Created in COMSOL Multiphysics 6.2

Transformation Diagram Computation

Introduction

During quenching of steel, the austenite decomposes into destination phases such as ferrite, pearlite, bainite, and martensite. The resulting phase composition depends to a large extent on the temperature history, and also on the chemical composition and austenite grain size. A common way to illustrate the phase transformation characteristics is to use transformation diagrams. Two of the most commonly used diagram types are the CCT (continuous cooling transformation) and the TTT (time-temperature transformation) diagrams. In the former, the austenitized material is cooled at a constant temperature rate, while in the latter, the material is kept at a constant temperature. Figure 1 shows an example CCT diagram, with temperature on the vertical axis, and logarithmic time on the horizontal. F_s, P_s, and B_s represent the start temperatures, at a given cooling rate, for the formation of, respectively, ferrite, pearlite, and bainite. The example CCT diagram shows that a cooling rate of 10 K/s is sufficient to suppress the formation of pearlite, whereas 1 K/s is not.

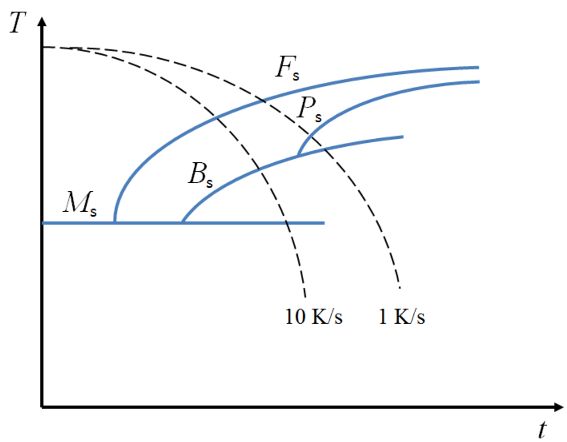

Figure 1: A CCT diagram.

A TTT diagram differs from a CCT diagram in that the austenite is rapidly cooled to a given initial temperature T_0, and then kept at that temperature, see Figure 2. This is performed for a range of start temperatures, and the transformation curves are constructed from the different times required to form a given phase. In a practical quenching situation, it is unlikely that material points will experience either of the two temperature histories that the CCT and TTT diagrams use, and instead experience varying temperature rates.

Nevertheless, the diagrams can give useful insights into the phase transformation behavior of a certain material.

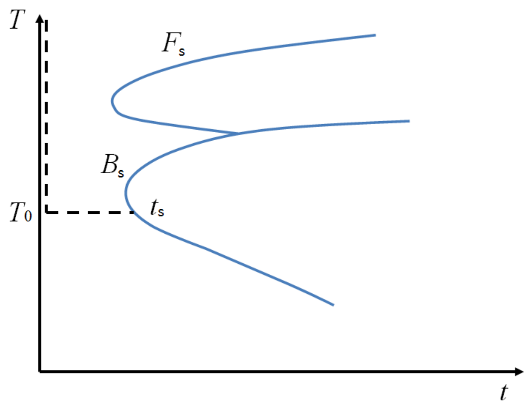

Figure 2: A TTT diagram.

In this model, CCT and TTT diagrams are constructed from a set of phase-transformation model data using the methods described above.

Model Definition

In order to compute transformation diagrams, no geometry is required, and suitable temperature histories can be accomplished without the need for a full heat-transfer analysis. The temperature is imposed as a parameter in the analysis. A number of parameters are used to compute the CCT and TTT diagrams. The diagrams are computed over a range of temperatures bounded by a lowest and a highest temperature. In the case of the CCT diagram computation, the cooling rate is additionally bounded by a lowest and a highest rate. The time-temperature combinations that illustrate the start of transformation in the CCT and TTT diagrams are obtained when a given phase reaches a defined (small) fraction. Table 1 shows these parameters.

TABLE 1: PARAMETERS USED IN THE MODEL DEFINITION.

Name	**Value**	**Description**
`highT`	900 °C	Highest transformation temperature
`lowT`	100 °C	Lowest transformation temperature
`startFraction`	0.01	Phase fraction indicating transformation start

TABLE 1: PARAMETERS USED IN THE MODEL DEFINITION.

Name	Value	Description
highRate	100 K/s	Highest cooling rate for CCT
lowRate	0.01 K/s	Lowest cooling rate for CCT

PHASE TRANSFORMATIONS

For simplicity, the model only considers austenite decomposition into a combination of ferrite and bainite, but it can straightforwardly be extended to include other destination phases as well.

