Created in COMSOL Multiphysics 6.2

Phase Transformations in a Round Bar

Introduction

In this model, phase transformations in a round steel bar are analyzed using a 2D model of its cross section. The bar is initially held at 900 °C, and at this temperature, the material is in an austenitic state. A transient heat transfer analysis is performed to simulate quenching in oil, where the source austenite decomposes into different destination phases. The quenching oil is modeled using a heat flux boundary condition. The resulting phase composition and its distribution in the radial direction of the bar are shown. This is a simple model that shows how to define a set of simultaneous metallurgical phase transformations, and how to use them in a thermal analysis.

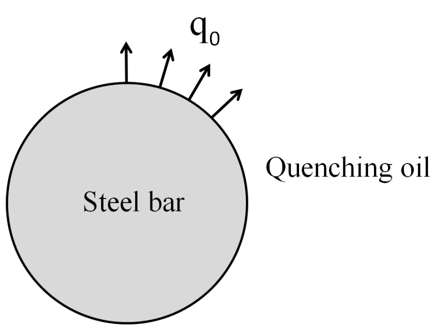

Figure 1: The 2D model of the round bar.

Model Definition

The model of the round bar is shown in Figure 2. The radius of the bar is 4 cm and a 15°-sector is considered.

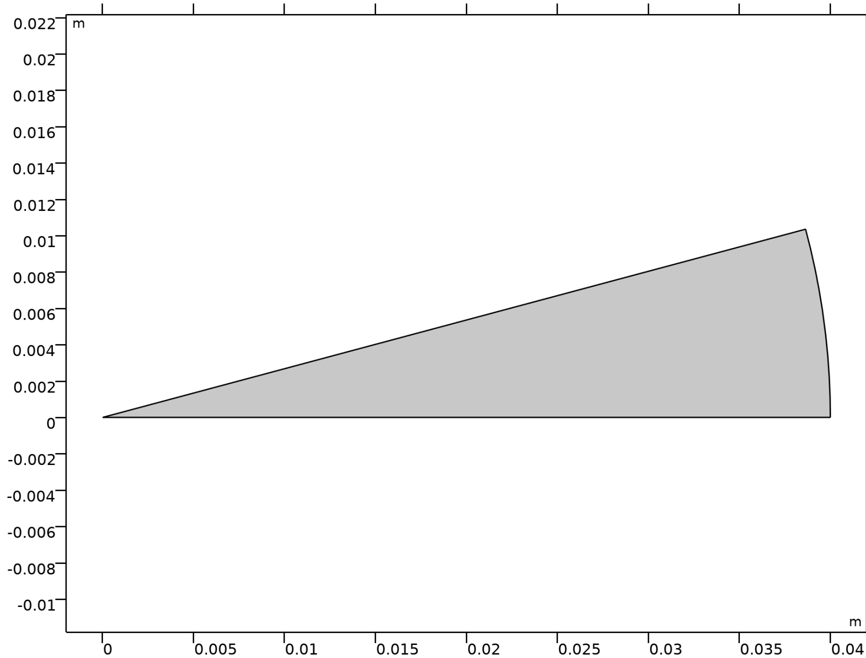

Figure 2: The 2D model of the round bar.

PHASE TRANSFORMATION ANALYSIS

When the bar is cooled from its austenitic state, several destination phases can form. The phase composition at a material point in the bar will depend on the characteristics of each possible phase transformation, together with the thermal history that the material point undergoes. In this model, we consider three phase transformations. These are listed in Table 1, where their respective type and phase transformation model are also indicated.

TABLE 1: POSSIBLE PHASE TRANSFORMATIONS.

Phase transformation	Type	Phase transformation model
Austenite to Ferrite/Pearlite	Diffusive	Leblond-Devaux
Austenite to Bainite	Diffusive	Leblond-Devaux
Austenite to Martensite	Displacive	Koistinen-Marburger

Austenite to Ferrite/Pearlite

The phase transformations from austenite to ferrite and/or pearlite is combined into a single phase transformation following Ref. 1. Because of its diffusive nature, it is modeled using the Leblond-Devaux phase transformation model. The temperature dependent functions describing the phase transformation are given in Table 2.

TABLE 2: AUSTENITE TO FERRITE / PEARLITE, TEMPERATURE DEPENDENT FUNCTIONS.

