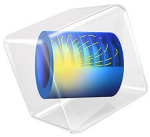

Calibration Against TTT Data

Introduction

During component quenching, austenite decomposes into a combination of other phases such as ferrite, pearlite, bainite, and martensite. The final phase composition inside a quenched component depends on the thermal history during cooling, and also on the alloying of the steel itself. The variations in quenching characteristics between steels can be significant, and each steel has to be characterized with respect to how phase transformations occur during a thermal transient. A common way to illustrate the phase transformation characteristics is through 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 CCT case, the austenitized material is cooled at varying constant temperature rates, and fractions of the emerging phases formed are plotted as points in time-temperature space. In the TTT case, the material is first rapidly cooled, and than held at a constant temperature. Figure 1 shows a schematic of a TTT diagram, in which a single phase transformation is considered. It is customary to plot a curve denoting the start of formation of the destination phase, in this case when the destination phase reaches a fraction of 1%. In other words, the curve shows the time it takes, at a fixed temperature, to form 1% of the destination phase. To complete the diagram, other curves are typically included. In this example, the 50% and 90% curves are also drawn. When several curves are used, phase transformation models can be readily fitted for the isothermal case.

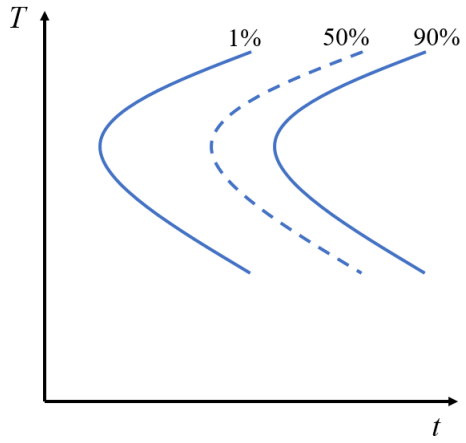

Figure 1: A TTT diagram.

In this model, TTT diagram data is used to calibrate the Johnson–Mehl–Avrami–Kolmogorov (JMAK) phase transformation model. Using the calibration result, a TTT diagram is computed and compared to the original TTT diagram data.

Model Definition

This model considers a set of experimental TTT data for a single phase transformation. The data is given in Table 1. The table shows, for each temperature, the times it takes to form 1%, 50%, and 90% of the phase.

TABLE 1: EXPERIMENTAL TTT DATA.

Temperature (K)	Time to 1% (s)	Time to 50% (s)	Time to 90% (s)
853	320	1100	1530
893	210	735	1020
933	180	620	860
973	210	710	990
1013	420	1450	2000

In order to calibrate a phase transformation model to this experimental data, no geometry is required, and the temperature field can be replaced by a temperature parameter. For each temperature in Table 1, a least-squares problem is solved to find a set of phase transformation model parameters such that the evolution of the phase fraction matches the experimental data.

PHASE TRANSFORMATION

The model only considers a single phase transformation, and it is described by the JMAK model. This model requires three parameters:

- An equilibrium phase fraction ξ_{eq}
- A time constant τ
- An Avrami exponent n

In general, all these parameters can be used to calibrate the phase transformation against experimental data, but this model considers a special case where the phase fraction tends toward one, and where the Avrami exponent is considered constant and equal to three. For each temperature under consideration, the goal is to find the value of τ that produces the best least squares fit. The JMAK model is integrated using a time-dependent study step, and the phase fraction of the forming phase (the destination phase) can then be schematically expressed as $\xi(t,\tau)$, where t is time, and τ is the time constant.

OPTIMIZATION

The purpose of the optimization, at a given temperature, is to find the optimal value for the phase transformation model parameter τ such that the phase fraction, that evolves over time, best reproduces the experimental data. An objective function can be expressed as

$$\theta = \sum_{k=1}^{N} \left(\frac{\xi(t_k, \tau)}{\xi_k} - 1 \right)^2$$

where the experimental data is given by N points, t_k is the time at which ξ_k of the phase has formed. This objective function is minimized for each temperature to find τ.

Results and Discussion

The purpose of calibrating phase transformation models is to be able to use them to describe phase transformations that occur, for example, during component quenching. In this example, the JMAK phase transformation model was calibrated against TTT data. The result from the calibration procedure is the temperature-dependent parameter τ. The parameter is shown in Figure 2. The figure shows that the value of τ is high toward the ends of the temperature range, and smaller in the center of the range. The parameter τ represents a characteristic time for phase transformation, and the experimental data confirms that the phase transformation is most rapid at the intermediate temperatures. When the calibrated phase transformation model is used to compute a TTT diagram, you can compare the resulting diagram to the experimental (input) data. This is done in Figure 3. By merely using τ as a fitting parameter, the 1%, 50%, and 90% lines are reproduced well. For an even better fit to the experimental data, the Avrami exponent, here considered a constant, could be added as a free parameter of the optimization problem.