Austenite to Ferrite

The phase transformation is modeled using the Leblond-Devaux phase transformation model. The temperature dependent functions describing this transformation are given in Table 2.

TABLE 2: AUSTENITE TO FERRITE, TEMPERATURE DEPENDENT FUNCTIONS.

Temperature (°C)	K (1/s)	L (1/s)
550	0	
600		0
620	0.002	0.0002
700	0.001	
750	0	
800		0.002
1000		0.002

Austenite to Bainite

The phase transformation is modeled using the Leblond–Devaux phase transformation model. Compared to the ferritic transformation, the bainitic transformation is active at lower temperatures. The temperature dependent functions describing the bainitic transformation are given in Table 3.

TABLE 3: AUSTENITE TO BAINITE, TEMPERATURE DEPENDENT FUNCTIONS.

Temperature (°C)	K (1/s)	L (1/s)
380	0	
400	0.0005	0
490	0.005	
500		0.0002

TABLE 3: AUSTENITE TO BAINITE, TEMPERATURE DEPENDENT FUNCTIONS.

Temperature (°C)	**K (1/s)**	**L (1/s)**
580	0.00005	0.002
600	0	0.002

Note that the tabulated values are example values that define ferritic and bainitic transformations. Variations in alloying elements of the steel would cause the functions to be different.

Results and Discussion

The computed CCT is shown in Figure 3. Three cooling curves are shown, corresponding to the cooling rates 100 K/s, 10 K/s, and 1 K/s. The CCT diagram shows the time and temperature when a phase begins to form, given a cooling rate. In this example, a cooling rate of 10 K/s causes bainite to form after about 40 seconds, and at a temperature of 520 °C. At a rate of 100 K/s, neither ferrite nor bainite form. Note that in practice, this type of very rapid cooling would be used to obtain a martensitic structure, because the martensitic transformation only depends on the undercooling below the martensite start temperature, and not on time. The diffusionless martensitic transformation is not considered here.

If an experimentally obtained CCT diagram exists, it can be compared to the computed version to calibrate and verify the temperature dependent functions that describe each phase transformation. What complicates any calibration procedure is that the formation of one destination phase (such as ferrite) reduces the available fraction of source phase (austenite) to form other destination phases (such as bainite). The phase transformations are intrinsically coupled, and it is difficult to treat one phase transformation separate from another. An experimentally obtained CCT diagram is therefore best compared to a computed CCT diagram that includes all relevant phase transformations.

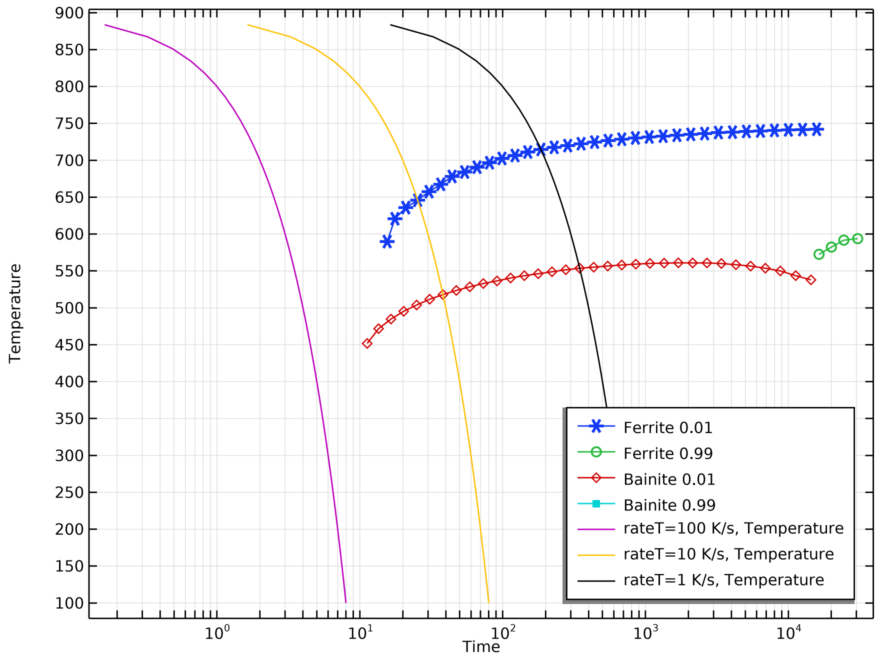

Figure 3: Computed CCT diagram showing the curves for 1% formed fraction of ferrite and bainite.

