Machine Learning Steel Heat Treatment Simulation

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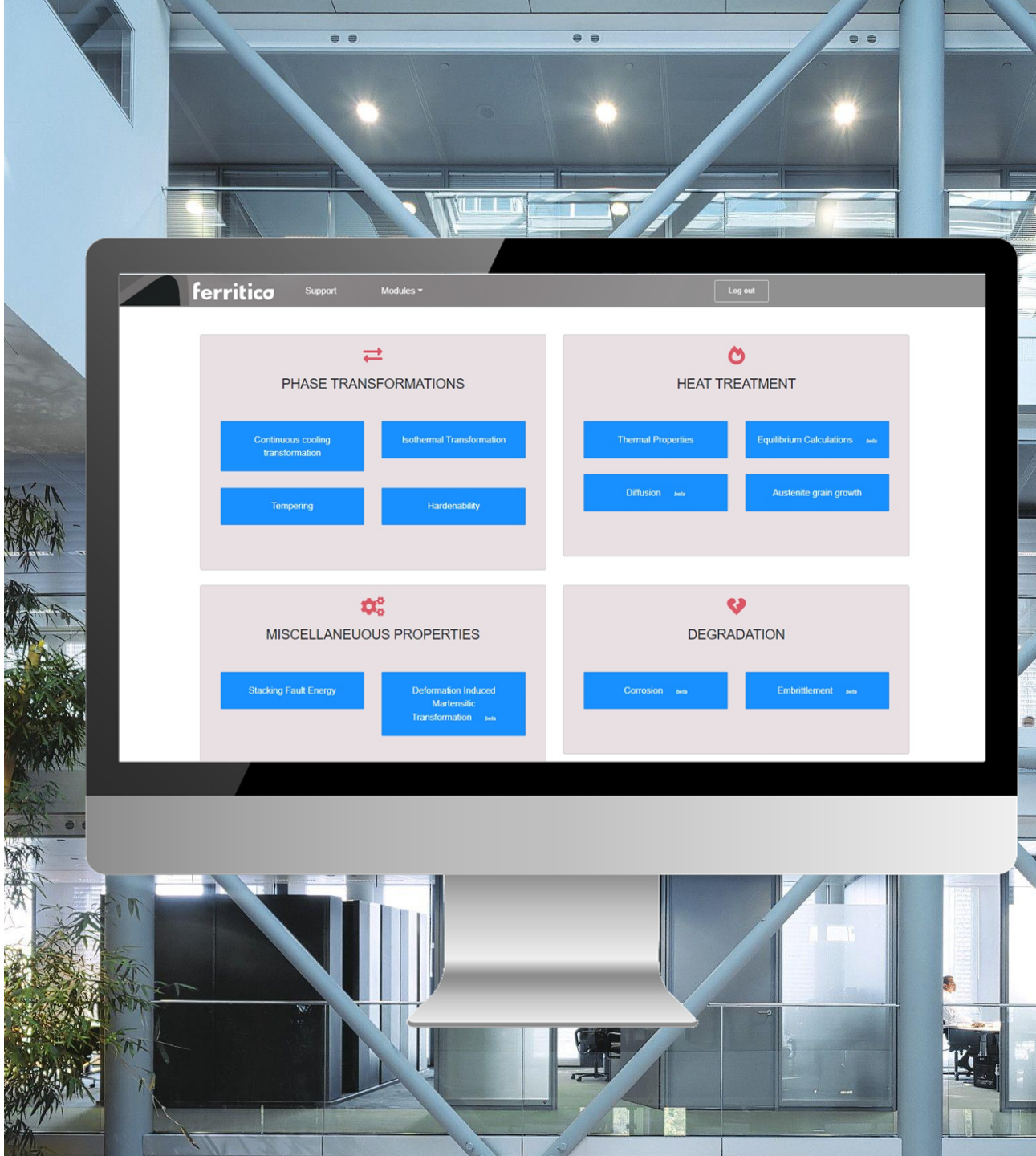
ABOUT FERRITICO

- Spinoff from steel research at KTH Royal Institute of Technology
- Steel simulation SaaS based on machine learning and physical modelling
- Contracted in ICME projects to develop customized materials simulation models



SITUATION –
POTENTIAL IN OPTIMIZATION

- High cost of developing steel when using trial-and-error and physical testing
- Simulation software enables digital steel development at lower cost
- Conventional simulation software accuracy and speed is limited and cannot support all industry use cases

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TRIAL-AND-ERROR PROCESS OPTIMIZATION

1 - NOVEL STEEL DEVELOPMENT

Reducing trial-and-error, time-to-market and cost for developing novel steel
- Interpretation -> prediction -> Optimization simulation support
- Generate steel recipes based on property prioritization order

2 - PRODUCT & PROCESS DEVELOPMENT

Steel product/ component simulation (e.g. FEM) needed to benchmark steel grades for a specific application :
- Need of ferritico simulated steel data sets for novel steels, taking steel grade tolerances and chemical composition deviations into consideration

3 - STEEL & COMPONENT MANUFACTURING

Conventional manufacturing and AM optimization through:
- Simulation support needed to efficiently ramp-up pilot material and component manufacturing to full scale production
- Ferritico global models needed to support simulation of major process engineering initiatives not supported by digital twins

4 - IMPLEMENTATION

Need for materials data as input to FEM simulation of implementation processes:
- Joining
- Shaping
- Additive manufacturing

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FERRITICO MACHINE LEARNING STEEL SIMULATION

SIMULATED PROPERTIES (OUTPUT)

- Thermal properties
- Electro Magnetic properties
- Mechanical properties
- Phase transformations
- Flow curves
- Steel degradation
- Upstream CO_2 footprint
- Alloy composition cost

COMPOSITION (INPUT 1)

96.5%	Iron (Fe)
0.5%	Carbon (C)
1.5%	Chromium (Cr)
1.5%	Nickel (Ni)

HEAT TREATMENT (INPUT 2)

Heat the alloy to 950 °C

Cool the alloy to room temperature at cooling rate 100°C per minute

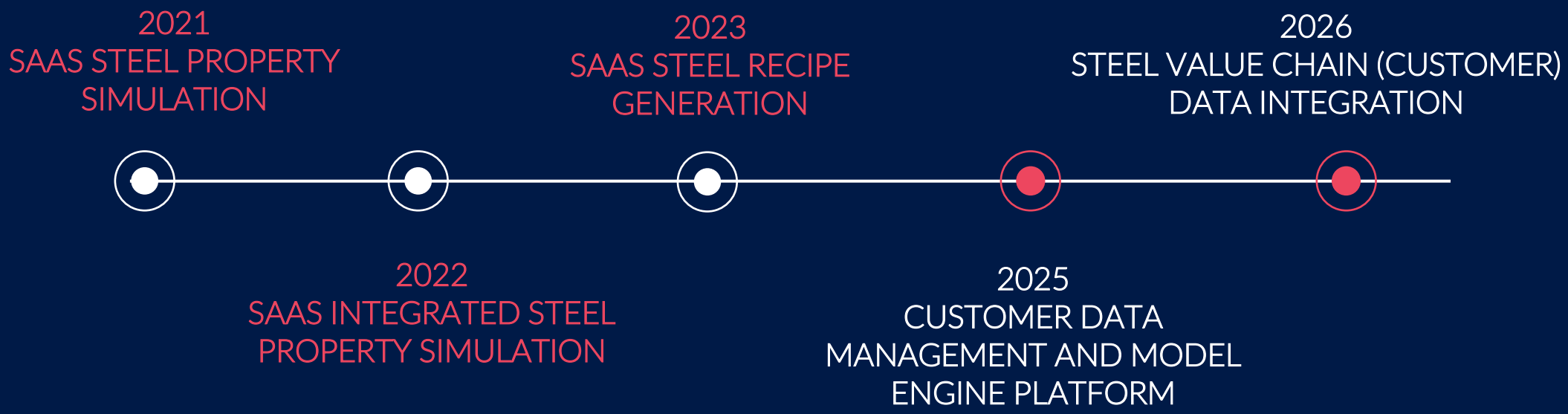
SOFTWARE FEATURES –
HOW DO WE HELP THE USER?

- **Accuracy** – simulate steel with higher accuracy than conventional software enabling new simulation use cases
- **Speed** – simulate steel properties within 20 sec while competing software sometimes need hours
- **Generative** – e.g. get alloy composition and/or process metric adjustment proposals enabling material property optimization, i.e. recipe generation

FERRITICO VALUE PROPOSITION –
HOW DO WE BOOST THE BUSINESS?

- **Time-to-market -** speeds up steel development, design and implementation
- **Product quality** - enables optimization implying increased margins and competitive advantage
- **Cost cutting** – helps identify material replacement and energy reduction possibilities
- **Sustainability –** products can be optimized for increased durability and decreased CO2 footprint
- **Creativity -** happier employees releasing the force of creativity instead of struggling with trial-and-error!

