

Improving the ML-based framework for predicting CCT diagram, phase fractions, and steel hardenability

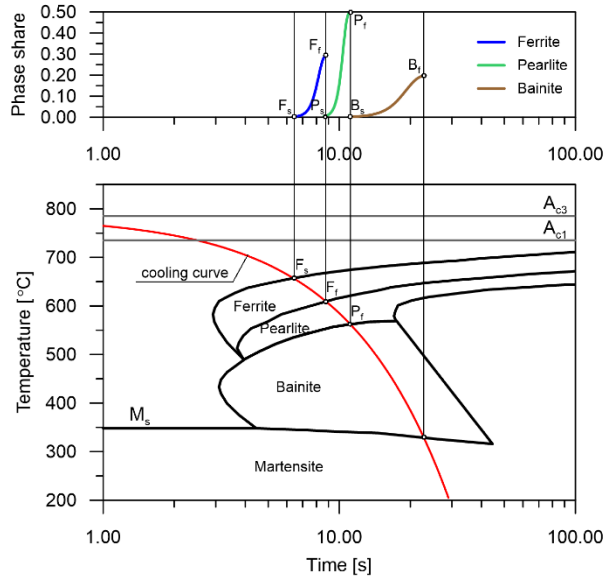
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TOFA 

20th DISCUSSION MEETING ON THERMODYNAMICS OF ALLOYS
20 - 24 September 2026
BLAD - SLOVENIA

Continuous Cooling Transformation (CCT) Diagrams



Kulawik, materials, 14 (2021) 4492.

How to obtain or predict a CCT diagram?

	Experiments	Kinetic Sim.	Empirical model
Accuracy	★★★★★	★★	★
Time efficiency	★	★★★★	★★★★★
Cost efficiency	★	★★★★	★★★★★
Specific alloy composition	★★	★★★★	★★★★★
Specific AUS temperature	★★	★★★★	★★★★★
Specific AUS time	★★	★★★★	★★★★★

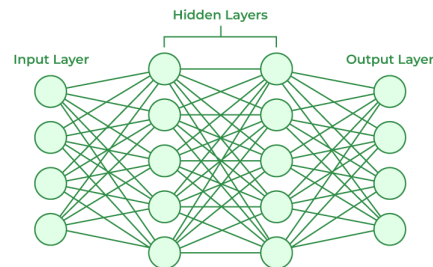
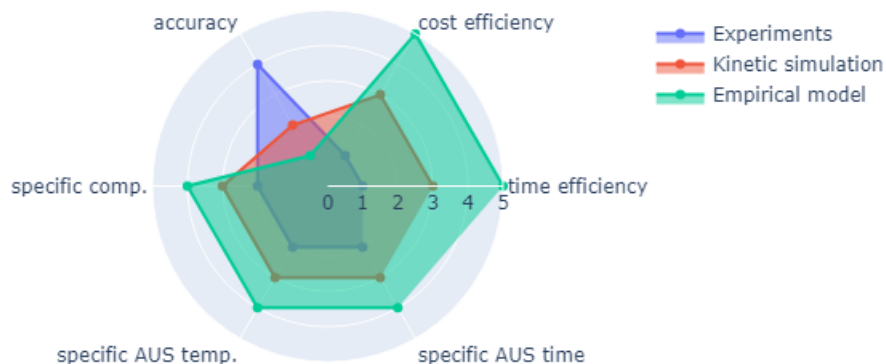


A CCT diagram is often used for an average composition within a given specification and an approximate austenitization condition, if we rely on inefficient means for generating such diagrams.

- Guide heat treatments
- Predict microstructures
- Predict properties
- for alloys, especially steels

Background

How to obtain or predict a CCT diagram?



Many groups have applied ANNs to this problem, but often:

- did not generate complete CCT diagrams,
- oversimplified the diagram representations,
- overcomplicated architectures, with up to 17 individual models.

Why Artificial Neural Networks?

- Capture complex nonlinear relationships
- Provide flexible architectures and training strategies
- Support customized loss functions and regularization
- Model interactions among multiple input variables

Why a shallow architecture?

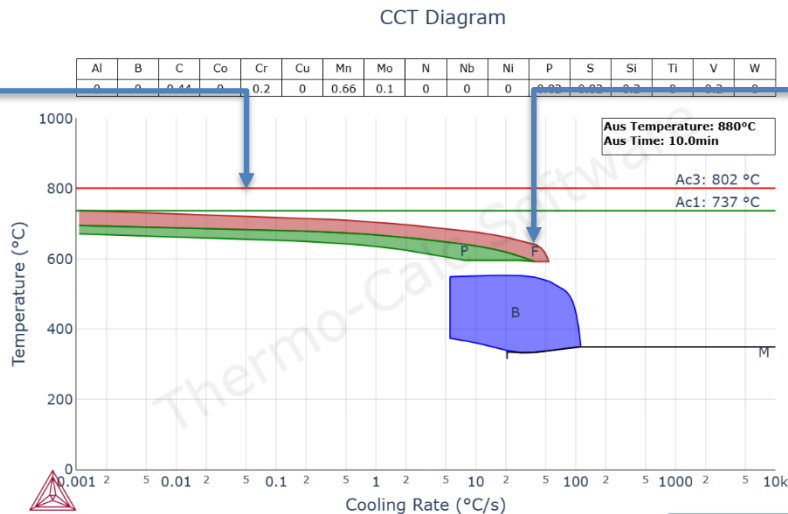
- Sufficient capacity for the expected relationships
- Lower computational cost
- Lower overfitting risk than deeper architectures
- Can be trained reliably with medium-sized datasets

Architecture and algorithm

Modeling objectives and prediction quantities

Ac temperatures

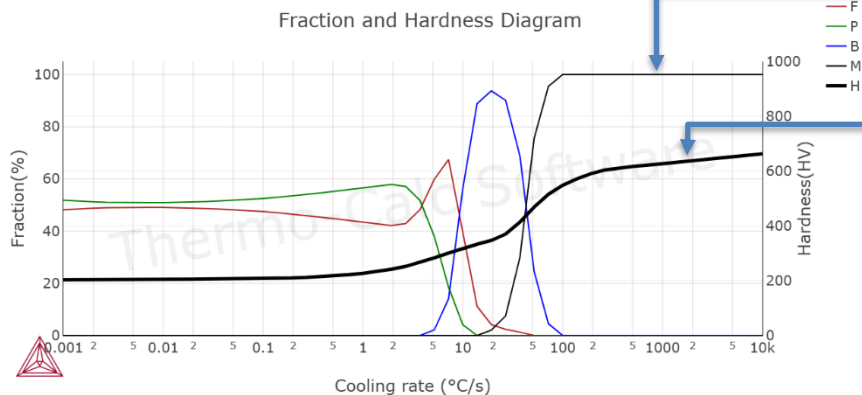
Transformation temperatures



14 quantities explicitly presented in a diagram:

A_{c1} , A_{c3} , F_s , F_f , P_s , P_f , B_s , B_f , M_s , f_F , f_P , f_B , f_M , hardness