Temperature (°C)	**K (1/s)**	**L (1/s)**
600	0.0001	0
620	0.0018	0.0002
800	0	0.002

The time rate of change of the fraction of the destination phase (ferrite and pearlite), formed at the expense of the available source phase (austenite), is then given by

$$\dot{\xi}^{\mathrm{d}} = K(T)\xi^{\mathrm{s}} - L(T)\xi^{\mathrm{d}}$$

Austenite to Bainite

The phase transformation from austenite to bainite is diffusive, but in addition to being temperature dependent, also depends on the temperature rate, following Ref. 1. The temperature dependent functions are given in Table 3 and the temperature rate dependent functions in Table 4.

TABLE 3: AUSTENITE TO BAINITE, TEMPERATURE DEPENDENT FUNCTIONS.

Temperature (°C)	**F (1/s)**	**G (1/s)**
340	0	
350	0.014	
450	0.067	0
550	0	0.067

TABLE 4: AUSTENITE TO BAINITE, TEMPERATURE RATE DEPENDENT FUNCTIONS.

Temperature rate (K/h)	**H (1)**
-43000	0.2
-15000	1
-7200	1.5
-1500	0.22
-700	0.1
-70	0.0044

The time rate of change of the fraction of the destination phase (bainite), formed at the expense of the available source phase (austenite), is then given by

$$\dot{\xi}^{\mathrm{d}} = F(T)H(\dot{T})\xi^{\mathrm{s}} - G(T)H(\dot{T})\xi^{\mathrm{d}}$$

Austenite to Martensite

Unlike the diffusive phase transformations above, the martensitic phase transformation is displacive, and the fraction of formed martensite is proportional to the undercooling below the martensite start temperature M_{s}. The transformation can be well described by the Koistinen-Marburger model; see Ref. 2. The time rate of change of the destination phase (martensite) is given by

$$\dot{\xi}^{\mathrm{d}} = -\xi^{\mathrm{s}}\beta\dot{T}$$

with the parameters given in Table 5. Martensite forms at the expense of the available fraction of source phase (austenite).

TABLE 5: AUSTENITE TO MARTENSITE PARAMETERS.

Parameter	**Value**
M_{s}	370°C
β	0.011 /K

Phase Transformation Latent Heat

When the austenite decomposes into the destination phases, latent heat is released. For simplicity, the phase transformation latent heat is taken to be independent of destination phase, with the value ΔH = 670,000 kJ/m^3.

THERMAL ANALYSIS

The heat transport in the bar is described by the heat equation:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k\nabla T) = Q$$

where T is the temperature, k represents the thermal conductivity, ρ is the density, C_p denotes the specific heat capacity, and Q is a heat source, here the rate of phase transformation latent heat. The thermal conductivity, the density, and the specific heat capacity are in general temperature dependent, but in the presence of metallurgical phase transformations, they also depend on the current phase composition. For example, the thermal conductivity of austenite is different from that of ferrite, and as the fractions of these phases evolve, so will the thermal conductivity of the compound material. The material properties in the heat equation therefore represent the effective (averaged) values of the constituent phases making up the compound material at a given instant in time.

Two simplifications are made regarding the material properties of the different phases: First, the temperature dependence of the phase material properties is neglected. Second, the properties of ferrite/pearlite, bainite, and martensite are taken to be equal.

TABLE 6: MATERIAL PROPERTIES OF THE PHASES.

Phase	**Thermal conductivity (W/(m·K))**	**Density (kg/m^3)**	**Specific heat capacity (J/(kg·K))**
Austenite	25	7900	550
Ferrite/Pearlite	45	7800	700
Bainite	45	7800	700
Martensite	45	7800	700

Boundary Conditions

Quenching of the round bar is modeled by applying a convective heat flux to the boundary of the domain following

$$q_0 = h(T)(T_{\mathrm{ext}} - T)$$

where $h(T)$ is the temperature dependent heat transfer coefficient. The quenching oil is taken to be at a constant temperature T_{ext} = 80°C. The temperature dependent heat transfer coefficient is given in Table 7. The table shows that there is a distinct peak in the heat transfer coefficient which corresponds to nucleate boiling.

TABLE 7: TEMPERATURE DEPENDENT HEAT TRANSFER COEFFICIENT.