The methodology in this example can be used sequentially to calibrate several phase transformation models, one phase transformation at a time. A natural next step, once every relevant phase transformation has been characterized, is to simulate continuous cooling, and produce a CCT diagram. Good agreement between a computed CCT diagram with its experimental counterpart may require adjusting the phase transformation model parameters.

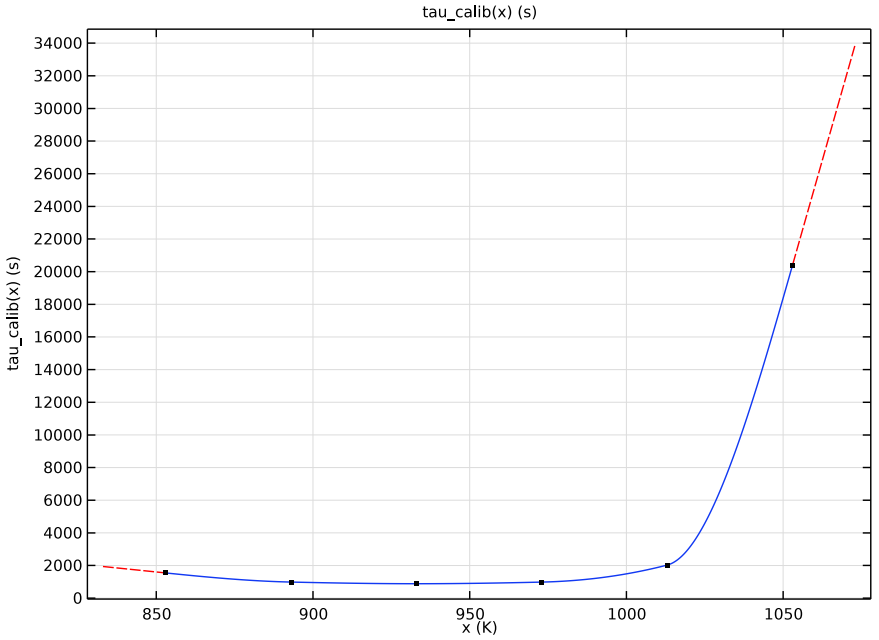

Figure 2: The temperature dependent phase transformation model parameter τ.

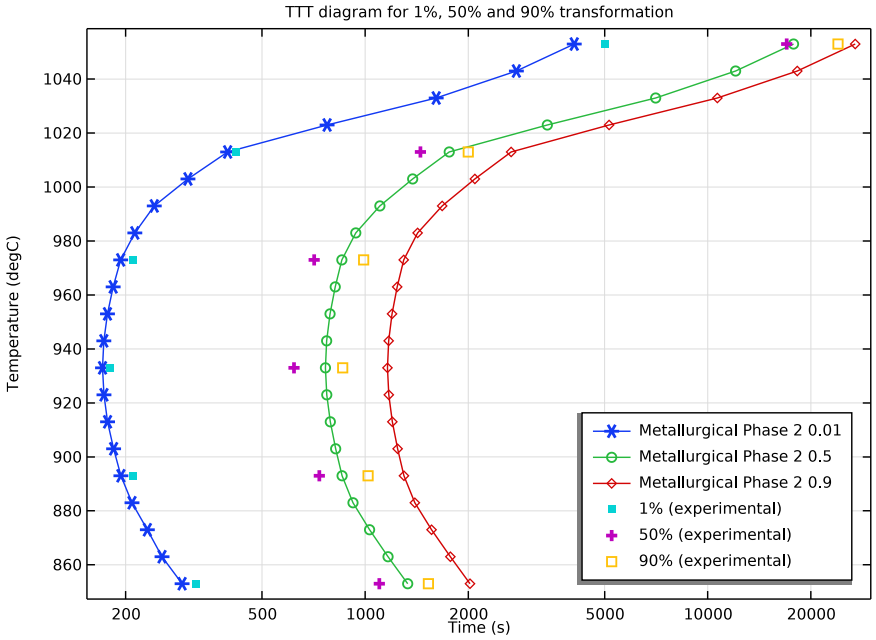

Figure 3: Comparison of the computed TTT diagram and experimental data, for the 1%, 50% and 90% lines.

