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Advanced Process Simulation of Solidification and Melting

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Abstract: At some stage in the production of every metal part or product, the metal material has been melted and solidified to form the primary or final shape as well as the as-cast structure. Quantitative prediction and control of solidification and melting has been, and remains, the most critical issue in the metallurgical industry. Example questions currently raised by the Austrian metallurgical industry, which is one of the key economic sectors of this country, are as follows: in thin-slab casting, how does the solid shell form and interact with turbulent flow? How can the electro-slag-remelting (ESR) process be better understood and controlled (stabilized)? How can metallurgical imperfections (macrosegregation, porosity, non-metallic inclusion, surface crack, etc.) in castings be predicted and minimized? Therefore, a Christian-Doppler laboratory—Advanced Process Simulation of Solidification and Melting was established in July 2011 with the final goal to address the questions mentioned above. This article reports on some progresses.

Keywords: Process simulation, Solidification, Melting, Thin slab casting, Electro-slag-remelting

Prozesssimulation von Erstarrungs- und Umschmelzvorgängen

Zusammenfassung: So gut wie jeder metallische Werkstoff wurde im Laufe seines Herstellprozesses ein- oder mehrmals er- bzw. umgeschmolzen und anschließend erstarrt. Dabei bildete sich ein Gussgefüge mit charakteristischen Gefügemerkmalen (Korngröße, Textur, Lunker, Poren, Seigerung, usw.), welche die Gebrauchseigenschaften des Produkts wesentlich beeinflussen. Quantitative Prognosen zur Kontrolle von Schmelz- und Erstarrungsvorgängen sind deshalb in der gesamten metallurgischen Industrie von entscheidender Bedeutung. Beispielsweise werden folgende Fragen von der österreichischen metallurgischen Industrie, welche als einer der ökonomischen Schlüsselsektoren des Landes gilt, aufgeworfen. Wie bildet sich die Strangschale von Strangguss im Kokillenbereich und wie interagiert diese mit der turbulenten Strömung? Wie kann der Elektro-Schlacke-Umschmelzen (ESU) Prozess besser verstanden und gesteuert (stabilisiert) werden? Wie können die metallurgisch unerwünschten Imperfektionen in den Gussteilen vorhergesagt und minimiert werden? Zur Klärung dieser Fragen wurde im Juli 2011 ein Christian Doppler Labor für Prozesssimulation von Erstarrungs- und Umschmelzvorgängen eingerichtet. Über diesbezügliche Forschungsfortschritte wird im Rahmen dieses Artikels berichtet.

Schlüsselwörter: Prozesssimulation, Erstarrung, Schmelzen, Dünnbrammengießen, Elektro-Schlacke-Umschmelzen

1. Introduction

1.1 State-of-the-Art

One of the major scientific challenges in developing a solidification and/or melting model lies in the requirement to bridge the length scales, i.e. to incorporate and account for small-scale physical phenomena in large-scale models or vice versa. This multi-scale/multi-phase/multi-physics nature of solidification and melting can be seen schematically in Fig. 1. In the last decades, numerous numerical models of solidification processes have been proposed [1–6], but no single model has been able to span the entire range of length scales from the process level of industrial interest (~m) down to the atomic scale (~Å) due to the

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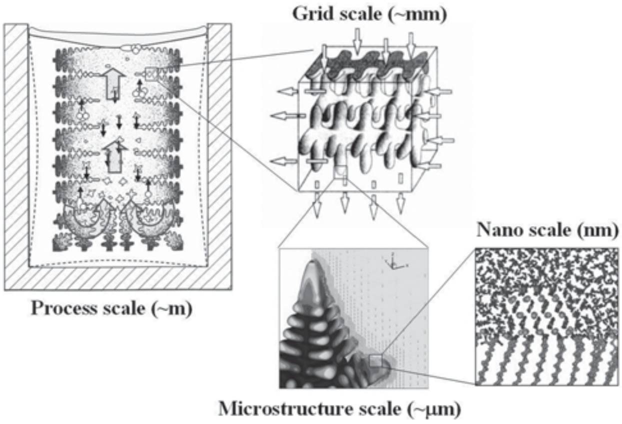


Fig. 1: Solidification—multiphase and multiple length scale problem

limitation of computational capacities. Therefore, a trend for the process-modelling of solidification/melting is to incorporate the interfacial phenomena occurring locally below the micro-structural scale into the global solidification process with a volume averaging approach [1, 2, 7].

