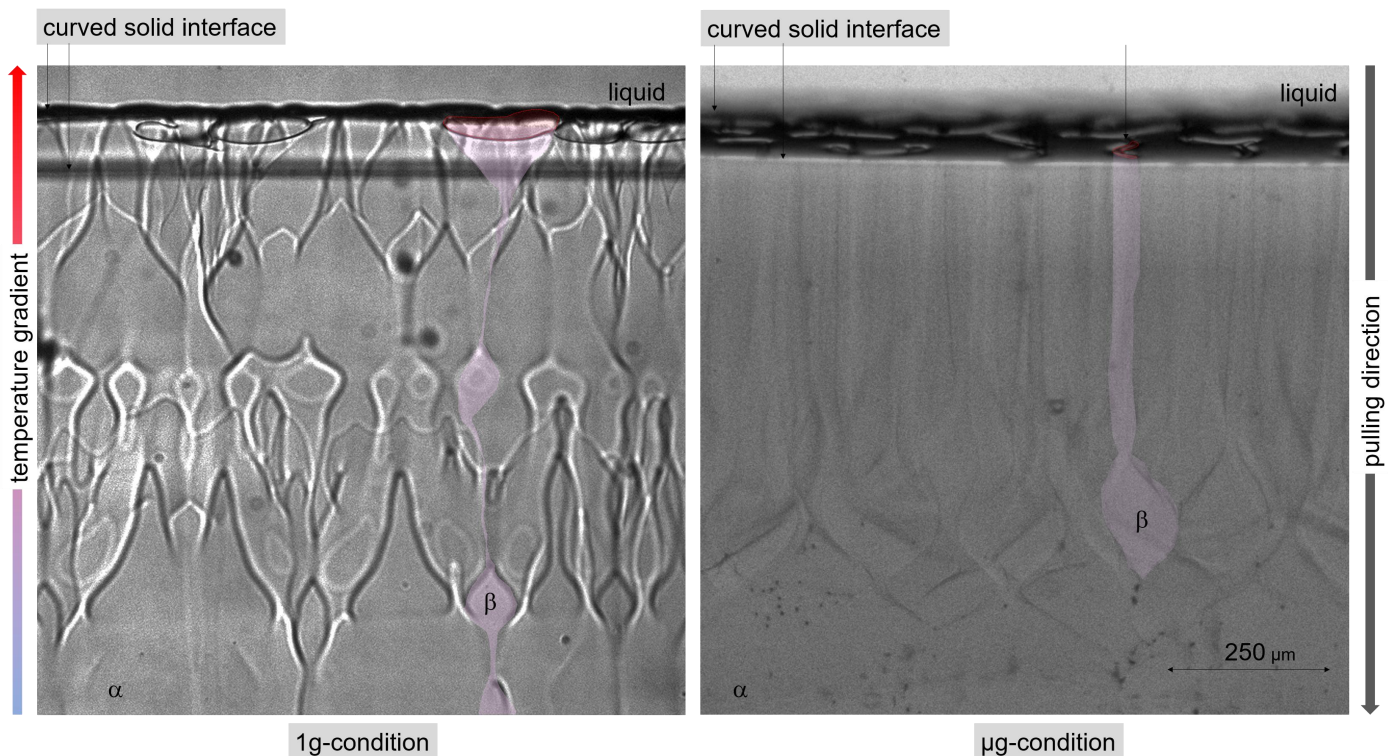


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Effect of the Thermo-solute Convection on Peritectic Layered Solidification Patterns

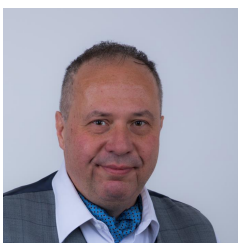
The aim of the ESA-METCOMP/FFG-METTRANS project is to gain a comprehensive fundamental understanding of metastable peritectic layered solidification patterns. In order to observe the solidification patterns in real time, the transparent peritectic organic model system TRIS-NPG was used instead of a metal alloy. The metastable coupled peritectic solidification reacts sensitively to solute convection due to density differences in the melt ahead of the solidification front. Therefore, the TRIS-NPG model system was processed under terrestrial conditions at the Montanuniversität Leoben as well and under microgravity conditions on board the International Space Station. Several concentrations were slowly solidified (Bridgman technique) in a implemented temperature gradient, $G_T = 4 \pm 0.2$ K, at varied pulling velocities, $V_p = 0.09 \pm 0.03$ $\mu\text{m/s}$.



The patterns observed under different gravitational conditions show the influence of solute convection on solidification. In both cases, the pro-peritectic alpha phase as well as the peritectic beta phase grow lamellar, similar to eutectic growth. Under terrestrial conditions, the preferred phase changes during competitive growth. This leads to an oscillating lamellar width, shown in color in the images. Without solute convection, this effect is severely limited.



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Research topics

- solidification morphologies
- organic model systems
- numerical simulation

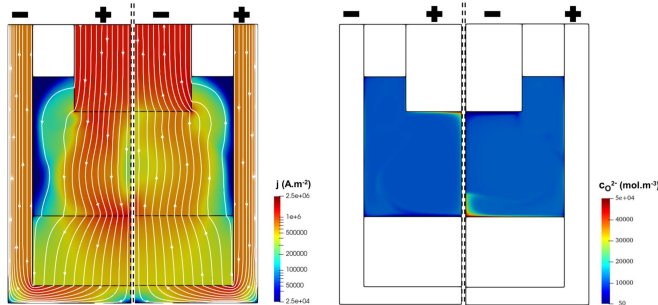


Multiphysics Simulations for Electrochemical Processing of Materials

Electrochemical refining (electrometallurgy), involving electromagnetics, fluid mechanics, and chemistry, is a multidisciplinary approach used in refining (extraction or purification) of metals and alloys through electrolysis. Processes include electrowinning, electrorefining, electroplating, and electroforming. Herein, simulation results showcasing the utilization of multiphysics modeling to comprehend those processes are illustrated.