Application Library path: `Metal_Processing_Module/Transformation_Diagrams/calibration_against_ttt_data`

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> Metal Phase Transformation (metp)**.

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
xieq	1	1	Equilibrium phase fraction
tau	1[s]	1 s	Time constant
n	3	3	Avrami exponent
Tsw	1[K]	1 K	Temperature sweep parameter
T	1[K]	1 K	Temperature

METAL PHASE TRANSFORMATION (METP)

Metallurgical Phase 2

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**, locate the **Transformation Times** section.

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

4 In the table, enter the following settings:

Target phase fractions (1)
0.01
0.5

5 Click **Add**.

6 In the table, enter the following settings:

Target phase fractions (1)
0.01
0.5
0.9

Phase Transformation 1

1 In the **Model Builder** window, click **Phase Transformation 1**.

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

3 From the **Phase transformation model** list, choose **Johnson–Mehl–Avrami–Kolmogorov (JMAK)**.

4 In the ξ_{eq}^{d} text field, type `xieq`.

5 In the $\tau_{s \rightarrow d}$ text field, type `tau`.

6 In the $n_{s \rightarrow d}$ text field, type `n`.

COMPONENT 1 (COMP1)

Global Least-Squares Objective 1

1 In the **Physics** toolbar, click **Optimization** and choose **Parameter Estimation**.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Experimental Data** section.

3 In the **Filename** text field, type `calibration_against_ttt_data_ttt001.txt`.

4 Click **Import**.

5 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 2.

6 In the table, enter the following settings:

Columns	Type	Settings
Column 1	Parameter	Name=T
Column 2	Value	Model expression=1, Variable name=col2
Column 3	Value	Model expression=1, Variable name=col3

7 From the **Name** list, choose **T (Temperature)**.

8 In the **Unit** text field, type K.

9 In the table, click to select the cell at row number 3 and column number 2.

10 In the table, enter the following settings:

Columns	Type	Settings
Column 1	Parameter	Name=T
Column 2	Time	Time unit=s
Column 3	Value	Model expression=metp.phase2.xi, Variable name=col3

11 In the **Model expression** text field, type `metp.phase2.xi`.

12 In the **Variable name** text field, type `col3a`.

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

14 In the **Scale value** text field, type `0.01`.

15 Right-click **Global Least-Squares Objective 1** and choose **Duplicate**.

Global Least-Squares Objective 2

1 In the **Model Builder** window, click **Global Least-Squares Objective 2**.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Experimental Data** section.

3 Find the **Data imported into model** subsection. Click **Discard**.

4 In the **Filename** text field, type `calibration_against_ttt_data_ttt050.txt`.

5 Click  **Import**.

6 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 3 and column number 2.

7 In the **Variable name** text field, type `col3b`.

8 In the **Scale value** text field, type `0.5`.

9 Right-click **Global Least-Squares Objective 2** and choose **Duplicate**.

Global Least-Squares Objective 3

1 In the **Model Builder** window, click **Global Least-Squares Objective 3**.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Experimental Data** section.

3 Find the **Data imported into model** subsection. Click **Discard**.

4 In the **Filename** text field, type `calibration_against_ttt_data_ttt090.txt`.

5 Click  **Import**.

6 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 3 and column number 2.

7 In the **Variable name** text field, type `col3c`.

8 In the **Scale value** text field, type `0.9`.

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(0,50,28000)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `0.001`.

6 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

7 Click + **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T (Temperature)	Tsw	K

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
Tsw (Temperature sweep parameter)	853 893 933 973 1013 1053	K

Parameter Estimation

1 In the **Study** toolbar, click **Optimization** and choose **Parameter Estimation**.

2 In the **Settings** window for **Parameter Estimation**, locate the **Experimental Data** section.

3 From the **Data source** list, choose **Selected Least-Squares objectives**.

4 Locate the **Objective Function** section. In the table, select the **Active** check boxes for **Global Least-Squares Objective 1**, **Global Least-Squares Objective 2**, and **Global Least-Squares Objective 3**.

5 Locate the **Estimated Parameters** section. Click + **Add**.

6 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
tau (Time constant)	2000[s]	1000	700[s]	28000[s]

7 Locate the **Parameter Estimation Method** section. Find the **Solver settings** subsection. From the **Least-squares time/parameter method** list, choose **Merge within manual range**.

8 In the **Optimality tolerance** text field, type `0.0001`.

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

RESULTS

Parameter estimation, Parameter estimation 1, Parameter estimation 2, Phase Composition (metp), Transformation Diagram (metp)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Phase Composition (metp)**, **Transformation Diagram (metp)**, **Parameter estimation**, **Parameter estimation 1**, and **Parameter estimation 2**.

