressure is related to the temperature as described by the *van't Hoff* equation (Ref. 4):

$$p_{\mathrm{eq}}(T, XH) = p_{\mathrm{iso}}(T_{\mathrm{iso}}, XH)\exp\left(\frac{\Delta H}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{iso}}}\right)\right), \tag{3}$$

where ΔH (J/mol) is the entropy change due to absorption. The hydrogen pressure at isothermal conditions, $p_{\mathrm{iso}}$, and the resulting absorbed hydrogen content ($XH$) comes from experimental data (Ref. 5).

The reaction rate of forming metal hydride $R_{\mathrm{MH}}$ (mol H /($\mathrm{m}^3$·s)) (Reaction (1)) can be expressed as a function of the absorption rate in Equation 2

$$R_1 = R_{\mathrm{MH}} = c_{\mathrm{M}}\frac{\partial}{\partial t}XH. \tag{4}$$

$c_{\mathrm{M}}$ is the concentration of metal sites (M) in the solid phase that hydrogen atoms can react with (mol M/$\mathrm{m}^3$)

$$c_{\mathrm{M}} = -\rho_{\mathrm{s}}\mathrm{M}_{\mathrm{M}}. \tag{5}$$

From stoichiometry, the reaction rate for $H_2$ (mol $H_2$/($\mathrm{m}^3$·s)) is

$$R_{\mathrm{H2}} = -\frac{R_{\mathrm{MH}}}{2}. \tag{6}$$

As hydrogen is absorbed and metal hydride is formed, heat (W/$\mathrm{m}^3$) is released according to

$$Q_{\mathrm{abs}} = -R_{\mathrm{MH}}\Delta H. \tag{7}$$

Finally, the maximum mass fraction of hydrogen atoms in the modeled alloy (M) is derived like this:

$$w_{\mathrm{H,\,max}} = \frac{\mathrm{XH}_{\max}\mathrm{M}_{\mathrm{H}}}{\mathrm{M}_{\mathrm{M}} + \mathrm{XH}_{\max}\mathrm{M}_{\mathrm{H}}} = 0{,}0059, \tag{8}$$

where $M_i$ is the molar mass for species $i$ and $XH_{max}$ is 6 (mol H/mol M).

### FLUID FLOW

The fluid flow of water in the cooling jacket is modeled as incompressible laminar flow. The inlet flow is assumed to be fully developed and an average inlet velocity is given. There is no slip at the jacket walls. The outlet has a pressure boundary condition with a static relative pressure equal to zero. There is no backflow at the outlet.

The fluid flow of hydrogen gas is modeled as a compressible, laminar flow, and described by the Navier-Stokes equations in the free flow parts, and the Brinkman equations in the porous material domain. The **Porous slip** formulation is used on boundaries adjacent to solid walls. This introduces slip velocity and relaxes the need for resolving the thin shear layer at the wall. A Darcian flow model is used in the porous domain.

The inlet of the gas has a pressure boundary condition. Normal flow and no backflow is enforced. The inlet pressure is gradually increased by 6 atm over 5 minutes. This improves the convergence rate of the system.

Symmetry boundary conditions are applied on each side of the modeled geometry.

### MASS TRANSFER

The incoming gas consists of mainly hydrogen. As absorption progresses, the hydrogen is removed from the gas, until mainly nitrogen remains. Since the gas phase consists of two species with comparative mole fractions, the system is described by the **Transport of Concentrated Species in Porous Media** interface. This interface solves for the mass transfer in the free flow domains and the porous domains. In the porous domains the conservation equations for hydrogen and nitrogen are:

$$\begin{aligned} \varepsilon_p \rho \frac{\partial \omega_{H2}}{\partial t} + \nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_{H2} &= (\varepsilon_p - \omega_{H2})Q_{mass} \\ \varepsilon_p \rho \frac{\partial \omega_{N2}}{\partial t} + \nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_{N2} &= -\omega_{N2} Q_{mass} \end{aligned}, \tag{9}$$

where $\varepsilon_p$ is the porosity, $\omega_i$ is the mass fraction of species $i$, $\mathbf{j}_i$ is the mass flux (kg/m$^3$), $\mathbf{u}$ is the velocity vector (m/s), and $Q_{mass}$ is the mass source (kg/(m$^3$·s)) due to absorption (see Equation 10). The terms in the mass conservation equations for the free flow domains are the same as for the porous domain except that the porosity is one and there are no mass sources.

The mass flux in the system consists of convective and diffusive flux. The diffusive flux is described with the **Mixture-averaged** diffusion model. This model is a simplification of the

Maxwell-Stefan model, and it is suitable when the multicomponent diffusion can be assumed to be constant as a function of partial pressure and temperature. In the porous domain the diffusivity is affected by the porosity. The resulting effective diffusivity is described by the **Bruggeman model**.

As mentioned, the reaction source is only defined in the porous domain. The mass source (kg $H_2/(m^3 \cdot s)$ of hydrogen gas being absorbed into the solid matrix is

$$Q_{\text{mass}} = \varepsilon M_{H2} R_{H2}, \tag{10}$$

where $\varepsilon$ is the porosity of the alloy, and $R_{H2}$ is given by Equation 6. This mass source is automatically added as a mass source to the fluid flow interface by the **Reacting Flow** multiphysics coupling.

The gas inflow has a given mole fraction as the boundary condition. As for the fluid flow description, symmetry boundaries for the mass transfer are used to reduce the modeling domain.

### HEAT TRANSFER

Heat transfer through convection and conduction is modeled by the **Heat Transfer In Porous Media** interface. In the porous domains, **Local thermal equilibrium** is assumed, which means that the temperatures of the solid and the fluid are assumed to be the same. The energy balance for the system is

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \rho_f C_{pf} \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{\text{eff}} \nabla T) + Q_{\text{abs}}, \tag{11}$$

where $\rho_f$ (kg/m$^3$) is the fluid density, $C_{pf}$ (J/(kg·K)) is the fluid heat capacity, $(\rho C_p)_{\text{eff}}$ (J/(m$^3$·K)) is the effective volumetric heat capacity, and $k_{\text{eff}}$ (W/(m·K)) is the effective thermal conductivity. Furthermore, $\mathbf{u}$ (m/s) is the fluid velocity field, derived by the fluid flow interface. $Q_{\text{abs}}$ (W/m$^3$) is the heat released as hydrogen is absorbed into the solid alloy and reacts to form metal hydride (Equation 7). This heat source is automatically added to the heat transfer interface by the **Reacting Flow** multiphysics coupling.

The effective conductivity of the solid-fluid system, $k_{\text{eff}}$, is related to the conductivity of the solid, $k_s$, and to the conductivity of the fluid, $k_f$, by

$$k_{\text{eff}} = \Theta_s k_s + \Theta_f k_f$$

Here $\Theta_s$ denotes the solid material's volume fraction, which is related to the volume fraction of the fluid $\Theta_f$ (or porosity) by

$$\Theta_f + \Theta_s = 1$$

The heat transfer interface sets up Equation 11 in the gas and porous media domains. For the solid alloy in the tank, only heat transfer by conduction applies:

$$-\nabla \cdot (k_s \nabla T) = 0 \tag{12}$$

where $k_s$ (SI unit: W/(m·K)) is the thermal conductivity of the solid.

To increase the absorption rate, the reactor is cooled by a water filled cooling jacket. **Inflow** and **Outflow** boundary conditions define this flow. The initial temperature in the tank is 15°C, while the inflow temperature in the cooling jacket is 5.5°C.

## *Results and Discussion*

Figure 3 shows the temperature and the absorbed hydrogen content in the reactor after 3600 s of charging. The absorbed hydrogen content is highest in the top bed closest to the gas inlet due to the highest concentration of hydrogen gas here. Since absorption releases heat, the temperature is also highest in this region. In each bed the absorption is

uneven. As the central part of the beds are not cooled down as efficiently as the beds' edges, the absorbed hydrogen content is lower at the centers.