Possible auxiliary quantities required for constructing the diagram



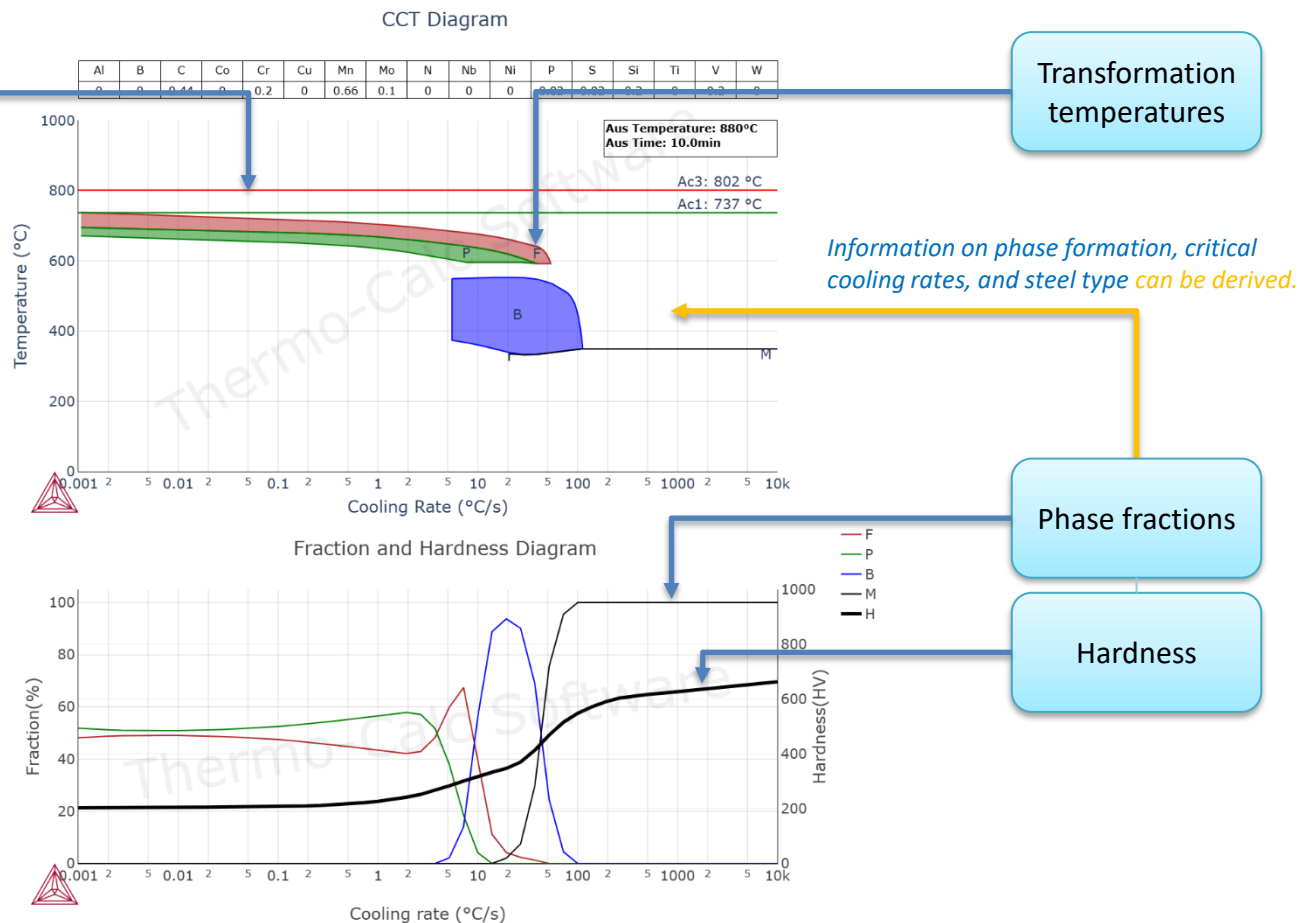
Architecture and algorithm

- 3 specialized ANN models + an advanced Assembly algorithm

14 quantities explicitly presented in a diagram:

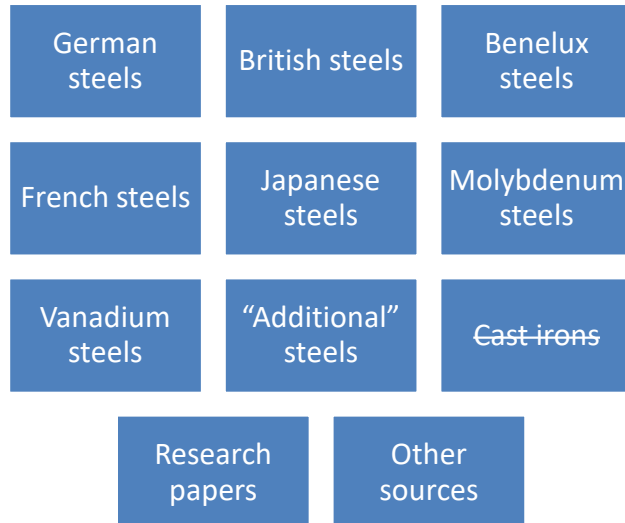
A_{c1} , A_{c3} , F_s , F_f , P_s , P_f , B_s , B_f , M_s , f_F , f_P , f_B , f_M , hardness

Zero auxiliary quantity required for constructing the diagram



Data curation, augmentation, synthesis

- *Data quantity and quality are crucial.*



transtemp_released_v2.1.0_metadata_v1.0.0.yaml	✓
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We decoupled ML dataset releases from diagram-level data updates.

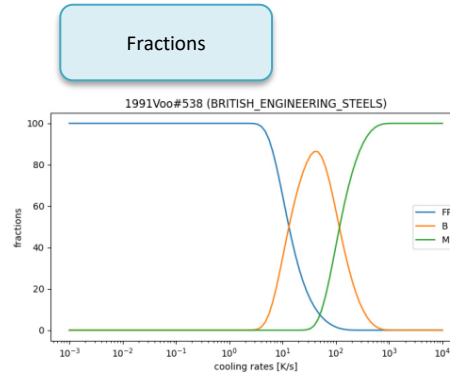
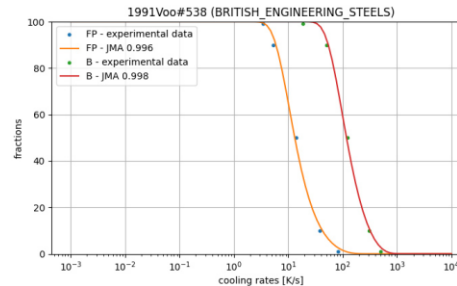
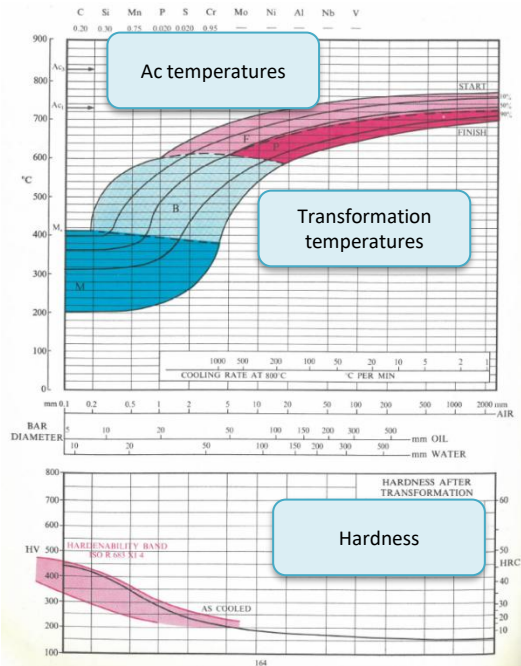
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- *Data management*

We began to adopt [FAIR Data Principles](#) in our projects to ensure our research assets are fully findable, accessible, interoperable, and reusable.