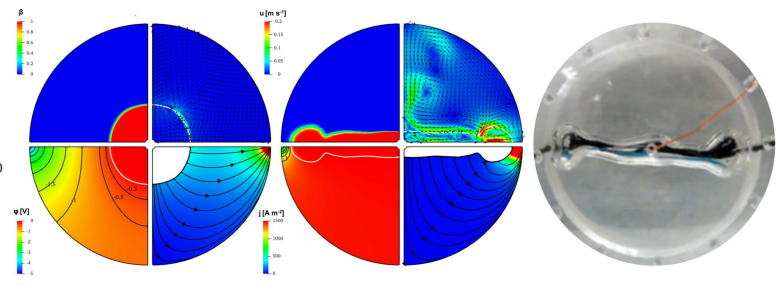
Electrorefining in the ESR process

The slag (electrolyte) in the ESR process is an ionic conductor composed of several ions, like Ca^{2+} , O^{2-} , Al^{3+} , Fe^{2+} , etc. As shown in the figure, the polarity of the electrode/ingot impacts the electric current density field and concentration of O^{2-} in the slag and at the ingot top [1].



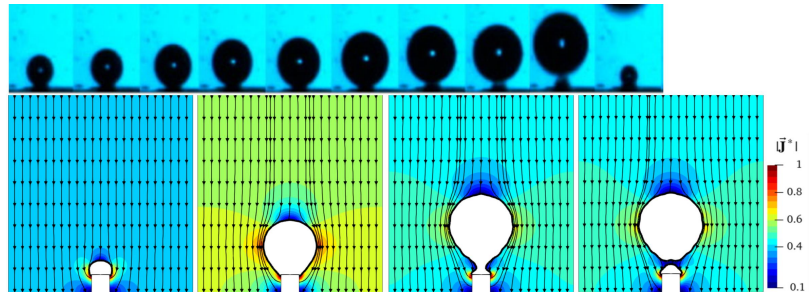
Electroforming

Electrochemically generated Marangoni flow is utilized for active control of interfacial dynamics, with diverse applications in prosthetics, soft robotics, and electrochemical sensors. The figure below illustrates transient field structures during the elongation of the eutectic gallium-indium (EGaIn) droplet toward the cathode in an actuator [2].



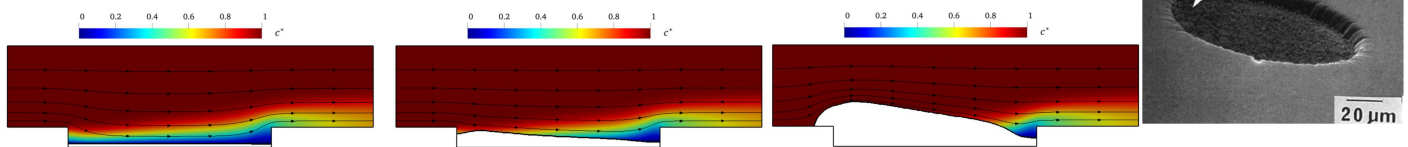
Electrolytic gas flow

Electrogenerated gas bubbles are commonly observed in metallurgical processes such as aluminium electrolysis or chemical processes like alkaline water electrolysis. Illustrated snapshots capture the electric current density field during the growth and detachment of the hydrogen bubble.



Electrodeposition

The electrodeposition process is extensively used to manufacture micro-electromechanical systems (MEMS). The transient shape evolution and concentration of the reactant ion (Cu^{2+}) during the electrodeposition of copper in a cavity, which has applications to microelectronics, are shown in the figure below [3].



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- [3] E. Karimi-Sibaki, et al., *J. Electrochem. Soc.* 170 (2023), 072501.



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Magnetohydrodynamics (MHD)
Electrometallurgy
Electrochemistry



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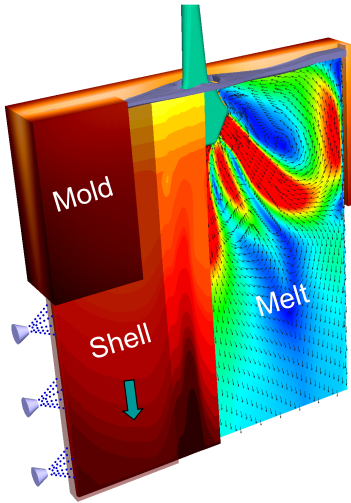


Multiphase Modelling of Thin Slab Continuous Casting under Applied Electromagnetic Braking

The thin slab casting (TSC) is a breakthrough near-net-shape technique for flat products accompanied by rapid casting and solidification rates. The TSC quality hinges on the turbulence, free-surface waving, super-heat flow and growth of the solidified shell. The electromagnetic brake (EMBr) is commonly applied to control the fresh melt flow after feeding through a submerged entry nozzle (SEN). Numerical modelling is employed as a perfect tool to investigate the multiphase phenomena in the continuous casting (CC) considering different scenarios with and without applied EMBr.

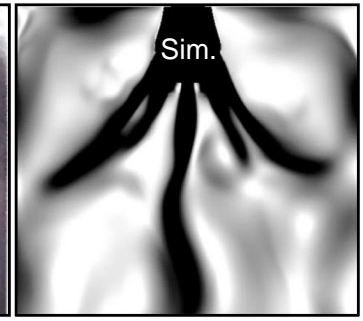
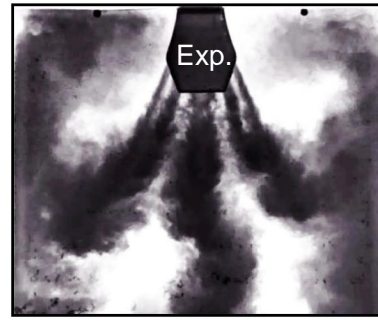
Heat transfer and solidification in TSC process

A solid shell growth against the walls of a funnel-type TSC mold is defined by the heat transfer through the water-cooled copper plates including thermal resistance of a slag skin and air gap [1] and influences the final slab quality.



