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# Instant Hydrogen And Carbon Production Via Thermal Plasma Pyrolysis

## Introduction

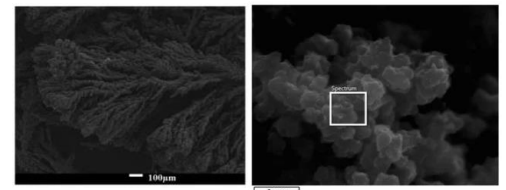
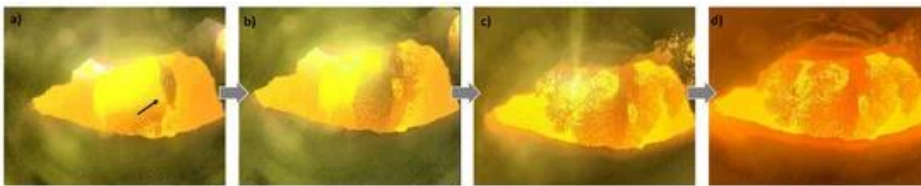
The pressing necessity to transition toward a climate-neutral industry underscores the importance of exploring CO<sub>2</sub>-free alternatives for hydrogen (H<sub>2</sub>) production. Recent advancements suggest that plasma technology holds promise in this endeavor. This study investigates H<sub>2</sub> production through methane pyrolysis using a laboratory-scale plasma furnace.

## Experimental setup

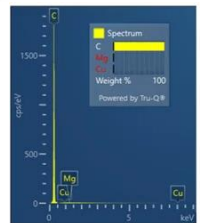
The plasma furnace features a DC-transferred thermal plasma arc system. The plasma gas comprises Ar and CH<sub>4</sub>, introduced into the reaction zone through the graphite hollow cathode positioned above a graphite anode pin. The off-gas is channeled for further analysis, while the plasma arc is recorded by a camera installed on the top lid.

## Hydrogen and carbon production

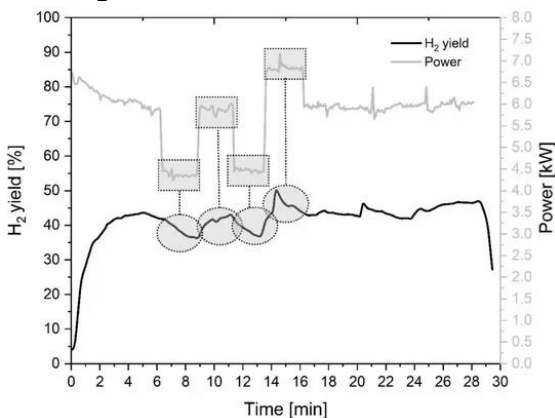
The progressive dendritic growth of carbon begins with a coral-shaped carbon structure forming from the cathode edge. The challenge in the process arises when the deposited carbon interferes with the plasma arc, creating new surfaces that divert the discharge away from the anode.



SEM and EDX analysis of the produced carbon reveal fluffy, pure solid carbon powder.



The H<sub>2</sub> yield is affected by various process parameters. For example, elevating the power input from 4 to 7 kW leads to an approximate 10% rise in the H<sub>2</sub> yield.



## Summary

Overall, the process demonstrates a high H<sub>2</sub> yield ranging up to 100%. A stable process is facilitated by higher power and lower CH<sub>4</sub> input, contributing to a higher H<sub>2</sub> yield. Conversely, increasing gas flow leads to a shorter gas residence time, resulting in reduced H<sub>2</sub> yield. The images of the plasma arc zone vividly illustrate the formation and growth of carbon, causing disruptive interruptions in the arc and declining efficiency. The produced solid carbon exhibits high purity with a fluffy and fine structure. This study concludes that further optimization and development of the process are necessary to achieve stable continuous operation with high utilization efficiency.

Daghagheleh, O.; Schenk, J.; Zarl, M.A.; Lehner, M.; Farkas, M.; Zheng, H. Feasibility of a Plasma Furnace for Methane Pyrolysis: Hydrogen and Carbon Production. *Energies* 2024, 17, 167. <https://doi.org/10.3390/en17010167>



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# Enhancing Steel Cleanness

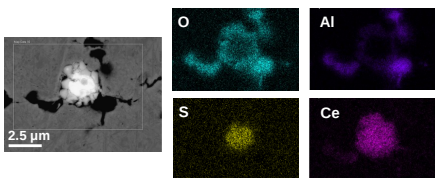
## Tracing Non-Metallic Inclusions with Modern Analytical Techniques

### Motivation

Microscopic non-metallic inclusions (NMIs) in steel production, typically sized between 1 and 15  $\mu\text{m}$ , can significantly influence product quality and process efficiency. Tracing techniques, including **active** and **passive methods**, provide valuable insights into **NMIs origin, formation** and **modification** throughout the process. These methods facilitate the detection and monitoring of NMIs, enabling process optimization and quality enhancement. Due to the transformation to **carbon-free steel production**, it is essential to identify the source of newly formed NMIs.

### Active Tracing

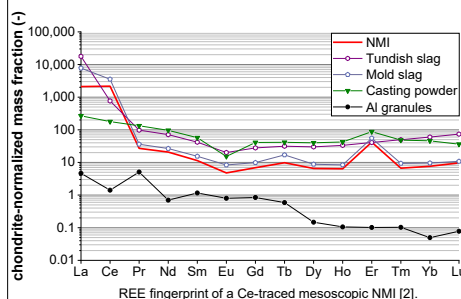
The leading method for NMI tracing is the direct addition of rare earth elements (REEs), such as La and Ce, to the liquid steel. Deoxidation products are **partly reduced**, making traced NMIs appear **brighter** in backscattered electron images at scanning electron microscopy [1]. REEs **influence** the **properties** and **behavior** of NMIs, necessitating alternative tracing techniques.



SEM image of Ce-traced mesoscopic NMI.

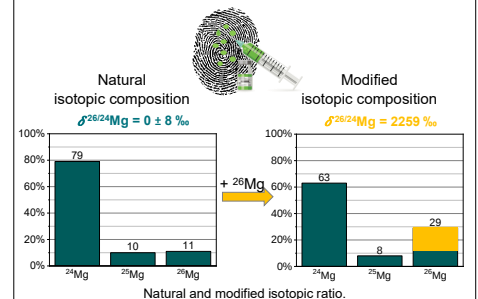
### Passive Tracing Elemental Fingerprint

REE fingerprints of auxiliaries and mesoscopic NMIs were determined by an inductively coupled plasma-mass spectrometer (ICP-MS). By comparing REE patterns of the investigated materials, potential sources of NMIs can be identified since each material is expected to have a **unique REE fingerprint**.



### Passive Tracing Isotopic Fingerprint

The **isotopic composition** of a potential NMI source is intentionally **modified** to differentiate from other ones of the same element. This **distinct signature** allows for tracking the isotopic composition of single NMIs and observing the evolution of NMIs originating from this source throughout the process.



### Summary

Active tracing by direct alloying REEs influences NMIs, while NMIs remain unchanged by passive methods. Elemental and isotopic fingerprinting enable the identification of the source for NMIs and a real-time tracking of their modifications over the process. Hence, countermeasures can be developed to improve the steel cleanness and the product quality.

#### Sources:

[1] K. Thiele, P. Presoly, D. Ernst, S.R. Babu and S.K. Michelic, Evaluation of different alloying concepts to trace non-metallic inclusions by adding rare earths on a laboratory scale. *Ironmaking and Steelmaking*. Vol.32 50 (2023), 5, pp. 507–516. doi:10.1080/03019233.2022.2124816

[2] K. Thiele, C. Truschner, C. Walkner, T.C. Meisel, S. Ilie, R. Rössler and S.K. Michelic, Investigating the Origin of Non-Metallic Inclusions in Ti-Stabilized ULC Steels Using Different Tracing Techniques. *Metals* 14 (2024), 1, pp. 103. doi:10.3390/met14010103



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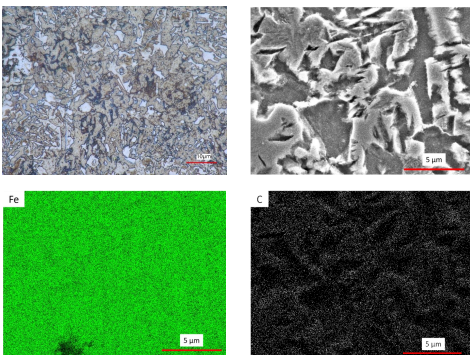
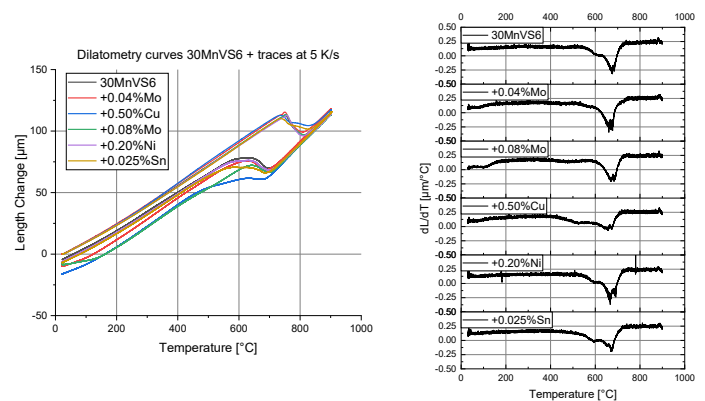
# Influence of Selected Trace Elements on the Phase Transformation in a Medium-Carbon Steel

## Introduction

The iron and steel industry is responsible for **5 % of the EU's total CO<sub>2</sub> emissions** [1]. Steel production via electric arc furnace (EAF) could potentially reduce the steel industry's CO<sub>2</sub> emissions by up to 75 % [2]. Increased usage of this aggregate leads to **accumulation of certain elements** – alloying or tramp – in the steel cycle over time [3]. To investigate certain tramp elements' influence on critical temperatures, phase transformation and the resulting microstructure, 30MnVS6 steel alloyed with tramp elements was tested in a quenching dilatometer from 900 °C to room temperature with a cooling rate of 5 K/s and exemplarily metallographically analyzed.