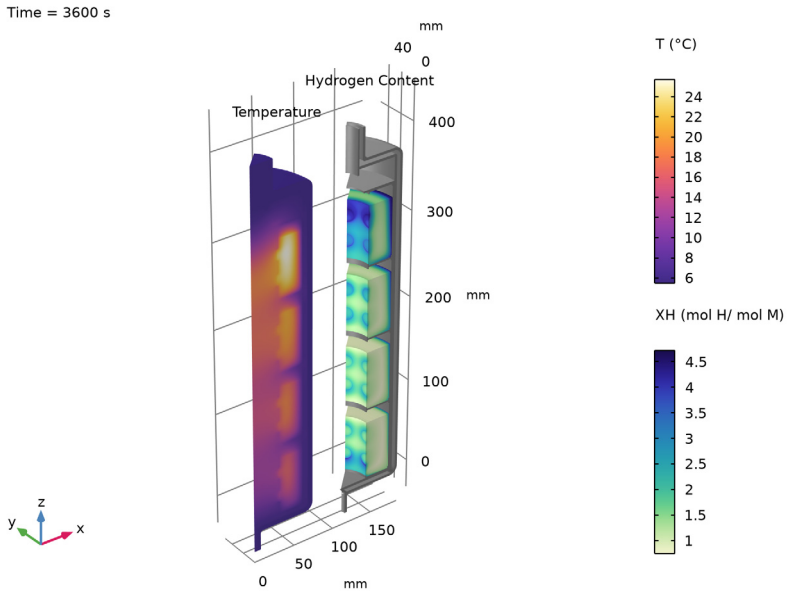


*Figure 3: Temperature and hydrogen content XH at 3600 s.*

Figure 4 shows the mass profile of hydrogen over time in the gas as well as in the solid phase. During the ramp up of the gas inflow pressure, the hydrogen content is increasing despite concurrent absorption. After 300 s when the ramping is complete, the gas phase

concentration and the absorption rate both decrease. At the end of the simulation 23 g of hydrogen has been absorbed into the metal alloy.

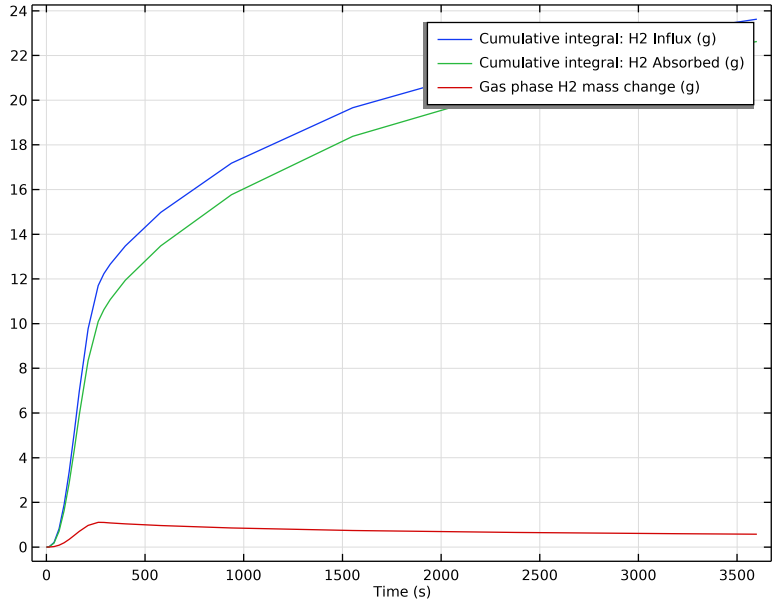


*Figure 4: Hydrogen mass profile over time in the gas as well as in the solid phase.*

Figure 5 shows the gas phase temperature, the bed temperature, and the charged hydrogen content *XH* over time. All three quantities are averaged over the respective domains. The hydride temperature increases throughout the loading. The gas temperature on the other initially decreases due to the water cooling. After about 12 s the temperature rises in the gas too. The average temperature in the hydride reaches 28°C, and the

temperature in the gas reaches 22°C, before both start to level off after the pressure loading finishes at 300 s.

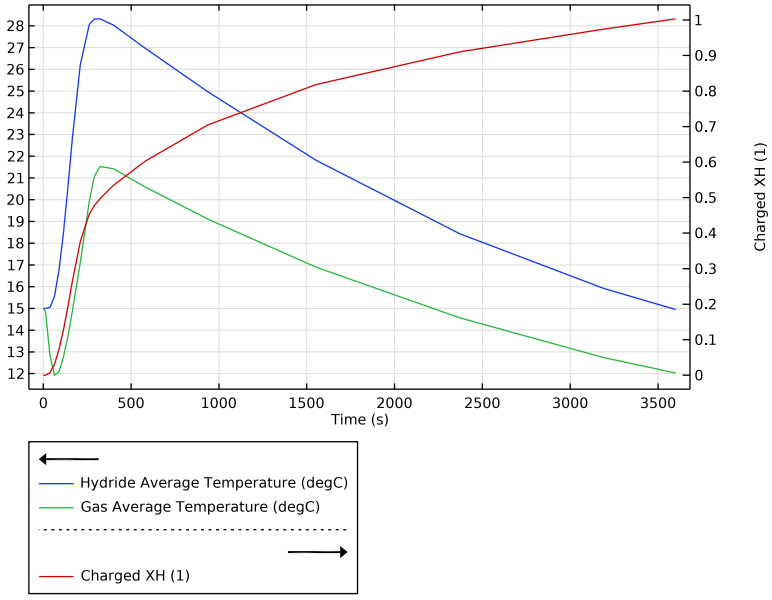


*Figure 5: Gas phase temperature, bed temperature, and charged hydrogen content* ***XH*** *over time.*

## *References*


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2. D.O. Lazarev and K.B. Minko, "Simulation of Hydrogen Desorption Processes in the Metal-Hydride Accumulator-Fuel Cell System," *Therm. Eng.*, vol. 57, no. 14, pp. 1222–1226, 2010.

3. U. Mayer, M. Groll, and W. Supper, "Heat and Mass Transfer in Metal Hydride Reaction Beds: Experimental and Theoretical Results", *J. Less-Common Met.*, vol. 131, pp. 235–244, 1987.

4. D. Lazarev, V. Artemov, G. Yankov, and K.B. Minko, "Numerical Simulation of Heat and Mass Transfer in Metal Hydride Hydrogen Accumulators of Different Complex

Designs," *Proceedings of the 14th International Heat Transfer Conference (IHTC14)*, IHTC14-22561, August 8–13, Washington, DC, USA.

5. V.N. Verbetsky, S.P. Malyshenko, S.V. Mitrokhin, V.V. Solovei, and Yu.F. Shmal'ko, "Metal Hydrides: Properties and Practical Applications. Review of the Works in CIS-Countries," *Int. J. Hydrogen Energy*, vol. 23, no. 12, pp. 1165–1177, 1998

**Application Library path:** `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/metal_hydride_tank`

## *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 **3D**.

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

3 Click **Add**.

4 In the **Velocity field (m/s)** text field, type `u_c`.

5 In the **Velocity field components** table, enter the following settings:

| |
|---|
| `u_c` |
| `v_c` |
| `w_c` |

6 In the **Pressure (Pa)** text field, type `p_c`.

7 In the **Select Physics** tree, select **Mathematics** > **ODE and DAE Interfaces** > **Domain ODEs and DAEs (dode)**.

8 Click **Add**.

9 In the **Field name (1)** text field, type `XH`.

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

| |
|---|
| `XH` |

11 Click **Define Source Term Unit**.

12 In the **Source term quantity** table, enter the following settings:

| Source term quantity | Unit |
|---|---|
| Custom unit | 1/s |

13 In the **Select Physics** tree, select **Chemical Species Transport** > **Nonisothermal Reacting Flow** > **Porous Media Flow** > **Brinkman Equations**.

14 Click **Add**.

15 In the **Added physics interfaces** tree, select **Transport of Concentrated Species in Porous Media (tcs)**.

16 In the **Mass fractions (1)** table, enter the following settings:

| |
|---|
| wH2 |
| wN2 |

17 Click **Study**.

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

19 Click **Done**.

## GLOBAL DEFINITIONS

### *Model Parameters*

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

2 In the **Settings** window for **Parameters**, type `Model Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Notice that some of the loaded parameters contain constants that has not yet been defined in the model. These will be added later.

### *Kinetic Model Parameters*

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Kinetic Model Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

*p_iso(Tiso,XH) (Experimental pressure-composition-isotherm curve at 20 degC)*

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global** > **Interpolation**.