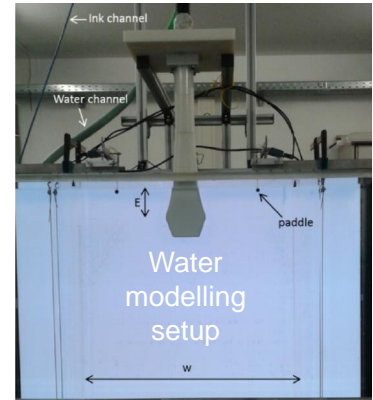
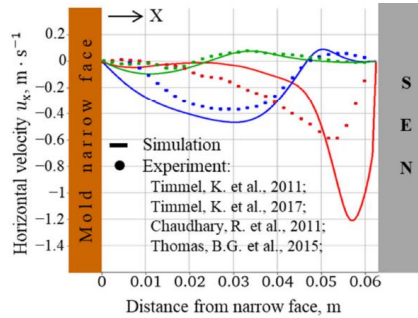
Turbulent melt flow

Water modelling experiments, including the SEN, mold, and strand Plexiglas segments with the paddle-type sensors were instrumented to measure the submeniscus velocity supported by videorecording of the dye injections to provide both qualitative and quantitative verification of the turbulent melt flow simulations [2].



MHD effects

To account for EMBr effects, solidification is coupled with a model for the turbulent free surface flow inside our in-house MHD code, which is experimentally verified [3].

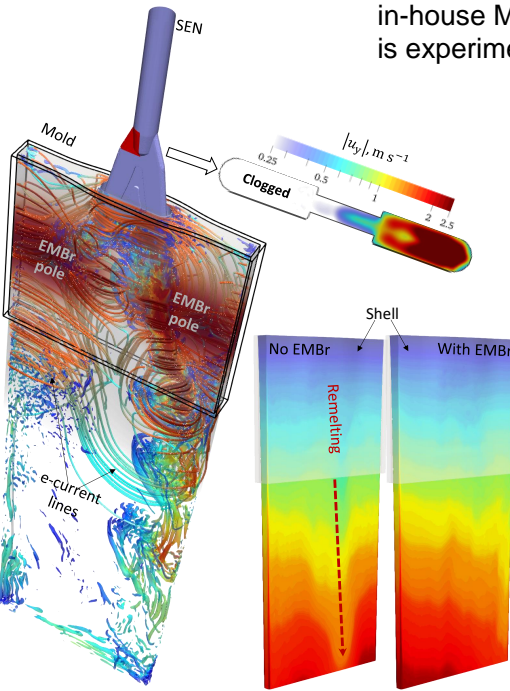
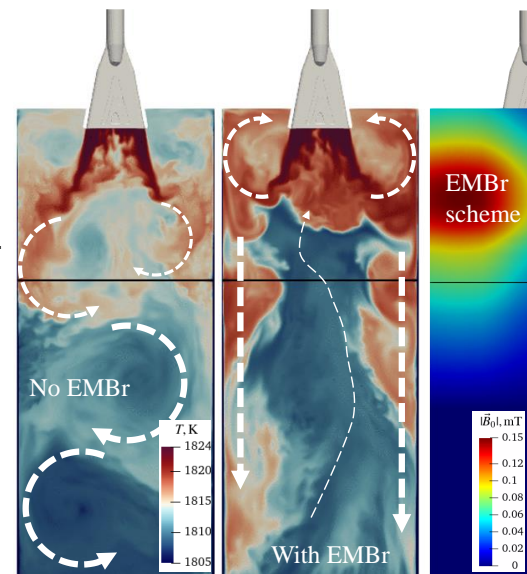


Applications to industrial process

Developed multiphase model is widely applied to investigate different practical issues during TSC. For example, they can be related to the asymmetric melt flow with a partially blocked SEN (left figures) [4] or caused by the mean flow fluctuations and instability (right figures).

References

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- [4] A. Vakhrushev, et al., Steel Res. Int. 2022, 93, 220088.



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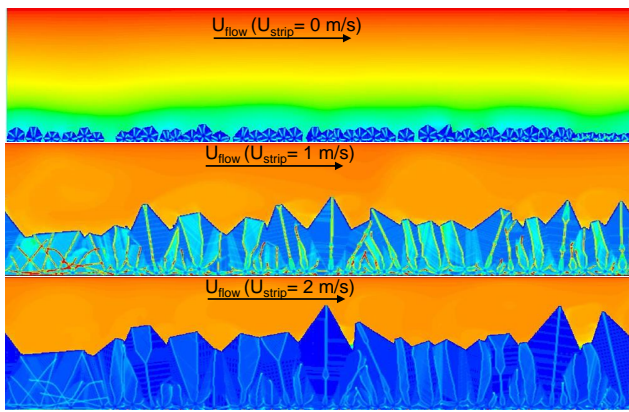


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Hydrodynamic influence on the build-up growth in the Galvanizing Industry

Motivation

Fe_2Al_5 faceted crystals (the so-called build-up) grow during the Galvanizing process, on the Zinc bath hardware. In the industry their occurrence is a problem and therefore it should be limited. The growth difference between the stationary and moving bath hardware suggests that the melt flow plays an important role. The aim of this work is to get a better understanding of the conditions which enhance the build-up growth.



Build-up growth together with Fe concentration field in the liquid.

Discussions

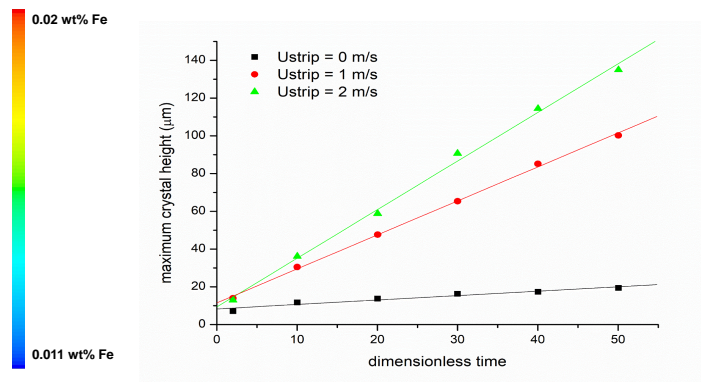
- A linear growth of the crystals can be observed for all cases.
- Faster steel strip velocities are related to faster growth of dross build-up.
- Many eddies will transport liquid zinc with high concentration in Fe and Al to the close vicinity of the crystals.
- This phenomenon enhances strongly the mass transfer, and therefore the growth.
- Competition between crystals growth was put in evidence, some crystals are overtook by others which grow faster.
- Good qualitative comparison was observed with the experimental results.
- For a quantitative comparison the numerical model needs accurate values for the interfacial kinetic coefficient as well as for the growth law.