With the volume averaging approach, a casting of industrial interest can be divided (discretized) into the representative volume elements (grid scale ~ mm). The macroscopic transport phenomena, such as mass, enthalpy, and species, are numerically solved based on these volume elements. All the microscopic phenomena occurring at the interfacial scale, such as the mass transfer due to solidification/melting, solute partitioning at the interface, release of latent heat, momentum exchange between phases with relative motion, will be volume-averaged in the representative volume element. Solidification kinetics and multiphase hydrodynamics will be coupled. A series of volume-averaging solidification/melting models have been developed by different researchers in the last decades. Significant contributions have been made by the current authors. Some of these models are summarized in Table 1.

In comparison to solidification, research on melting is relatively scarce [39]. In the past few years, remelting technologies have played an increasingly important role in the metallurgical industry, and the number of Electro-Slag-Remelting (ESR) and Vacuum Arc Remelting (VAR) units is increasing. Currently, ESR and VAR are commonly used; however, far-reaching investigations at the industrial scale in particular have rarely been published. There is still a great demand for more knowledge on these processes, and how to optimize the production processes regarding to the alloy quality and energy efficiency is still a remaining question. Some modelling efforts have also been made [40–44]. We know that the ESR is a process which involves two liquids: liquid steel and liquid slag. From a fluid dynamic point of view, the ESR process is a multiphase process, with a free interface (liquid steel/liquid slag), and with a mixed area (slag and falling steel droplets). The authors recently used the magneto-hydrodynamics (MHD) method to study the ESR process with a special focus on the multiphase flow phenomena in the slag and melt pool [45–47]. The full coupling between the phase distribution and the electric current gives answers to many questions and permits modelling not only the averaged behavior of the process but also its dynamic behavior.

1.2 Faced Challenges and Planned Modules

Quantitative prediction and control of solidification/melting has been, and remains, the most critical issue in the metallurgical industry. This Christian-Doppler laboratory is going to apply the solidification models mentioned above to investigate the solidification/melting related issues raised from industry. Examples of questions from the metallurgy industry are as follows: in thin-slab casting, how does the solid shell form and interact with turbulent flow? How can the electro-slag-remelting (ESR) process be better understood and controlled (stabilized)? How can metallurgical imperfections (macrosegregation, non-metallic inclusion, surface crack, etc.) in castings be predicted and minimized? Following the priority of the industry demands, two projects, here called 'Modules', are initially run.

Module I: Hydrodynamics in thin slab casting. Thin slab casting (TSC) has a great potential to replace the conventional slab casting for producing flat/strip products. The industry practices, however, have shown some drawbacks: sensitivity to breakout, edge cracks, and so on. The goals of this module are to refine and apply a mixture solidification model to predict the shell formation in the thin slab casting, with a focus on the turbulent flow and its impact on the two-phase mushy zone; to use this model to study the interaction between the melt flow and surface slag, including the transport phenomenon of the torn slag in the melt; and finally to assist the industry in optimization of the submerged entry nozzle (SEN) and mold design. The industry partner of this module is RHI AG.

Module II: Electromagnetic processing of dual-phase fluids. Electro-slag-remelting (ESR) is an advanced technique for producing high quality steel ingots. Understanding of the remelting process and the ability to model it, including the complicated interaction between the molten steel and liquid slag, is critical for controlling the ESR process. In the early stage, a previously developed numerical model will be evaluated with experimental data. In the late stage process, simulations will be performed to aid industry in optimization of the remelting process with respect to both energy efficiency and ingot quality. The industry partner of this module is INTECO special melting technologies GmbH.