Data curation, augmentation, synthesis

Data Curation

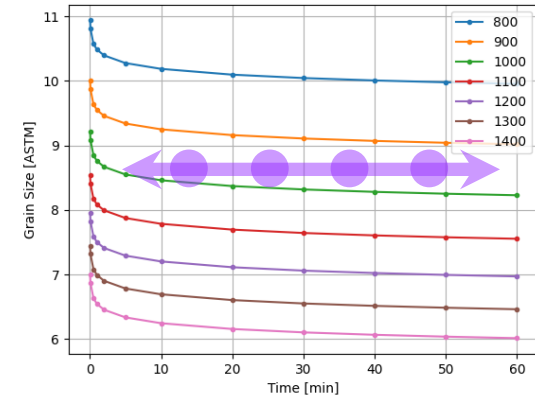


Data Augmentation

- Equivalent austenitization conditions (T, t)

$$\gamma = \frac{A}{T} + B \cdot \ln(t) + C$$

- T in Kelvin
- t in hour
- Grain size γ in ASTM scale



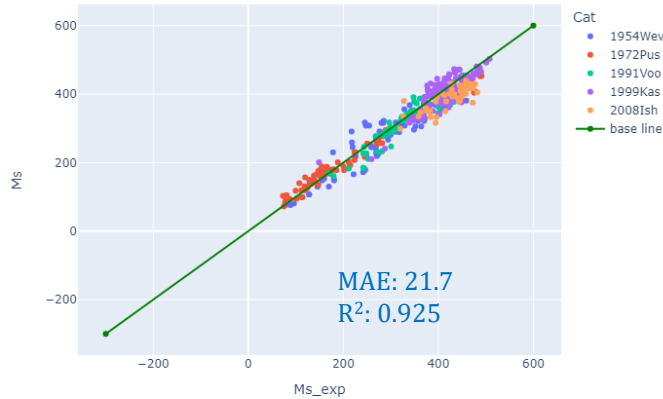
- Impacts of austenitization temperatures
- Composition variation

Data curation, augmentation, synthesis

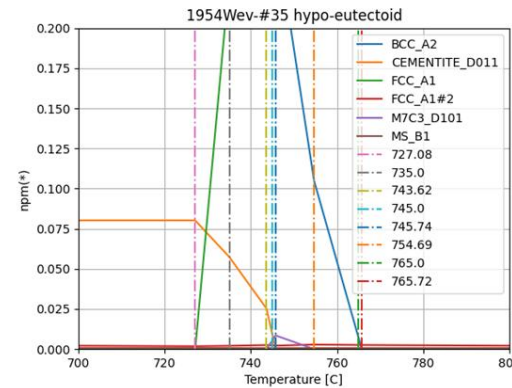
■ Data Calculation and Synthesis

- Martensite start temperatures at high cooling rates
- TC-Python (or Property Model Calculator)
- Considering intercritical annealing

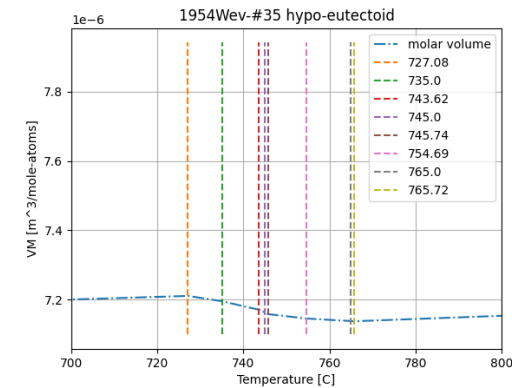
- Critical transformation temperatures
- In theory, $Ae_3 < Ac_3$ & $Ae_1 < Ac_1$. Fs approaches Ae_3 and Ps approaches Ae_1 during slow cooling.
- Ferrite and Pearlite fractions
- Equilibrium estimation, corresponding to very slow cooling



calc. vs exp. Ms temperatures



Individual phase fractions



Molar volume of the steel

- to clarify controversies
- to estimate missing data
- to synthesize data

TC-Python + customized algorithm for
evaluating Ae_1 , Ae_3 , $frac_F$, and $frac_P$

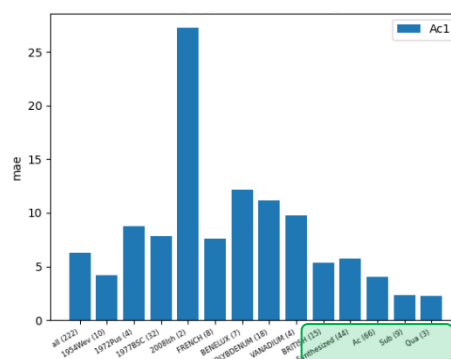
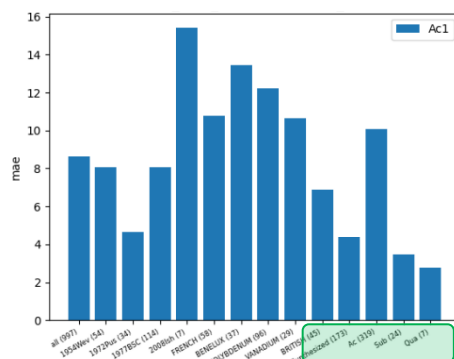
Critical temperatures

■ Ac1 and Ac3

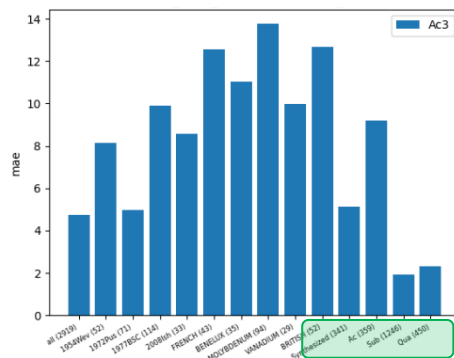
- Simple, conventional neural networks
- Steel compositions as features
- *Augmented with Thermo-Calc calculations*

■ Elemental descriptors not used

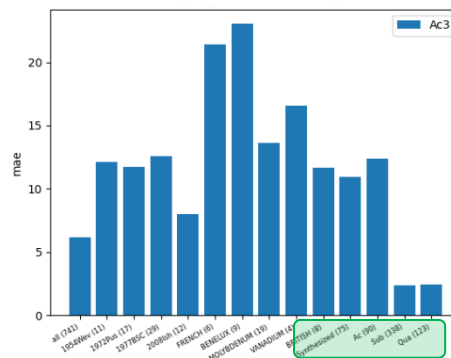
- M-D interactions require a sophisticated representation,
- with a complex architecture, e.g., graph-based models.
- Such models require a large amount of reliable training data.



Ac1



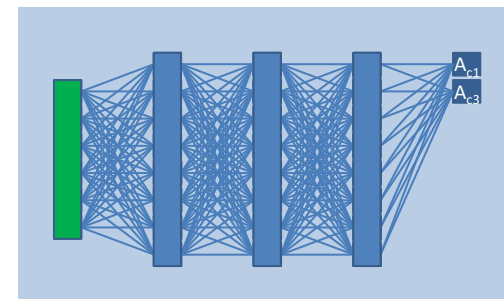
Training



Validation

Ac3

	Train	Validation
Overall	5.7 °C	6.2 °C
Ac1	8.6 °C	6.3 °C
Ac3	4.7 °C	6.2 °C



A conceptual illustration

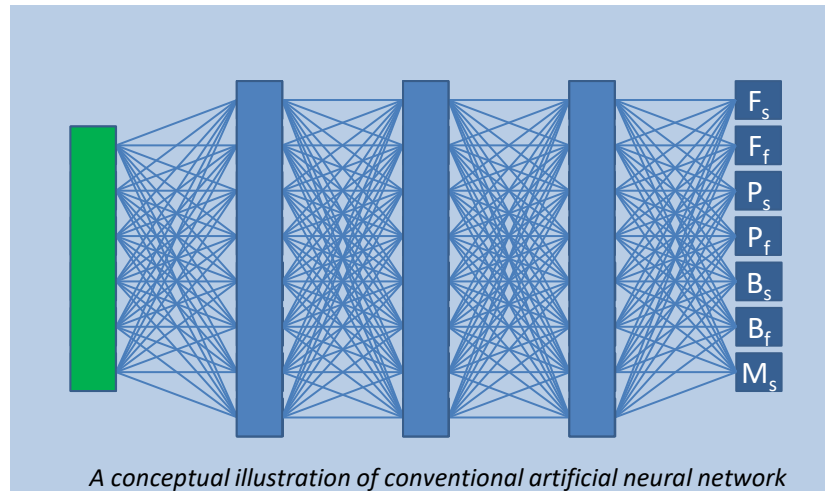
Transformation temperatures

- **Conventional network**
- For start and finish transformation temperatures of Ferrite, Pearlite, and Bainite, as well as Martensite start temperatures
- Composition, austenitization conditions, and cooling rates as input features