TECHNOLOGY ROADMAP



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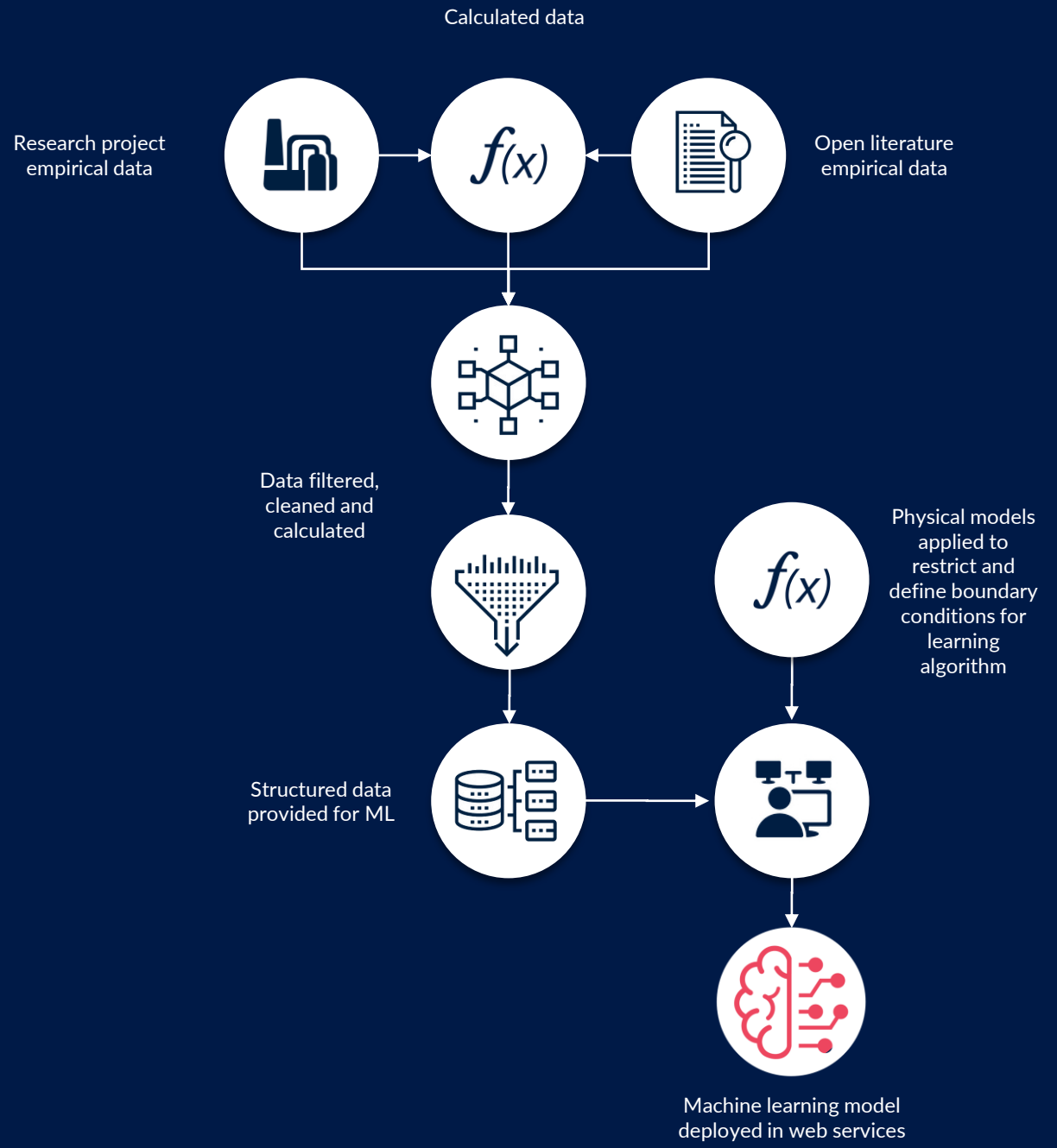
METHODOLOGY

- Information retrieval and extraction techniques used to collect and structure open literature data
- Partner empirical data is pooled
- Physical models are used to generate high quality synthetic data and generate complete data sets
- Ferritico simulation modules are used to generate intermediate features from raw data sets
- Well defined physical relationships are used to support ML algorithms. “Do not learn what we already know”



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FERRITICO MACHINE LEARNING SERVICES

FERRITICO STEEL SIMULATION SAAS

Generic module-based SaaS, built on open literature, partner pooled and in-house generated data and offered out-of-the-box

DIGITAL TWINS – RESEARCH PROJECT COLLABORATIONS

Customized modules “Digital twins” developed in collaboration with research projects based on project data sets. Combined with Ferritico SaaS if steel related project

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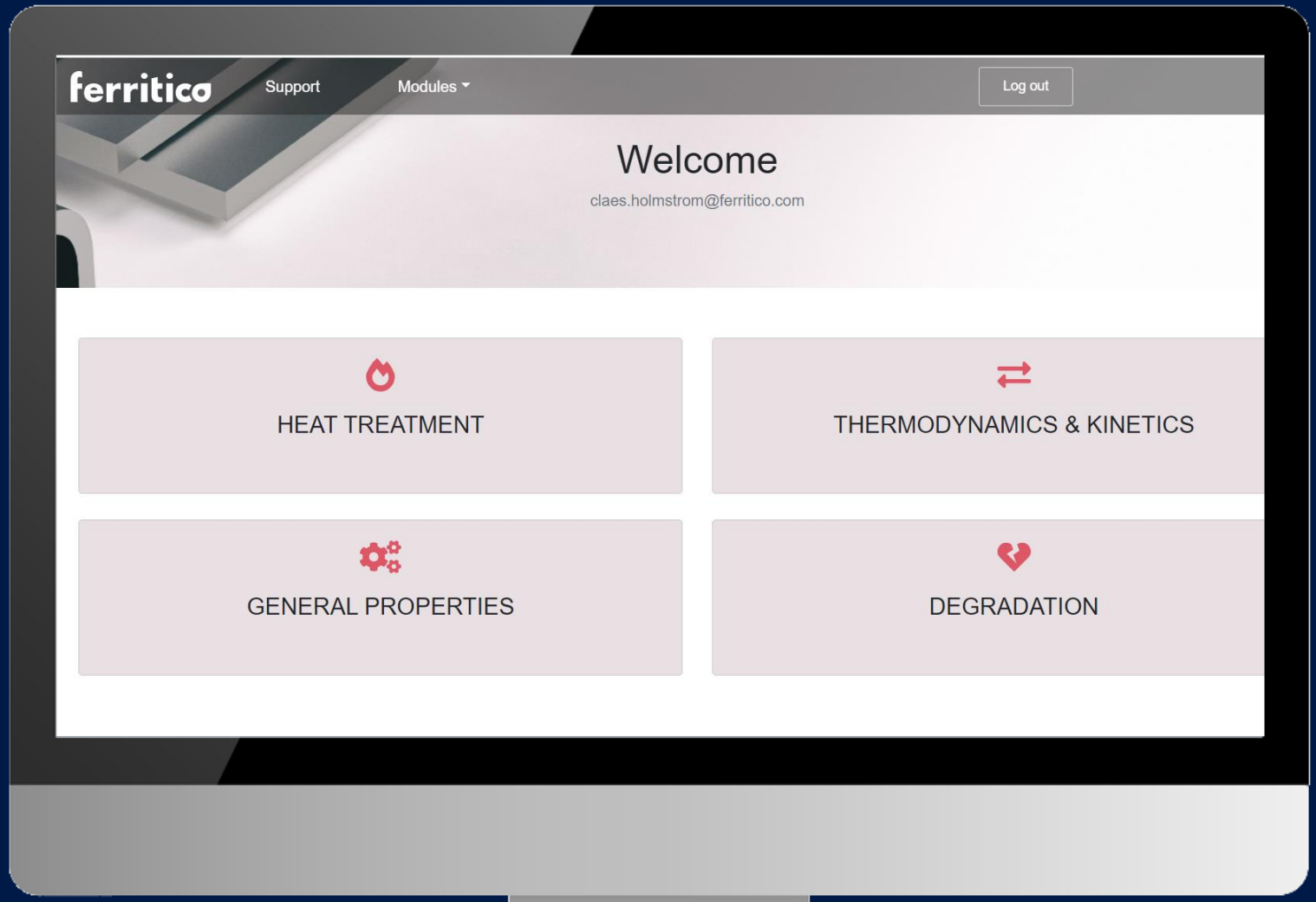
FERRITICO SAAS



