



Model created in COMSOL Multiphysics 6.4

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 then 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.

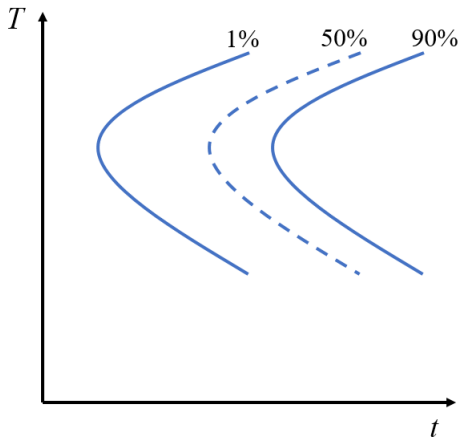


Figure 1: A TTT diagram.

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, which 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, and 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.

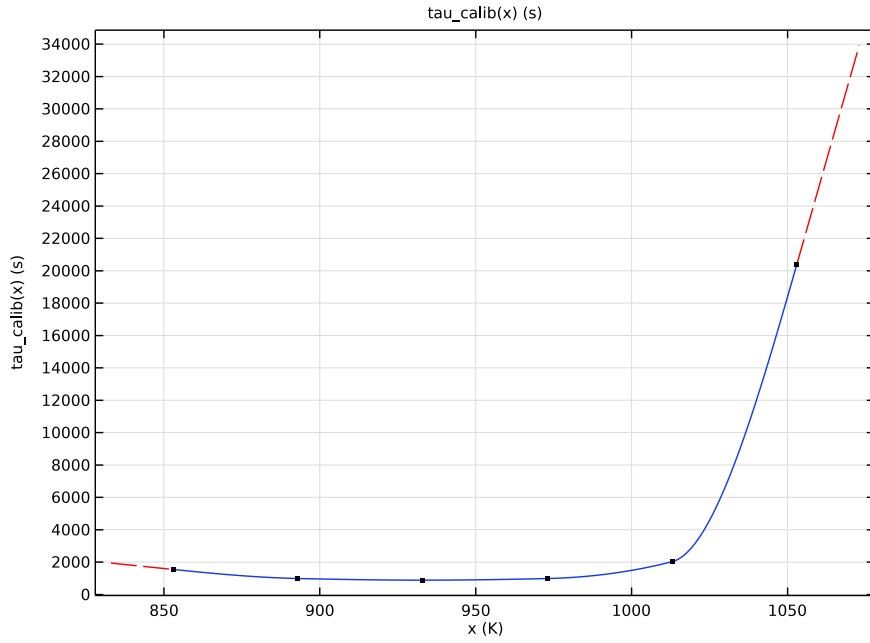


Figure 2: The temperature-dependent phase transformation model parameter τ .

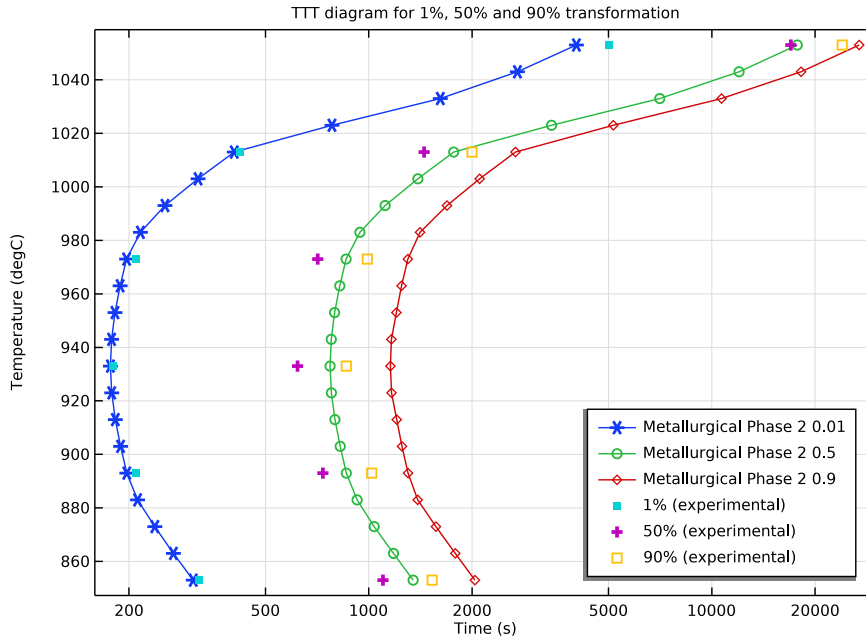



Figure 3: Comparison of the computed TTT diagram and experimental data for the 1%, 50%, and 90% lines.

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  **OD**.