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

Evaluation Group 1

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 1/Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (t, T)** list, choose **Last**.

Global Evaluation 1

1 Right-click **Evaluation Group 1** and choose **Global Evaluation**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
tau	s	Time constant

4 In the **Evaluation Group 1** toolbar, click **Evaluate**.

You can now save the calibrated values into a text file, for example into a file called calibration_against_ttt_data_tau_calib.txt.

Table 1

1 In the **Results** toolbar, click **Data** and choose **Table**.

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

3 From the **Source** list, choose **Evaluation group**.

4 Locate the **Output** section. In the **Filename** text field, type `calibration_against_ttt_data_tau_calib.txt`.

DEFINITIONS

Interpolation 1 (int1)

1 In the **Home** toolbar, click **Functions** and choose **Local>Interpolation**.

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

3 From the **Data source** list, choose **File**.

Assuming that the calibrated values for the phase transformation model have been stored in a file, the values can be imported as an interpolation function.

4 Click **Browse**.

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

6 In the **Number of arguments** text field, type 1.

7 Find the **Functions** subsection. In the table, enter the following settings:

Function name	Position in file
tau_calib	4

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

9 From the **Extrapolation** list, choose **Linear**.

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

Argument	Unit
Column 1	K

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

Function	Unit
tau_calib	s

12 Click **Plot**.

13 Click **Plot**.

ADD PHYSICS

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

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

3 In the tree, select **Recently Used>Metal Phase Transformation (metp)**.

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

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

METAL PHASE TRANSFORMATION 2 (METP2)

Metallurgical Phase 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Metal Phase Transformation 2 (metp2)** click **Metallurgical Phase 2**.

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

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

4 In the table, enter the following settings:

Target phase fractions (1)
0.01
0.5

5 Click **Add**.

6 In the table, enter the following settings:

Target phase fractions (1)
0.01
0.5
0.9

7 In the **Model Builder** window, click **Metal Phase Transformation 2 (metp2)**.

8 In the **Settings** window for **Metal Phase Transformation**, locate the **Temperature** section.

9 In the T text field, type T.

Phase Transformation 1

1 In the **Model Builder** window, click **Phase Transformation 1**.

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

3 From the **Phase transformation model** list, choose **Johnson–Mehl–Avrami–Kolmogorov (JMAK)**.

4 In the ξ_{eq}^{d} text field, type `xieq`.

5 In the $\tau_{s \to d}$ text field, type `tau_calib(metp2.T)`.

6 In the $n_{s \to d}$ text field, type `n`.

ADD STUDY

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

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

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

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

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

STUDY 2

Step 1: Time Dependent

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

2 In the **Output times** text field, type `range(0,25,28000)`.

3 From the **Tolerance** list, choose **User controlled**.

4 In the **Relative tolerance** text field, type `0.001`.

5 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Metal Phase Transformation (metp)**.

6 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T (Temperature)	`range(853,10,1053)`	K

9 In the **Home** toolbar, click **Compute**.

RESULTS

Experiment (1%)

1 In the **Model Builder** window, expand the **Results>Tables** node.

2 Right-click **Results>Tables** and choose **Table**.

3 In the **Settings** window for **Table**, type `Experiment (1%)` in the **Label** text field.

4 Locate the **Data** section. Click **Import**.

5 Browse to the model's Application Libraries folder and double-click the file `calibration_against_ttt_data_ttt001.txt`.

Experiment (50%)

1 In the **Results** toolbar, click  **Table**.

2 In the **Settings** window for **Table**, type `Experiment (50%)` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `calibration_against_ttt_data_ttt050.txt`.

Experiment (90%)

1 In the **Results** toolbar, click  **Table**.

2 In the **Settings** window for **Table**, type `Experiment (90%)` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `calibration_against_ttt_data_ttt090.txt`.

Transformation Diagram (metp2)

1 In the **Model Builder** window, under **Results** click **Transformation Diagram (metp2)**.

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

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

4 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Time (s)`.

5 In the **y-axis label** text field, type `Temperature (degC)`.

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

7 In the **Title** text area, type `TTT diagram for 1%, 50% and 90% transformation`.

Table Graph 1

1 Right-click **Transformation Diagram (metp2)** and choose **Table Graph**.

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

3 From the **Table** list, choose **Experiment (1%)**.

4 From the **x-axis data** list, choose **Column 2**.

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

6 In the **Columns** list, select **Column 1**.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

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

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

11 In the table, enter the following settings:

Legends
1% (experimental)

Duplicate the table graph twice, and create the 50% and 90% lines.