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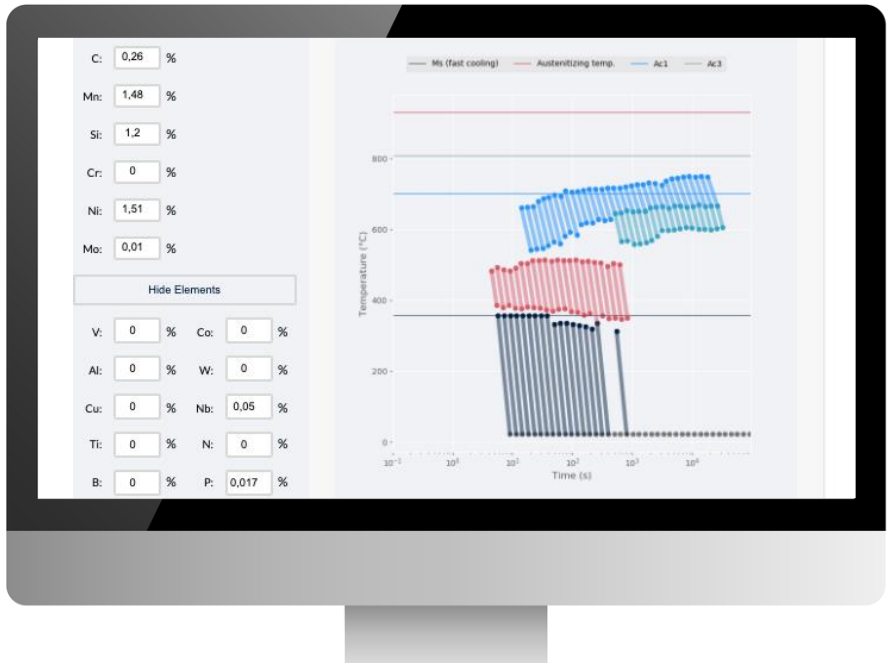
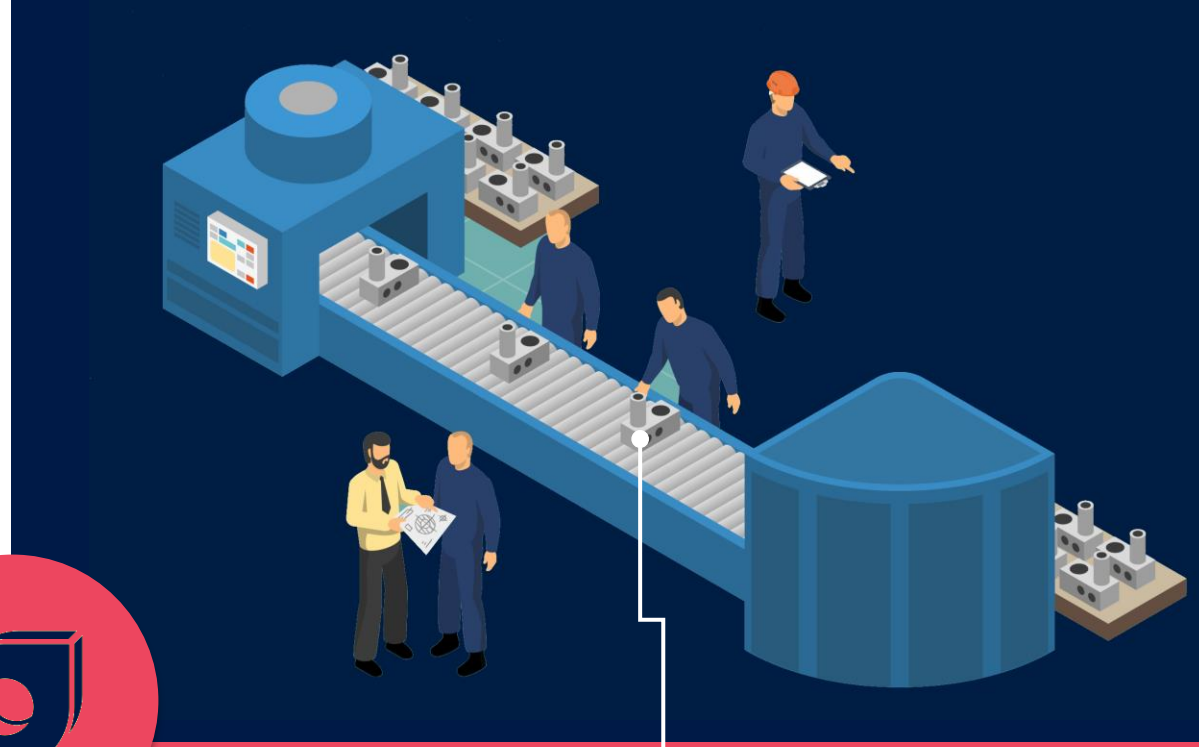
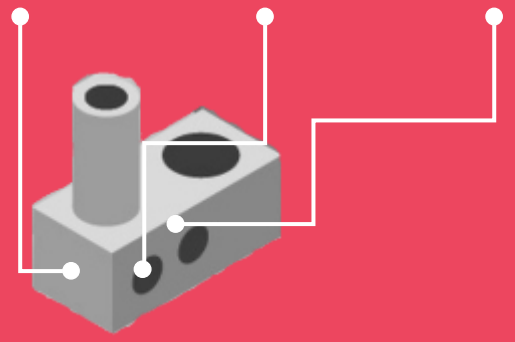
FERRITICO CCT MODULE –
HEAT TREATMENT DIGITALIZATION

- Input - Composition, aus temp, time and cooling rates
- Output - CCT diagrams, phase fractions, hardness, AC1, AC3 etc.
- Method – Combination of 18 ML classification and regression models built on DB with 2.200 CCT diagrams.





Phase	CR 100 °C /min	CR 20 °C /min	CR 10 °C /min
Austenite	0%	0%	0%
Ferrite	5%	0%	60%
Pearlie	0%	40%	40%
Bainite	15%	60%	0%
Martensite	80%	0%	0%



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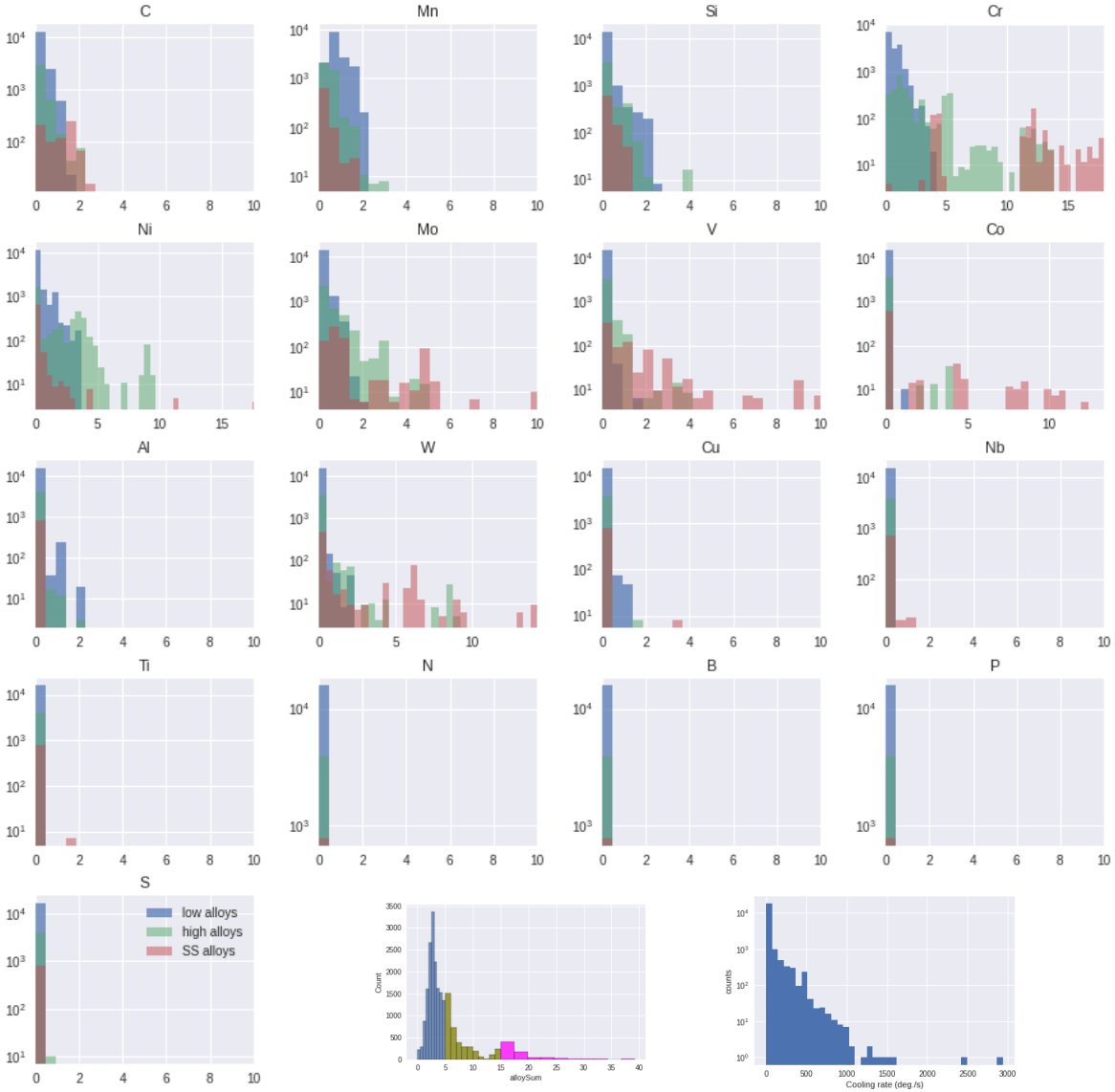
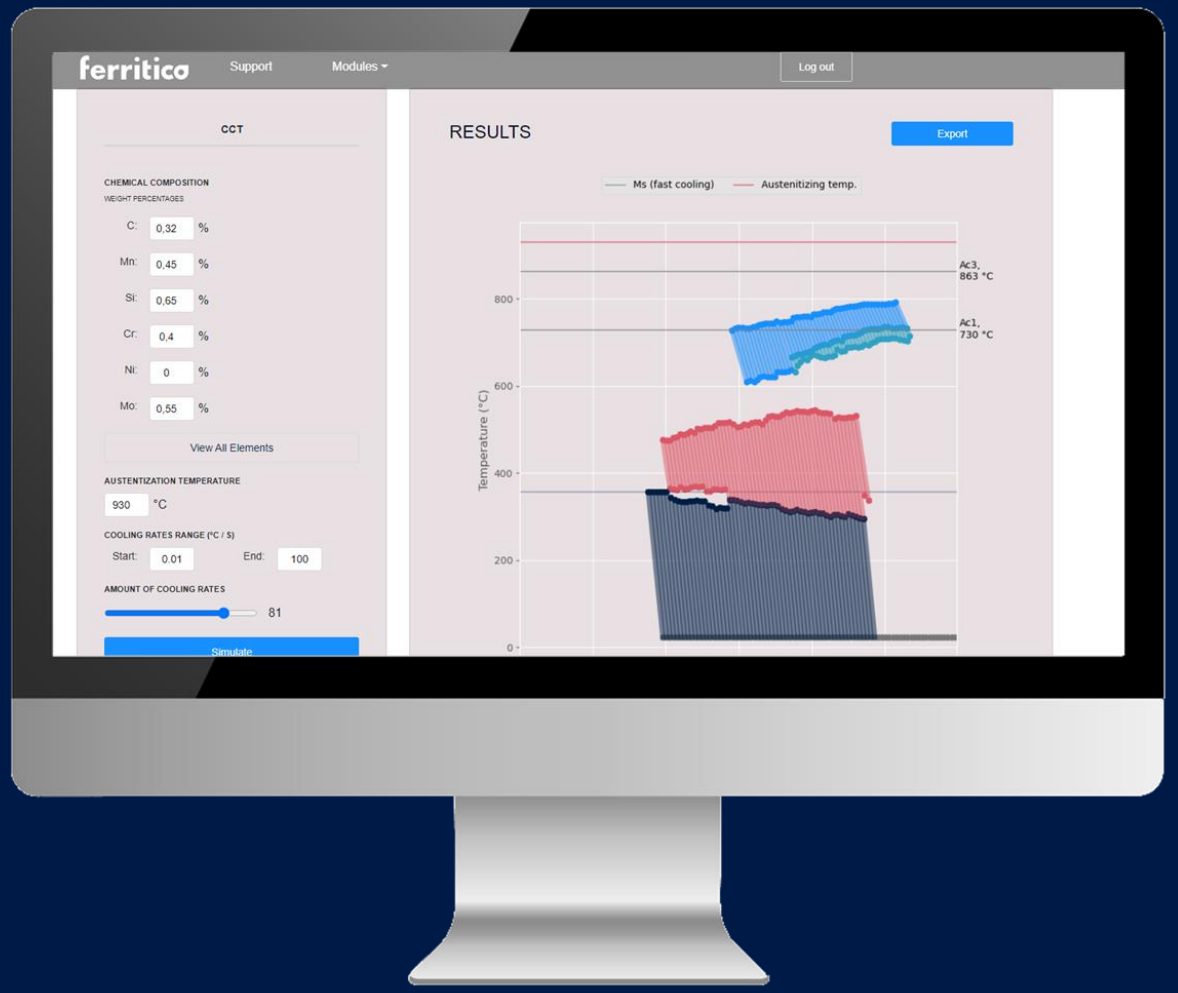
CCT V 2.0 DB





