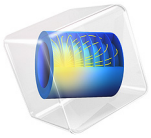

Model created in COMSOL Multiphysics 6.4

Dilatometry Curves from CCT

Introduction

Simulation of quenching of a steel component requires phase transformation data that describes how the austenite decomposes into a combination of ferrite, pearlite, bainite, and martensite. This data is generally temperature-dependent, and must be obtained from literature resources, from performing experiments, or using computational methods. Similarly, material properties are also temperature-dependent, vary between metallurgical phases, and must be obtained in some manner. This example imports computed phase transformation data and phase material properties for a general steel to compute a CCT diagram and dilatometry curves across a range of cooling rates.

Model Definition

In order to simulate phase transformations during cooling from an austenitic state, various aspects of the problem have to be accounted for. The most important aspects are discussed below.

CONTINUOUS COOLING TRANSFORMATION

In this example, a fully austenitic base structure is cooled from 900°C to room temperature, across a range of constant cooling rates. Rates from 0.001 K/s to 1000 K/s are used, in ten increments per decade.

PHASE TRANSFORMATIONS

Phase transformation data and metallurgical phase material properties for general steels can be exported from JMatPro® (Ref. 1), and imported into COMSOL Multiphysics. Every phase transformation model in the Metal Processing Module is of the general form:

$$\dot{\xi}^{\mathrm{d}} = -\dot{\xi}^{\mathrm{s}} = A_{\mathrm{s}\to\mathrm{d}}$$

where the rate term $A_{\mathrm{s}\to\mathrm{d}}$ describes the rate at which a destination phase forms at the expense of a source phase. Each built-in phase transformation model in the Metal Processing Module is of this form, and the difference between models lies in the functional form for the rate term. When phase transformations are imported, applicable phase transformation models in the Metal Processing Module are automatically configured, that is, their respective rate terms are configured using the imported data. For diffusive phase transformations, this means that the Lebond–Devaux, the Johnson–Mehl–Avrami–Kolmogorov, and the Kirkaldy–Venugopalan, simplified phase transformation models are configured (using TTT data), and for the displacive martensitic phase transformation, the Koistinen–Marburger phase transformation model is configured. For the diffusive phase

transformations, the imported data is additionally processed into a temperature-dependent interpolation function (rate term) A that makes no a-priori assumption as to an underlying phase transformation model structure. It has the form

$$\dot{\xi}^{d} = -\dot{\xi}^{s} = A\left(T, \frac{\xi^{d}}{\xi^{d}_{eq}(T)}\right)$$

where $\xi^{d}_{eq}(T)$ is the temperature-dependent equilibrium phase fraction of the destination phase. This "phase transformation model free" formulation is selected by default for diffusive phase transformations imported from JMatPro®, as it generally provides the best fit.

In this example, we use an example file from JMatPro® containing phase transformation data for a hypoeutectoid steel. Austenite decomposition into ferrite, pearlite, bainite, and martensite is included in the file that is imported.

THERMAL STRAINS

In the phase transformation physics interfaces of the Metal Processing Module, thermal strains can be computed either using thermal expansion coefficients and volume reference temperatures of the different metallurgical phases, or using temperature-dependent densities of the different metallurgical phases. In this example, we use the density-based approach. The axial thermal strain measure is defined as

$$\varepsilon_{th} = \frac{1}{3}\left(\frac{\rho}{\rho_{th}} - 1\right)$$

where ρ is the phase fraction averaged density of the steel, evaluated at the initial phase composition and the volume reference temperature, and ρ_{th} is the phase fraction averaged density of the steel, evaluated at the current phase composition and the current temperature.

This model uses an example file from JMatPro® containing phase material property data for a hypoeutectoid steel, including temperature-dependent density functions for austenite, ferrite, pearlite, bainite, and martensite.

Results and Discussion

A common way to characterize, or illustrate, the phase transformation behavior of steels is through a CCT diagram, in which each curve corresponds to the time required to reach a certain phase fraction of a certain phase, at different cooling rates. Figure 1 shows the CCT diagram resulting from the imported phase transformation data. The red curve

corresponds to 1% of ferrite having formed, and so on. The blue curve corresponds in this case effectively to the cessation of all phase transformations, as it represents the 1% line of (available) austenite.