Summary

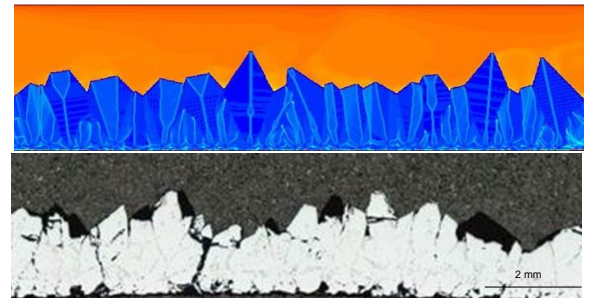
- An increase of the steel strip velocity from 1 to 2 m/s results in a 30% faster build-up growth.
- The diffusion and mass transfer are increased by the strong melt flow and therefore the growth of crystals is faster.
- The enhancement of the mass transfer due to higher strip velocities plays an important role in the build-up growth.
- A qualitative good agreement was found in the comparison of the shape of simulated and experimentally observed build-up growth.

Method

A 2D cellular-automaton model with a front-tracking method was used for the numerical simulations. Different cases were simulated where the steel strip velocity was varied from 0 m/s to 2 m/s. The corresponding flow velocities were applied at the top wall. These cases reproduce the industrial conditions of the build-up growth on the stationary hardware and on the rotating bath hardware. Periodic boundary conditions were applied at the left and right walls of the simulation domain.



Maximum crystal size vs time for different flow velocities.



Comparison of crystal's shape between simulation results (up) and experimental observation (down).



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Modeling freeze-lining formation: a case study in the slag fuming process

Abstract: Slag fuming is an innovative process designed to recycle Zn-containing slags from industrial waste materials. To protect the reactor from the corrosive molten slag, a as-solidified slag layer, known as freeze-lining (FL), is formed on the reactor walls. To capture the complex multiphase flow dynamics, heat transfer, and FL formation in the slag fuming process, a sophisticated CFD model was created. The simulation results provide valuable insights into the fuming process, particularly the evolution of the slag bath temperature, slag splashing dynamics, FL formation (in slag bath and in freeboard), heat fluxes through the reactor walls, and global net energy balance.

Introduction

FL formation on furnace walls, achieved through the solidification of slag, constitutes an important consideration in the design of pyrometallurgical vessels. The FL shields refractories from direct degradation caused by the corrosive molten slags and minimizes energy consumption. However, the exact mechanisms of FL formation remain unclear.

To help in our understanding of the mechanisms behind FL formation, a CFD model was developed. The model was used to simulate a batch-type, plasma-driven slag fuming furnace process (Fig. 1), like the ones operated at Aurubis-Beerse. Our goal was to shed some lights on the phenomena taking place inside the furnace, understand the mechanisms behind FL formation and their impact on energy savings.

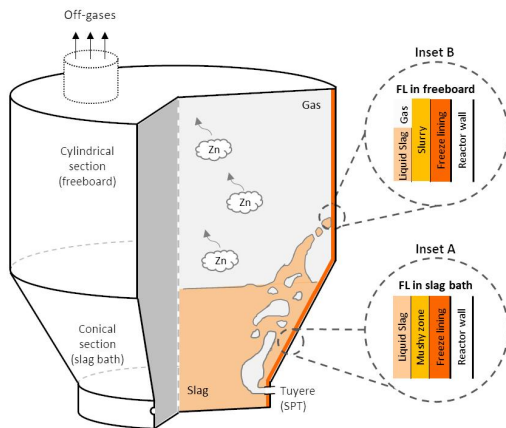


Figure 1. Schematic of water-cooled slag fuming furnace with submerged plasma torches. Insets highlight different types of FLs.

Results

Our simulations reveal complex flow dynamics in the slag bath (Fig. 2a) as well as frequent splashing of slag onto the freeboard. These splashing events are crucial for the

FL formation in the freeboard region (Fig. 2b).

The average FL thickness measured in an industrial furnace operated by Aurubis-Beerse was 3 cm. Our simulation results agree well with this value (Fig. 3).

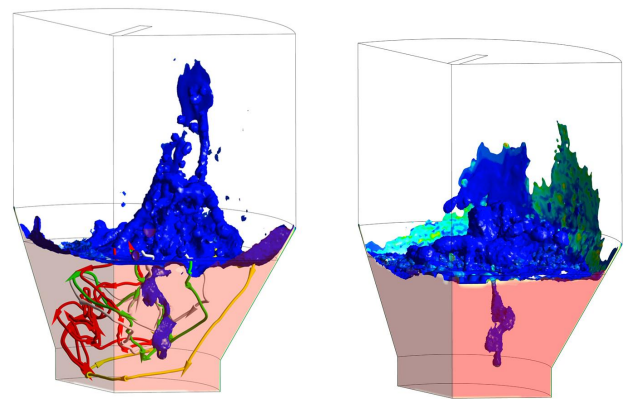


Figure 2. Simulation results of a) flow in slag bath and b) slag splashing with corresponding FL formation in freeboard.