Load experimental data that will be used to derive the equilibrium hydrogen pressure as a function of temperature and absorption degree.

2 In the **Settings** window for **Interpolation**, type `p_iso(Tiso,XH) (Experimental pressure-composition-isotherm curve at 20 degC)` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `p_iso`.

4 Click **Load from File**.

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

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

| Function | Unit |
|---|---|
| p_iso | atm |

8 In the **Argument** table, enter the following settings:

| Argument | Unit |
|---|---|
| t | 1 |

Add a function for the equilibrium hydrogen pressure as a function of temperature and absorbed amount hydrogen.

*p_eq(T,XH) (Equilibrium Hydrogen Pressure)*

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global** > **Analytic**.

2 In the **Settings** window for **Analytic**, type `p_eq(T,XH) (Equilibrium Hydrogen Pressure)` in the **Label** text field.

3 In the **Function name** text field, type `p_eq`.

4 Locate the **Definition** section. In the **Expression** text field, type `p_iso(XH)*exp(deltaH/R_const*(1/T-1/293.15[K]))`.

5 In the **Arguments** text field, type `XH, T`.

6 Locate the **Units** section. In the **Function** text field, type `Pa`.

7 In the table, enter the following settings:

| Argument | Unit |
|---|---|
| XH | 1 |
| T | K |

### GEOMETRY 1

Import a file with the reactor geometry. Symmetry reduces the modeling domain to 1/8th of the real tank geometry.

1 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `metal_hydride_tank_geom_sequence.mph`.

3 In the **Geometry** toolbar, click **Build All**.

Add materials to the model. The materials that will be added are: Structural steel, Gas mixture, Water (liquid), and Intermetallic Alloy (the metal hydride).

### ADD MATERIAL

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

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

3 In the **Search** text field, type `structural steel`.

4 Click **Search**.

5 In the tree, select **Built-in** > **Structural steel**.

6 Click the **Add to Component** button in the window toolbar.

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

### MATERIALS

*Structural steel (mat1)*

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

2 From the **Selection** list, choose **Tank Walls**.

*Gas Mixture*

1 In the **Materials** toolbar, click **Blank Material**.

2 In the **Settings** window for **Material**, type `Gas Mixture` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Gas**.

4 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** > **Gas Mixture (mat2)** node, then click **Basic (def)**.

5 In the **Settings** window for **Basic**, locate the **Output Properties** section.

6 Click + **Select Quantity**.

7 In the **Physical Quantity** dialog, type `dynam` in the text field.

8 In the tree, select **Transport** > **Dynamic viscosity (Pa*s)**.

9 Click **OK**.

10 In the **Settings** window for **Basic**, locate the **Output Properties** section.

11 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Dynamic viscosity | mu | `chem.eta` | Pa·s | 1x1 |

12 Click + **Select Quantity**.

13 In the **Physical Quantity** dialog, type `heat` in the text field.

14 In the tree, select **Transport** > **Heat capacity at constant pressure (J/(kg*K))**.

15 Click **OK**.

16 In the **Settings** window for **Basic**, locate the **Output Properties** section.

17 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Heat capacity at constant pressure | Cp | `chem.Cptot` | J/(kg·K) | 1x1 |

18 Click + **Select Quantity**.

19 In the **Physical Quantity** dialog, type `thermal` in the text field.

20 In the tree, select **Transport** > **Thermal conductivity (W/(m*K))**.

21 Click **OK**.

22 In the **Settings** window for **Basic**, locate the **Output Properties** section.

23 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Thermal conductivity | k_iso ; kii = k_iso, kij = 0 | `chem.kval` | W/(m·K) | 3x3 |

*Intermetallic Alloy*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** click **Porous Material 1 (pmat1)**.

2 In the **Settings** window for **Porous Material**, type `Intermetallic Alloy` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Metal Hydride**.

*Fluid 1 (pmat1.fluid1)*

1 Right-click **Intermetallic Alloy** and choose **Fluid**.

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

3 From the **Material** list, choose **Gas Mixture (mat2)**.

*Solid (pmat1.solid)*

1 In the **Model Builder** window, click **Solid (pmat1.solid)**.

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

3 In the $\theta_s$ text field, type `1-porM`.

4 In the **Model Builder** window, expand the **Solid (pmat1.solid)** node, then click **Basic (def)**.

5 In the **Settings** window for **Basic**, locate the **Output Properties** section.

6 Click + **Select Quantity**.

7 In the **Physical Quantity** dialog, type `density` in the text field.

8 In the tree, select **General** > **Density (kg/m^3)**.

9 Click **OK**.

10 In the **Settings** window for **Basic**, locate the **Output Properties** section.

11 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Density | rho | `rhoM` | kg/m³ | 1x1 |

12 Click + **Select Quantity**.

13 In the **Physical Quantity** dialog, type `heat capa` in the text field.

14 In the tree, select **Transport** > **Heat capacity at constant pressure (J/(kg*K))**.

15 Click **OK**.

16 In the **Settings** window for **Basic**, locate the **Output Properties** section.

17 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Heat capacity at constant pressure | Cp | CpM | J/(kg·K) | 1x1 |

18 Click + **Select Quantity**.

19 In the **Physical Quantity** dialog, type `mean` in the text field.

20 In the tree, select **Transport** > **Mean molar mass (kg/mol)**.

21 Click **OK**.

22 In the **Settings** window for **Basic**, locate the **Output Properties** section.

23 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Mean molar mass | Mn | MnM | kg/mol | 1x1 |

24 Locate the **Local Properties** section. In the **Local properties** table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| dp | 10[um] | m | Mean particle diameter |
| cM | rhoM/MnM | mol/m³ | Concentration of metal sites that can absorb hydrogen atoms |

*Intermetallic Alloy (pmat1)*

1 In the **Model Builder** window, click **Basic (def)**.

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

3 Click + **Select Quantity**.

4 In the **Physical Quantity** dialog, type `ther` in the text field.

5 In the tree, select **Transport** > **Thermal conductivity (W/(m*K))**.

6 Click **OK**.

7 In the **Settings** window for **Basic**, locate the **Output Properties** section.

8 In the table, enter the following settings:

| Property | Variable | Expression | Unit | Size |
|---|---|---|---|---|
| Thermal conductivity | k_iso ; kii = k_iso, kij = 0 | chem.kval/pmat1.porosity^3 | W/(m·K) | 3x3 |

### ADD MATERIAL

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

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

3 In the **Search** text field, type `water, liquid`.

4 Click **Search**.

5 In the tree, select **Built-in** > **Water, liquid**.

6 Click the **Add to Component** button in the window toolbar.

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

### MATERIALS

*Water, liquid (mat3)*

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

2 From the **Selection** list, choose **Cooling Channel**.

### DEFINITIONS (COMP1)

*XH_source (Absorption rate)*

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

2 Right-click **Component 1 (comp1)** > **Definitions** and choose **Local Variables**.

Add an expression for the absorption rate.

3 In the **Settings** window for **Variables**, type `XH_source (Absorption rate)` in the **Label** text field.

4 Locate the **Variables** section. Click **Load from File**.

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

*Step 1 (step1)*

1 In the **Definitions** toolbar, click **More Functions** and choose **Step**.

2 In the **Settings** window for **Step**, click to expand the **Smoothing** section.

3 In the **Size of transition zone** text field, type `t_ramp_gas`.

4 From the **Location definition** list, choose **Beginning of step**.

*Step 2 (step2)*

1 In the **Definitions** toolbar, click **More Functions** and choose **Step**.

2 In the **Settings** window for **Step**, locate the **Smoothing** section.

3 From the **Location definition** list, choose **Beginning of step**.

4 In the **Size of transition zone** text field, type `t_ramp_liquid`.

To define this model, several thermodynamic properties needs to be defined. All of the needed properties could be provided by adding a **Thermodynamic System**. By adding such a system and plotting the property functions, we saw that these properties are practically constant for the modeled process conditions. Therefore, a **Thermodynamic System** is not used in this model. By using constant values for the properties, the computational time is decreased.

Set up the chemistry interface that declares the reaction rate and thermodynamic properties.

### CHEMISTRY (CHEM)

*Reaction 1*

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

The chemical equation for formation of metal hydride could be described as hydrogen atoms disappearing from the gas phase. The reaction rate of forming metal hydride is expressed as the concentration of metal that can absorb hydrogen atoms times the hydrogen atom absorption rate.