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FERRITICO CCT BENCHMARKING

Phase formation

The aggregated average percentage error for simulation of whether the phases Ferrite, Pearlite, Bainite and Martensite are formed. The benchmark is based on empirically measured CCT diagrams for 14 steel grades (some chemical compositions listed below) that are not included in the machine learning database and where benchmarking CCT data is available for 8-12 cooling rates.

	Ferritico %-error	Competitor %-error
Ferrite	8.1 %	20.7 %
Pearlite	18.9 %	27.0 %
Bainite	23.4 %	27.9 %
Martensite	22.5 %	27.0 %

Phase transformation temperatures

The aggregated average error for simulation of the temperatures on which transformation of the phases Ferrite, Pearlite, Bainite and Martensite are starting and finishing respectively. The benchmark is based on empirically measured CCT diagrams for 14 steel grades (some chemical compositions listed below) that are not included in the machine learning database and where benchmarking CCT data is available for 8-12 cooling rates. In the table, _s and _f refer to the start and finish temperature of the transformation of a phase, e.g. Fe_s being Ferrite start temperature.

	Ferritico error	Competitor error
Fe_s	34.9 °C	49.0 °C
Fe_f	45.7 °C	77.5 °C
P_s	28.4 °C	68.0 °C
P_f	55.2 °C	117.1 °C
B_s	53.6 °C	74.3 °C
B_f	40.1 °C	93.4 °C
M_s	39.6 °C	47.8 °C

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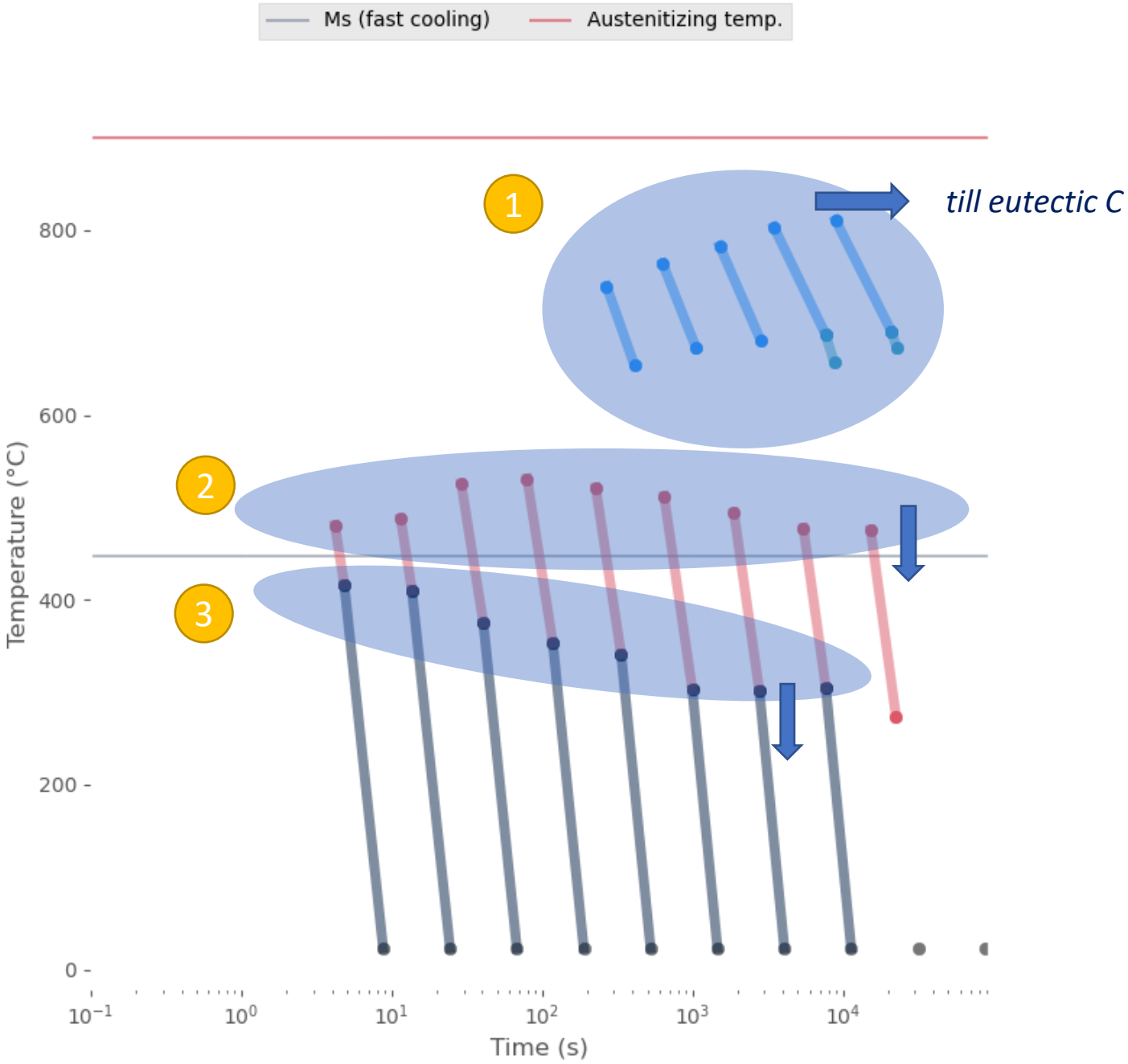
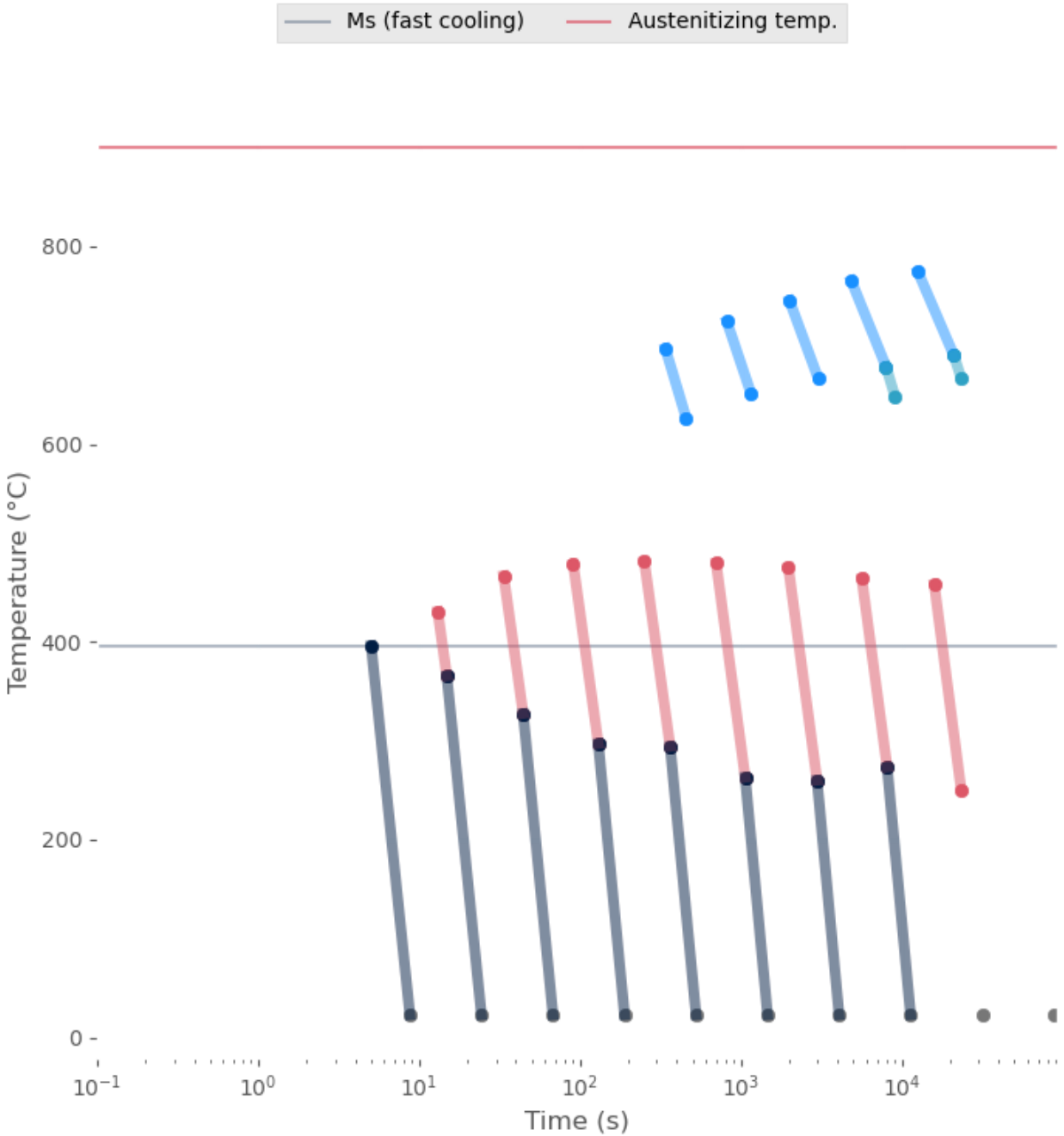
Trends in CCT