Composition



Condition



- Soft constraints to reduce inconsistencies among prediction targets
- Customized loss function and metrics

Fractions and hardness

- **Custom network architecture**
- Composition, austenitization conditions, and cooling rates as input features
- Causal dependencies between phase fractions and hardness
- Soft constraints to promote physically consistent predictions

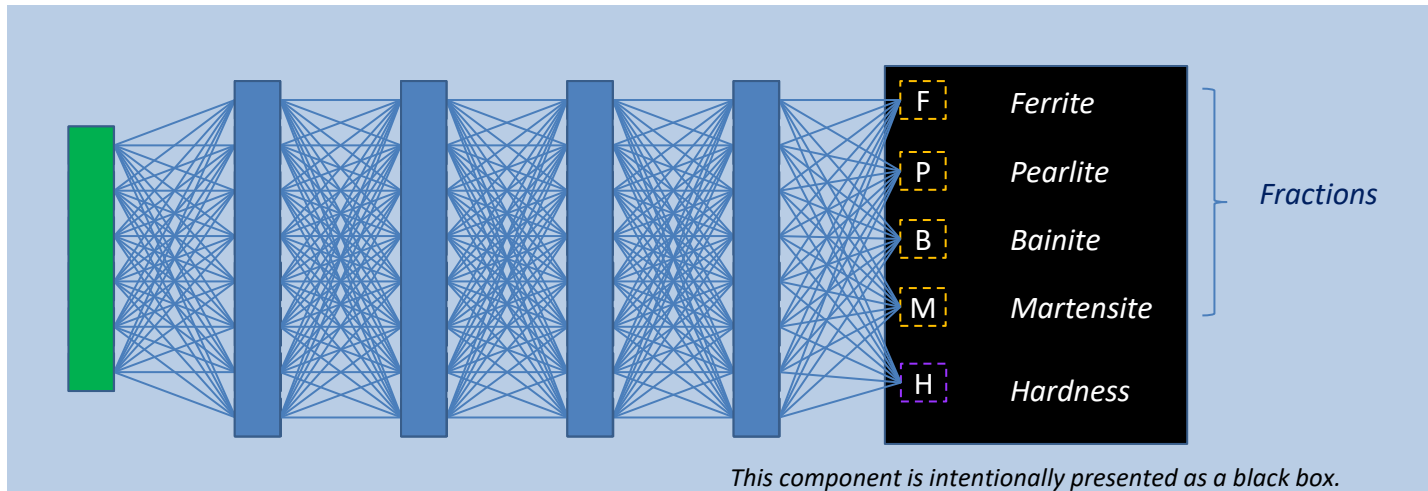
Composition



Condition



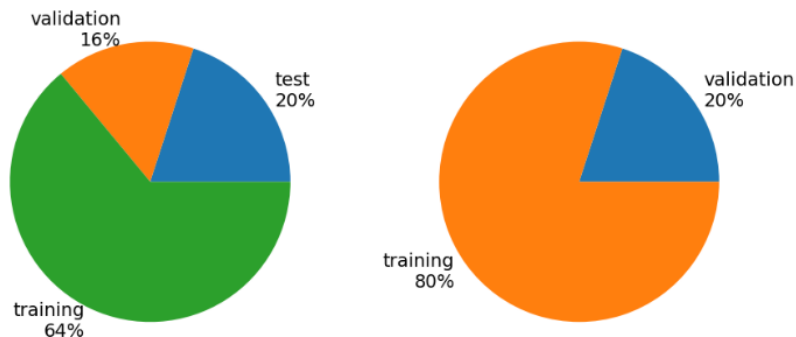
Fractions



Validate model prediction

Validation-Set Statistics

- Limited, uncertain, and heterogeneous data → no independent test set.
- A new random validation subset was selected for each modeling run. Performance was evaluated statistically across repeated random splits.
- Scores may be optimistic but are adequate for internal model ranking.



- Statistics for individual types of quantities

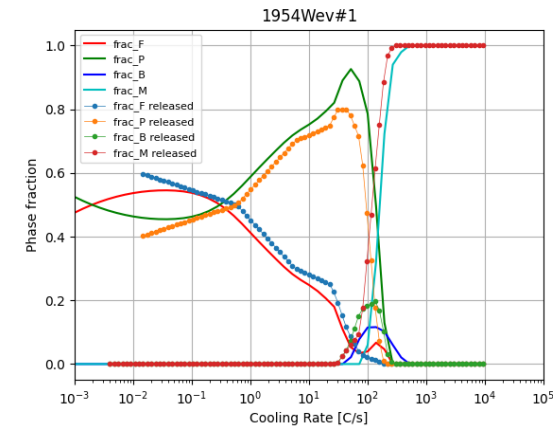
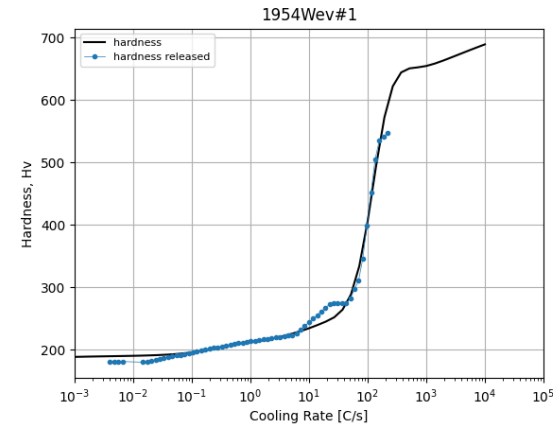
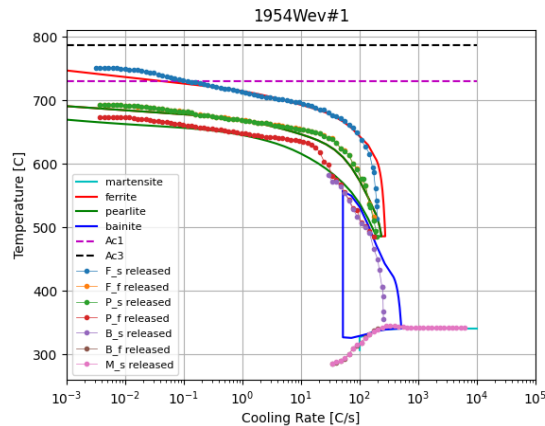
MAE	Train	val
Trans. Temperature	15 °C	23 °C
Ac1 and Ac3 temperatures	6 °C	6 °C
Phase fractions	0.01	0.04
Hardness	15 Hv	37 Hv