## Dilatometry – Phase Transformation

Trace amounts of **copper** and especially **molybdenum** significantly **delay phase transformation** in 30MnVS6 steel. The transformation curve and its first derivative suggest that the microstructure is ferritic-pearlitic. The effect of nickel and tin on the cooling behavior on phase transformation of this steel is less pronounced than for example molybdenum's and if further investigations are to be made, they should include higher amounts of especially tin in the steel.



Light microscope & SEM image (above), Elemental mappings (below)

## Microstructure

30MnVS6 with an addition of 0.50 wt.% copper could not be accurately quantified under the light microscope. In the secondary electron image the brighter areas are higher which indicates that the material has been **selectively etched**. The elemental mappings suggest that there is no variation in the iron distribution but shows a network-like structure in carbon. These are strong indicators of a ferritic-pearlitic structure. Beraha I etching solution forms a **film on the material** and thus one can assume that the etching solution was too viscous to penetrate into the pearlite lamellae. Instead, the solution has deposited over the whole of the pearlitic area.

## Summary

Copper delays phase transformation and thus carbon has a smaller time frame to enter the cementite areas in the pearlite resulting in **narrowing of the lamellae** – thus the film of etching solution over the lamellae. This supports the notion that already trace amounts of copper delay phase transformation noticeably.

In the dilatometry curves it is evident that also trace amounts of molybdenum already delay phase transformation. The dilatometry curves of the nickel- and tin-alloyed steels are not distinctly altered which suggests that phase transformation is not significantly affected by trace amounts of these elements.

Sources: [1] The European Steel Association (EUROFER) AISBL, Making a success of the EU Green Deal, Brussels, 2020. [2] C. Broadbent, Steel's recyclability: demonstrating the benefits of recycling steel to achieve a circular economy, Int J Life Cycle Assess 21 (2016) 1658–1665. [3] K. Daehn, Copper contamination in end-of-life steel recycling, developing a new strategy from million-tonnes to milligrams. Dissertation, 2019.



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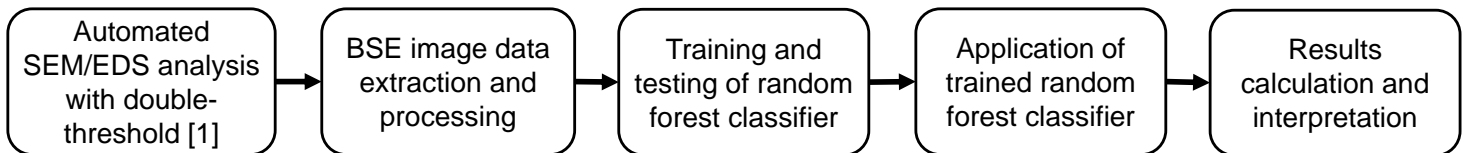
# AI Assisted Steel Cleanness Evaluation

## Morphology Classification of Traced Non-Metallic Inclusions

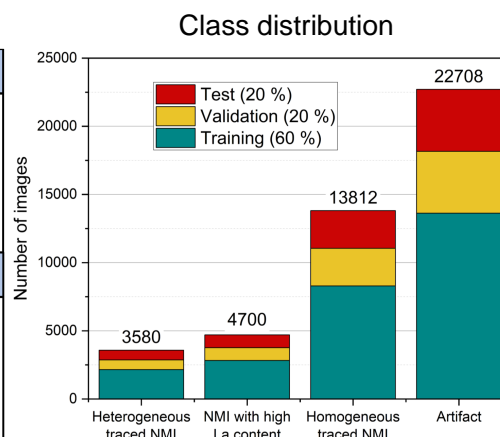
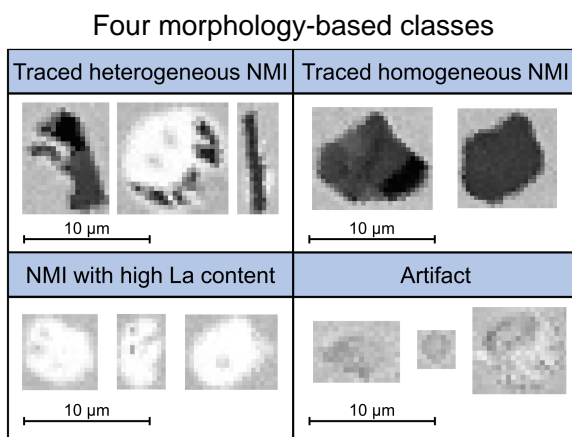
### Motivation

Non-metallic inclusions (NMIs) play a crucial role in determining the chemical and physical properties of the final steel product. The active tracing technique allows for investigating the formation and modification mechanisms of detrimental NMIs throughout the steelmaking process by adding rare earth elements (REEs) directly to the melt. The interaction of REEs with NMIs results in the modification to **traced multiphase particles**. Obtaining information about the **REE distribution in traced NMIs** advances the existing steel cleanness evaluation by automated scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS). **Artificial intelligence (AI)** is used to gain access to this morphological information from backscattered electron (BSE) images, leading to a **better process understanding** and a **more in-depth evaluation** of tracing experiments.

### Workflow



### Dataset



### Achieved performance metrics

Evaluating the random forest classifier with the test set:

Accuracy = 92,8 %

Precision = 90,6 %

Recall = 86,0 %

### Summary

Application of artificial intelligence for image classification enhances the existing steel cleanness evaluation by gaining access to additional information about the morphology of REE-traced NMIs. More data can be extracted from tracing experiments, thereby enabling a better understanding of the process. Hence, AI appears to be a very promising tool to support manual and automated steel cleanness evaluation in future.

#### Sources:

[1] K. Thiele, R. Musi, S. Ramesh Babu and S.K. Michelic, Optimization of the Two- and Three-Dimensional Characterization of Rare Earth-Traced Deoxidation Products. Adv Eng Mater 25 (2023), 11. doi:10.1002/adem.202201748



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# Physics-Driven Models

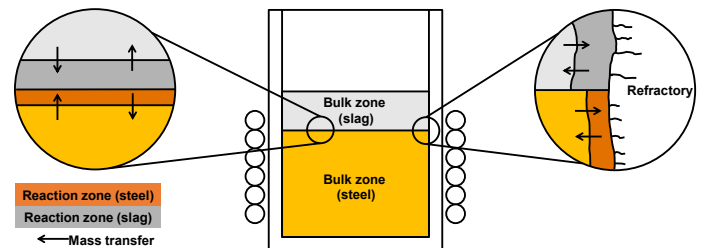
## Modeling of Inclusion Modifications in Complex Metallurgical Systems

### Motivation

The increasing demands on material properties and process efficiency necessitate advanced modeling techniques, such as physics-driven models in metallurgy. Such models can be used to map complex interactions within metallurgical processes. To model the specific case of non-metallic inclusion (NMI) modification across processes, it is necessary to determine and include metallurgical phenomena acting on them. This approach provides an understanding of how NMIs evolve towards a negative state for material properties.

### Thermodynamic/Kinetic Interaction

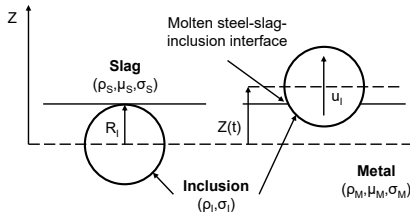
To describe the reactions between the phases in a metallurgical system (steel, slag, refractories, NMIs), the Effective Equilibrium Reaction Zone Model (EERZ) is used. In a defined time step, a certain amount of one phase enters an imaginary reaction zone at the interface of two phases (kinetics) and reacts there towards equilibrium (thermodynamics). The change in the composition of the individual phases can thus be mapped [1].



Representation of the reaction zones and mass flows in an example metallurgical system

### Inclusion Separation

The separation of NMIs at the steel-slag interface can be described by a system of differential equations based on a force equilibrium [2].