Temperature (°C)	**Heat transfer coefficient (W/(m^2·K))**	**Heat transfer mechanism**
300	200	Convection
500	3000	Nucleate boiling
650	700	Film boiling (vapor blanket)

Results and Discussion

When the steel bar is cooled by the quenching oil, the thermal history for points along the bar radius varies as shown in Figure 3. This is expected, because the heat transfer at the boundary is governed by the heat flux from the bar to the oil, while the heat transport inside the bar is controlled by the thermal diffusivity of the material. A practical implication is that even if the quenching intensity could be fully controlled, the rate of cooling of the interior of a component cannot. The distribution of the destination phases are shown in Figure 4, Figure 5, and Figure 6. Figure 7 shows the radial distribution of the destination phases. In this particular situation, the final phase composition is mainly bainitic with only a few percent ferrite/pearlite, and with the largest amount of martensite having formed at the surface of the bar.

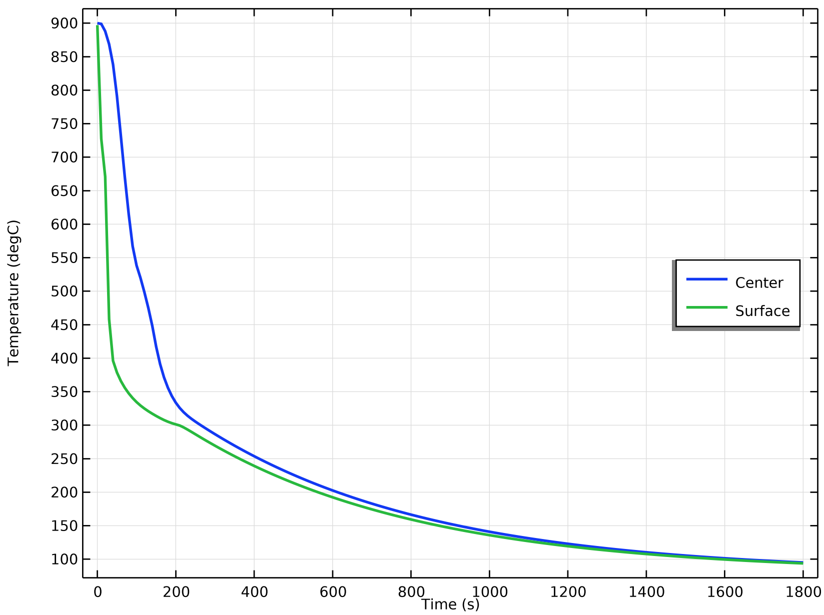

Figure 3: Temperature history at the center and at the surface of the bar.

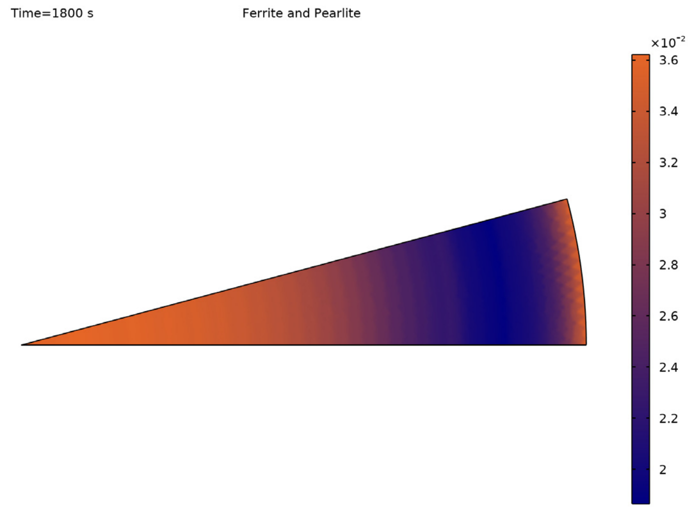

Figure 4: Fraction of ferrite / pearlite.

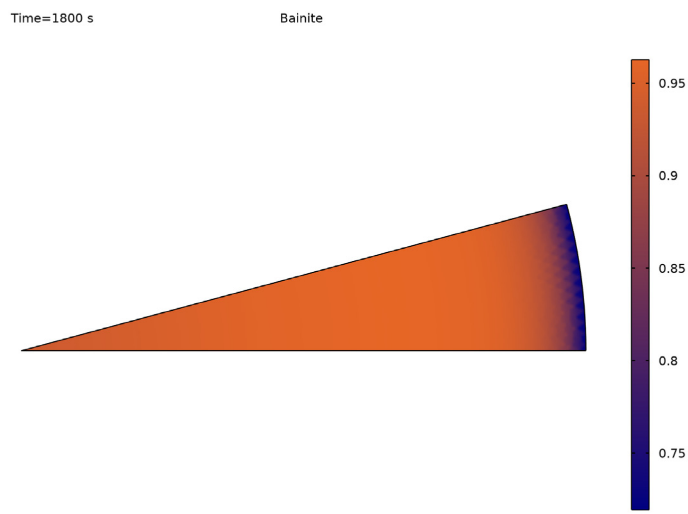

Figure 5: Fraction of bainite.