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

3 In the **Formula** text field, type `0.5 H2 => 0 H2`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. In the $r_j$ text field, type `pmat1.solid.def.cM* XH_source`.

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

7 In the $H$ text field, type `deltaH`.

*Species: H2*

1 In the **Model Builder** window, click **Species: H2**.

2 In the **Settings** window for **Species**, click to expand the **Transport Expressions** section.

3 From the **Thermal conductivity** list, choose **User defined**.

4 In the $k$ text field, type `kH2`.

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

6 In the $C_p$ text field, type `CpH2`.

*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 `N2`.

4 Locate the **Transport Expressions** section. From the **Thermal conductivity** list, choose **User defined**.

5 In the $k$ text field, type `kN2`.

6 Locate the **Thermodynamic Expressions** section. From the list, choose **User defined**.

7 In the $C_p$ text field, type `CpN2`.

Match the species in **Chemistry** with the same species in the mass transfer interface, and define the mass transfer parameters for the gas mixture.

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

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

10 Find the **Bulk species** subsection. From the **Species solved for** list, choose **Transport of Concentrated Species in Porous Media**.

11 In the table, enter the following settings:

| Species | Type | Mass fraction | Value (1) |
|---|---|---|---|
| H2 | Variable | wH2 | Solved for |
| N2 | Free species | wN2 | Solved for |

12 Click to expand the **Calculate Transport Properties** section. From the **Ratio of specific heats** list, choose **User defined**.

13 In the $\gamma$ text field, type `1.4`.

14 From the **Dynamic viscosity** list, choose **User defined**.

15 In the $\mu$ text field, type `visc`.

Define the expression for the absorption rate of hydrogen atoms per metal atom (1/s), and set the initial value.

### ABSORBED HYDROGEN ATOMS PER METAL ATOM, XH

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Domain ODEs and DAEs (dode)**.

2 In the **Settings** window for **Domain ODEs and DAEs**, type `Absorbed Hydrogen Atoms Per Metal Atom, XH` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Metal Hydride**.

4 Click to expand the **Discretization** section. From the **Shape function type** list, choose **Lagrange**.

5 From the **Element order** list, choose **Linear**.

*Distributed ODE 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Absorbed Hydrogen Atoms Per Metal Atom, XH (dode)** click **Distributed ODE 1**.

2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.

3 In the *f* text field, type `XH_source`.

*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 *XH* text field, type `XH0`.

The chemical properties of the gas system, the absorption rate of hydrogen, the metal hydride formation, as well as the material properties has been defined. Continue by defining the fluid flow in the tank. The **Brinkman Equations** interface is used to describe the gas flow both in the fluid domains, and in the porous domains.

### BRINKMAN EQUATIONS (BR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Brinkman Equations (br)**.

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

3 From the **Selection** list, choose **Flow Region**.

4 Locate the **Physical Model** section. From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

5 Clear the **Neglect inertial term (Stokes flow)** checkbox.

6 In the $p_{\text{ref}}$ text field, type `P0`.

7 Click to expand the **Discretization** section. From the **Discretization of fluids** list, choose **P1+P1**.

*Fluid Properties 1*

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

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

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

*Porous Matrix 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Brinkman Equations (br)** > **Porous Medium 1** click **Porous Matrix 1**.

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

3 From the **Permeability model** list, choose **Kozeny-Carman**.

4 In the $d_p$ text field, type `pmat1.solid.def.dp`.

*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 **Boundary Selection** section. From the **Selection** list, choose **Gas Inflow**.

5 Locate the **Pressure Conditions** section. In the $p_0$ text field, type `Pin*step1(t)`.

*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 **Symmetry**.

## HEAT TRANSFER IN POROUS MEDIA (HT)

*Porous Medium 1*

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

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

3 From the **Effective thermal conductivity** list, choose **Equivalent thermal conductivity**.

*Initial Values 1*

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

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

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

*Fluid 1*

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

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

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

*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 **Tank Walls**.

*Inflow 1*

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

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

3 From the **Selection** list, choose **Gas Inflow**.

4 Locate the **Upstream Properties** section. In the $T_{\mathrm{ustr}}$ text field, type `T0`.

Define the heat transfer in the system.

*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 **Tank Shell**.

4 Locate the **Heat Flux** section. From the **Flux type** list, choose **Convective heat flux**.

5 In the $h$ text field, type `2[W(m^2/K)]`.

6 In the $T_{\mathrm{ext}}$ text field, type `T0`.

*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 **Symmetry**.

*Fluid 2*

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

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

3 From the **Selection** list, choose **Cooling Channel**.

4 Locate the **Model Input** section. Click **Make All Model Inputs Editable** in the upper-right corner of the section.

5 Locate the **Heat Convection** section. From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

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

7 From the $\gamma$ list, choose **User defined**. In the associated text field, type `1.4`.

*Cooling Water Inflow*

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

2 In the **Settings** window for **Inflow**, type `Cooling Water Inflow` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Cooling Water Inflow**.

4 Locate the **Upstream Properties** section. In the $T_{\mathrm{ustr}}$ text field, type `Tcooling*step2(t)+T0*(1-step2(t))`.

*Cooling Water Outflow*

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

2 In the **Settings** window for **Outflow**, type `Cooling Water Outflow` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Cooling Water Outflow**.

Now define the mass transfer in the system. This is done with a **Transport of Concentrated Species in Porous Media** interface.

### TRANSPORT OF CONCENTRATED SPECIES IN POROUS MEDIA (TCS)

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

2 In the **Settings** window for **Transport of Concentrated Species in Porous Media**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Flow Region**.

*Fluid 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport of Concentrated Species in Porous Media (tcs)** > **Porous Medium 1** click **Fluid 1**.

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

3 In the table, enter the following settings:

| Species 1 | Species 2 | Diffusivity | Diffusion coefficient (m^2/s) |
|---|---|---|---|
| wH2 | wN2 | User defined | D_H2_N2 |

4 From the **Effective diffusivity model** list, choose **Bruggeman model**.

*Initial Values 1*

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

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

3 From the **Mixture specification** list, choose **Mole fractions**.

4 In the $x_{0,\mathrm{wN2}}$ text field, type `x0_N2`.

*Fluid 1*

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

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

3 In the table, enter the following settings:

| Species 1 | Species 2 | Diffusivity | Diffusion coefficient (m^2/s) |
|---|---|---|---|
| wH2 | wN2 | User defined | D_H2_N2 |

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

*Reaction Sources 1*

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

Define the mass source of hydrogen leaving the gas phase in the pores.

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

3 From the **Selection** list, choose **Metal Hydride**.

4 Locate the **Reactions** section. Select the **Mass transfer to other phases** checkbox.

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

6 From the $R_{\mathrm{wN2}}$ list, choose **Reaction rate for species N2 (chem)**.

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

*Inflow 1*

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

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

3 From the **Selection** list, choose **Gas Inflow**.

4 Locate the **Inflow** section. From the **Mixture specification** list, choose **Mole fractions**.

5 In the $x_{0,\mathrm{wN2}}$ text field, type `x0_N2`.

*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 **Symmetry**.

Use the **Laminar Flow** interface to define the flow of cooling water.

### LAMINAR FLOW - COOLING

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 - Cooling` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Cooling Channel**.

*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 **Cooling Water Inflow**.

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

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

*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 **Cooling Water Outflow**.

*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 **Symmetry**.

The cooling flow simulation is sensitive to disturbances during the solution. Use pseudo time-stepping for a more robust solution process. To enable this, use the **Show more option** button and select to show **Advanced Physics Options**.

4 Click the **Show More Options** button in the **Model Builder** toolbar.

5 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

6 Click **OK**.

Enable pseudo time-stepping in the **Advanced Settings** section.

7 In the **Model Builder** window, click **Laminar Flow - Cooling (spf)**.

8 In the **Settings** window for **Laminar Flow**, click to expand the **Advanced Settings** section.

9 Find the **Pseudo time stepping** subsection. From the **Use pseudo time stepping for stationary equation form** list, choose **On**.

Now move on to mesh the geometry.

Now move on to mesh the geometry.

### MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Fine**.

4 Right-click **Component 1 (comp1)** > **Mesh 1** and choose **Edit Physics-Induced Sequence**.

*Size - Gas Domains*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size 1**.

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

3 From the **Selection** list, choose **Flow Region**.

4 In the **Label** text field, type `Size - Gas Domains`.

*Size - Gas Wall Boundaries*

1 In the **Model Builder** window, click **Size 2**.

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

3 From the **Selection** list, choose **Metal Hydride and Wall Boundary**.

4 In the **Label** text field, type `Size - Gas Wall Boundaries`.

5 Locate the **Element Size** section. Click the **Predefined** button.

6 From the **Predefined** list, choose **Fine**.

7 Click the **Custom** button.

8 Locate the **Element Size Parameters** section.

9 Select the **Maximum element size** checkbox. In the associated text field, type `3.5`.

10 Select the **Minimum element size** checkbox. In the associated text field, type `0.76`.

11 Select the **Maximum element growth rate** checkbox.

12 Select the **Curvature factor** checkbox.

13 Select the **Resolution of narrow regions** checkbox.

14 Click  **Build Selected**.

*Size - Metal Hydride Domains*

1 In the **Model Builder** window, click **Size 3**.

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

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

4 From the **Selection** list, choose **Metal Hydride**.

5 In the **Label** text field, type `Size - Metal Hydride Domains`.

6 Locate the **Element Size** section. Click the **Predefined** button.

7 From the **Predefined** list, choose **Normal**.

8 Click the **Custom** button.

9 Locate the **Element Size Parameters** section.

10 Select the **Maximum element size** checkbox. In the associated text field, type `2.5`.

11 Click  **Build Selected**.

*Size - Metal Hydride Boundaries*

1 In the **Model Builder** window, right-click **Size - Gas Wall Boundaries** and choose **Duplicate**.

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

3 From the **Selection** list, choose **Metal Hydride Boundary**.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `2.0`.

5 Clear the **Minimum element size** checkbox.

6 In the **Maximum element growth rate** text field, type `1.1`.

7 Clear the **Curvature factor** checkbox.

8 Clear the **Resolution of narrow regions** checkbox.

9 In the **Label** text field, type `Size - Metal Hydride Boundaries`.

10 Click  **Build Selected**.

*Size - Cooling Channel Outlet*

1 In the **Model Builder** window, right-click **Size - Gas Domains** and choose **Duplicate**.

2 In the **Settings** window for **Size**, type `Size - Cooling Channel Outlet` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. Click  **Clear Selection**.

4 Select Domains 1 and 2 only.

5 Locate the **Element Size** section. Click the **Predefined** button.

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

7 Click the **Custom** button.

8 Locate the **Element Size Parameters** section.

9 Select the **Maximum element size** checkbox. In the associated text field, type `1.3`.

10 Select the **Minimum element size** checkbox. In the associated text field, type `0.11`.

11 Select the **Maximum element growth rate** checkbox.

12 Select the **Curvature factor** checkbox.

13 Select the **Resolution of narrow regions** checkbox.

14 Click **Build Selected**.

*Mapped 1*

1 In the **Mesh** toolbar, click **More Generators** and choose **Mapped**.

2 Select Boundary 58 only.

*Distribution 1*

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Edges 100 and 101 only.

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

4 In the **Number of elements** text field, type `6`.

*Distribution 2*

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Edges 99 and 282 only.

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

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

5 In the **Number of elements** text field, type `15`.

6 In the **Element ratio** text field, type `3`.

7 Click **Build Selected**.

*Mapped 2*

1 In the **Mesh** toolbar, click **More Generators** and choose **Mapped**.

2 Select Boundary 370 only.

*Distribution 1*

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Edges 694 and 696 only.

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

4 In the **Number of elements** text field, type `6`.

*Distribution 2*

1 In the **Mesh** toolbar, click  **Distribution**.

2 Select Edges 693 and 698 only.

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

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

5 In the **Number of elements** text field, type 150.

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

7 Select the **Symmetric distribution** checkbox.

8 Click  **Build Selected**.

*Mapped 3*

1 In the **Mesh** toolbar, click  **More Generators** and choose **Mapped**.

2 Select Boundary 45 only.

*Distribution 1*

1 In the **Mesh** toolbar, click  **Distribution**.

2 Select Edges 70 and 637 only.

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

4 In the **Number of elements** text field, type 6.

*Distribution 2*

1 In the **Mesh** toolbar, click  **Distribution**.

2 Select Edges 71 and 72 only.

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

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

5 In the **Number of elements** text field, type 45.

6 In the **Element ratio** text field, type 5.

7 Select the **Symmetric distribution** checkbox.

8 Click  **Build Selected**.

*Free Triangular 1*

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

2 Select Boundaries 57, 286, 364, and 365 only.

*Size 1*

1 In the **Mesh** toolbar, click **Size Attribute** and choose **Finer**.

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

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 Click the **Custom** button.

5 Locate the **Element Size Parameters** section. Select the **Maximum element size** checkbox.

6 Click in the associated text field, then press Ctrl+Space. From the menu, choose **Parameters** > **dCoolingChannel - Thickness, cooling channel - m**.

7 In the **Maximum element size** text field, type `dCoolingChannel/5`.

8 Select the **Minimum element size** checkbox. In the associated text field, type `0.32`.

9 Select the **Maximum element growth rate** checkbox.

10 Select the **Curvature factor** checkbox.

11 Select the **Resolution of narrow regions** checkbox.

12 Click **Build Selected**.

*Swept 1*

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

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

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

4 Select Domains 7–9, 39, 54, 55, and 60 only.

*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 `15`.

4 Click **Build Selected**.

*Free Tetrahedral 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Free Tetrahedral 1**.

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

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

4 From the **Selection** list, choose **Metal Hydride**.

5 Click **Build Selected**.

*Swept 2*

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

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

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

4 From the **Selection** list, choose **Hole Domains**.

*Distribution 1*

1 In the **Mesh** toolbar, click  **Distribution**.

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

3 In the **Number of elements** text field, type 4.

4 Click  **Build Selected**.

*Free Tetrahedral 2*

1 In the **Mesh** toolbar, click  **Free Tetrahedral**.

2 In the **Settings** window for **Free Tetrahedral**, click  **Build Selected**.

*Boundary Layers 1*

1 In the **Model Builder** window, click **Boundary Layers 1**.

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

3 From the **Selection** list, choose **Cooling Channel**.

*Boundary Layer Properties 1*

1 In the **Model Builder** window, expand the **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.

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

3 From the **Selection** list, choose **Cooling Channel Walls**.

4 Locate the **Layers** section. In the **Number of layers** text field, type 6.

5 In the **Thickness adjustment factor** text field, type 2.

6 Click  **Build Selected**.

*Boundary Layers 2*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** right-click **Boundary Layers 1** and choose **Duplicate**.

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

3 From the **Selection** list, choose **Metal Hydride**.

*Boundary Layer Properties 1*

1 In the **Model Builder** window, expand the **Boundary Layers 2** node, then click **Boundary Layer Properties 1**.

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

3 From the **Selection** list, choose **Metal Hydride Boundary**.

4 Locate the **Layers** section. In the **Number of layers** text field, type `5`.

5 Click **Build Selected**.

*Boundary Layer Properties 2*

In the **Model Builder** window, right-click **Boundary Layer Properties 2** and choose **Delete**.

*Boundary Layers 2*

In the **Model Builder** window, right-click **Boundary Layers 2** and choose **Build Selected**.

*Boundary Layers 3*

1 Right-click **Component 1 (comp1)** > **Mesh 1** > **Boundary Layers 2** and choose **Duplicate**.

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

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

*Boundary Layer Properties 1*

1 In the **Model Builder** window, expand the **Boundary Layers 3** node, then click **Boundary Layer Properties 1**.

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

3 From the **Selection** list, choose **Metal Hydride and Wall Boundary**.

4 Locate the **Layers** section. In the **Number of layers** text field, type `3`.

5 In the **Thickness adjustment factor** text field, type `4`.

6 Click **Build Selected**.

Compute the first study solving for the cooling flow inside the walls of the reactor.

Compute the first study that solves for the water flow inside the cooling jacket.