Overview of an NMI at the steel/slag interface

$$\frac{d^2Z}{dt^2} = 2 \frac{\rho_S * A(Z, \rho_M, \rho_S) - \rho_I}{\rho_S * A(Z, \rho_M, \rho_S) + 2\rho_I} - 3 * D(Z, R_I, \rho_S, \rho_I) *$$

$$B(Z, \sigma_{IM}, \sigma_{IS}, \sigma_{MS}) - \frac{9}{E(Z, R_I, \rho_S, \rho_I, \mu_S)} * C(Z, \mu_M, \mu_S) * \frac{dZ}{dt}$$

Sources:

- [1] Van Ende, Marie-Aline, et al. "A kinetic model for the Ruhrstahl Heraeus (RH) degassing process." Metallurgical and materials transactions B 42 (2011): 477-489.
- [2] Strandh, Jenny, et al. "Solid inclusion transfer at a steel-slag interface with focus on tundish conditions." ISIJ international 45.11 (2005): 1597-1606.
- [3] Lei, Hong, Keiji Nakajima, and Ji-Cheng He. "Mathematical model for nucleation, Ostwald ripening and growth of inclusion in molten steel." ISIJ international 50.12 (2010): 1735-1745.

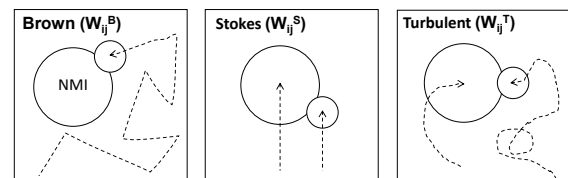
### Inclusion Nucleation

The phenomenon of homogeneous nucleation can be described thermodynamically. For a spherical particle with the radius  $R_I$ , the surface energy  $\gamma$  and the free energy of the bulk crystal  $\Delta G_V$ , give the total free energy  $\Delta G$  [3].

$$\Delta G = 4\pi R_I^2 \gamma + \frac{4}{3} \pi R_I^3 \Delta G_V$$

### Inclusion Agglomeration

Description of the probability  $W_{ij}^{TC}$  of two inclusions (inclusion i and inclusion j) meeting through various flow phenomena [3].



Agglomeration phenomena included in the description

$$W_{ij}^{TC} = W_{ij}^B + W_{ij}^S + W_{ij}^T$$



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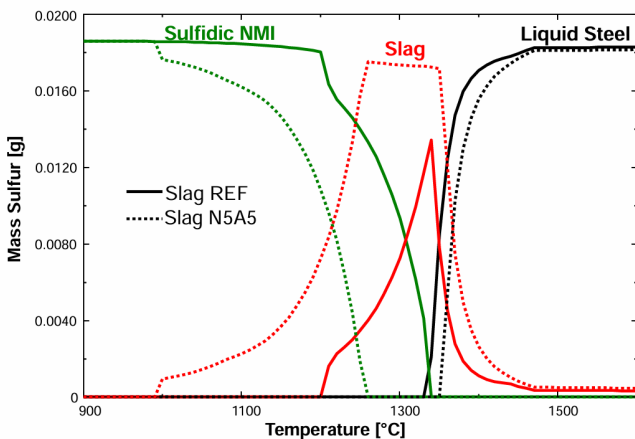
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# Impact of Na<sub>2</sub>O-Slags on Non-metallic Inclusions

## Thermodynamic and experimental investigation

### Introduction

During the analysis of experimental data acquired to investigate the **effects of alkali-metal oxides in slags** for the secondary metallurgy of steels **on non-metallic inclusions (NMIs)**, unexpected results were observed. Instead of decreasing the amount of oxidic particles, as expected from previous work, a drastic increase of oxidic particles accompanied by an equally substantial **decrease in the amount of sulfides** in the samples was found. This result contrasts thermodynamic calculations, which did not predict a significant change in the population of sulfidic NMIs in steel due to changes in the slag's chemical composition. Additional thermodynamic calculations are performed, and accompanying experiments are conducted to clarify this matter. With this, the desulfurization effect can be tied to the **cooling conditions** during the experiments, substantially improving the further design of experimental work in this field.



Sulfur solubility depending on temperature and Na-content in Steel-Slag systems [1]

### Thermodynamic Considerations

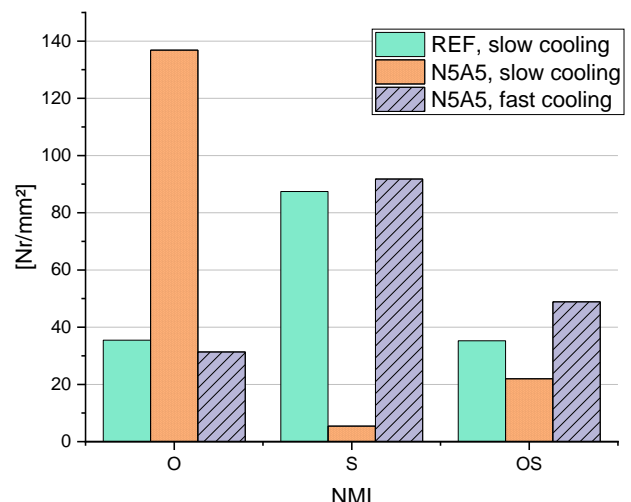
Thermodynamic calculations were conducted to examine the presence of sulfur in solidified samples. Slag N5A5, containing 5 wt.% of sodium, enhances **sulfur solubility** in the slag phase and expands the temperature range in which sulfur is stable in the slag, as indicated in the figure on the left by the red lines. This range corresponds with the solidus temperature of the steel (1340°C). As a result, during steel solidification, **sulfur migrates to the slag phase** and does not form sulfides in the steel matrix, particularly with sodium contents in the slag. Conversely, rapid cooling or quenching hinders this migration to the slag phase and facilitates sulfide formation in the steel phase.

### Summary

By using a modified experimental set-up, **faster cooling rates** can be achieved for the steel-slag system. Analysis of the NMI landscape, shown in the figure on the right, suggests that faster cooling rates can maintain the same level of sulfidic NMIs in steels after contact with Na-containing slag N5A5 as with slow cooling after contact with Na-free slag REF. This confirms the assumption made from thermodynamic calculations. In previous experiments, slower cooling rates likely caused sulfur removal from steel due to higher solubility in the slag phase.

Source:

[1] C. W. Bale, E. Bélisle, P. Chartrand, S. A. Deckerov, G. Eriksson, A.E. Gheribi, K. Hack, I. H. Jung, Y. B. Kang, J. Melançon, A. D. Pelton, S. Petersen, C. Robelin, J. Sangster, P. Spencer and M-A. Van Ende, FactSage Thermochemical Software and Databases - 2010 - 2016, Calphad, vol. 54, pp 35-53, 2016 <[www.factsage.com](http://www.factsage.com)>



Sulfur solubility depending on Na-content in Steel-Slag system



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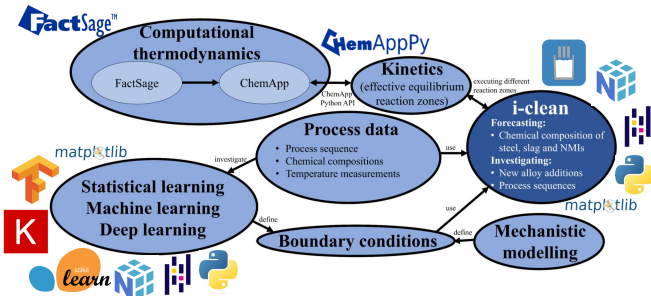
# Hybrid thermodynamic and statistical modeling of secondary metallurgical processes

## Abstract

This study combines traditional metallurgical modeling with statistical learning to investigate the chemical interactions among steel, slag, and non-metallic inclusions during **secondary steelmaking**. The process of predicting the composition of each phase from Basic Oxygen Furnace (BOF) tapping to ladle furnace (LF) processing is conducted using the **Effective Equilibrium Reaction Zone (EERZ)** method. This is done by utilizing the **ChemApp™/FactSage™ thermodynamic software** and extensive data from an industrial partner. Furthermore, the research involves a detailed **statistical analysis of production data**, chemical analysis of **steel samples**, and **temperature measurements** to define boundary conditions.

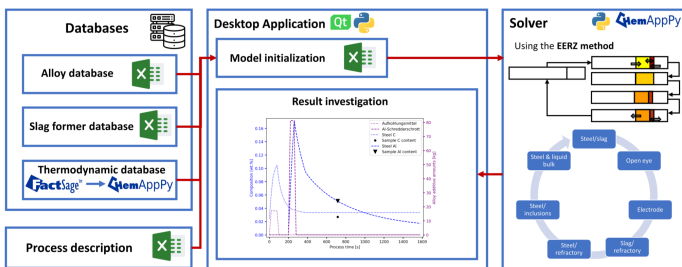
## Concept of the project work

The **EERZ method** is used to describe the **reaction kinetics**. The **thermodynamic equilibrium** is calculated using the **ChemApp™ Python API** and **FactSage™ databases**. The boundary conditions of all processes implemented into the **developed software "i-clean"** are based on **statistical/machine learning** methods, semi-empirical values, and mechanistic models.