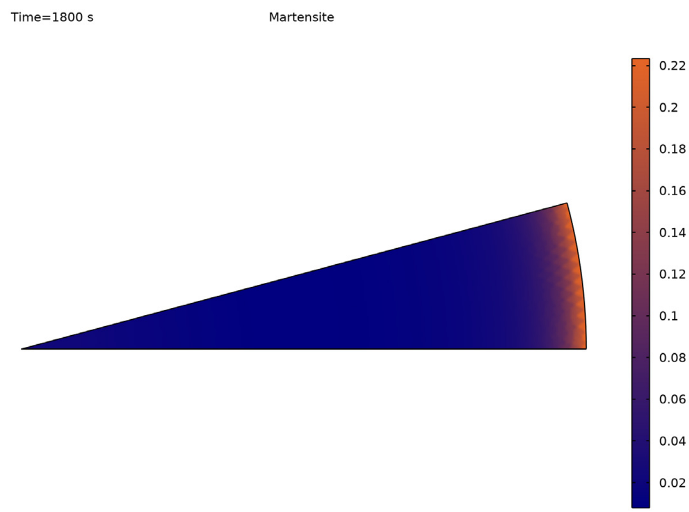

Figure 6: Fraction of martensite.

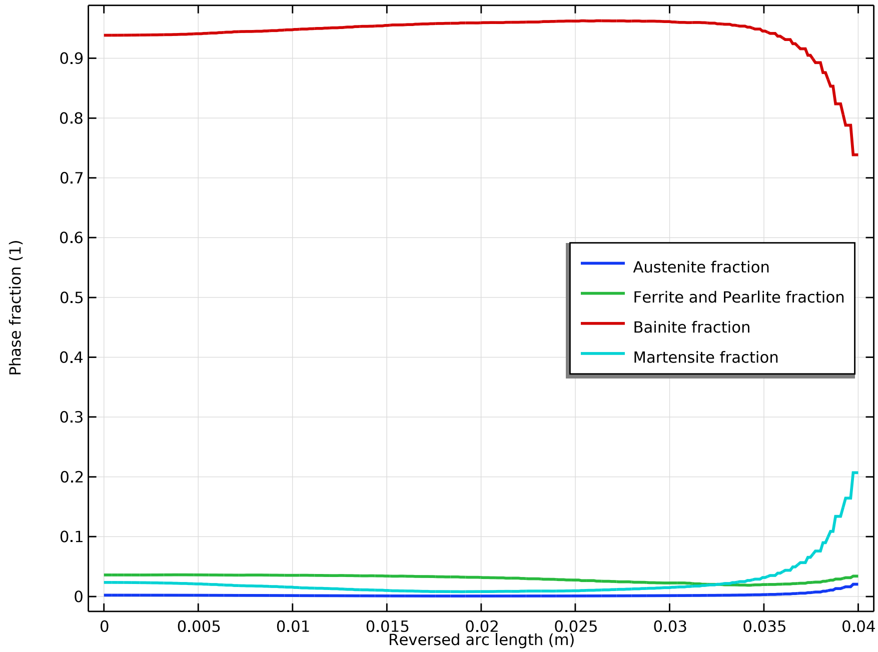

Figure 7: The radial distribution of the phase composition.

References

1. J.B. Leblond and J. Devaux, "A new kinetic model for anisothermal metallurgical transformations in steels including effect of austenite grain size," *Acta Metall.*, vol. 32, no. 1, pp. 137–146, 1984.

2. D. Koistinen and R. Marburger, "A general equation prescribing the extent of the austenite-martensite transformation in pure iron-carbon alloys and plain carbon steels," *Acta Metall.*, vol. 7, p. 59–60, 1959.

Application Library path: `Metal_Processing_Module/Tutorial_Examples/phase_transformations_in_a_round_bar`

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 **2D**.
2 In the **Select Physics** tree, select **Heat Transfer>Metal Processing> Heat Transfer with Phase Transformations**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select Study** tree, select **General Studies>Time Dependent**.
6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
3 In the table, enter the following settings:

Name	Expression	Value	Description
r	0.04[m]	0.04 m	Bar radius
latheat	670000[kJ/m^3]	6.7E8 J/m³	Phase transformation latent heat

GEOMETRY 1

Circle 1 (c1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node.
2 Right-click **Geometry 1** and choose **Circle**.
3 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
4 In the **Radius** text field, type r.
5 In the **Sector angle** text field, type 15.
6 Click **Build All Objects**.