- *Not the best individual models in terms of validation-set statistics. Choices made also based on extensive diagram-level review.*

Validate model prediction

Diagram-Level Review

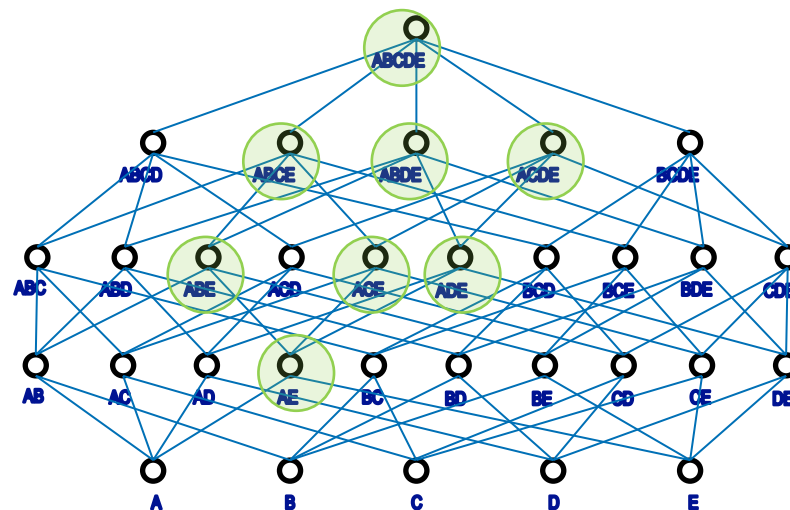
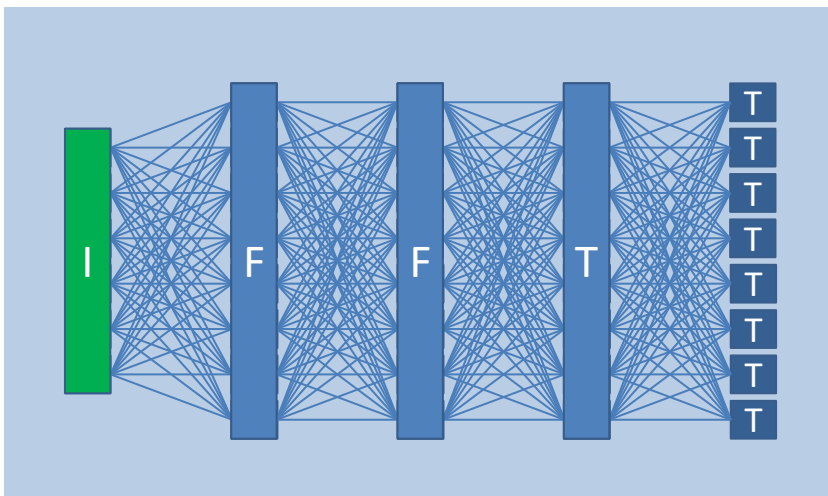
- Statistical metrics evaluate only individual predictions (A_{C1} , A_{C3} , F_s , F_f , P_s , P_f , B_s , B_f , M_s , f_F , f_P , f_B , f_M , H), whereas the final outputs are assembled CCT and supplementary diagrams.
- Diagram-level review is therefore required to evaluate continuity, trends across cooling rates, physical plausibility, and cross-quantity consistency.



Fine-tuning ANN models

- Fine-tune the baseline model using the expanded dataset instead of rebuilding it from scratch.
- Preserve established relationships and balanced performance (across compositions and predicted quantities), while learning from the newly added data.

- Update a CALPHAD database in a controlled way, where modifications are focused on the most relevant systems, phases, and parameters.

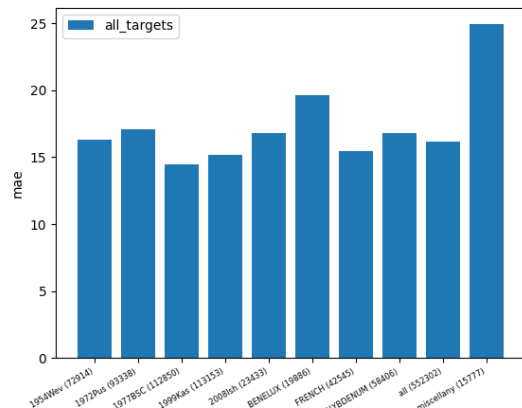


Fine-tuning an ML model vs updating a CALPHAD database

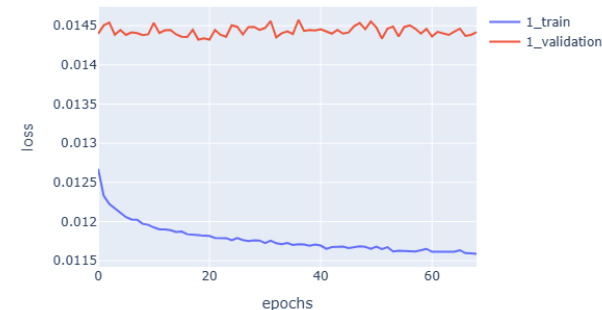
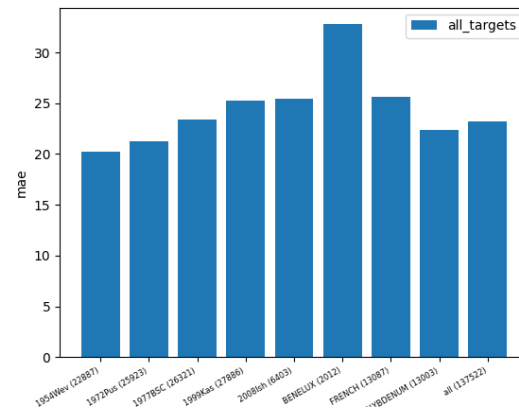
Fine tuning transformation temperatures

- All targets | The same validation set

Training

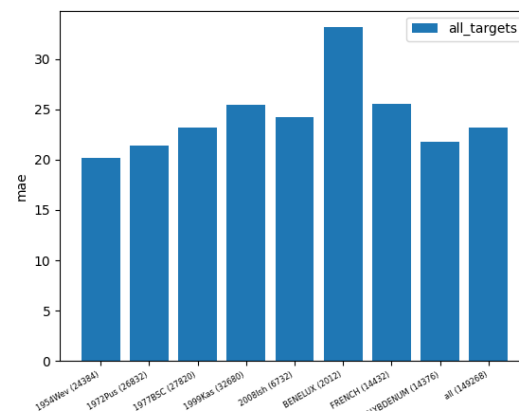
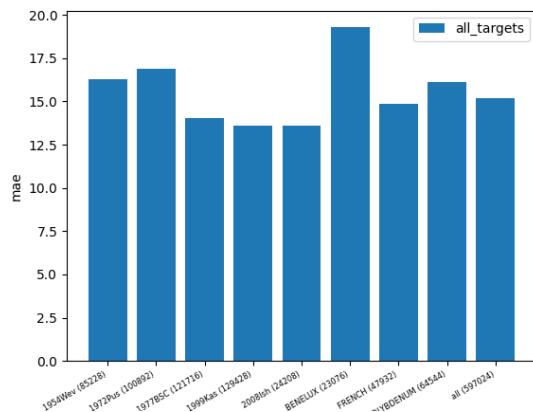