Increase in C

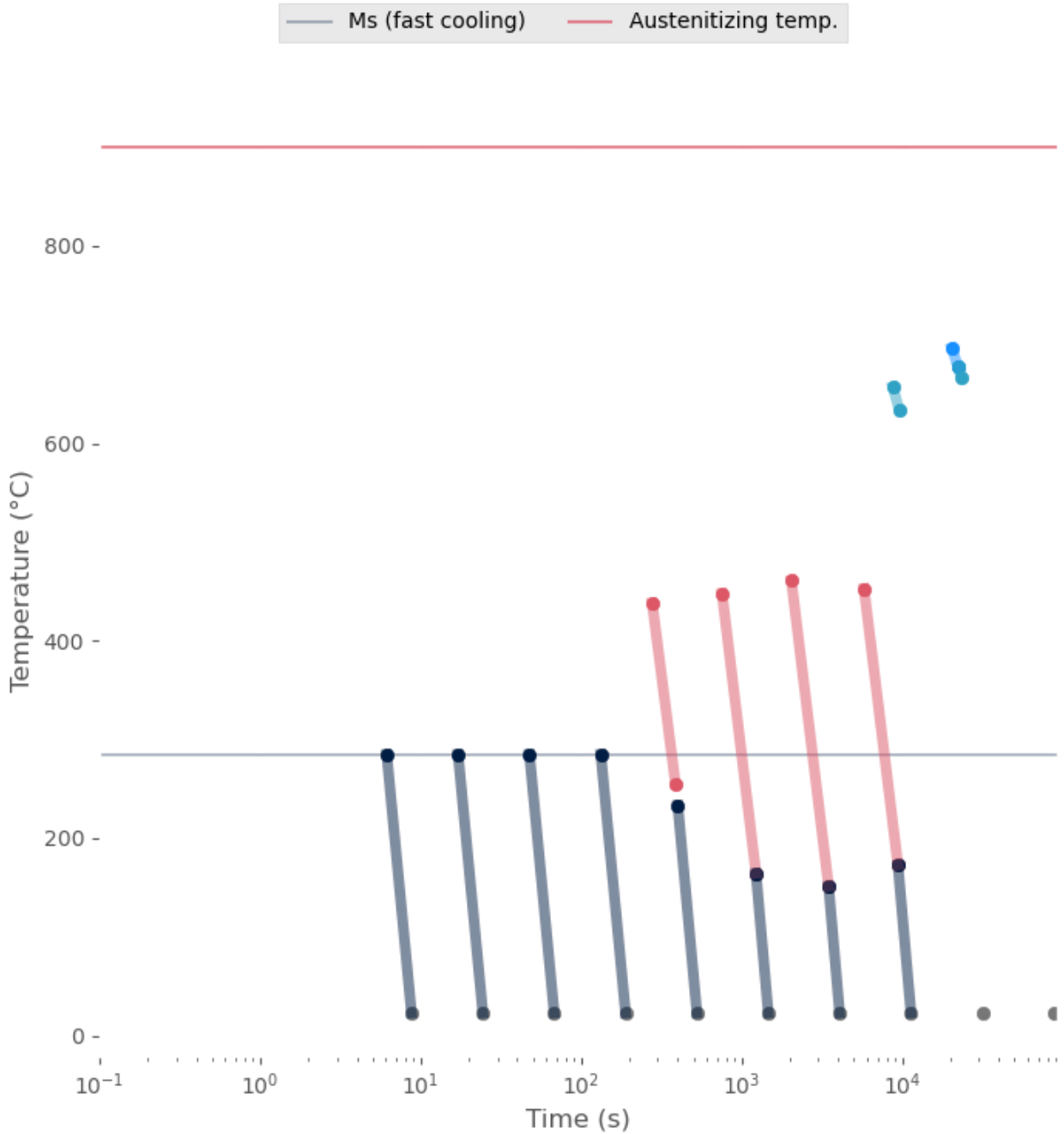
0.07 C



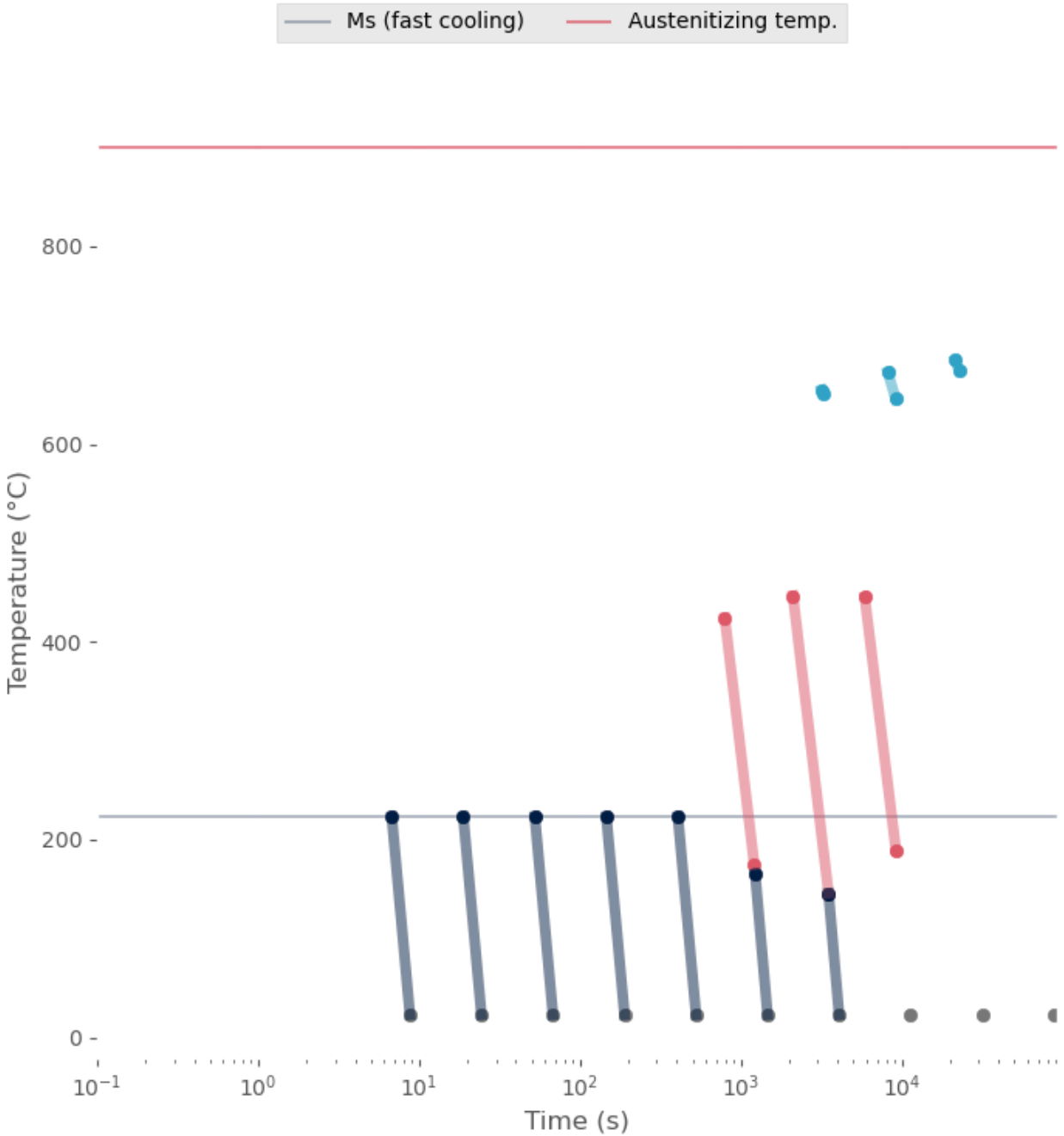
0.25 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