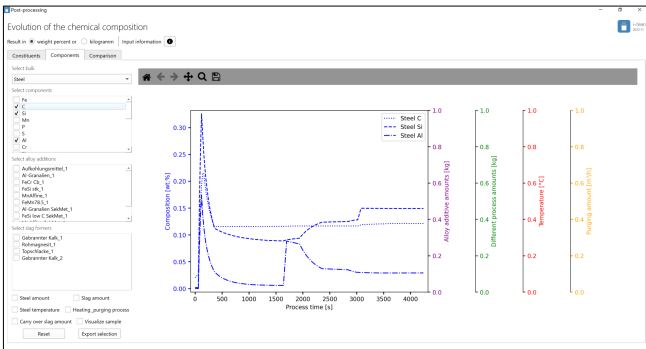
## Software architecture of the developed Python application "i-clean"

The software can be divided into three segments: **Pre-processing** is dedicated to define the databases and each process step (e.g., alloying, heating, purging, ...). The **solver** calculates the chemical composition during the secondary refining. In **post-processing**, one can investigate the simulation results for the whole secondary metallurgical treatment.



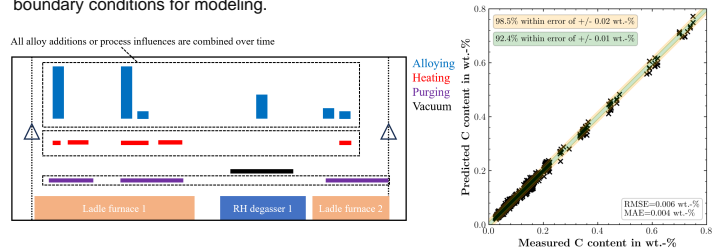
## Investigating the simulation results

The developed **user-friendly GUI** lets one intuitively define boundary conditions, start simulations, and examine the results. Thus, in post-processing, the **development of individual elements/components** in the various process phases can be displayed over the duration of the process. Process influences (e.g., alloying, heating, rinsing, ...) can also be depicted. Moreover, the calculations can be **compared to actual measurements**.



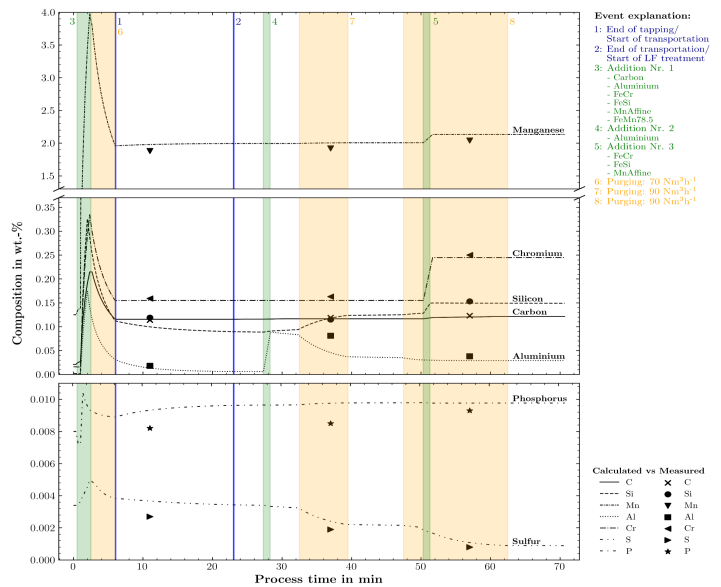
## Statistical analysis of the production data

Through **comprehensive descriptive data analyses**, followed by various **data cleansing** steps and **regression modeling** (e.g., MLR, LASSO, Random Forest, etc.), **new insights** regarding the alloy yield rate are gained from the process data, which can be used as boundary conditions for modeling.



## Exemplary simulation results and knowledge gain

With the help of "i-clean" software, it becomes possible to **simulate complete process sequences** of secondary metallurgy and test new process routes. This approach **generates new knowledge and possibilities** for future metallurgical refining treatments. If one defines the initial conditions (e.g., tapped steel mass, amount of carry-over slag, ...) and process schedule (e.g., material additions, transport phases of the ladle, amounts of heating and purging gas) according to the carried-out treatment in the steel plant, the simulation results are close to the measured steel and slag compositions. This is one potential of the software to **investigate the phenomena** occurring in the ladle.



## Summary and Outlook

The development of "i-clean" software enables comprehensive investigations into the changes in the **chemical composition of the steel, slag, and non-metallic inclusions** throughout the secondary metallurgical process using the **EERZ** method and the thermodynamic database **FactSage™**. With the help of **data-driven approaches**, process boundary conditions (e.g., the yield rate of alloy additions) can be estimated for the simulation. With the **user-friendly GUI**, one can define starting conditions according to the specific use case and examine the simulation results in the post-processing. Future work will deal with the hybrid determination of temperature or the detailed description of various metallurgical treatments (e.g., desulfurization via top slag).



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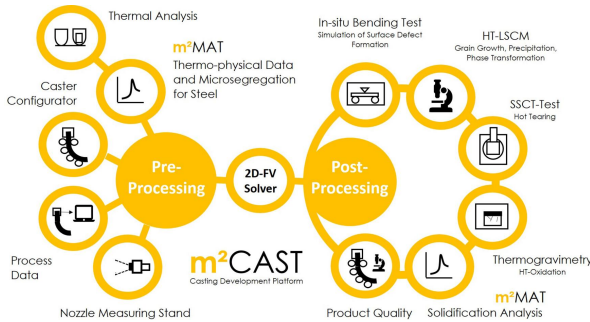
# Real-time Modeling of Continuous Casting Processes

## Abstract

Ongoing efforts are being made to create **online quality prediction systems** based on metallurgical fundamentals with **online capable fast runtimes**. This research presents a **2D heat transfer model** named **m<sup>2</sup>CAST** that can be used to advance the **slab casting process**. An implicit **finite volume method (FVM)** based on the **Tridiagonal Matrix Algorithm (TDMA)** and the **Alternating Direction Implicit (ADI)** method was developed. Additionally, the introduction of a **non-uniform grid** further accelerated the simulation. To describe the boundary conditions in the secondary cooling zone (SCZ), measurements are taken at the **Nozzle Measuring Stand (NMS)**. The developed model enables the examination of all heat transfer coefficients on the surface, the temperature field, and the shell growth of the steel strand. Finally, the simulation results were validated with plant measurements at a slab caster.

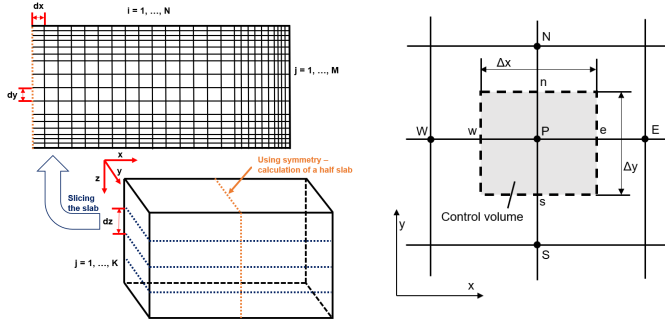
## Introduction and motivation

Montanuniversity Leoben's M<sup>2</sup>CC group uses **experimental and numerical simulations** to study **continuous casting's quality aspects**. The goal is to create a platform to exchange information gained from plant process conditions and laboratory tests. The "casting development platform" **m<sup>2</sup>CAST**, using numerical methods, thermodynamic databases, and experimental data, represents a cornerstone of the project.



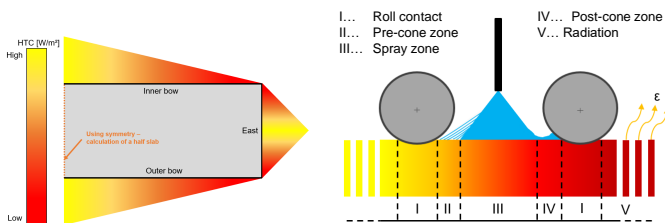
## Discretization and numerical modeling

Accurate surface simulations in slab casting require **fine meshing**, especially since large grid spacing distorts early mold calculations due to high heat transfer and temperature gradients. A **non-uniform grid** was developed to balance accuracy and computing time, matching fine mesh results and **cutting computation time by up to 95 %**. A 2D FVM for heat conduction was implemented and optimized using the TDMA and ADI methods for more computational efficiency.



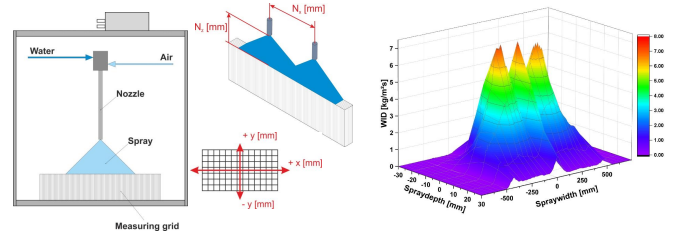
## Thermal boundary conditions definition

Heat **transfer boundary conditions** for the continuous casting simulation are divided into the **primary cooling zone** and a **five-zone secondary cooling process**. Inside the mold, only conduction takes place between the steel strand and the surroundings. Within the secondary cooling zone, different phenomena occur. A combination of heat conduction, radiation, and convection must be considered while modeling the boundary conditions.