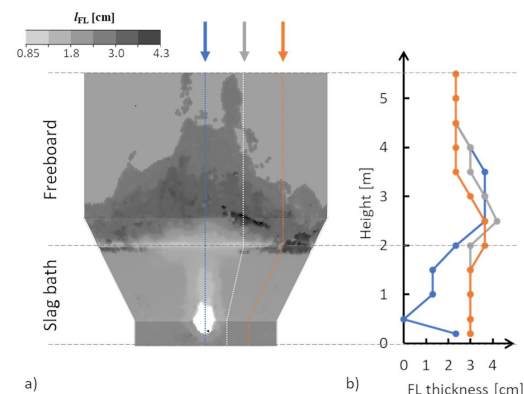
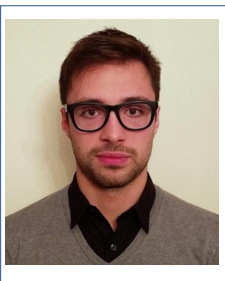


Figure 3. Simulation results of a) FL distribution across the reactor wall, b) FL thickness variation along the reactor height. Average FL thickness in industrial furnace operated at Aurubis-Beerse was 3 cm.



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SMMP

Solidification of Aluminum Alloy: Space Experiments and Numerical Modeling

A scientific team MICAST, led by European Space Agency (ESA), used both experimental and modeling methods to study the alloy solidification under controlled flow conditions onboard the International Space Station (ISS).

10 solidification experiments were planned to be carried out onboard the ISS. Aluminum alloys with different compositions were designed by industry. With the excellent microgravity condition, the flow effect on the solidification can be well controlled via rotational magnetic field (RMF). The experimental results can be used to develop numerical model.

Figure 1 shows the astronaut performing the experiments onboard, and some experiment facilities, solidification samples and metallographic analysis of the microstructure.

Among 10 experiments, 6 were performed in spring 2022; another 4 are scheduled for 2024/2025.

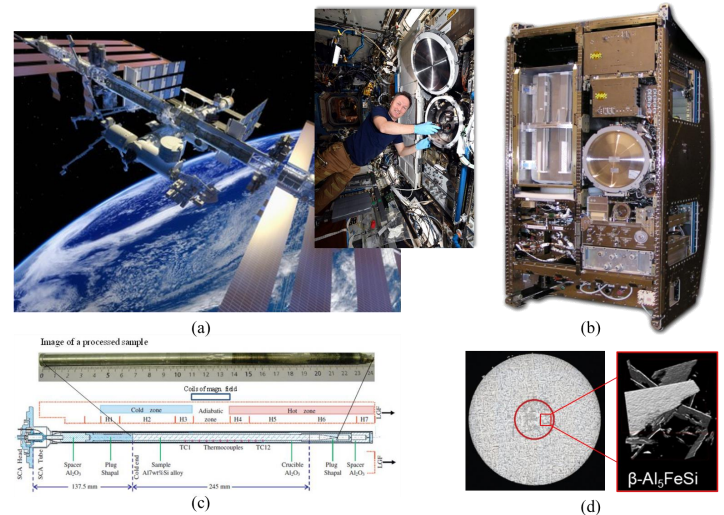


Figure 1. MICAST space solidification experiments of AlSi7Fe1 alloy. (a) ISS with inset photo: the astronaut (Matthias Maurer) was exchanging MSL MICAST SCA 3# 10 (ESA). (b) MSL (ESA) in MSRR-1 (NASA). (c) Setup of the sample carriage inserted in the furnace. (d) Microstructure of the downloaded AlSi7Fe1 sample.

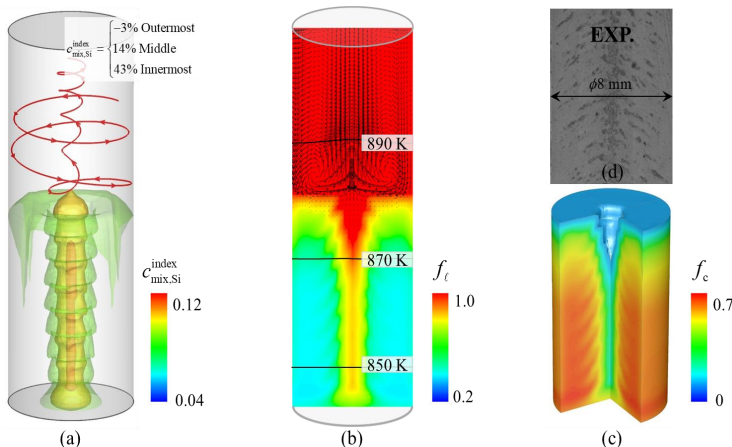


Figure 2. Typical solidification results of the AlSi7Fe1 under rotating magnetic field (RMF) at 550 s. (a) Iso-surfaces of Si macrosegregation index ($C_{mix,Si}^{index}$). (b) Contour of liquid fraction (f_l) along the center of the longitudinal section, overlaid with isotherms and vectors of the meridional flow. (c) Contour of the columnar phase fraction (f_c) in two vertical sections and one iso-surface of $f_c = 0.01$ on the top indicating the position of the columnar tip front. (d) The as-solidified structure on the vertical section of the sample.

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- 2 H. Zhang, M. Wu, C.M.G. Rodrigues, A. Ludwig, and A. Kharicha: *Metall. Mater. Trans. A*, 2021, vol. 52, pp. 3007–22.



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Influence of the Coriolis force on the solidification of a Fe-0.82wt.%C alloy

Abstract: A 3D numerical simulation model of the solidification of Fe-0.82wt.%C steel alloy under thermosolutal convection is presented. The simulated domain is in a rotating frame of reference, and rotates with a constant speed. This involves considering fictitious forces such as Centrifugal and Coriolis forces. The aim is to analyze the impact of the Coriolis force on flow, and segregation patterns. Results indicate that the Coriolis force disrupts thermosolutal convection, significantly influencing the final macro-segregation pattern. Aligned flow and segregation structures are observed at different horizontal planes, likely due to the Coriolis force. Marangoni flow competes with the Coriolis force at the end of solidification, leading to different segregation patterns at various horizontal cut planes.

Introduction

Horizontal Centrifugal Casting (HCC) is a specialized casting technique used to produce cylindrical metal components. In this study, a steel molten metal is contained in a 3D rotating geometry (Fig. 1) initially at a temperature above the liquidus to simulate the solidification process during HCC.