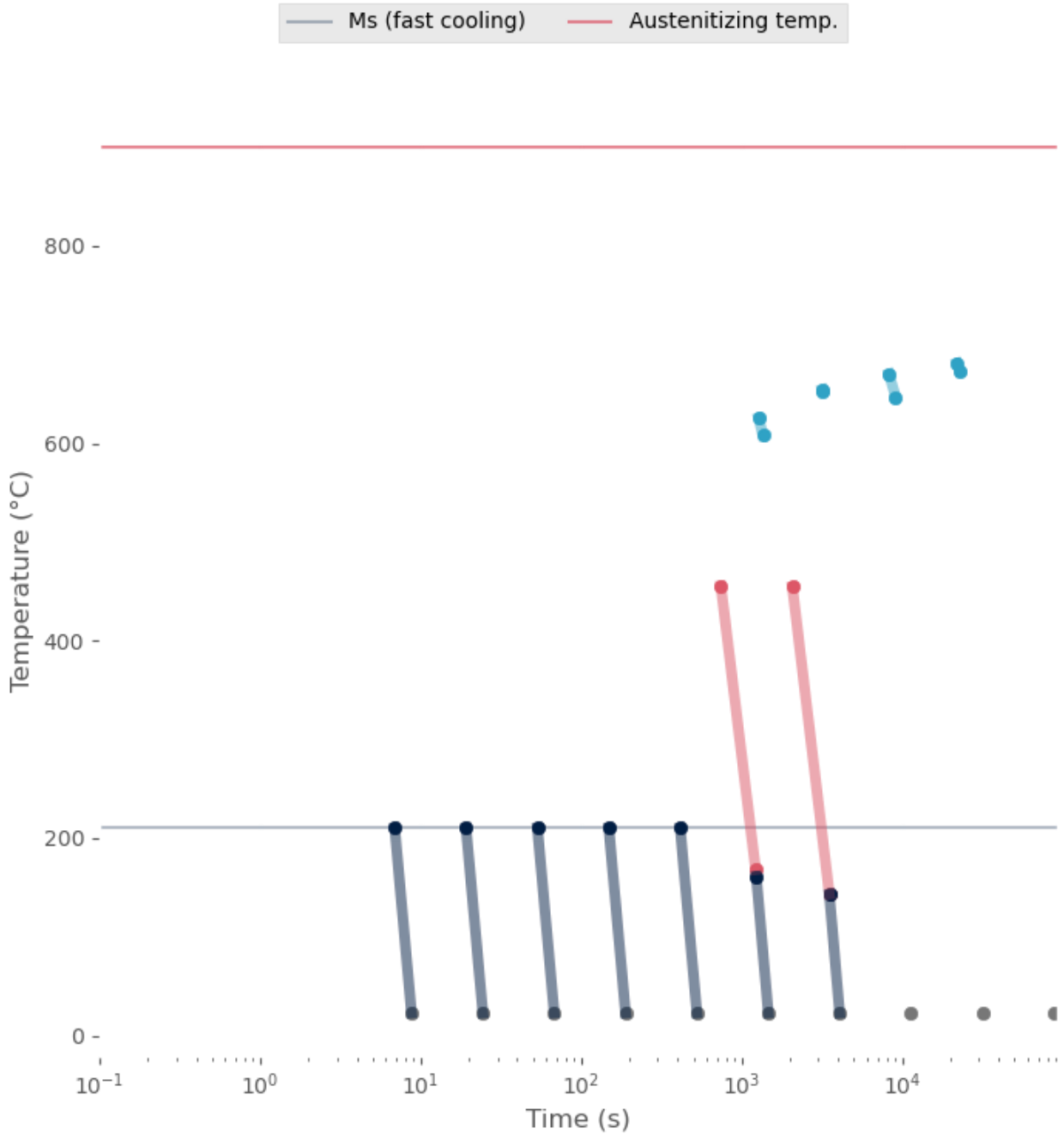
0.5 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

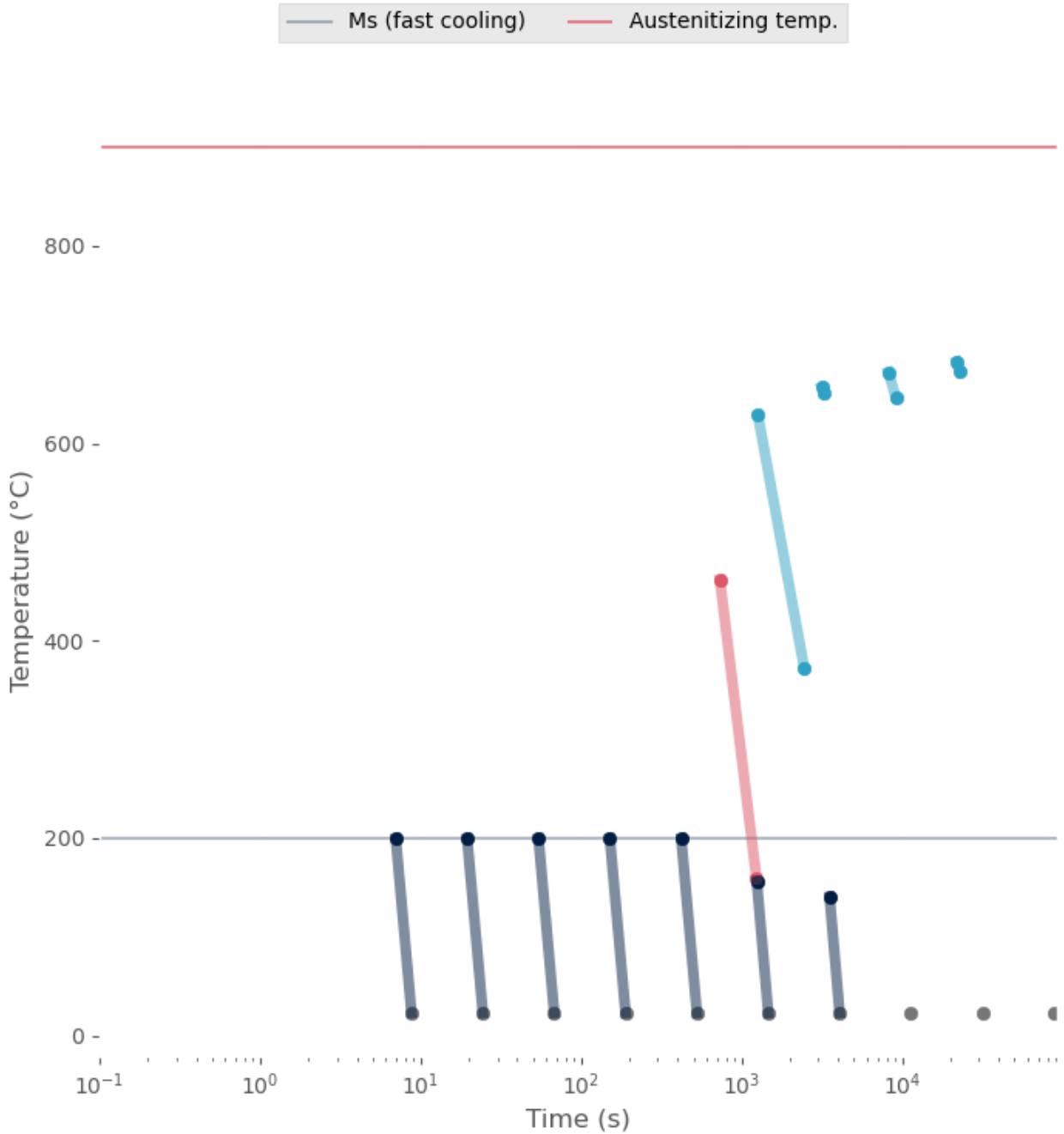
0.7 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

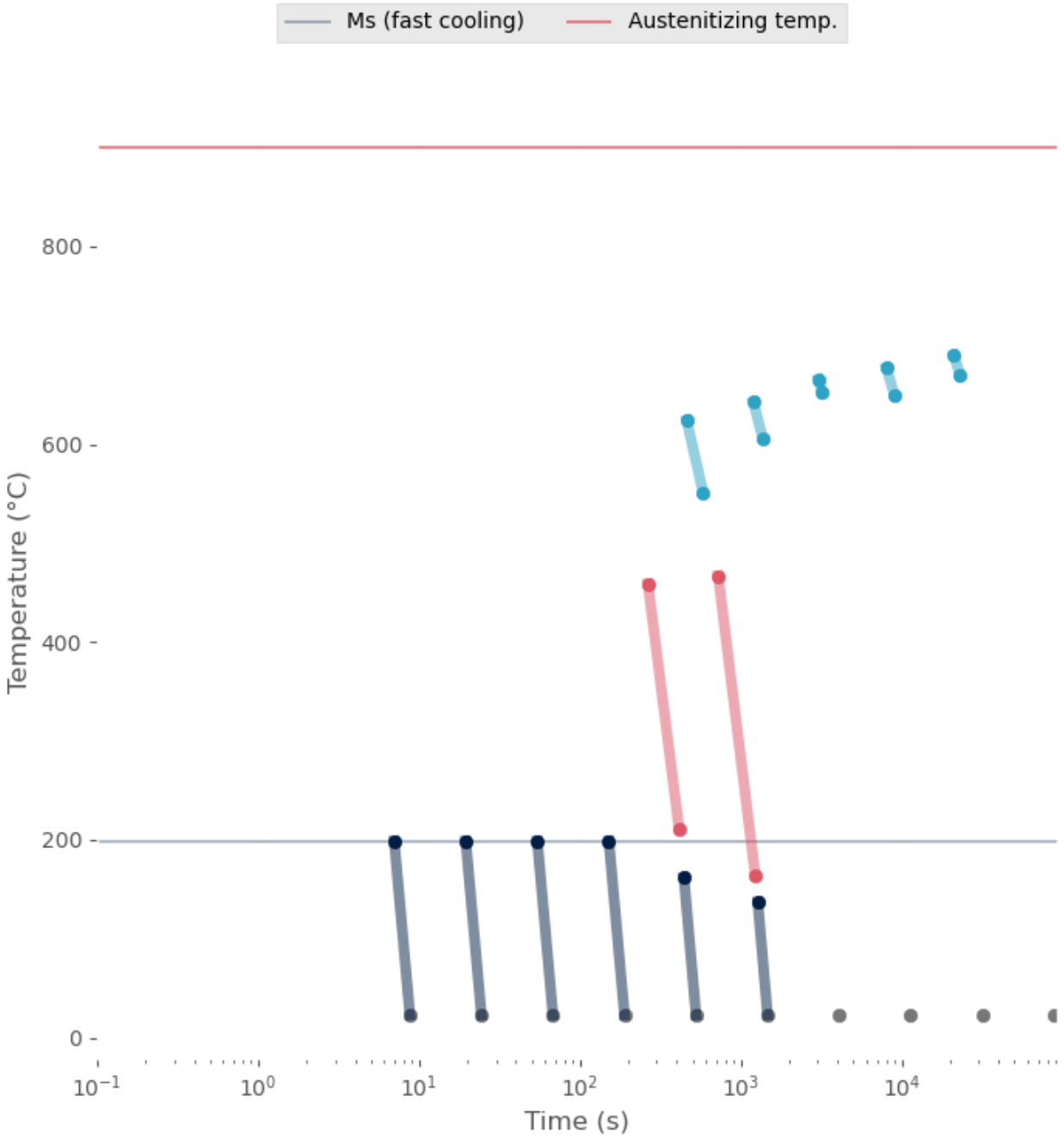
0.8 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