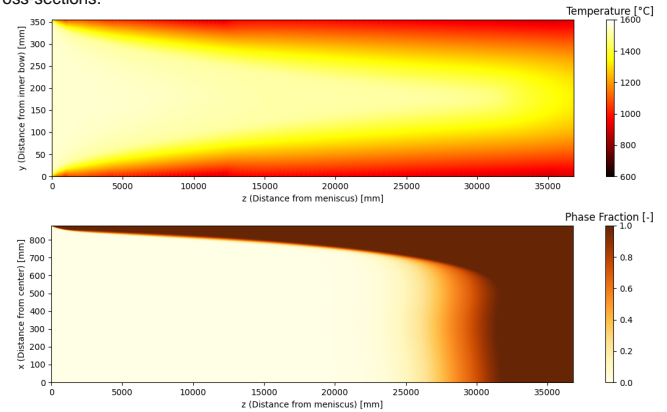
## Nozzle measuring stand (NMS)

The **water impact density** measurement setup uses a transparent grid to capture the nozzle spray. It is adjustable for different distances and can be set up in a single or dual configuration. Visual analysis of the filled grid cells provides a water distribution profile, as illustrated in the 3D graph.

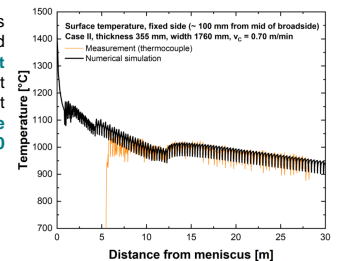


## Simulation of temperature field and solidification progress

The **m<sup>2</sup>CAST** software enables detailed analysis of **temperature profiles**, **shell growth**, and **heat transfer coefficients** by slicing the slab at user-defined positions for visualization. This method allows the **examination of three-dimensional solidification patterns** and offers detailed 2D temperature field analysis through horizontal or vertical cross-sections.



The figure on the right-hand side shows the outer bow's measured and calculated surface temperature profiles. **Excellent agreement** between the drag element measurements and the software result could be confirmed. The **calculation time** for the whole slab was approximately **90 seconds**.



## Summary and outlook

The poster outlines the use of **m<sup>2</sup>CAST** software to enhance evaluations in continuous casting. It emphasizes the efficiency of a **non-uniform grid** for faster results, details **primary and secondary cooling zone conditions**, and showcases a **nozzle measuring stand** for water impact density assessment. Temperature is validated using drag element measurements, revealing the software's **high accuracy** in temperature profiling. Future work will concentrate on implementing metallurgical models to predict the strand quality under real-time conditions.



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ONE STEP AHEAD.

# HT-LSCM in steel research

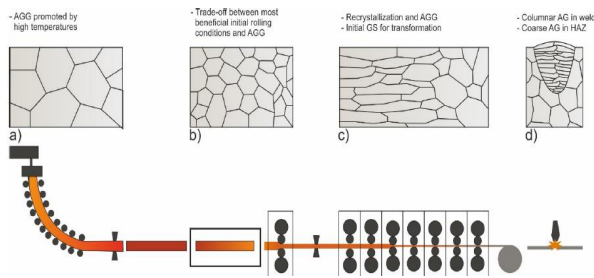
## Austenite grain growth and phase transformation observations

### HT-LSCM

High-Temperature Laser Scanning Confocal Microscope is a thermo-optical method for surface investigations of specified samples. The aim is to investigate, validate and/or quantify relevant metallurgical mechanisms for scientific knowledge or to improve industrial processes. Samples are investigated under argon or helium atmosphere with a maximum heating rate of 1200 °C/min to 1600 °C and a maximum cooling rate of -500 °C/min. Beside steel, other binary alloys, ceramics and non-ferrous metals can be examined.

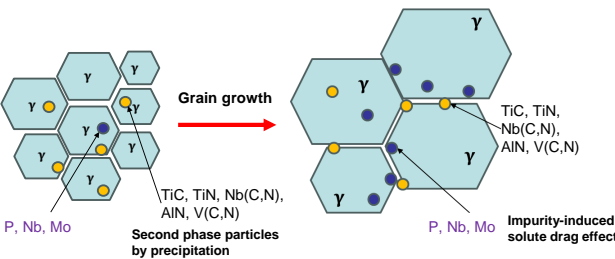
### Relevance of solid-state phenomena in steel processing

Continuous casting of steel is the most dominant process in steelmaking as nearly 97 % of the annual steel production is continuously cast to slabs, billets or blooms. During the process, austenite grain growth and phase transformation occurring during cooling at the strand surface may affect to product quality related to surface cracks. The initial average austenite grain size influences the final microstructures and phase transformations throughout the entire processing of steel i.e.: reheating, rolling mill and heat treatments.



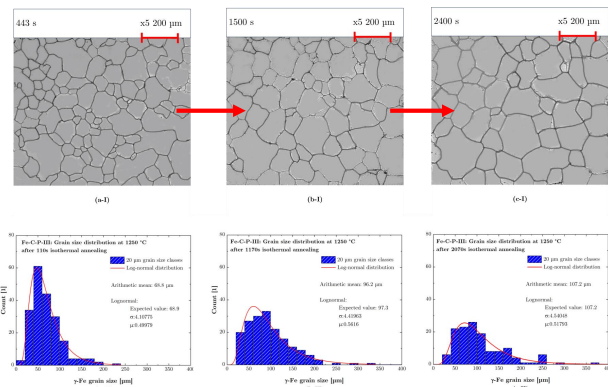
### Austenite grain growth – (AGG)

The average austenite grain size is a relevant parameter for continuous casting, as controls the working volume of further processing and the mechanical properties. The two most important grain growth inhibiting mechanisms associated with AGG are the **solute drag effect**, where impurities segregate to the grain boundaries and **Zener pinning forces** by precipitated second phase particles i.e.: Nb(C,N), AlN, V(C,N). By quantifying the mean grain size as a function of temperature and chemical composition, it is possible to investigate the influence of both mechanisms on the austenite grain growth kinetics at elevated temperatures.



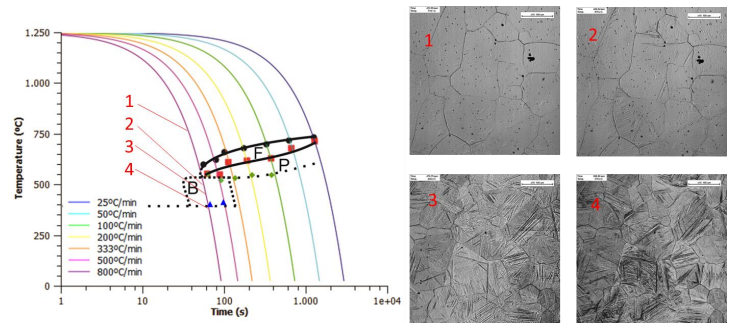
### Example: Austenite grain growth in a ternary Fe-C-P alloy

The figure shows the isothermal microstructure evolution with the corresponding grain size distribution in a sample containing 0.20 wt.-%C and 0.15 wt.-%P at 1250 °C.



### Phase transformations during cooling

Due to the versatility of steel and its allotropic behavior, time-temperature transformation diagrams are essential for the cooling strategies to obtain the desired microstructure and further mechanical properties. HT-LSCM enables the investigation of phase transformations in real time from austenite to non-equilibrium phases. It is also possible to study the effect of austenite grain size on phase transformation.



### Summary and outlook

HT-LSCM is a valuable tool for in situ observation of metallurgical phenomena on the surface of steel samples. Currently, the role of C, N and P as well as Nb(C,N) on grain growth inhibition is investigated. In future research, the focus will be placed on green steel transformation including the analysis of tramp elements.



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ONE STEP AHEAD.

# Hydrogen Plasma Smelting Reduction of Iron Ore

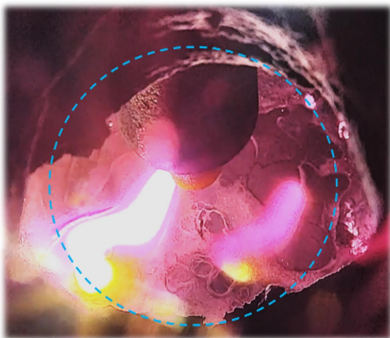
## A Pathway to a Sustainable Steel Industry

### Motivation

Driven by global climate agreements like the Paris Agreement and the European Green Deal, there's an urgent need for greener steel production. The Hydrogen Plasma Smelting Reduction (HPSR) process offers a solution that significantly reduces carbon emissions during steel production. Since the HPSR process utilizes excited hydrogen species with a much higher reduction potential, it constitutes a promising pathway for sustainable steel manufacturing. With its ability to use diverse iron ore feedstocks, it promotes resource efficiency and resilience in steel production, enabling a one-step process from iron ore to steel.