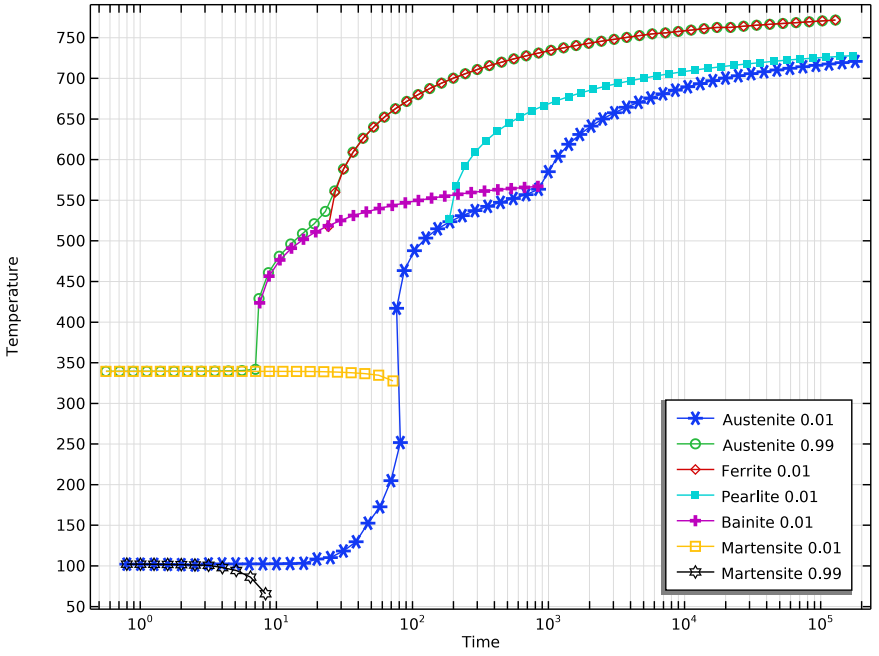

Figure 1: Computed CCT diagram based on the imported phase transformation data.

The different metallurgical phases are of different, and temperature-dependent, densities. This is shown in Figure 2. Notably, the density curve for austenite is higher than other phases, suggesting that as the steel phase transforms during cooling, there is should be a density decrease, which should manifest itself as a thermal expansion. In the figure, the evolving effective density of the steel is shown. At the highest cooling rate (1000 K/s), the austenite decomposes fully into martensite, and the figure shows how the effective density transitions from the density of pure austenite, to that of pure martensite (the black curve). The effective density curves corresponding to lower cooling rates, where the resulting phase composition is a mixture of destination phases, all originate as pure austenite, but subsequently display various kinks corresponding to different phase transformations taking place. From the effective density, a thermal strain measure can be defined. Figure 3 shows, for a selection of cooling rates, the resulting (axial) thermal strain based on the evolving effective density of the steel. Note here, that since the computation started at an elevated

temperature of 900°C, while the volume reference temperature of the phases was set to room temperature, this will appear as an initial strain (an offset).