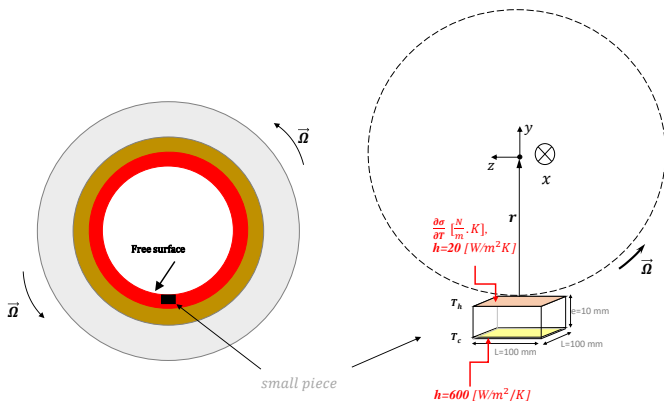


Figure 1. Top: Picture of Horizontal Centrifugal Casting process. Bottom: Schematic of the simulated domain during HCC.

Results

The main results are as follows:

- Marangoni flow produces hexagonal patterns (Fig. 2).
- Coriolis force reorganizes the flow and segregation into aligned structures with the rotation (Fig. 3).

- The Marangoni flow produces convective and segregated cells near the free surface (Figs. 2 and 3 (a)).

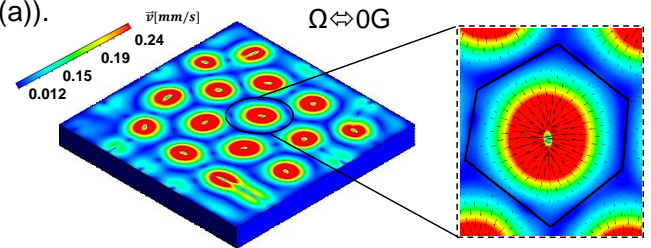


Figure 2. Hexagonal patterns produced by Marangoni flow for $\Omega \leftrightarrow 0\text{G}$.

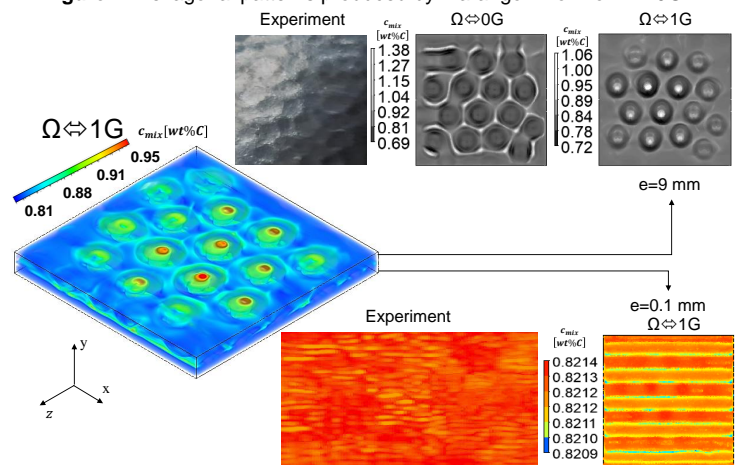
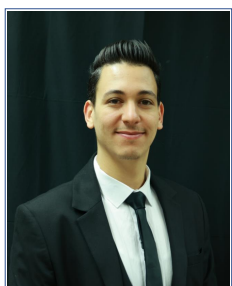


Figure 3. Qualitative comparison between experimental and numerical results in terms of segregation at $e=0.1\text{ mm}$ and $e=9\text{ mm}$ for the static case and $\Omega \leftrightarrow 1\text{G}$.

Conclusion

The present results are summarized as follows:

- Coriolis force produces aligned flow and segregation structures.
- Marangoni flow was able to compete with Coriolis near the free surface by producing hexagonal patterns.



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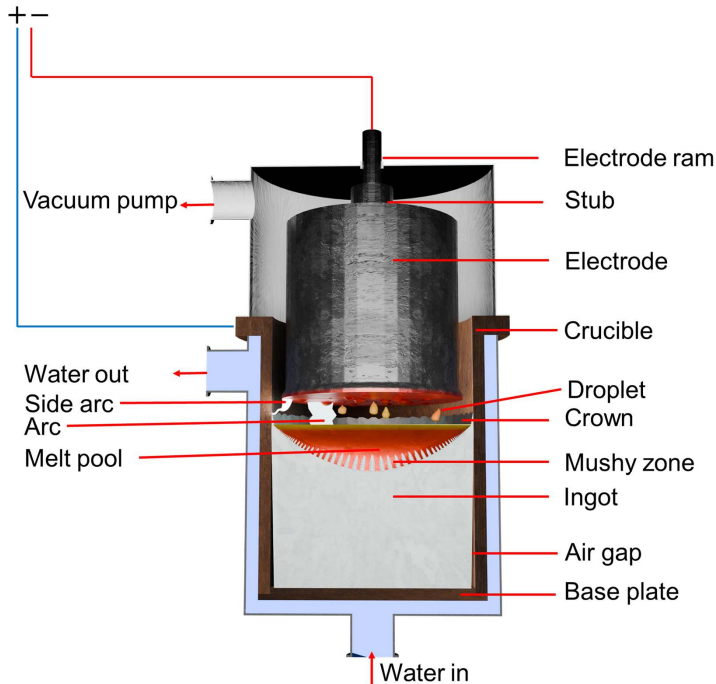
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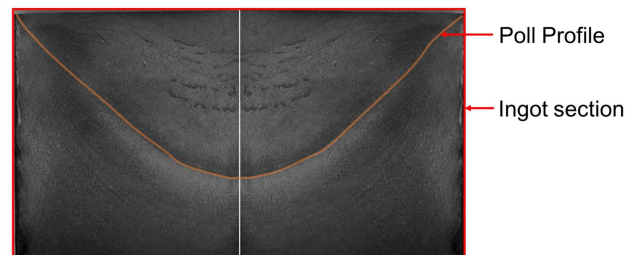
Molding Transport Phenomena in Vacuum Arc Remelting

Vacuum Arc Remelting (VAR) is a refining method commonly used in the production of high-quality alloys, particularly for aerospace applications such as Stainless Steel, Titanium, and Nickel superalloys. This process involves melting an electrode within a vacuum environment by creating an arc between the electrode and a base plate placed within the mold. As the electrode's tip melts, droplets form and then pass through the vacuum to join the molten pool. Subsequently, the molten pool solidifies within a water-cooled mold, resulting in a high-grade, ultra-clean alloy with minimized oxide inclusions.