- 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** checkbox.
- 4 Click  **Add**.
- 5 In the **Target phase fractions** table, enter the following settings:

| |
|------|
| 0.01 |
| 0.5 |
| 0.9 |



Phase Transformation

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

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

COMPONENT 1 (COMP1)

Least-Squares Objective 1

- 1 In the **Physics** toolbar, click  **Optimization** and choose **Parameter Estimation**.
- 2 In the **Settings** window for **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, enter the following settings:

| Columns | Type | Settings |
|----------|-----------|---|
| Column 1 | Parameter | |
| Column 2 | Value | Model expression=1, Name=col2, Weight=1 |
| Column 3 | Value | Model expression=1, Name=col3, Weight=1 |


- 6 In the table, click to select the cell at row number 1 and column number 2.
- 7 From the **Name** list, choose **T (Temperature)**.
- 8 In the **Unit** text field, type K .
- 9 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=1, Name=col3, Weight=1 |


- 10 In the table, click to select the cell at row number 3 and column number 2.
- 11 In the **Model expression** text field, type `metp.phase2.xi`.
- 12 In the **Column name** text field, type `col3a`.
- 13 From the **Scale** list, choose **Manual**.

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

Least-Squares Objective 2


- 1 Right-click **Least-Squares Objective 1** and choose **Duplicate**.
- 2 In the **Settings** window for **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 **Column name** text field, type col3b.
- 8 In the **Scale value** text field, type 0.5.

Least-Squares Objective 3

- 1 Right-click **Least-Squares Objective 2** and choose **Duplicate**.
- 2 In the **Settings** window for **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 **Column name** text field, type col3c.
- 8 In the **Scale value** text field, type 0.9.

STUDY I


Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study I** 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, choose **Logarithmic** from the **Entry method** list.
- 5 In the **Start** text field, type 0.1.
- 6 In the **Stop** text field, type 1e5.
- 7 In the **Steps per decade** text field, type 10.
- 8 Click **Replace**.

- 9 In the **Settings** window for **Time Dependent**, click to expand the **Study Extensions** section.
- 10 Select the **Auxiliary sweep** checkbox.
- 11 Click **+ Add**.
- 12 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** checkboxes for **Least-Squares Objective 1**, **Least-Squares Objective 2**, and **Least-Squares Objective 3**.
- 5 Locate the **Estimated Parameters** section. Click **+ Add**.
- 6 In the table, enter the following settings:

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


- 7 Locate the **Parameter Estimation Method** section. From the **Method** list, choose **BOBYQA**.
- 8 From the **Least-squares time/parameter list method** list, choose **Merge within manual range**.
- 9 In the **Optimality tolerance** text field, type 0.0001.
- 10 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 **Definitions** toolbar, click  **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 Locate the **Data Column Settings** section. In the table, enter the following settings:

| Columns | Type | Settings |
|-------------------|-----------------|--------------------|
| tau | Ignored column | |
| T | Ignored column | |
| Time | Ignored column | |
| Time constant (s) | Function values | Function name=intl |

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

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

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

10 In the **Name** text field, type `tau_calib`.

11 In the **Unit** text field, type s.


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

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

14 Click  **Plot**.

15 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 the **Add to Component 1** button 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 **Settings** window for **Metallurgical Phase**, locate the **Transformation Times** section.
- 2 Select the **Compute transformation times** checkbox.
- 3 Click  **Add**.
- 4 In the **Target phase fractions** table, enter the following settings:



| |
|------|
| 0.01 |
| 0.5 |
| 0.9 |

- 5 In the **Model Builder** window, click **Metal Phase Transformation 2 (metp2)**.
- 6 In the **Settings** window for **Metal Phase Transformation**, locate the **Temperature** section.
- 7 In the T text field, type T .

Phase Transformation



- 1 In the **Model Builder** window, click **Phase Transformation**.
- 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 $\xi_{\text{eq}}^{\text{d}}$ text field, type xieq .
- 5 In the $\tau_{\text{s} \rightarrow \text{d}}$ text field, type $\text{tau_calib}(\text{metp2}.T)$.
- 6 In the $n_{\text{s} \rightarrow \text{d}}$ 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 the **Add Study** button 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 Click  **Range**.
- 3 In the **Range** dialog, choose **Logarithmic** from the **Entry method** list.
- 4 In the **Start** text field, type 0.1.
- 5 In the **Stop** text field, type 1e5.
- 6 In the **Steps per decade** text field, type 10.
- 7 Click **Replace**.
- 8 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.
- 9 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Metal Phase Transformation (metp)**.
- 10 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 11 Click  **Add**.
- 12 In the table, enter the following settings:

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


- 13 In the **Study** 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 **ID 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 box, 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** checkbox.
- 10 From the **Legends** list, choose **Manual**.

II In the table, enter the following settings:

Legends

1% (experimental)

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