The computed TTT diagram is shown in Figure 4. Unlike the CCT diagram, the TTT diagram is more straightforwardly used to calibrate phase transformation models. In contrast, the CCT diagram is more likely to realistically represent a quenching process. During a process of constant temperature, a certain phase transformation can be calibrated more easily, as the temperature dependent functions in Table 2 and Table 3 become constants. The CCT and TTT diagrams are computed using the same set of data for the phase transformations involved.

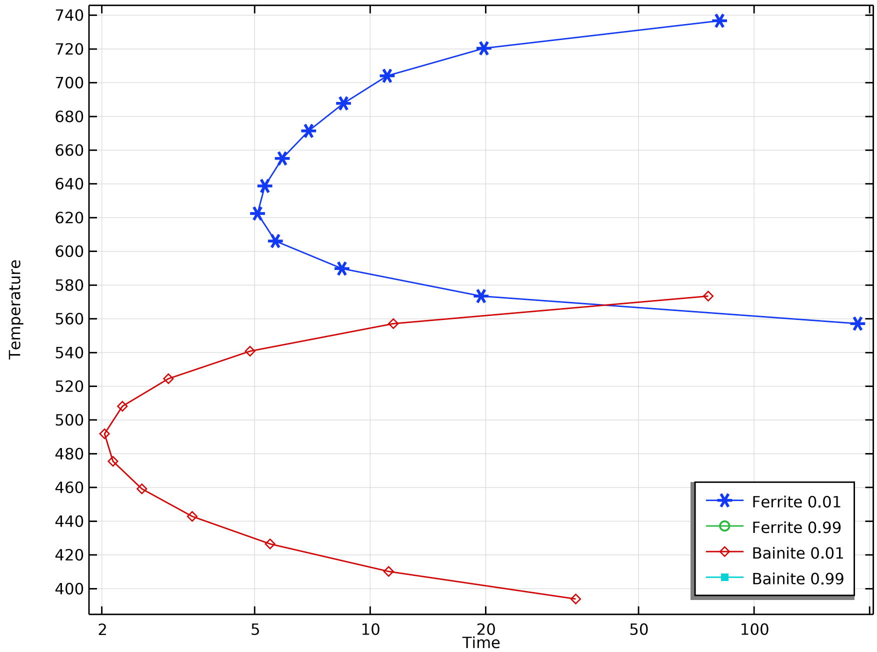

Figure 4: Computed TTT diagram showing the curves for 1% formed fraction of ferrite and bainite.

Reference

1. B. Liscic, H.M. Tensi, L.C.F. Canale, and G.E. Totten (Eds.), "Quenching theory and technology," *CRC Press, Taylor & Francis Group*, 2010.

Application Library path: `Metal_Processing_Module/Transformation_Diagrams/transformation_diagram_computation`

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 Click **Load from File**.
4 Browse to the model's Application Libraries folder and double-click the file `transformation_diagram_computation_parameters.txt`.

DEFINITIONS

Add two definitions for the temperature used in the CCT and TTT computations.

CCT

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.
2 Right-click **Definitions** and choose **Variables**.
3 In the **Settings** window for **Variables**, type `CCT` in the **Label** text field.
4 Locate the **Variables** section. In the table, enter the following settings:

Name	**Expression**	**Unit**	**Description**
`T`	`T0-rateT*t`	K	`Temperature for CCT`

TTT

1 Right-click **Definitions** and choose **Variables**.
2 In the **Settings** window for **Variables**, type `TTT` in the **Label** text field.
3 Locate the **Variables** section. In the table, enter the following settings:

Name	**Expression**	**Unit**	**Description**
`T`	`T0`	K	`Temperature for TTT`

Interpolation 1 (int1)

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 `K_Austenite_to_Ferrite`.

4 Click **Load from File**.

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

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

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

Argument	Unit
t	degC

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

Function	Unit
K_Austenite_to_Ferrite	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_Austenite_to_Ferrite`.

4 Click **Load from File**.

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

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

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

Argument	Unit
t	degC

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

Function	Unit
L_Austenite_to_Ferrite	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 `K_Austenite_to_Bainite`.

4 Click **Load from File**.

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

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

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

Argument	Unit
t	degC

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

Function	Unit
K_Austenite_to_Bainite	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 `L_Austenite_to_Bainite`.

4 Click **Load from File**.

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

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

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

Argument	Unit
t	degC

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

Function	Unit
L_Austenite_to_Bainite	1/s

AUSTENITE DECOMPOSITION (AUDC)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Austenite Decomposition (audc)**.