Experimental validation

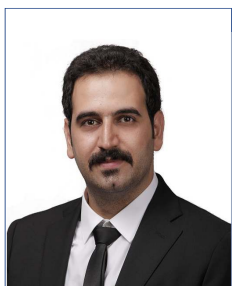
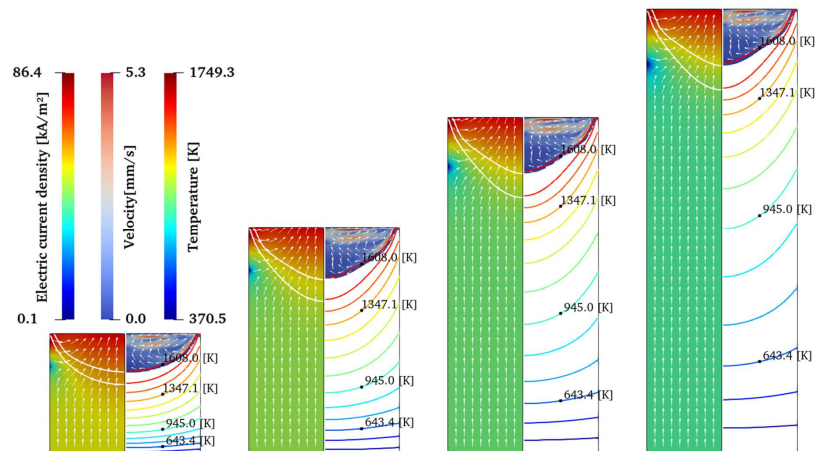
One effective method for validating simulation results in VAR is through pool marking. This technique involves adding different particles to the liquid pool during the process. Due to gravity, these added particles sink down and become embedded within the solidification front of ingot. After the process is complete and the ingot is cut, the location of these added particles reveals the pool profile of the ingot. By comparing this profile with simulation results, we can verify the accuracy of the simulation and ensure its reliability for predicting real-world outcomes in VAR operations.



Modeling of VAR

Modeling VAR requires considerable complexity, primarily due to the complex coupling of multiple physical phenomena, such as heat transfer, mass transfer, solidification, electromagnetism, flow dynamics, plasma arc, and cathode spots. Additionally, achieving accurate transient simulation results relies on particular attention to boundary conditions to precisely capture the evolving phenomena during the ingot's growth. Despite the challenges, employing computational fluid dynamics (CFD) provides invaluable insights, enabling process optimization and accurate prediction of ingot quality.

Transient simulation result



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NH₄Cl-H₂O solidification in a larger containment: searching for avalanches

Abstract

This investigation searches for crystal avalanches during the solidification of an ammonium chloride-water solution that contains 29.57 weight percent NH₄Cl. We demonstrate that four stages and relatively large areas of mushy regions slide downward under certain conditions and form spectacular crystal avalanches.

Experimental conditions

A container (0.6 m height, 0.4 m wide, and 0.06 m depth) was filled with a 29.57 wt.pct Ammonium chloride-water solution. The lateral walls are made of brass, and the front and back walls are made of commercial PMMA. The solution was prepared by mixing NH₄Cl powder with distillate water. We started with an alloy at a temperature of $T_0 = 333$ K (60 °C), which was then cooled down to $T_{inf} = 278$ K (5 °C) via the side walls.

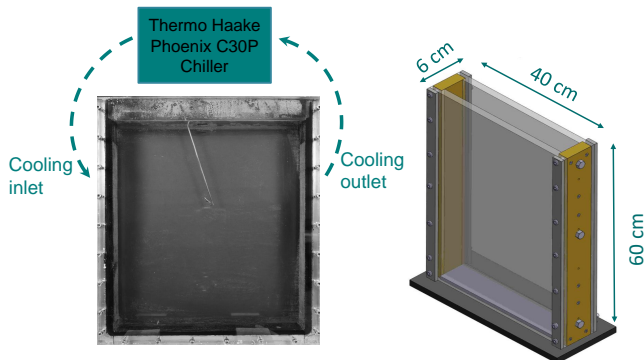


Fig.1. container. The container is cooled from two sides with a predefined cooling rate.

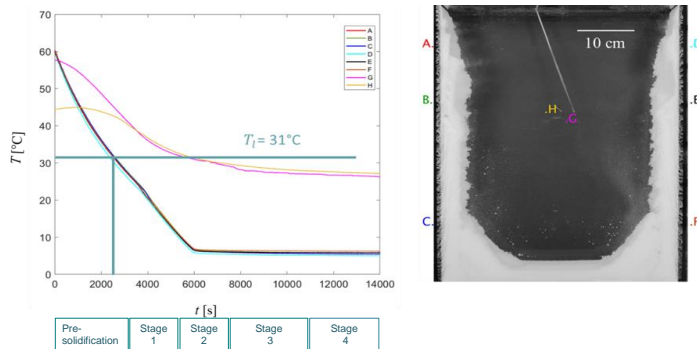


Fig.2. Temperature curves. Temperatures were measured with 8 thermocouples on the brass surfaces (A, B, C, D, E, F, G) at different positions, inside the cell (G) and on the Plexiglass (H).