0.9 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

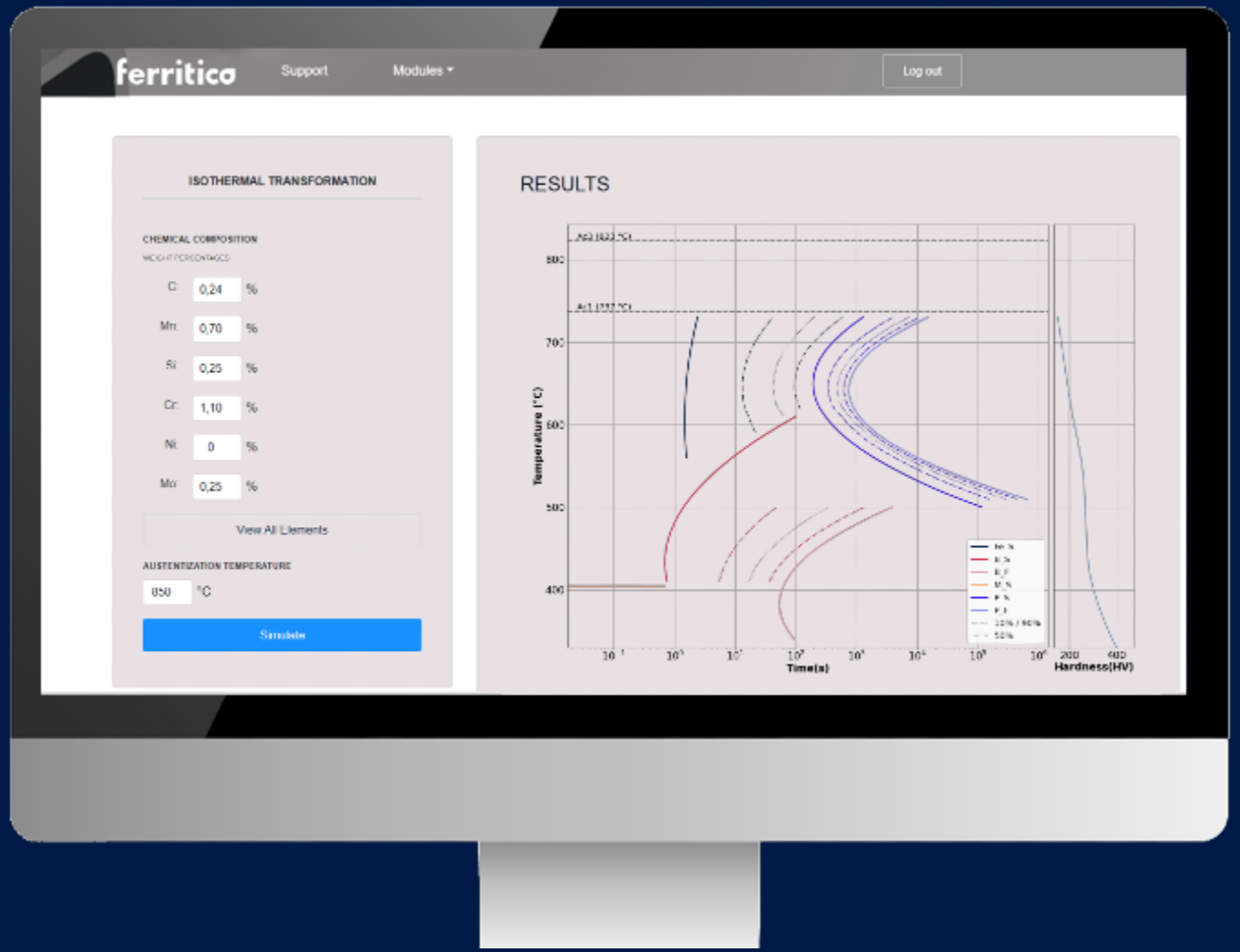
1.1 C


Ms (fast cooling)
Austenitizing temp.
800
600
400
200
0
Temperature (°C)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Time (s)

3/3

	C	Mn	Cr	Ni	Mo	Co	AT
Trend scores	3/3	2/4	3/4	3/4	4/4	0/3	1/1

FERRITICO ISOTHERMAL TRANSFORMATION MODULE



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FERRITICO TTT BENCHMARKING

Phase formation

The aggregated average percentage error for simulation of whether the phases Ferrite, Pearlite, Bainite and Martensite are formed. The benchmark is based on empirically measured TTT diagrams for 14 steel grades (chemical compositions listed below) that are not included in the machine learning database and where benchmarking TTT data is extracted for randomly selected temperatures .

	Ferritico %-error	Competitor %-error
Ferrite start	5.07 %	23.04 %
Pearlite start	4.91 %	31.13 %
Bainite start	7.60 %	4.17 %
Martensite start	28.85 %	0.00 %
Ferrite end	4.91 %	31.13 %
Pearlite end	3.37 %	27.73 %
Bainite end	12.75 %	12.43 %
Martensite end	NA	NA

Phase transformation time

The aggregated average error for simulation of the time in seconds on which transformation of the phases Ferrite, Pearlite, Bainite and Martensite are starting and finishing respectively. The benchmark is based on empirically measured TTT diagrams for 14 steel grades (chemical compositions listed below) that are not included in the machine learning database and where benchmarking TTT data has been extracted for randomly selected temperatures. In the table, _s and _f refer to the start and finish time of the transformation of a phase, e.g. Fe_s being Ferrite start time. TTT M_s model is temporary and will be improved in V 2.0 when consuming the main ferritico Ms model.

	Ferritico error	Competitor error
Fe_s	3.57	9.14
Fe_f	3.06	3.26
P_s	3.06	3.26
P_f	4.69	8.22
B_s	3.55	2.26
B_f	4.10	3.90
M_s	*17.37 °C*	13.52 °C

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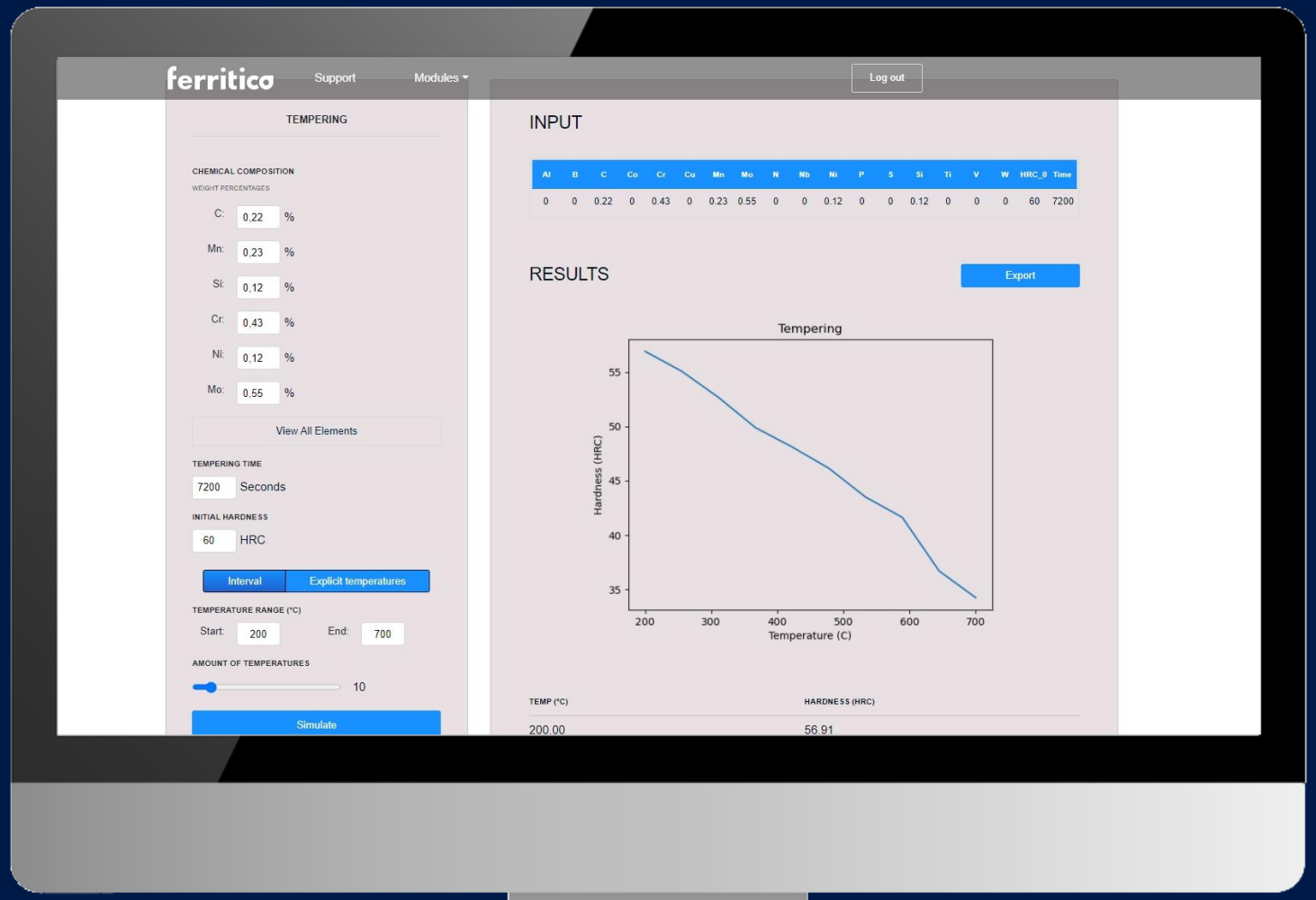
FERRITICO TEMPERING MODULE