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

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

Ferrite

1 In the **Model Builder** window, under **Component 1 (comp1)> Austenite Decomposition (audc)** click **Ferrite**.

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

3 Select the **Compute transformation times** check box.

Bainite

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

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

3 Select the **Compute transformation times** check box.

Austenite to Ferrite

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

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

3 In the $K_{\mathrm{s} \rightarrow \mathrm{d}}$ text field, type `K_Austenite_to_Ferrite(audc.T)`.

4 In the $L_{\mathrm{s} \rightarrow \mathrm{d}}$ text field, type `L_Austenite_to_Ferrite(audc.T)`.

Austenite to Bainite

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

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

3 In the $K_{\mathrm{s} \rightarrow \mathrm{d}}$ text field, type `K_Austenite_to_Bainite(audc.T)`.

4 In the $L_{\mathrm{s} \rightarrow \mathrm{d}}$ text field, type `L_Austenite_to_Bainite(audc.T)`.

Austenite to Pearlite

In the **Model Builder** window, right-click **Austenite to Pearlite** and choose **Disable**.

Pearlite

In the **Model Builder** window, right-click **Pearlite** and choose **Disable**.

Austenite to Martensite

In the **Model Builder** window, right-click **Austenite to Martensite** and choose **Disable**.

Martensite

In the **Model Builder** window, right-click **Martensite** and choose **Disable**.

CCT

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

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

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

5 In the table, enter the following settings:

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

6 Click **Range**.

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

8 In the **Start** text field, type `highRate`.

9 In the **Stop** text field, type `lowRate`.

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

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 Click **Range**.

4 In the **Range** dialog box, choose **Number of values** from the **Entry method** list.

5 In the **Stop** text field, type `(T0-lowT)/rateT`.

6 In the **Number of values** text field, type `50`.

7 Click **Replace**.

8 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

9 Select the **Modify model configuration for study step** check box.

10 In the tree, select **Component 1 (comp1)>Definitions>TTT**.

11 Right-click and choose **Disable**.

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

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 **Add Study** in the window toolbar.

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

TTT

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

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

Parametric Sweep

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

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

3 From the **Sweep type** list, choose **All combinations**.

4 Click **+ Add**.

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

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T0 (Cooling temperature parameter)		K

7 Click **Range**.

8 In the **Range** dialog box, choose **Number of values** from the **Entry method** list.

9 In the **Start** text field, type `highT`.

10 In the **Stop** text field, type `lowT`.

11 In the **Number of values** text field, type `nTemps`.

12 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,maxTime/99,maxTime)`.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

5 In the tree, select **Component 1 (comp1)>Definitions>CCT**.

6 Right-click and choose **Disable**.

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

RESULTS

Global 5

1 In the **Model Builder** window, expand the **Results>Transformation Diagram (audc)** node.

2 Right-click **Transformation Diagram (audc)** and choose **Global**.

3 In the **Settings** window for **Global**, locate the **Data** section.

4 From the **Dataset** list, choose **CCT/Parametric Solutions 1 (sol2)**.

5 From the **Parameter selection (rateT)** list, choose **From list**.

6 In the **Parameter values (rateT (K/s))** list, select **100**.

7 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
audc.T	degC	Temperature

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

9 Right-click **Global 5** and choose **Duplicate**.

Global 6

1 In the **Model Builder** window, click **Global 6**.

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

3 In the **Parameter values (rateT (K/s))** list, select **10**.

4 Right-click **Global 6** and choose **Duplicate**.

Global 7

1 In the **Model Builder** window, click **Global 7**.

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

3 In the **Parameter values (rateT (K/s))** list, select **1**.

4 In the **Transformation Diagram (audc)** toolbar, click **Plot**.

Global 1

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

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

3 In the table, enter the following settings:

Expression	Unit	Description
`audc.phase2.temperature_1`	`degC`	`Temperature 1`

Change the temperature unit to degrees Celsius in the remaining CCT plots as well.

Change the temperature unit to degrees Celsius in the TTT plots.

Global 1

1 In the **Model Builder** window, expand the **Transformation Diagram (audc) 1** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`audc.phase2.temperature_1`	`degC`	`Temperature 1`

Global 3

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

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

3 In the table, enter the following settings:

Expression	Unit	Description
`audc.phase4.temperature_1`	`degC`	`Temperature 1`

4 In the **Transformation Diagram (audc) 1** toolbar, click **Plot**.