Validation



Fine tuning

Train	Validation
16 °C	23 °C



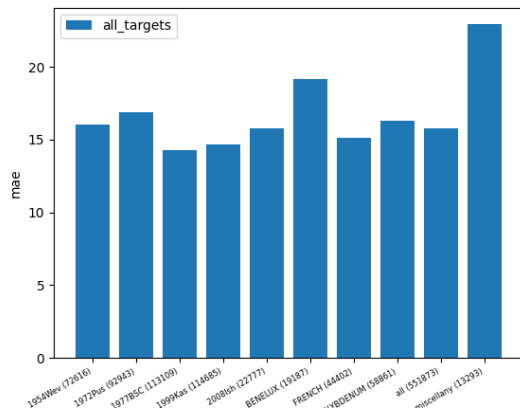
Train	Validation
15 °C	23 °C

Baseline model

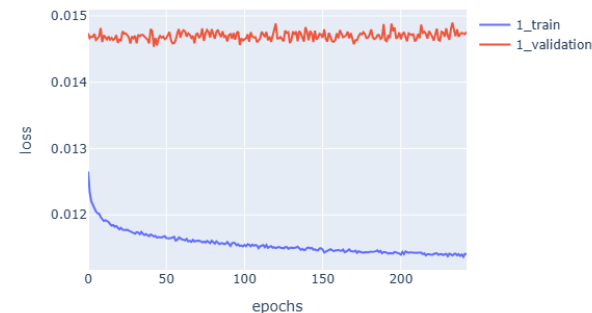
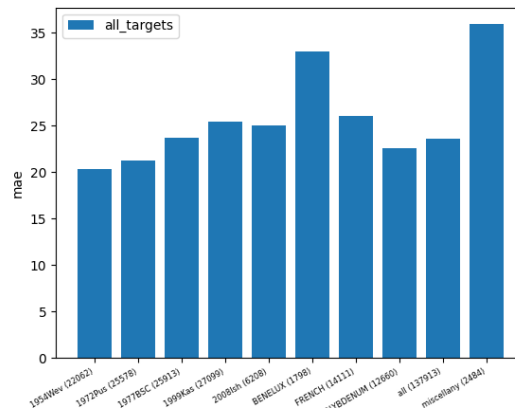
Fine tuning transformation temperatures

■ All targets | Extended validation set

Training

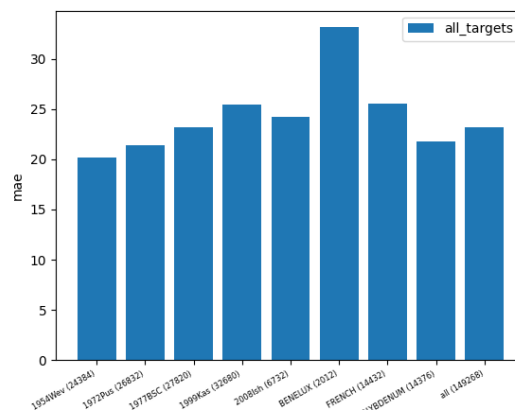
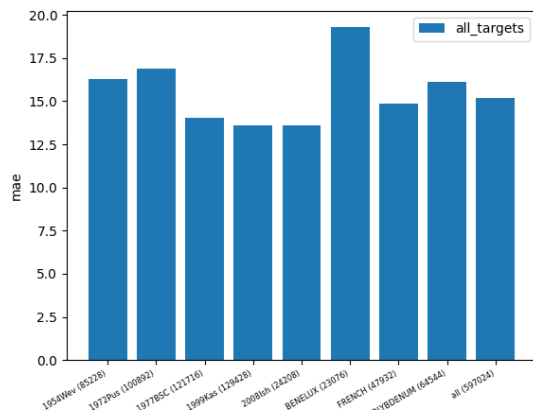


Validation



Fine tuning

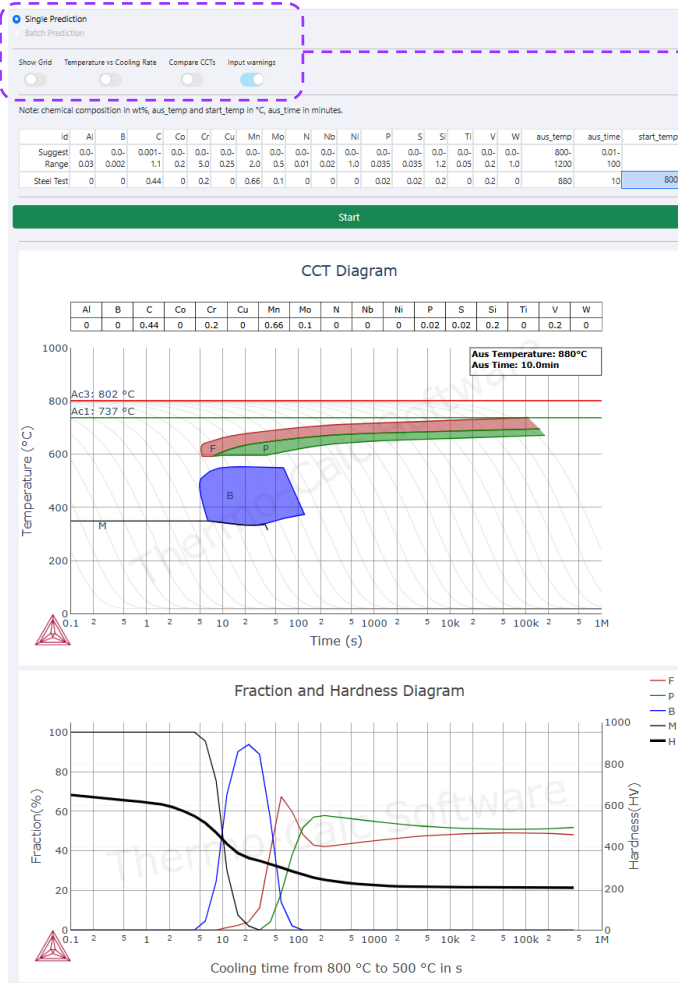
Train	Validation
16 °C	24 °C



Train	Validation
15 °C	23 °C

Baseline model

Deployment



Single Prediction

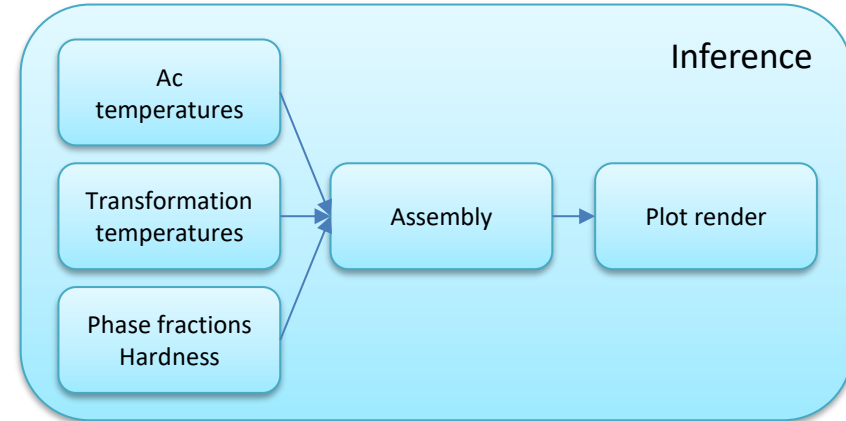
Batch Prediction

Show Grid

Temperature vs Cooling Rate

Compare CCTs

Input warnings

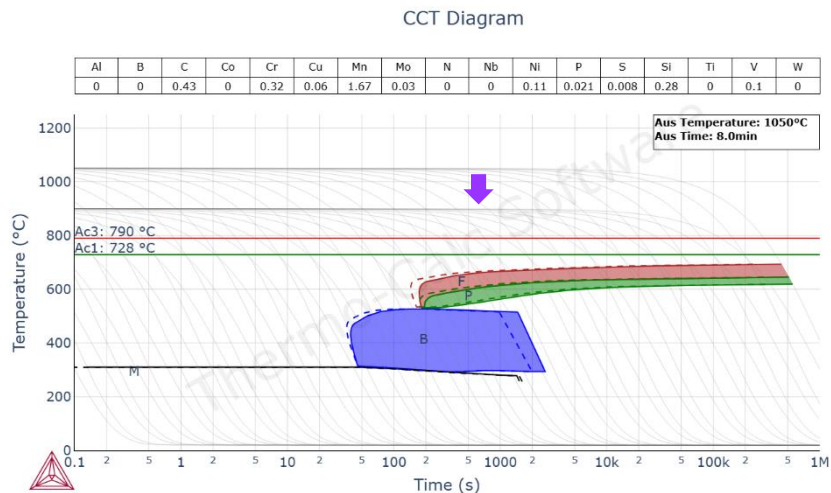


Diagrams are generated in under 0.2 seconds on a standard PC.
Deployed as a web application. Beta-tested for a couple of years.
Will soon be integrated into Thermo-Calc and released.