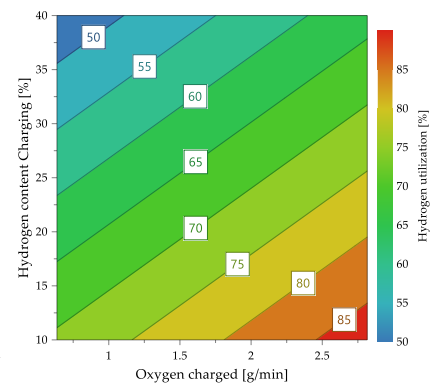
### Enhancing Efficiency through Optimal Material Charging

Key findings include the influence of **charging rates** and **hydrogen concentration** on oxygen removal and the importance of optimizing hydrogen concentration for the overall process times, particularly with **high iron ore feed rates**.



### Impact of Plasma Stability on HPSR

The stability of the plasma arc during the reduction significantly affects the economic and ecological efficiency of the process. Research has demonstrated that both the **gas composition** of the plasma and the **electrode tip geometry** influence arc stability in a wide range.



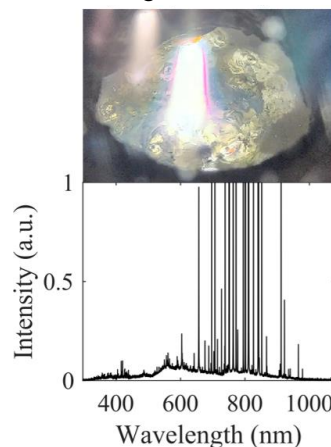
### Summary

Through a combination of research findings on the effects of feed rate and hydrogen supply on reduction behavior, as well as maintaining a stable arc and improving the understanding of plasma composition, electron density and species temperatures due to OES measurements, progress can be made in refining the hydrogen plasma smelting reduction process. These advancements pave the way for subsequent scale-up efforts toward industrial implementation.

Source: Daniel Ernst, Strategies for optimizing process parameters of hydrogen plasma smelting reduction plants. Dissertation (2023)

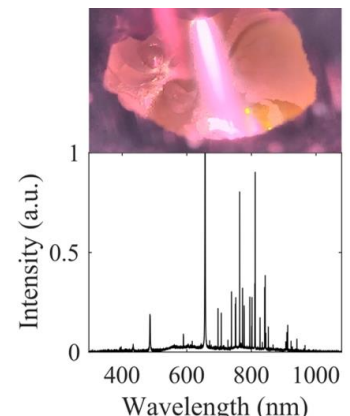
### Optical Emission Spectroscopy (OES)

Argon-Plasma



Wide range of emission lines from **670** to **900 nm**

Hydrogen-Argon-Plasma



Two strong emission lines **H $\alpha$**  (656 nm), **H $\beta$**  (483 nm)



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ONE STEP AHEAD.

# Development of thermodynamic databases for solidification of advanced steels with FactSage™

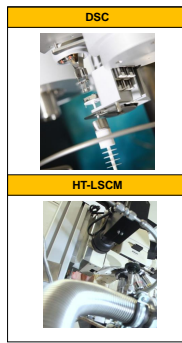
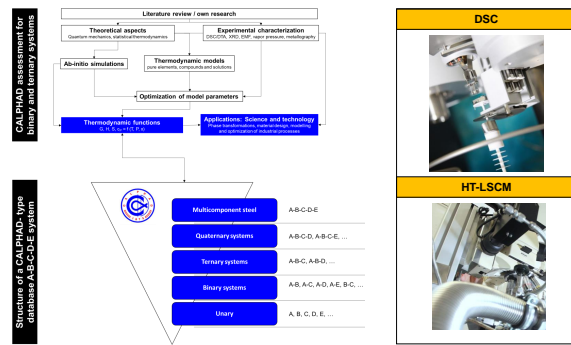
## Metallurgical thermodynamics and CALPHAD

The **CAL**culaton of **PH**ase **DI**agrams (**CALPHAD**) approach is widely used in scientific and industrial computation of thermodynamic properties of alloys. In steelmaking, the development of self-consistent databases started in the 1960s and is these days often directly coupled to process models, e.g. secondary metallurgy and continuous casting, for predictive quality control and to support metallurgical models with fundamental information on phase equilibria and Gibbs energy related data, e.g. heat capacity. This work deals with the development of a database for Fe-C-Si-Mn-Al high-alloyed steels.

### Introduction to the CALPHAD approach

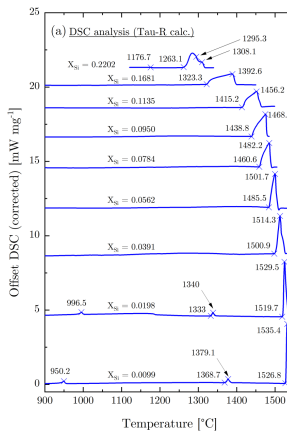
The development of a thermodynamic database can be described as an inverse pyramid. Starting from pure elements, the database is rapidly growing by adding binary and ternary systems. In general, literature data are critically assessed in the first step and considered in modeling the Gibbs energy of each stable phase.

A specific advantage is the possibility of own measurements that can be included, e.g., phase equilibrium temperatures or thermodynamic data. At the Chair of Ferrous Metallurgy, Differential Scanning Calorimetry (DSC) and High-Temperature Laser Scanning Confocal Microscopy (HT-LSCM) are used to generate experimental data.

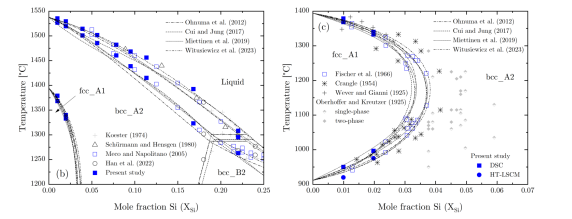


### Experimental study and thermodynamic modeling of the Fe-Si phase diagram

The Fe-Si system was experimentally investigated by DSC, analyzing 9 samples with varying Si content from  $X_{Si} \sim 0.01 - 0.22$  (0.5 - 12 mass pct.). DSC is a proven method to record phase transitions associated with an exothermic or endothermic enthalpy change.



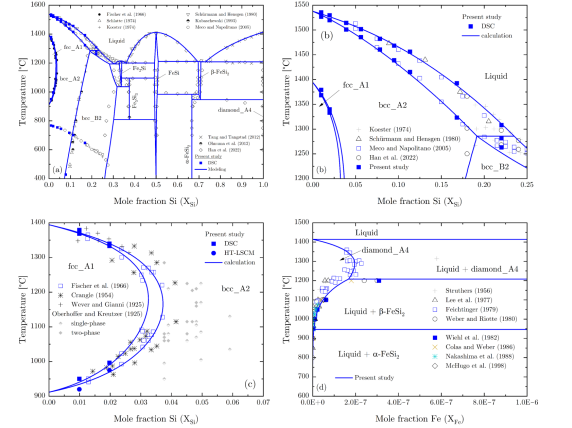
By comparing the newly gained DSC data with existing assessments from the literature, it is clear that the melting of BCC in the Fe-rich part is poorly described in the majority of publications. The accurate knowledge of this phase equilibrium is of significant importance for practical aspects of continuous casting of high-alloyed Si-steels.



The figure shows the thermodynamic model for the liquid phase using FactSage™ software, along with experimental data from the literature and the DSC analysis.

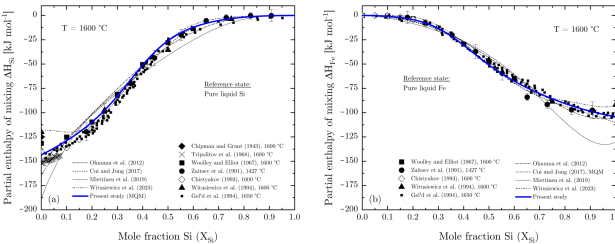
The following aspects could be significantly improved in the new database:

- Accuracy of ferrite (BCC) melting and solid-state phase equilibria (FCC/BCC) in the Fe-rich part.
- Solubility of Fe and Si in compounds, e.g.,  $Fe_2Si$ ,  $FeSi$  and  $\beta-FeSi_2$ .



### Thermodynamic model for the liquid phase using FactSage™ software

For solidification calculation, the proper modeling of the melt must be guaranteed. In case of short-range-ordering (SRO) tendency, which is particularly the case in metal/non-metal and metal/semi-metal systems, the Modified Quasichemical Model (MQM) gives best results for data related to the enthalpy of mixing, this fact can be seen in the Fe-Si melt at 1600 °C (see following figures).



### Summary and outlook

The CALPHAD approach is a valuable tool to create self-consistent databases for thermodynamic calculations of steel. Combined with advanced in-house experimental techniques, e.g. DSC, new findings on phase equilibria of steel can be implemented into an effective algorithm for calculating phase transformation and enthalpy related data of innovative steels using FactSage™ thermochemical software.



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We Innovate Materials



Promoting Innovation.