### STUDY 1: COOLING FLOW

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

2 In the **Settings** window for **Study**, type `Study 1: Cooling Flow` in the **Label** text field.

*Step 1: Stationary*

1 In the **Model Builder** window, under **Study 1: Cooling Flow** click **Step 1: Stationary**.

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

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Absorbed Hydrogen Atoms Per Metal Atom, XH (dode)**, **Chemistry (chem)**, **Transport of Concentrated Species in Porous Media (tcs)**, **Brinkman Equations (br)**, and **Heat Transfer in Porous Media (ht)**.

4 In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkbox for **Reacting Flow 1 (nirf1)**.

5 In the **Study** toolbar, click **= Compute**.

## RESULTS

*Streamline 1*

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

2 Right-click **Velocity (spf)** and choose **Streamline**.

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

4 From the **Selection** list, choose **Cooling Water Inflow**.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

6 In the **Tube radius expression** text field, type `0.15`.

7 Select the **Radius scale factor** checkbox.

8 Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

*Color Expression 1*

Right-click **Streamline 1** and choose **Color Expression**.

*Slice*

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

*Volume 1*

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

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

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

*Selection 1*

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

2 Select Domain 6 only.

*Material Appearance 1*

In the **Model Builder** window, right-click **Volume 1** and choose **Material Appearance**.

*Velocity (spf)*

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

2 Clear the **Plot dataset edges** checkbox.

3 In the **Velocity (spf)** toolbar, click **Plot**.

*Pressure (spf), Velocity (spf)*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Velocity (spf)** and **Pressure (spf)**.

2 Right-click and choose **Group**.

*Cooling Flow*

1 In the **Settings** window for **Group**, type `Cooling Flow` in the **Label** text field.

2 Drag and drop below **Tables**.

Add a second study that solves for the absorption.

### ADD STUDY

1 In the **Study** 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** > **Time Dependent**.

4 Click the **Add Study** button in the window toolbar.

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

### STUDY 2: ABSORPTION

In the **Settings** window for **Study**, type `Study 2: Absorption` in the **Label** text field.

*Step 1: Time Dependent*

1 In the **Model Builder** window, under **Study 2: Absorption** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `0 3600`.

4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Laminar Flow - Cooling (spf)**.

5 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

6 From the **Method** list, choose **Solution**.

7 From the **Study** list, choose **Study 1: Cooling Flow, Stationary**.

Use **Get Initial Value** to generate the default solver, and derive the initial values.

8 In the **Model Builder** window, click **Study 2: Absorption**.

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

10 Clear the **Generate default plots** checkbox.

11 In the **Study** toolbar, click **Get Initial Value**.

For a time dependent analysis it is a good practice to use manual scales for the dependent variables that has known magnitude. Give manual scales for those variables.

*Solution 2 (sol2)*

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

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.

3 In the **Model Builder** window, expand the **Study 2: Absorption** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** node, then click **Pressure (comp1.p)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Scale** text field, type `P0`.

7 In the **Model Builder** window, click **Temperature (comp1.T)**.

8 In the **Settings** window for **Field**, locate the **Scaling** section.

9 From the **Method** list, choose **Manual**.

10 In the **Scale** text field, type `T0`.

11 In the **Model Builder** window, click **Velocity Field (comp1.u)**.

12 In the **Settings** window for **Field**, locate the **Scaling** section.

13 From the **Method** list, choose **Manual**.

14 In the **Model Builder** window, click **Mass Fraction (comp1.wN2)**.

15 In the **Settings** window for **Field**, locate the **Scaling** section.

16 From the **Method** list, choose **Manual**.

17 In the **Model Builder** window, click **Dependent Variable XH (comp1.XH)**.

18 In the **Settings** window for **Field**, locate the **Scaling** section.

19 From the **Method** list, choose **Manual**.

20 In the **Model Builder** window, click **Time-Dependent Solver 1**.

21 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

22 From the **Times to store** list, choose **Steps taken by solver**.

23 In the **Store every Nth step** text field, type `4`.

24 Click to expand the **Time Stepping** section.

25 Select the **Initial step** checkbox. In the associated text field, type `0.1`.

### RESULTS

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

2 In the **Settings** window for **Results**, locate the **Update of Results** section.

3 Select the **Only plot when requested** checkbox.

4 Locate the **Save Data in the Model** section. From the **Save plot data** list, choose **On**.

#### *U, H2, pA, T, XH*

1 In the **Results** toolbar, click **3D Plot Group**.

Set up a plot group that can be used to inspect the computations while solving. An array plot is convenient as it makes it possible to study several fields at the same time.

2 In the **Settings** window for **3D Plot Group**, type `U, H2, pA, T, XH` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Absorption/ Solution 2 (sol2)**.

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

5 In the **Parameter indicator** text field, type `Time = eval(t) s`.

6 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

7 Locate the **Color Legend** section. Select the **Show titles** checkbox.

8 From the **Position** list, choose **Right double**.

9 Click to expand the **Plot Array** section. Select the **Enable** checkbox.

10 In the **Relative padding** text field, type `0.5`.

#### *spf.U*

1 In the **U, H2, pA, T, XH** toolbar, click **Surface**.

2 In the **Settings** window for **Surface**, type `spf.U` in the **Label** text field.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `Water (m/s)`.

4 From the **Color table** list, choose **Acanthaster**.

*br.U*

1 Right-click **spf.U** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Brinkman Equations** > **Velocity and pressure** > **br.U - Velocity magnitude - m/s**.

3 In the **Label** text field, type `br.U`.

4 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `Gas (m/s)`.

5 From the **Color table** list, choose **Passiflora**.

6 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

*Velocity*

1 In the **Model Builder** window, right-click **U, H2, pA, T, XH** and choose **Annotation**.

2 In the **Settings** window for **Annotation**, type `Velocity` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `Velocity`.

4 Locate the **Position** section. In the **x** text field, type `rTank*0.5`.

5 In the **z** text field, type `1.2*hTank`.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

7 From the **Anchor point** list, choose **Lower middle**.

8 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

*U, H2, pA, T, XH*

In the **U, H2, pA, T, XH** toolbar, click  **Volume**.

*Walls*

1 In the **Settings** window for **Volume**, type `Walls` in the **Label** text field.

2 Locate the **Expression** section. In the **Expression** text field, type `1`.

3 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

*Selection 1*

1 In the **U, H2, pA, T, XH** toolbar, click  **Selection**.

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

3 From the **Selection** list, choose **Tank Walls**.

*Walls*

In the **Model Builder** window, click **Walls**.

*Material Appearance 1*

1 In the **U, H2, pA, T, XH** toolbar, click **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Steel (anodized)**.

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

6 In the **U, H2, pA, T, XH** toolbar, click **Plot**.

*U, H2, pA, T, XH*

In the **U, H2, pA, T, XH** toolbar, click **Surface**.

*tcs.x_wH2*

1 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species in Porous Media** > **Species wH2** > **tcs.x_wH2 - Mole fraction - 1**.

2 In the **Label** text field, type `tcs.x_wH2`.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `x_H2 (1)`.

4 From the **Color table** list, choose **Prionace**.

*Gas Phase H2*

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

2 In the **Settings** window for **Annotation**, type `Gas Phase H2` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `Gas Phase H2`.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

*Walls 1*

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

2 In the **Settings** window for **Volume**, locate the **Plot Array** section.

3 In the **Index** text field, type `1`.

4 In the **U, H2, pA, T, XH** toolbar, click **Plot**.

*U, H2, pA, T, XH*

In the **U, H2, pA, T, XH** toolbar, click **Surface**.

*br.pA*

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

2 In the **Expression** text field, type `br.pA`.

3 In the **Label** text field, type `br.pA`.

4 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `pA (Pa)`.

5 From the **Color table** list, choose **Cividis**.

6 From the **Color table transformation** list, choose **Reverse**.

*Gas Phase H2, Walls 1*

1 In the **Model Builder** window, under **Results** > **U, H2, pA, T, XH**, Ctrl-click to select **Gas Phase H2** and **Walls 1**.

2 Right-click and choose **Duplicate**.

*Pressure*

1 In the **Settings** window for **Annotation**, type `Pressure` in the **Label** text field.

2 Locate the **Annotation** section. In the **Text** text field, type `Pressure`.

3 Locate the **Plot Array** section. In the **Index** text field, type `2`.

*Walls 1.1*

1 In the **Model Builder** window, click **Walls 1.1**.

2 In the **Settings** window for **Volume**, locate the **Plot Array** section.

3 In the **Index** text field, type `2`.

4 In the **U, H2, pA, T, XH** toolbar, click  **Plot**.

*U, H2, pA, T, XH*

In the **U, H2, pA, T, XH** toolbar, click  **Surface**.