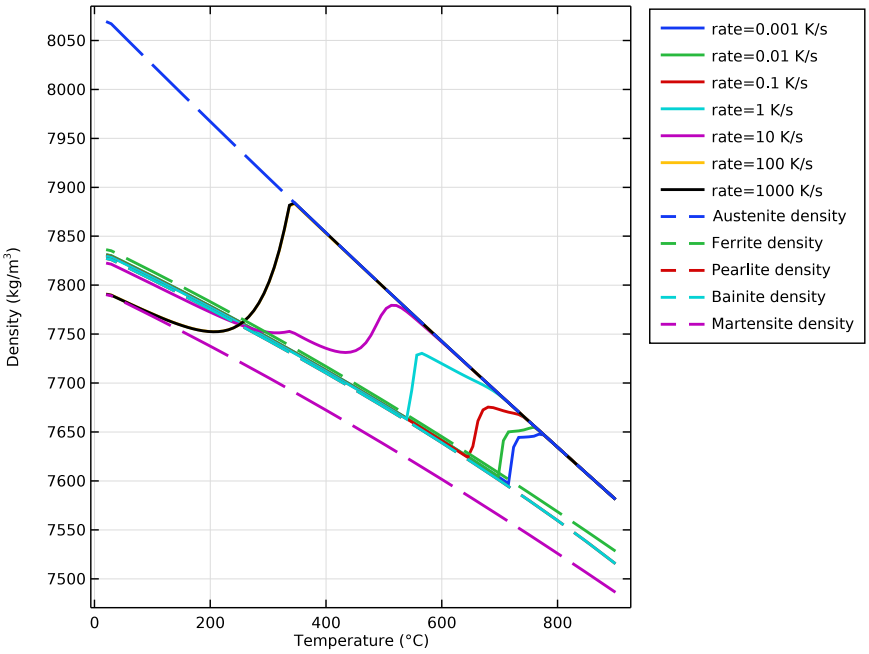

Figure 2: Temperature-dependent phase densities and the evolving effective density resulting from phase transformations, at different cooling rates.

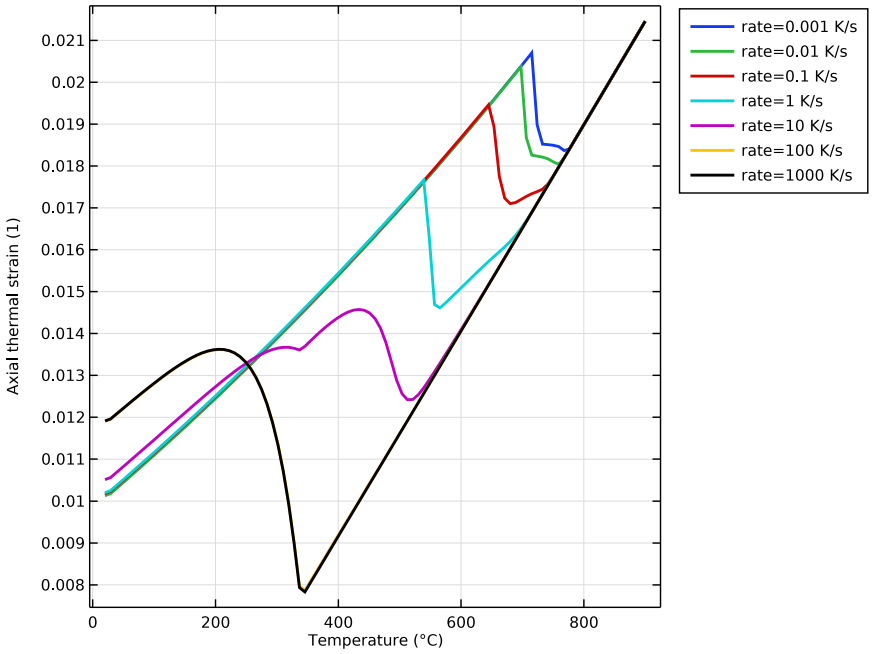

Figure 3: Axial thermal strain computed based on the evolving effective density, at different cooling rates.

Notes About the COMSOL Implementation

- The *Austenite Decomposition* is used in 0D, since we are prescribing cooling rates directly and do not model the heat transfer in a solid body.
- Phase transformation data is imported by selecting *Import Phase Transformations* in the physics interface context menu.
- Phase material properties are imported by selecting *Import Materials* from the *Materials* context menu under *Global Definitions* or under *Materials* at the component level (not available in 0D).

Reference

1. Sente Software, Ltd., United Kingdom.

Application Library path: `Metal_Processing_Module/Transformation_Diagrams/dilatometry_curves_from_cct`

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 **0D**.

2 In the **Select Physics** tree, select **Heat Transfer** > **Metal Processing** > **Austenite Decomposition (audc)**.

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
rate	1[K/s]	1 K/s	Cooling rate
Ts	900[degC]	1173.2 K	Start temperature
Tf	20[degC]	293.15 K	Finish temperature

4 In the **Materials** toolbar, click **Import Materials** and choose **Import Materials**.

5 In the **Import Materials** dialog, click **Browse**.

6 Browse to the model's Application Libraries folder and double-click the file `dilatometry_curves_from_cct_JMatPro_general_steel.xml`.