DEFINITIONS

Interpolation 1 (int1)

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

2 Right-click **Definitions** and choose **Functions>Interpolation**.

3 In the **Settings** window for **Interpolation**, locate the **Definition** section.

4 In the **Function name** text field, type K.

5 In the table, enter the following settings:

t	f(t)
600	0.0001
620	0.0018
800	0

6 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	degC

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

Function	Unit
K	1/s

Interpolation 2 (int2)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type L.

4 In the table, enter the following settings:

t	f(t)
600	0
620	0.0002
800	0.002

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

Argument	Unit
t	degC

6 In the **Function** table, enter the following settings:

Function	Unit
L	1/s

Interpolation 3 (int3)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type F.

4 In the table, enter the following settings:

t	f(t)
340	0
350	0.014
450	0.067
550	0

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

Argument	Unit
t	degC

6 In the **Function** table, enter the following settings:

Function	Unit
F	1/s

Interpolation 4 (int4)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type G.

4 In the table, enter the following settings:

t	f(t)
450	0
550	0.067

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

Argument	Unit
t	degC

6 In the **Function** table, enter the following settings:

Function	Unit
G	1/s

Interpolation 5 (int5)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

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

4 In the table, enter the following settings:

t	f(t)
-43000	0.2
-15000	1
-7200	1.5
-1500	0.22
-700	0.1
-70	0.0044

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

Argument	Unit
t	K/h

6 In the **Function** table, enter the following settings:

Function	Unit
H	1

Interpolation 6 (int6)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

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

4 In the table, enter the following settings:

t	f(t)
300	200
500	3000
650	700

5 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

6 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	`degC`

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

Function	Unit
htc	`W/(m^2*K)`

MATERIALS

Austenite

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

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

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	25	W/(m·K)	Basic
Density	rho	7900	kg/m³	Basic
Heat capacity at constant pressure	Cp	550	J/(kg·K)	Basic

4 Right-click **Austenite** and choose **Duplicate**.

Ferrite and Pearlite

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Austenite 1 (mat2)**.

2 In the **Settings** window for **Material**, type `Ferrite and Pearlite` in the **Label** text field.

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

Property	**Variable**	**Value**	**Unit**	**Property group**
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	45	W/(m·K)	Basic
Density	rho	7800	kg/m³	Basic
Heat capacity at constant pressure	Cp	700	J/(kg·K)	Basic

4 Right-click **Ferrite and Pearlite** and choose **Duplicate**.

Bainite

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Ferrite and Pearlite 1 (mat3)**.

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

3 Right-click **Bainite** and choose **Duplicate**.

Martensite

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Bainite 1 (mat4)**.

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

METAL PHASE TRANSFORMATION (METP)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Metal Phase Transformation (metp)**.

2 In the **Settings** window for **Metal Phase Transformation**, locate the **Material Properties** section.

3 Select the **Compute effective thermal properties** check box.

4 Click **Create Compound Material** in the upper-right corner of the **Material Properties** section.

Austenite

1 In the **Model Builder** window, under **Component 1 (comp1)>Metal Phase Transformation (metp)** click **Metallurgical Phase 1**.

2 In the **Settings** window for **Metallurgical Phase**, type `Austenite` in the **Label** text field.

3 Locate the **Phase Material** section. From the **Phase material** list, choose **Austenite (mat1)**.

Ferrite and Pearlite

1 In the **Model Builder** window, under **Component 1 (comp1)> Metal Phase Transformation (metp)** click **Metallurgical Phase 2**.
2 In the **Settings** window for **Metallurgical Phase**, type `Ferrite and Pearlite` in the **Label** text field.
3 Locate the **Phase Material** section. From the **Phase material** list, choose **Ferrite and Pearlite (mat2)**.

Bainite

1 In the **Physics** toolbar, click **Domains** and choose **Metallurgical Phase**.
2 In the **Settings** window for **Metallurgical Phase**, type `Bainite` in the **Label** text field.
3 Locate the **Phase Material** section. From the **Phase material** list, choose **Bainite (mat3)**.

Martensite

1 In the **Physics** toolbar, click **Domains** and choose **Metallurgical Phase**.
2 In the **Settings** window for **Metallurgical Phase**, type `Martensite` in the **Label** text field.
3 Locate the **Phase Material** section. From the **Phase material** list, choose **Martensite (mat4)**.