Result

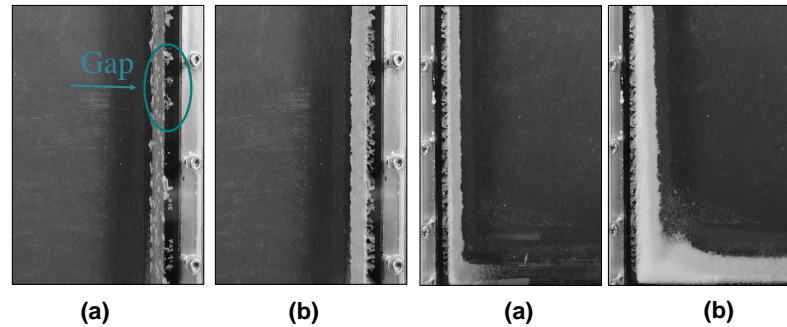


Fig.3. Stage 1: Nucleation and growth (a) Nucleation at the brass surface and in the gap between brass and Plexiglas happened around 3500 s after cooling was started. (b) 1000 s after that, the brass surface was completely filled with crystals.

Fig.4. stage 2: Corner-sedimentation (a) After 4500 s, the falling of Crystals from the sides started. (b) Crystals gradually filled the bottom corners as a result of sedimentation around 6000s. Crystals are most probably coming out from the columnar mushy region along the brass as a result of remelting or fragmentation.



Fig.5. Stage 3: Swinging of turbulent snowing. The left and right areas of heavy turbulent snowing interact with each other. That started at around 6800 s and lasted till around 10000 s. During this stage, numerous avalanches occurred and the sedimentation in the corner region got quite steep.

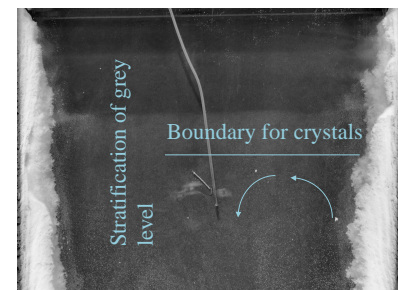


Fig.6. Stage 4: Stratified double-diffusive convection This stage started at around 9500 s and last till the end at around 13000 s. From the top towards the bottom, the flow got calm and evidently went from side to side. A stratification of the grey level indicated different levels of concentration.



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Research Focus

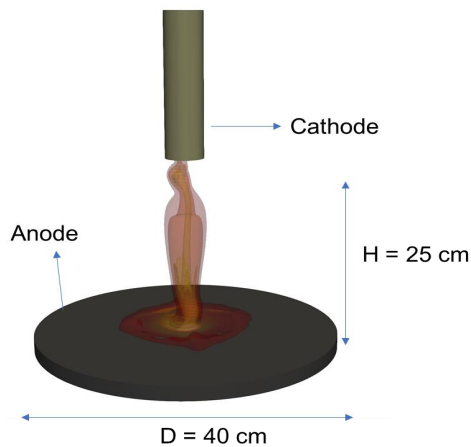
- Solidification experiment
- Crystal avalanches
- Stages during solidification



Dynamic Behavior of Hydrogen Electric Arc: a 3D Numerical Model

Abstract: We introduce a 3D numerical model designed to simulate the behavior of a hydrogen electric arc. This model couples the electromagnetic field of hydrogen plasma arc, with flow and heat transfer. The electric arc functions under atmospheric pressure conditions, utilizing direct current (DC) and operating in the local thermal equilibrium condition. The model reveals the spontaneous emergence of arc instabilities near the cathode, which then propagate downwards along the arc jet. Additionally, we observe instances of the arc spontaneously splitting into multiple arcs before merging back into a single arc.

Model: The 3D hydrogen arc is modeled under atmospheric conditions with a current of 5 kA. The model aims to mimic the behavior of hydrogen arcs inside electric arc furnaces. The geometry resembles a cylinder full of hydrogen gas. The current flows between two solid electrodes in contact with the cylinder's horizontal surfaces.



Schematic representation of the computational domain.

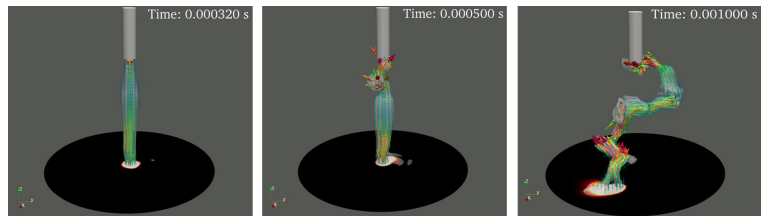
Results:

The main findings are:

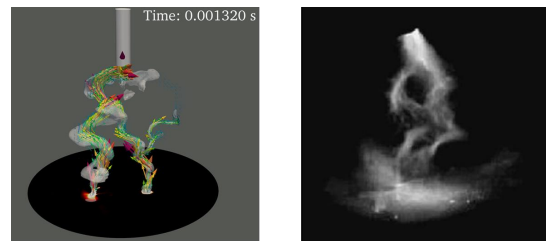
1. Arc is instable by nature without any external effects
2. The model results were comparable to experimental observation.
3. The arc splitting and recombination occurs simultaneously and very rapidly.

Conclusion: A magnetohydrodynamic 3D model is developed to study the instability and transient behavior of a high intensity hydrogen plasma arc. It is found that arc instabilities emerge spontaneously near the cathode before propagating downwards along the arc jet. Also, spontaneous splitting into several arcs is observed before merging again into one arc.

The instability occurs suddenly near the cathode electrode and propagates downwards along the arc. The arc structure is fully disturbed and transitions in 0.5 millisecond.



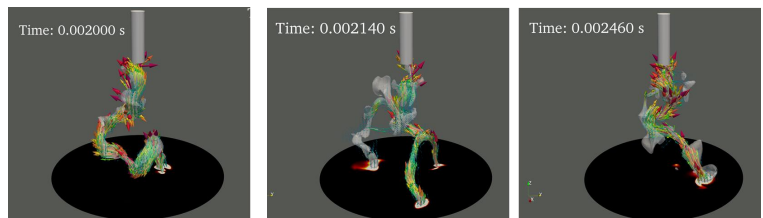
The model was predicted the structure of pretzel arc shape which was already been captured by experiments.



Simulation 5 kA

Experiment 7 kA
[Jones et al., Minerals Engineering, 2002]

The Arc splits into 3 different arcs. The splitting and recombination occurs in less than 0.5 millisecond



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Research focus : Magnetohydrodynamic flows inside Electric arc furnaces.

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