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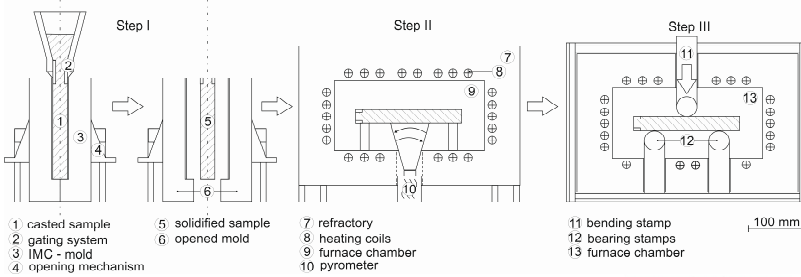
ONE STEP AHEAD.

# Simulation of straightening in continuous casting

## The role of increased levels of Cu, Sn and Ni and its interactions

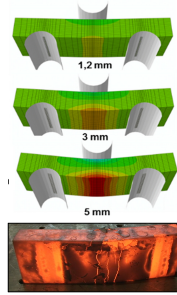
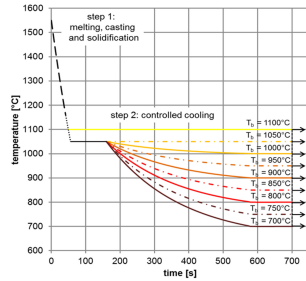
### Abstract

This study aims to investigate the relevance of Cu, Sn, and Ni and their effects on surface crack formation in continuous casting. Surface cracks can affect the quality and integrity of the final product, leading to costly reworking or production losses. Due to the increasing use of scrap, the content of Cu, Sn and Ni in steel will increase in the coming years. Understanding possible defect mechanisms is crucial to ensure the reliability of the continuous casting process. Benchmark experiments were performed under conditions close to continuous casting, in order to be capable of making assessments prior the industrial production.



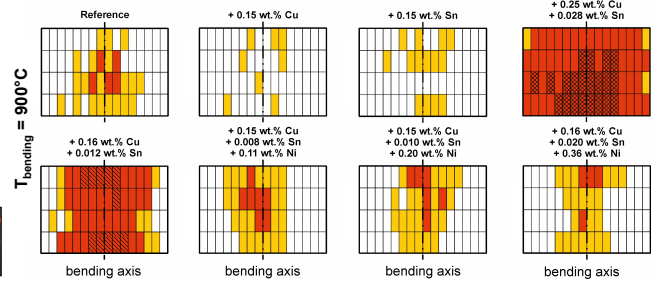
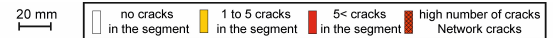
### Experimental method

Every sample is prepared in an induction furnace and cast into a mold to ensure that the microstructure corresponds to the one of the strand shell. Cooling to bending temperature can either be inert or oxidizing (H<sub>2</sub>O, Air). Mechanical deformation is attained by an isothermal three-point bending procedure. The experimental conditions are similar to continuous casting.

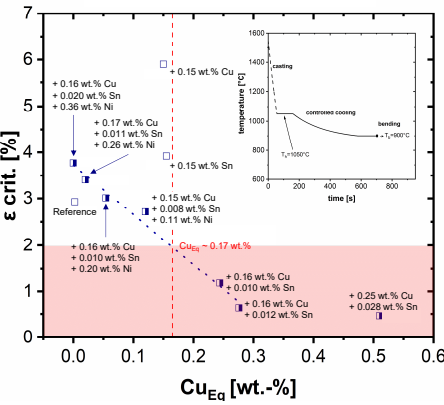


### Introduction and motivation

The increasing utilization of scrap leads to an increase of Cu, Sn and Ni in steel, resulting in new challenges with regard to surface crack formation in continuous casting. The IMC-B test was developed at Montanuniversität Leoben, representing a testing method for characterizing the material behavior of cast steel samples after controlled cooling in oxidizing atmospheres at elevated temperatures. The aim of the method is the experimental simulation of the susceptibility to surface defect formation for continuous casting processes.

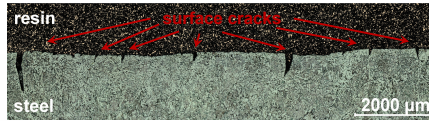


Chemical composition [wt.%]				
C	Si	Mn	Al	N
0.16-0.18	0.35-0.45	1.40-1.60	0.025-0.045	0.003-0.008



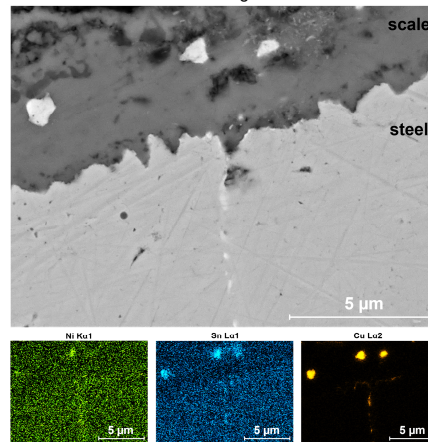
$$wt.\%Cu_{Eq} = wt.\%Cu + 10wt.\%Sn - wt.\%Ni - 2wt.\%S$$

The Cu<sub>eq</sub> is basically the effective Cu content, which increases or decreases with elements that strengthen or weaken this phenomenon.

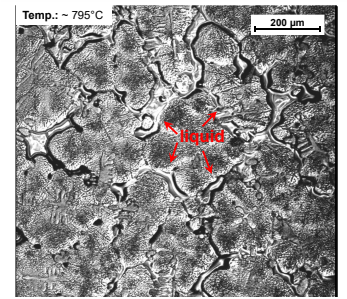
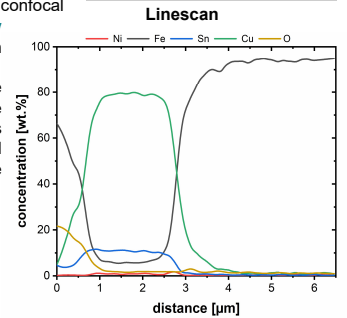
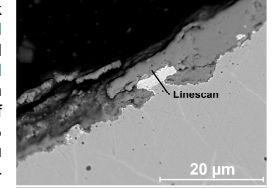


### Evaluation

The crack detection procedure provides the total number of intergranular cracks and the critical strain for first crack formation ε on the sample surface. For the continuous casting process the strains are smaller than 2%. "Reference" represents the standard composition of the investigated construction steel. Different contents of the tramp elements Cu, Sn and Ni were specifically alloyed to determine their influence on surface cracking. In particular, the joint addition of Cu and Sn leads to a drastic deterioration in terms of surface cracking. This can be effectively counteracted by adding Ni. A Cu<sub>eq</sub> higher than ~ 0.17 wt.% was identified as critical for straightening in continuous casting at 900°C.



The significant increase in crack formation in the presence of Cu and Sn is due to segregation and selective oxidation processes around the grain boundaries. A line scan indicated a composition of approximately 80 wt.% Cu, 10 wt.% Sn and 10 wt.% Fe. In-situ observations on the high-temperature laser scanning confocal microscope confirms a low melting phase with T<sub>solidus</sub> ~795°C. It can be concluded that the preferential cracking in the presence of Cu and Sn is due to partially liquid phases at the austenite grain boundaries.



80 wt.% Cu – 10 wt.% Sn – 10 wt.% Fe

### Summary and outlook

Summing up, it can be stated that increased tramp element levels have significant impact on surface cracking in the continuous casting process. The combined appearance of Cu and Sn is particularly harmful, whereas the additional presence of Ni leads to an improvement. In addition to the influences of the most common tramp elements Cu, Sn and Ni quantified here, other elements such as As, Sb and Mo, which are considered problematic, offer great potential for further investigations.

Source: Krobath et al.: steel research international 2020. Bernhard et al.: Manuscript submitted 03/24, steel research international. Lex C.: Master thesis, Leoben 2023.



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# High-temperature oxidation of steel

## Potential and opportunities to support the green transformation

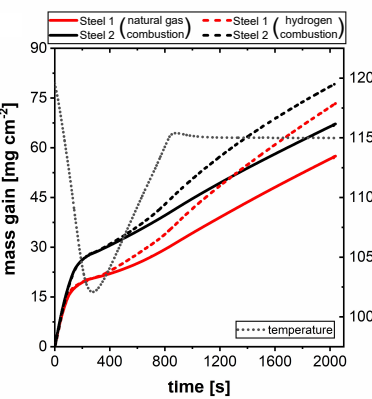
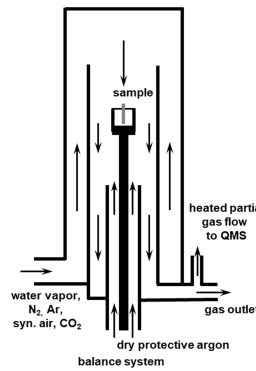
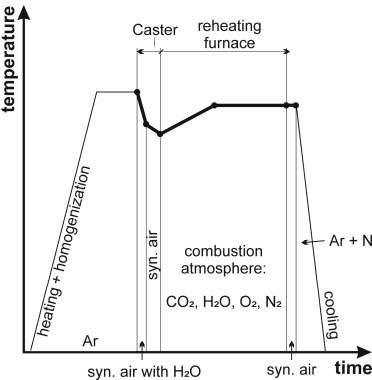
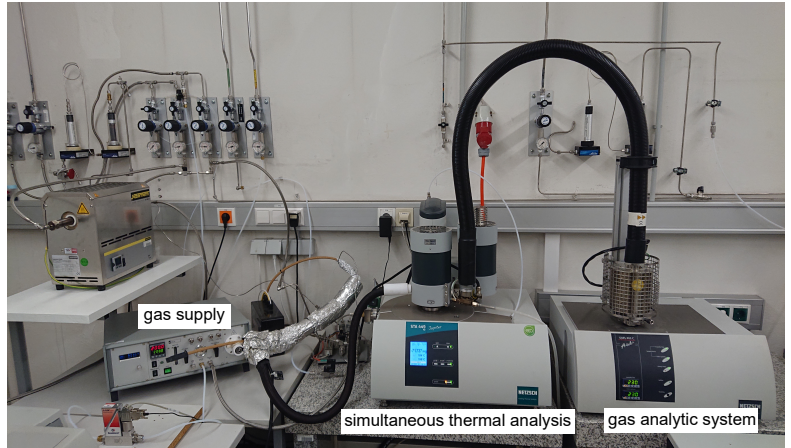
### Abstract