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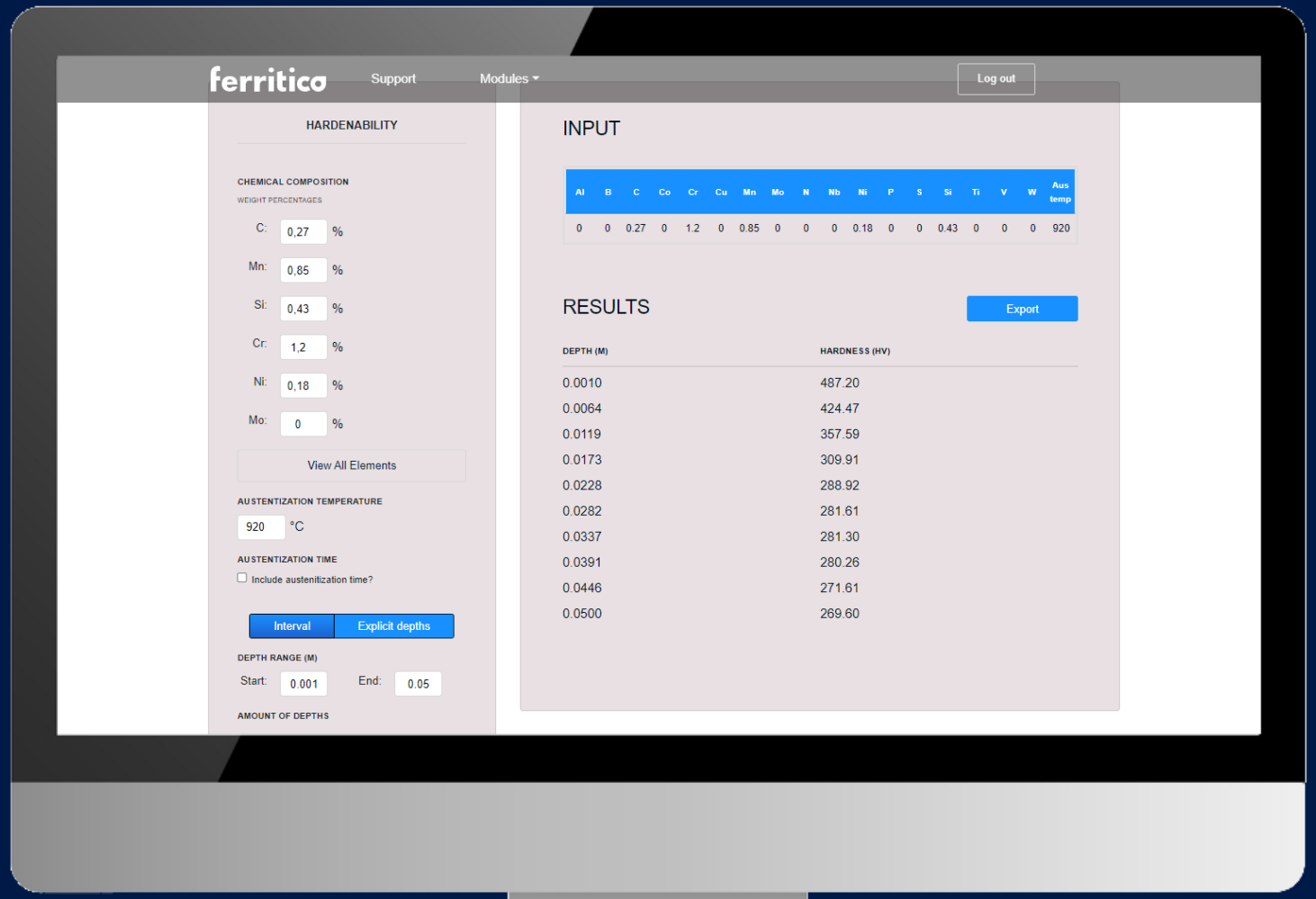
FERRITICO HARDENABILITY MODULE



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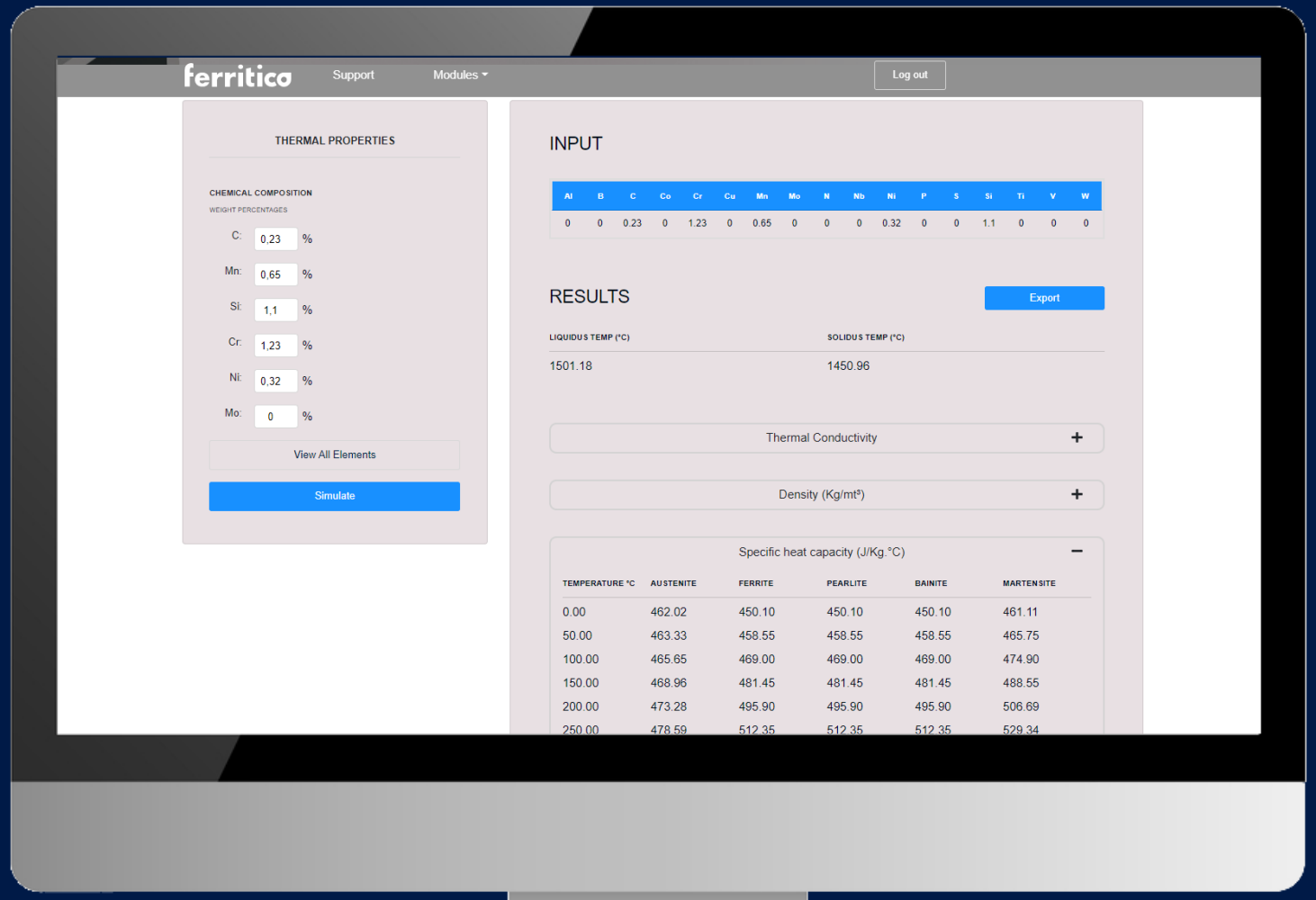
FERRITICO THERMAL PROPERTIES MODULE



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