*T*

1 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Default** > **T - Temperature - K**.

2 In the **Label** text field, type `T`.

3 Locate the **Expression** section. From the **Unit** list, choose **°C**.

4 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `T (°C)`.

5 From the **Color table** list, choose **HeatCameraLight**.

*Temperature*

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

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

3 Locate the **Annotation** section. In the **Text** text field, type `Temperature`.

4 Locate the **Plot Array** section. In the **Index** text field, type `3`.

5 In the **U, H2, pA, T, XH** toolbar, click **Plot**.

*U, H2, pA, T, XH*

In the **U, H2, pA, T, XH** toolbar, click **Surface**.

*XH*

1 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Default** > **XH - Dependent variable XH**.

2 In the **Label** text field, type `XH`.

3 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `XH (mol H/ mol M)`.

4 From the **Color table** list, choose **Cynanthus**.

*Pressure, Walls 1.1*

1 In the **Model Builder** window, under **Results** > **U, H2, pA, T, XH**, Ctrl-click to select **Pressure** and **Walls 1.1**.

2 Right-click and choose **Duplicate**.

*Hydrogen Content*

1 In the **Settings** window for **Annotation**, type `Hydrogen Content` in the **Label** text field.

2 Locate the **Annotation** section. In the **Text** text field, type `Hydrogen Content`.

3 Locate the **Plot Array** section. In the **Index** text field, type `4`.

*Walls 1.1.1*

1 In the **Model Builder** window, click **Walls 1.1.1**.

2 In the **Settings** window for **Volume**, locate the **Plot Array** section.

3 In the **Index** text field, type `4`.

4 In the **U, H2, pA, T, XH** toolbar, click **Plot**.

Compute the second study that solves for the complete system. Turn on plot while solving and select the prepared plot.

## STUDY 2: ABSORPTION

*Step 1: Time Dependent*

1 In the **Model Builder** window, under **Study 2: Absorption** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, click to expand the **Results While Solving** section.

3 Select the **Plot** checkbox.

4 From the **Plot group** list, choose **U, H2, pA, T, XH**.

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

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

**RESULTS**

*U, H2, pA, T, XH*

Set up result plots and evaluation groups. Begin with the gas phase concentrations.

**RESULT TEMPLATES**

1 In the **Home** toolbar, click **Windows** and choose **Result Templates**.

2 Go to the **Result Templates** window.

3 In the tree, select **Study 2: Absorption/Solution 2 (sol2)** > **Transport of Concentrated Species in Porous Media** > **Plot array: Concentrations, H2, N2 (tcs)**.

4 Click the **Add Result Template** button in the window toolbar.

5 In the **Results** toolbar, click **Result Templates** to close the **Result Templates** window.

**RESULTS**

*Concentrations, H2, N2 (tcs)*

1 In the **Settings** window for **3D Plot Group**, type `Concentrations, H2, N2 (tcs)` in the **Label** text field.

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

3 In the **Concentrations, H2, N2 (tcs)** toolbar, click **Plot**.

Continue with the temperature and the absorbed ratio XH.

*Temperature and XH*

1 In the **Model Builder** window, right-click **U, H2, pA, T, XH** and choose **Duplicate**.

2 In the **Model Builder** window, click **U, H2, pA, T, XH 1**.

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

*Gas Phase H2, Pressure, Velocity, Walls, Walls 1, Walls 1.1, br.U, br.pA, spf.U, tcs.x_wH2*

1 In the **Model Builder** window, under **Results** > **Temperature and XH**, Ctrl-click to select **spf.U**, **br.U**, **Velocity**, **Walls**, **tcs.x_wH2**, **Gas Phase H2**, **Walls 1**, **br.pA**, **Pressure**, and **Walls 1.1**.

2 Right-click and choose **Delete**.

*T*

1 In the **Settings** window for **Surface**, locate the **Plot Array** section.

2 Select the **Manual indexing** checkbox.

*Temperature*

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

2 In the **Settings** window for **Annotation**, locate the **Plot Array** section.

3 In the **Index** text field, type 0.

*XH*

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

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

3 Select the **Manual indexing** checkbox.

4 In the **Index** text field, type 1.

*Hydrogen Content*

1 In the **Model Builder** window, click **Hydrogen Content**.

2 In the **Settings** window for **Annotation**, locate the **Plot Array** section.

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

*Walls 1.1.1*

1 In the **Model Builder** window, click **Walls 1.1.1**.

2 In the **Settings** window for **Volume**, locate the **Plot Array** section.

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

*Selection 1*

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

2 In the **Model Builder** window, expand the **Walls 1.1.1** node, then click **Selection 1**.

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

4 Click to select the  **Activate Selection** toggle button.

5 Select Domains 3, 6, 10, 23, 26, 27, 30, 31, 34, 35, 38, and 56–59 only.

*Temperature and XH*

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

2 In the **Model Builder** window, under **Results** click **Temperature and XH**.

3 In the **Temperature and XH** toolbar, click  **Plot**.

Set up an **Evaluation Group** that can be used to illustrate the absorption process in the tank over time.

*Evaluation Group, H2 Absorption*

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

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

3 From the **Dataset** list, choose **Study 2: Absorption/Solution 2 (sol2)**.

4 In the **Label** text field, type `Evaluation Group, H2 Absorption`.

*H2 Influx*

1 Right-click **Evaluation Group, H2 Absorption** and choose **Integration** > **Surface Integration**.

2 In the **Settings** window for **Surface Integration**, type `H2 Influx` in the **Label** text field.

3 Locate the **Selection** section. From the **Selection** list, choose **Gas Inflow**.

4 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species in Porous Media** > **Species wH2** > **Fluxes** > **tcs.ntflux_wH2 - Normal total flux - kg/(m²·s)**.

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

| Expression | Unit | Description |
|---|---|---|
| `-tcs.ntflux_wH2*sectorNum` | `g/s` | `H2 Influx` |

6 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.

7 Select the **Cumulative** checkbox.

*Evaluation Group, H2 Absorption*

Right-click **H2 Influx** and choose **Volume Integration**.

*H2 Absorbed*

1 In the **Settings** window for **Volume Integration**, type `H2 Absorbed` in the **Label** text field.

2 Locate the **Selection** section. From the **Selection** list, choose **Metal Hydride**.

3 Locate the **Expressions** section. Click  **Clear Table**.

4 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species in Porous Media** > **Species wH2** > **tcs.R_wH2 - Total rate expression - kg/(m³·s)**.

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

| Expression | Unit | Description |
|---|---|---|
| `-tcs.R_wH2*sectorNum` | `g/s` | `H2 Absorbed` |

6 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.

7 Select the **Cumulative** checkbox.

*Gas phase H2 mass change*

1 In the **Model Builder** window, right-click **Evaluation Group, H2 Absorption** and choose **Integration** > **Volume Integration**.

2 In the **Settings** window for **Volume Integration**, type `Gas phase H2 mass change` in the **Label** text field.

3 Locate the **Selection** section. From the **Selection** list, choose **Flow Region**.

4 Locate the **Expressions** section. Click **Clear Table**.

5 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `tcs.epsilon_p*(tcs.rho*wH2-m0_H2)*sectorNum` | `g` | `Gas phase H2 mass change` |

*Evaluation Group, H2 Absorption*

1 In the **Model Builder** window, click **Evaluation Group, H2 Absorption**.

2 In the **Evaluation Group, H2 Absorption** toolbar, click **Evaluate**.

## EVALUATION GROUP, H2 ABSORPTION

1 Go to the **Evaluation Group, H2 Absorption** window.

2 Click the **Table Graph** button in the window toolbar.

## RESULTS

*Table Graph 1*

1 In the **Settings** window for **Table Graph**, locate the **Data** section.

2 From the **Plot columns** list, choose **Manual**.

3 In the **Columns** list, select **Cumulative integral: H2 Influx (g)**.

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

*Table Graph 2*

1 Right-click **Results** > **1D Plot Group 6** > **Table Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 In the **Columns** list, select **Cumulative integral: H2 Absorbed (g)**.