Austenite to Ferrite and Pearlite

1 In the **Model Builder** window, under **Component 1 (comp1)> Metal Phase Transformation (metp)** click **Phase Transformation 1**.
2 In the **Settings** window for **Phase Transformation**, type `Austenite to Ferrite and Pearlite` in the **Label** text field.
3 Locate the **Phase Transformation** section. In the $K_{\mathrm{s}\,->\,\mathrm{d}}$ text field, type `K(metp.T)`.
4 In the $L_{\mathrm{s}\,->\,\mathrm{d}}$ text field, type `L(metp.T)`.
5 Locate the **Phase Transformation Latent Heat** section. In the $\Delta H_{\mathrm{s}\,->\,\mathrm{d}}$ text field, type `latheat`.

Austenite to Bainite

1 In the **Physics** toolbar, click **Domains** and choose **Phase Transformation**.
2 In the **Settings** window for **Phase Transformation**, type `Austenite to Bainite` in the **Label** text field.
3 Locate the **Phase Transformation** section. From the ξ^{s} list, choose **Austenite**.
4 From the ξ^{d} list, choose **Bainite**.
5 In the $K_{\mathrm{s}\,->\,\mathrm{d}}$ text field, type `F(metp.T)*H(metp.Tt)`.
6 In the $L_{\mathrm{s}\,->\,\mathrm{d}}$ text field, type `G(metp.T)*H(metp.Tt)`.

7 Locate the **Phase Transformation Latent Heat** section. In the $\Delta H_{s\,->\,d}$ text field, type `latheat`.

Austenite to Martensite

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

2 In the **Settings** window for **Phase Transformation**, type `Austenite to Martensite` in the **Label** text field.

3 Locate the **Phase Transformation** section. From the ξ^{s} list, choose **Austenite**.

4 From the ξ^{d} list, choose **Martensite**.

5 From the **Phase transformation model** list, choose **Koistinen–Marburger**.

6 In the M_s text field, type `370[degC]`.

7 Locate the **Phase Transformation Latent Heat** section. In the $\Delta H_{s\,->\,d}$ text field, type `latheat`.

MATERIALS

Compound Material (metpmat)

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

2 Select Domain 1 only.

HEAT TRANSFER IN SOLIDS (HT)

Initial Values 1

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

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

3 In the T text field, type `900[degC]`.

Symmetry 1

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

2 Select Boundaries 1 and 2 only.

Heat Flux 1

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

2 Select Boundary 3 only.

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

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

5 In the h text field, type `htc(T)`.

6 In the T_{ext} text field, type `80[degC]`.

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 **Extra fine**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** 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 `range(0,10,1800)`.

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, under **Study 1>Solver Configurations>Solution 1 (sol1)** click **Time-Dependent Solver 1**.

4 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

5 From the **Steps taken by solver** list, choose **Intermediate**.

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

RESULTS

1D Plot Group 6

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

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

3 From the **Time selection** list, choose **Last**.

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

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

Line Graph 1

1 Right-click **1D Plot Group 6** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Metal Phase Transformation>Austenite>metp.phase1.xi - Phase fraction - 1**.

3 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Reversed arc length**.

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

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

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

7 In the table, enter the following settings:

Legends
`Austenite fraction`

8 Select Boundary 2 only.

9 Right-click **Line Graph 1** and choose **Duplicate**.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

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

3 In the **Expression** text field, type `metp.phase2.xi`.

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

Legends
`Ferrite and Pearlite fraction`

5 Right-click **Line Graph 2** and choose **Duplicate**.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

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

3 In the **Expression** text field, type `metp.phase3.xi`.

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

Legends
`Bainite fraction`

5 Right-click **Line Graph 3** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

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

3 In the table, enter the following settings:

Legends
fraction

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `metp.phase4.xi`.

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

Legends
Martensite fraction

1D Plot Group 7

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

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

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

4 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Point Graph 1

1 Right-click **1D Plot Group 7** and choose **Point Graph**.

2 Select Point 1 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 From the **Unit** list, choose **degC**.

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

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

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

8 In the table, enter the following settings:

Legends
Center

Point Graph 2

1 In the **Model Builder** window, right-click **1D Plot Group 7** and choose **Point Graph**.

2 Select Point 3 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 From the **Unit** list, choose **degC**.

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

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

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

8 In the table, enter the following settings:

Legends
Surface