Model prediction

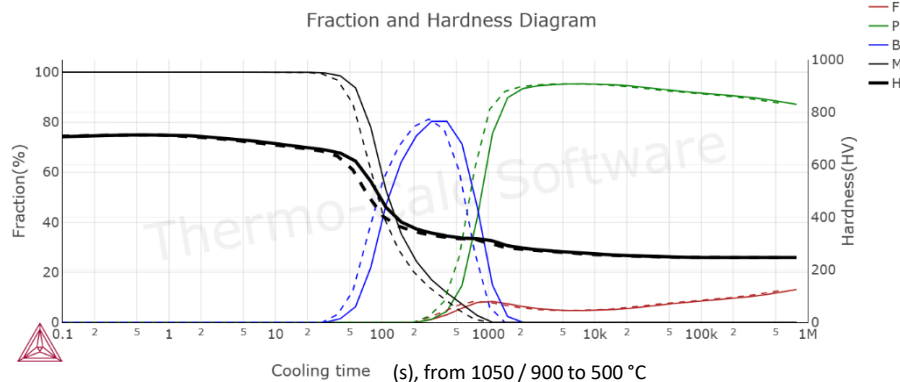
- The same diagram with different start temperatures

- *Efficient*
- *Flexible*



Start temperature:

- 1050°C (solid line)
- 900°C (dashed line)

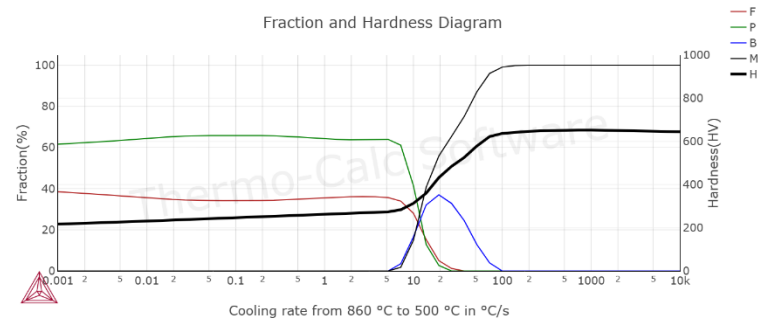
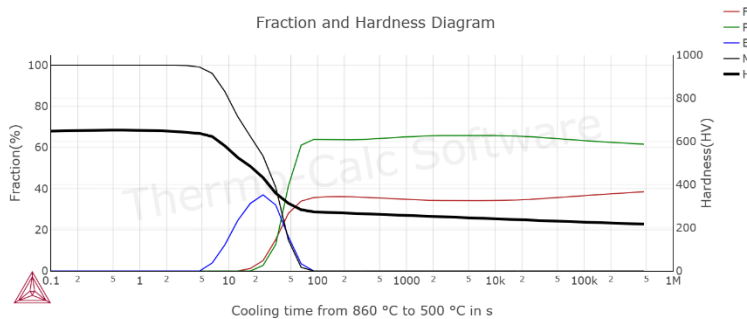
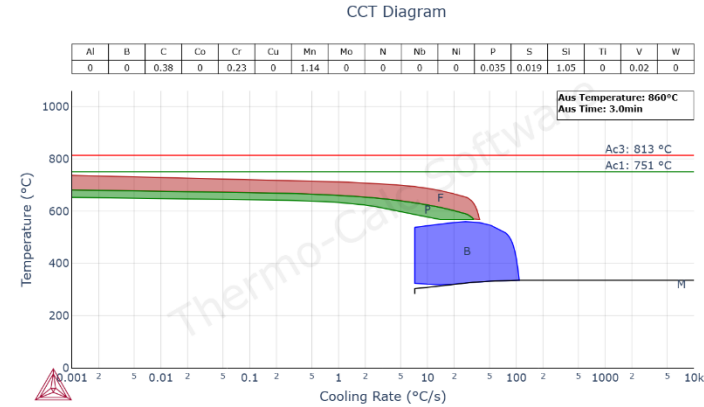
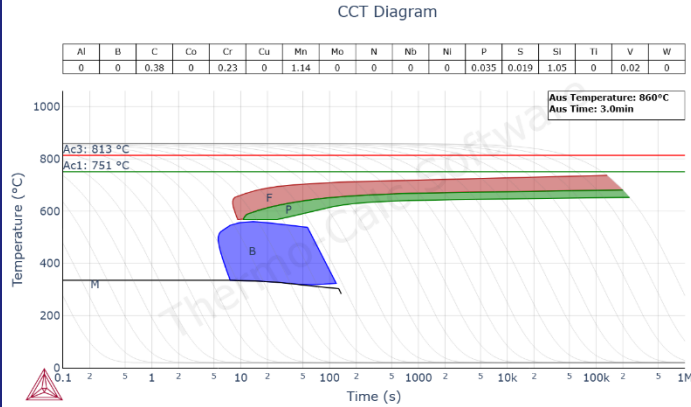


The Aus. temperature is often taken as the start temperature, but one can choose a different temperature. The same diagram can be instantly replotted as requested.

Model prediction

- The same diagram in two forms (vs time or cooling rate)

- *Efficient*
- *Flexible*

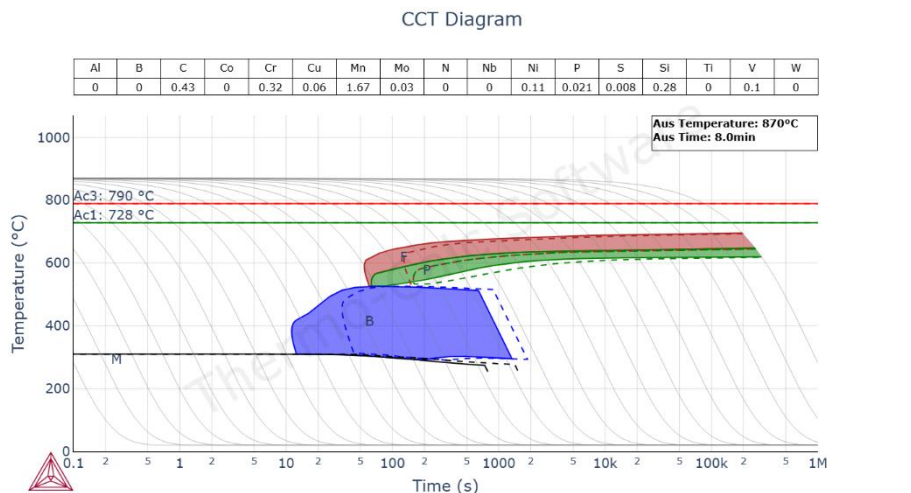


- Newtonian cooling is assumed. Each cooling curve is represented by the cooling rate at the start, which is taken at the austenitization temperature in this case.