*Table Graph 3*

1 Right-click **Table Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 In the **Columns** list, select **Gas phase H2 mass change (g)**.

4 In the **1D Plot Group 6** toolbar, click **Plot**.

*H2 Absorption*

1 In the **Model Builder** window, under **Results** click **1D Plot Group 6**.

2 In the **Settings** window for **1D Plot Group**, type `H2 Absorption` in the **Label** text field.

3 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.

4 In the table, enter the following settings:

| Plot | Plot on secondary y-axis |
|---|---|
| Table Graph 1 | |
| Table Graph 3 | √ |

5 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

6 In the **H2 Absorption** toolbar, click **Plot**.

Set up another **Evaluation Group** to illustrate the temperature and increase of XH in the tank over time.

*Evaluation Group 2*

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

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

3 From the **Dataset** list, choose **Study 2: Absorption/Solution 2 (sol2)**.

*Hydride Average Temperature*

1 Right-click **Evaluation Group 2** and choose **Average** > **Volume Average**.

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

3 From the **Selection** list, choose **Metal Hydride**.

4 Locate the **Expressions** section. Click **Clear Table**.

5 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| T | degC | Hydride Average Temperature |

6 In the **Label** text field, type `Hydride Average Temperature`.

*Gas Average Temperature*

1 Right-click **Hydride Average Temperature** and choose **Duplicate**.

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

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

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

| Expression | Unit | Description |
|---|---|---|
| T | degC | Gas Average Temperature |

5 In the **Label** text field, type `Gas Average Temperature`.

*Charged XH*

1 Right-click **Gas Average Temperature** and choose **Duplicate**.

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

3 From the **Selection** list, choose **Metal Hydride**.

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

| Expression | Unit | Description |
|---|---|---|
| XH-XH0 | 1 | Charged XH |

5 In the **Label** text field, type `Charged XH`.

*Evaluation Group, Average Temperature and Charged XH*

1 In the **Model Builder** window, under **Results** click **Evaluation Group 2**.

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group, Average Temperature and Charged XH` in the **Label** text field.

3 In the **Evaluation Group, Average Temperature and Charged XH** toolbar, click **Evaluate**.

### EVALUATION GROUP, AVERAGE TEMPERATURE AND CHARGED XH

1 Go to the **Evaluation Group, Average Temperature and Charged XH** window.

2 Click the **Table Graph** button in the window toolbar.

## RESULTS

*Average Temperature and Charged XH*

1 In the **Model Builder** window, under **Results** click **1D Plot Group 7**.

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

*Table Graph 1*

1 In the **Model Builder** window, click **Table Graph 1**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Plot columns** list, choose **Manual**.

4 In the **Columns** list, choose **Hydride Average Temperature (degC)** and **Gas Average Temperature (degC)**.

5 Locate the **Legends** section. Select the **Show legends** checkbox.

*Table Graph 2*

1 Right-click **Results** > **Average Temperature and Charged XH** > **Table Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 In the **Columns** list, select **Charged XH (1)**.

*Average Temperature and Charged XH*

1 In the **Model Builder** window, click **Average Temperature and Charged XH**.

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

3 Select the **Two y-axes** checkbox.

4 In the table, select the **Plot on secondary y-axis** checkbox for **Table Graph 2**.

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

6 From the **Position** list, choose **Bottom**.

7 In the **Number of rows** text field, type 2.

8 In the **Average Temperature and Charged XH** toolbar, click  **Plot**.

Check that the results are reasonable by performing some quick calculations in a **Parameters** node. For convenience, the parameters have been added to a file. Load the text-file and enter the values from the evaluation groups.

### GLOBAL DEFINITIONS

*Control Calculations*

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Control Calculations` in the **Label** text field.

3 Locate the **Parameters** section. Click the **Load** button. From the menu, choose **Load from File**.

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

Make sure that the values for `mabsH2` and `XHcharged` correspond to the values at 3600 s in the evaluation groups.

Finally, set up graphics that illustrate the metal tank with and without metal hydride beds. Begin by adding the necessary datasets.

### RESULTS

*Study 1: Cooling Flow/Solution 1 (3) (sol1)*

In the **Results** toolbar, click **More Datasets** and choose **Solution**.

*Study 1: Cooling Flow/Solution 1 (4) (sol1)*

In the **Results** toolbar, click **More Datasets** and choose **Solution**.

*Tank Walls*

1 In the **Model Builder** window, under **Results** > **Datasets** click **Study 1: Cooling Flow/Solution 1 (3) (sol1)**.

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

3 From the **Solution** list, choose **Solution 2 (sol2)**.

4 In the **Label** text field, type `Tank Walls`.

*Selection*

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

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

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

4 From the **Selection** list, choose **Tank Walls**.

*Tank Walls, 4/8 Sectors*

1 In the **Results** toolbar, click **More Datasets** and choose **Sector 3D**.

2 In the **Settings** window for **Sector 3D**, locate the **Data** section.

3 From the **Dataset** list, choose **Tank  Walls (sol2)**.

4 Locate the **Symmetry** section. In the **Number of sectors** text field, type `8`.

5 From the **Sectors to include** list, choose **Manual**.

6 In the **Number of sectors to include** text field, type `4`.

7 Click **Plot**.

8 In the **Label** text field, type `Tank Walls, 4/8 Sectors`.

*Tank Walls, 5/8 Sectors*

1 Right-click **Tank Walls, 4/8 Sectors** and choose **Duplicate**.

2 In the **Settings** window for **Sector 3D**, type `Tank Walls, 5/8 Sectors` in the **Label** text field.

3 Locate the **Symmetry** section. In the **Number of sectors to include** text field, type `5`.

*Tank, 4/8 Sectors*

1 Right-click **Tank Walls, 5/8 Sectors** and choose **Duplicate**.

2 In the **Settings** window for **Sector 3D**, type `Tank, 4/8 Sectors` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Absorption/ Solution 2 (sol2)**.

*Tank, 5/8 Sectors*

1 Right-click **Tank, 4/8 Sectors** and choose **Duplicate**.

2 In the **Settings** window for **Sector 3D**, type `Tank, 5/8 Sectors` in the **Label** text field.

Add a plot for the tank geometry.

*Tank Geometry*

1 In the **Results** toolbar, click **3D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Tank Walls, 5/8 Sectors**.

*Surface 1*

1 In the **Tank Geometry** toolbar, click **Surface**.

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

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

*Material Appearance 1*

1 Right-click **Surface 1** and choose **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Chrome**.

5 In the **Tank Geometry** toolbar, click **Plot**.

*Tank Geometry*

1 In the **Model Builder** window, under **Results** click **Tank Geometry**.

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

3 Clear the **Plot dataset edges** checkbox.

Use a dedicated view to visualize the tank without the need to zoom repeatedly.

4 From the **View** list, choose **New view**.

5 In the **Tank Geometry** toolbar, click **Plot** to create the view. Now give it a suitable name.

6 Click **Go to Source**.

*View Tank*

1 In the **Model Builder** window, under **Results** > **Views** click **View 3D 8**.

2 In the **Settings** window for **View 3D**, type `View Tank` in the **Label** text field.

Modify the camera according to your preferences. An example of settings for the added view can be seen by opening the Application Library model.

*Tank Geometry*

1 In the **Model Builder** window, under **Results** click **Tank Geometry**.

2 In the **Tank Geometry** toolbar, click **Plot**.

Now visualize the metal hydride beds in the reactor.

*Tank Geometry with Beds*

1 Right-click **Tank Geometry** and choose **Duplicate**.

2 In the **Model Builder** window, click **Tank Geometry 1**.

3 In the **Settings** window for **3D Plot Group**, type `Tank Geometry with Beds` in the **Label** text field.

*Volume 1*

1 Right-click **Tank Geometry with Beds** and choose **Volume**.

2 In the **Settings** window for **Volume**, locate the **Data** section.

3 From the **Dataset** list, choose **Tank, 5/8 Sectors**.

4 Locate the **Expression** section. In the **Expression** text field, type `XH`.

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

*Surface 1*

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

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

3 From the **Dataset** list, choose **Tank Walls, 4/8 Sectors**.

4 In the **Tank Geometry with Beds** toolbar, click **Plot**.