Oxidation processes are unavoidable in solid-steel processing leading to scale formation and internal oxidation phenomena. A deeper understanding of the occurring phenomena such as intergranular oxidation, decarburization and liquid metal infiltration of grain boundaries is essential to continuously improve the product quality. A decisive factor in high-temperature oxidation are tramp elements with a lower oxygen affinity than iron, such as Cu, Sn and Ni - as they do not oxidize but accumulate at the bulk/scale interface which may lead to additional quality problems. The issue of increasing tramp elements in steel will be a key topic of research and production due to higher recycling rates of steel.

### Experimental Setup and possibilities

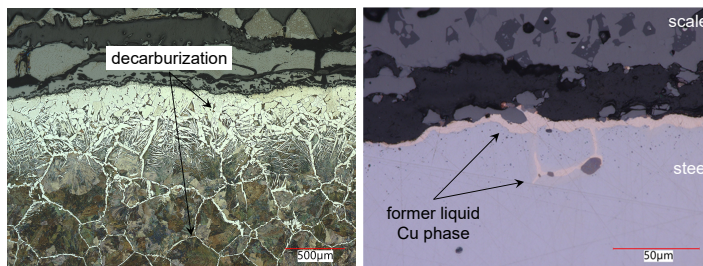
On the Chair of Ferrous Metallurgy, an experimental setup for investigating complex issues in the field of high-temperature oxidation was established. All experiments take place under perfectly controllable laboratory conditions. Requirements range from simple isothermal cycles to complex process simulations with heating, cooling and isothermal segments.

The mass gain during oxidation is recorded continuously by a high-sensitive balance system. In addition to a wide range of different gas atmospheres (CO<sub>2</sub>, up to 100 vol.% H<sub>2</sub>O, N<sub>2</sub>, O<sub>2</sub>, Ar), changing to an inert gas atmosphere is possible at any time. To achieve a high-purity inert Ar atmosphere, an external getter furnace is implemented (<10<sup>-15</sup> ppm O<sub>2</sub>). At the gas outlet, a partial gas flow is continuously analyzed by the mass spectrometer, to control the adjusted gas atmosphere.



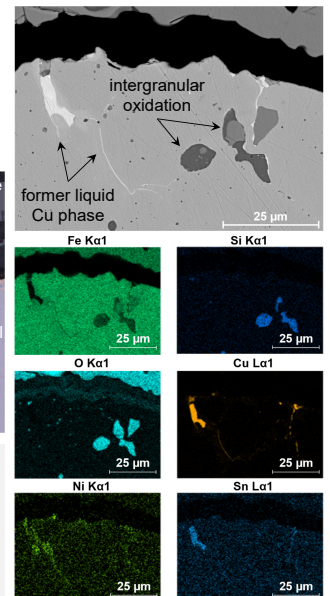
### Thermogravimetric evaluation

A precise statement about the scaling behavior is provided by the evaluation of the mass gain curve. The kinetic data obtained can be used to describe future experiments or industrial processes. This enables the estimation of how different parameters (e.g., oxidation atmosphere or steel composition) influence scaling and which production losses are to be expected.



### Metallographic evaluation

In addition to the scale layer thickness and morphology, the steel/scale interface is of particular interest. Specific phenomena such as surface decarburization, the formation of low-melting phases and infiltration of grain boundaries or the formation of oxide precipitations along grain boundaries (intergranular oxidation) can have a significant influence on the subsequent quality of the product.



### Summary and outlook

High-temperature oxidation experiments under controlled conditions are essential for understanding oxidation and decarburization mechanisms to enhance product quality and support the recycling of low quality scrap. The concept presented enables the investigation of specific oxidation phenomena and allows statements to be drawn about how steel composition, temperature or gas atmosphere influence oxidation. Of particular interest is how parameters can be specifically changed to either favor external oxidation (scaling, loss of material), which can lead to an improvement of the steel/scale interface (less internal/intergranular oxidation, less decarburization) or vice versa the internal oxidation.

Source: Gaiser et al.: Manuscript submitted 03/24, ISIJ International



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# In-situ Observation of Steel/Slag/Inclusion

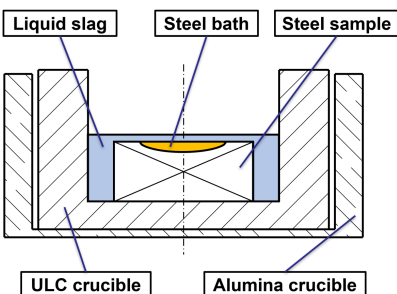
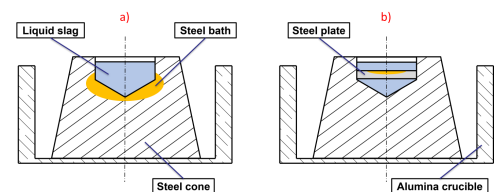
## Development of a Suitable Method for HT-CSLM

### Motivation

Non-metallic inclusions (NMIs) are inevitably present in steels. They heavily **influence material properties** such as fatigue strength, corrosion resistance, or polishability. Therefore, the amount and size of NMIs have to be as low as possible. The High-Temperature Confocal Scanning Laser Microscope (HT-CSLM) is a widely used tool in metallurgical and material research, including the investigation of several steel cleanliness-relevant topics such as **agglomeration** or **dissolution** of NMIs. However, a holistic observation of the behavior of NMIs in steel, at the steel/slag interface, and in the slag has yet to be reported. Hence, this work depicts the **development** of a suitable **method** for in-situ investigations.

### Early development stages

Different crucible materials can be used to conduct HT-CSLM experiments. Usually, alumina crucibles are used for metallic materials, while platinum crucibles are better suited for melting oxidic samples. Neither of these standard setups can be used for steel/slag experiments. Therefore, a dual **crucible concept was developed**. In the first experiments, a truncated steel cone placed in an alumina crucible was used as sample and to hold the slag. Later, a steel plate was inserted as sample

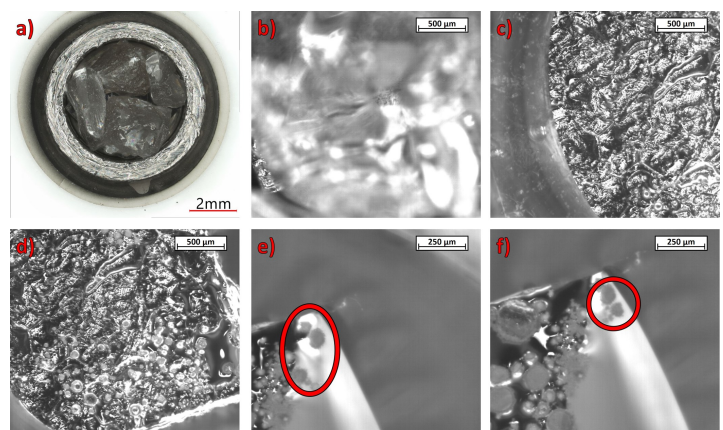


### Recent development steps

However, controlling the size of the liquid steel pool and focusing on the shifting surface of the melt proved to be complicated. In further experiments, a **shallow steel crucible** with a high melting point was used instead of the cone, and the steel sample to be investigated was placed inside. With this setup, the agglomeration of NMIs in the steel bath, the movement towards the steel/slag interface, and the detachment into the slag can be observed.

### Experimental results

The **dual concept** of an alumina and a steel crucible is shown in (a), which is filled with the steel sample and glassy slag chunks. During heating, the slag **softens** (b) and **melts** (c). The slag remains transparent and covers the steel sample partially. With further temperature increase the **steel** also starts to **melt** (d). As a liquid steel pool is formed, **NMIs appear** at the steel's surface (e), which **agglomerate** (f), move towards the steel/slag interface, and detach into the slag phase.



Source: Cejka, J.; Michelic, S.K. In-Situ Observation of Steel/Slag/Inclusion Interaction by Means of High-Temperature Confocal Scanning Laser Microscopy. *Metals* 2023, 13, 686. <https://doi.org/10.3390/met13040686>



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