Model prediction

Impact of austenitization temperature

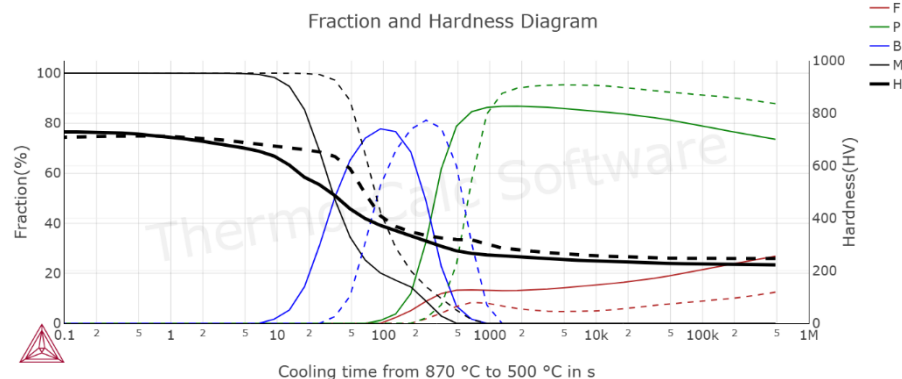
- *Efficient*
- *Specific*



Aus. temperature:

- 870°C (solid line)
- 1050°C (dashed line)

The start temperature is set at 870°C for both CCT diagrams for comparison.

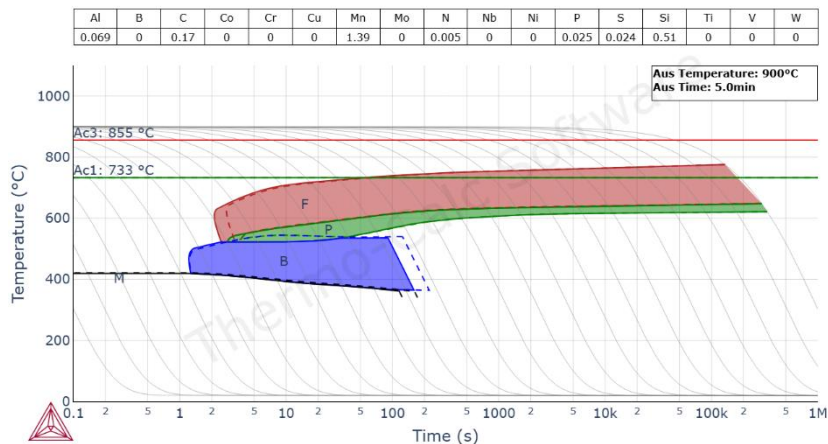


The model enables us to instantly generate a CCT diagram for any specific austenitization temperature.

Model prediction

Impact of austenitization time

CCT Diagram

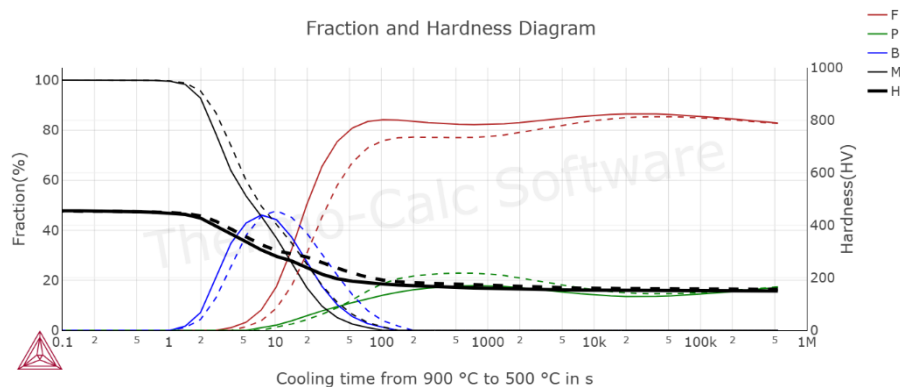


- *Efficient*
- *Specific*

Aus. time:

- 5 min (solid line)
- 15 min (dashed line)

Fraction and Hardness Diagram

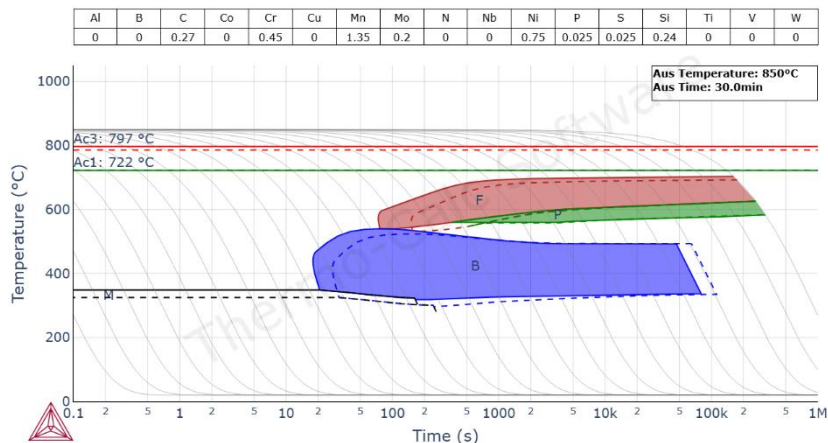


It enables us to instantly generate a CCT diagram for any specific austenitization time.

Model prediction

Impact of carbon content

CCT Diagram

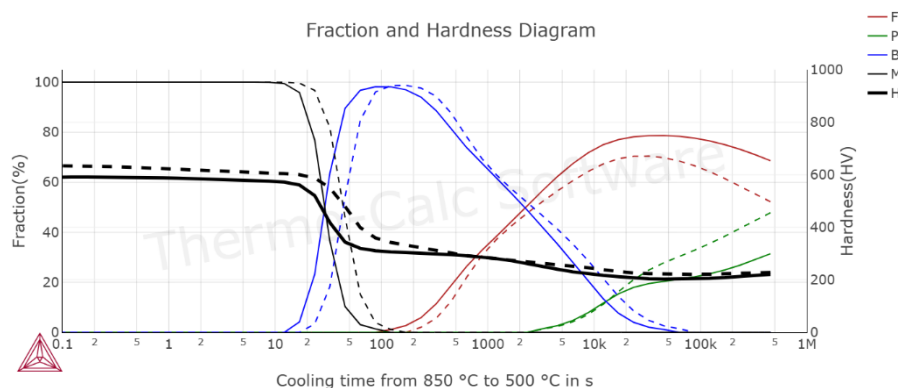


- *Efficient*
- *Specific*

- 0.27 wt.% C (solid line)
- 0.33 wt.% C (dashed line)

British Steels, 1977, BSC. #47 (solid line) and #48 (dashed line)

Fraction and Hardness Diagram



It enables us to instantly generate a CCT diagram for any specific composition.

Summary

Data collection, curation,
augmentation, synthesis



Framework architecture,
network design, model training



Rule-based algorithm for
assembling diagrams

The ML-based framework for predicting CCT diagram, phase fractions, and steel hardenability will soon be integrated into Thermo-Calc and released.

Continuous optimization:

- Data enhancement
- Network optimization
- Model training (Fine tuning)

Special thanks to Dr. Andre Schneider for his constructive insights, and to Jani Koljonen for the deployment on cloud.

Thank you all for your attention!