7 Click **OK**.

AUSTENITE DECOMPOSITION (AUDC)

General Steel, Austenite to Ferrite

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Austenite Decomposition (audc)** and choose **Import Phase Transformations**.

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

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

4 In the T text field, type `Ts-rate*t`.

5 Select the **Enable thermal strains** checkbox.

6 From the **Thermal strain formulation** list, choose **Density based**.

Austenite

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

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

3 From the **Phase material** list, choose **General Steel, Austenite (mat1)**.

4 Locate the **Transformation Times** section. Select the **Compute transformation times** checkbox.

5 Select the **Decreasing phase fraction** checkbox.

Ferrite

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

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

3 From the **Phase material** list, choose **General Steel, Ferrite (mat2)**.

4 Locate the **Transformation Times** section. Select the **Compute transformation times** checkbox.

Pearlite

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

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

3 From the **Phase material** list, choose **General Steel, Pearlite (mat3)**.

4 Locate the **Transformation Times** section. Select the **Compute transformation times** checkbox.

Bainite

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

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

3 From the **Phase material** list, choose **General Steel, Bainite (mat4)**.

4 Locate the **Transformation Times** section. Select the **Compute transformation times** checkbox.

Martensite

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

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

3 From the **Phase material** list, choose **General Steel, Martensite (mat5)**.

4 Locate the **Transformation Times** section. Select the **Compute transformation times** checkbox.

General Steel, Austenite to Ferrite

1 In the **Model Builder** window, click **General Steel, Austenite to Ferrite**.

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

3 From the ξ^s list, choose **Austenite**.

4 From the ξ^d list, choose **Ferrite**.

General Steel, Austenite to Pearlite

1 In the **Model Builder** window, click **General Steel, Austenite to Pearlite**.

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

3 From the ξ^s list, choose **Austenite**.

4 From the ξ^d list, choose **Pearlite**.

General Steel, Austenite to Bainite

1 In the **Model Builder** window, click **General Steel, Austenite to Bainite**.

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

3 From the ξ^s list, choose **Austenite**.

4 From the ξ^d list, choose **Bainite**.

General Steel, Austenite to Martensite

1 In the **Model Builder** window, click **General Steel, Austenite to Martensite**.

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

3 From the ξ^s list, choose **Austenite**.

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

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
rate (Cooling rate)		K/s

5 In the table, click to select the cell at row number 1 and column number 2.

6 Click **Range**.

7 In the **Range** dialog, choose **Logarithmic** from the **Entry method** list.

8 In the **Start** text field, type `1e-3`.

9 In the **Stop** text field, type `1e3`.

10 In the **Steps per decade** text field, type `10`.

11 Click **Add**.

Step 1: Time Dependent

1 In the **Model Builder** window, 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(0,0.01,1)*(Ts-Tf)/rate`.

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

Solution 1 (sol1)

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

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

3 In the **Model Builder** window, 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 **Strict**.

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

Set preferred units for result presentation.

RESULTS

Preferred Units 1

1 In the **Results** toolbar, click **Configurations** and choose **Preferred Units**.

2 In the **Settings** window for **Preferred Units**, locate the **Units** section.

3 Click **Add Physical Quantity**.

4 In the **Physical Quantity** dialog, select **General** > **Temperature (K)** in the tree.

5 Click **OK**.

6 In the **Settings** window for **Preferred Units**, locate the **Units** section.

7 In the table, enter the following settings:

Quantity	Unit	Preferred unit
Temperature	K	°C

8 Click **Apply**.

Axial Thermal Strain (audc)

1 In the **Model Builder** window, under **Results** click **Axial Thermal Strain (audc)**.

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

3 From the **Parameter selection (rate)** list, choose **From list**.

4 In the **Parameter values (rate (K/s))** list, choose **0.001**, **0.01**, **0.1**, **1**, **10**, **100**, and **1000**.

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

Global 1

1 In the **Model Builder** window, expand the **Axial Thermal Strain (audc)** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click to expand the **Coloring and Style** section.

3 From the **Width** list, choose **2**.

4 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

5 In the **Axial Thermal Strain (audc)** toolbar, click **Plot**.