2. Progress of the CD Laboratory: Selected Simulation Examples

2.1 Solidification of Thin Slab Casting (TSC)

A key issue for modelling the thin slab casting (TSC) is to consider the evolution of the solid shell, which strongly interacts with the turbulent flow and, in the meantime, is subject to continuous deformation due to the funnel-

TABLE 1:
Overview of volume-averaging solidification models

Models	Short descriptions of key features	Origins	Authors' contributions
Mixture solidification model	Enthalpy-based model; Mixture continuum for the mushy zone; A predefined solidification path; Turbulence effect	[8–14]	[15, 16] Application in CC slab and TSC slab; Model evaluations; Extension for the motion of solid phase
Globular equiaxed solidification model	Two phase: liquid and solid; Spherical crystal morphology; Diffusion governed crystal growth; Flotation and sedimentation of solid	[2, 17]	[18–20] Further refinements and extensions; Model evaluations
Cylindrical columnar solidification model	Two phases: liquid and solid; Cylindrical crystal morphology; Diffusion governed crystal growth; Interdendritic flow; Channel segregation; Bulging and softreduction in CC	[21, 22]	[23, 24] Model development; Functionality examination; Mechanisms of channel segregation; Application in continuous castings
Mixed columnar-equiaxed solidification model (non-dendritic)	Three phases: liquid, equiaxed and columnar; Cylindrical crystal morphology for columnar, and spherical for equiaxed; Columnar tip tracking; Diffusion governed crystal growth; Interdendritic flow and grain sedimentation; Columnar-to-equiaxed transition (CET); Different segregation phenomena in steel ingot		[25–30] Model development; Functionality examination; Mechanisms of segregation; Model evaluation; Application in steel ingots
Dendritic equiaxed solidification model	Three phases: solid dendrites, interdendritic and extradendritic melts; Dendritic crystal morphology; Shape factors for the grain envelope; Growth of envelope according to Lipton-Glicksman-Kurz model; Solidification of interdendritic melt according to diffusion	[31, 32]	[33, 34] Further refinements and extensions; Functionality examination; Model evaluation
Dendritic mixed columnar-equiaxed solidification model	Five phases: extradendritic melt, interdendritic melts in columnar and equiaxed grains, solid dendrites in columnar and equiaxed grains; Dendritic crystal morphology; Shape factors for the grain envelope; Growth of columnar primary dendrite tips (Kurz-Giovanola-Trivedi model); Growth of grain envelope (Lipton-Glicksman-Kurz model); Solidification of interdendritic melt according to diffusion; Columnar-to-equiaxed transition (CET)		[35–38] Model development; Functionality examination; Model evaluation

type mold. Here an enthalpy-based mixture solidification model that considers turbulent flow [12–14] is employed. This model is extended to include the motion of the solidifying and deforming solid shell [48]. The motion of the solid phase ($\vec{u}_s$) in the fully-solidified strand and partially-solidified mushy zone is estimated with a simplified volume-conserved Laplace's equation. A proper boundary condition is required, representing solid shell sliding along mold surface. The slab surface velocity is calculated with the assumption of a constant tangential moving velocity equal to casting velocity [49].

As an example, simulation results of a TSC of low alloy are shown in Fig. 2. With the four-port SEN design, 4-convection-roll flow pattern is developed. Roll A continuously transports superheat into the meniscus region to maintain a sufficiently high temperature and avoid premature solidification of the meniscus. Roll B is assumed to facilitate the penetration of liquid slag (dragged by the liquid melt) into the gap to form a slag film between the strand and the mold. Rolls C and D promote the mixing of superheat in the wide face region, hence enhancing uniformity of the shell in the wide face region. It is worth mentioning that a good resolution of the solidifying mushy zone is ensured with the help of developed numerical mesh adaptation algorithm. In the vicinity of the side jet impingement point, there are still about six grid points in the mushy zone (Fig. 2b, c). Shell formation is strongly influenced by the flow-solidification interactions. These interactions include the resistance of the solid dendrites to the interdendritic flow as well as the transport of the sensible and latent heat of the liquid phase by the interdendritic flow. The moving solid phase in mushy zone impedes the bulk flow, slowing down the bulk flow gradually through the mushy zone to the shell moving velocity. The strong impingement of the side jet on the solidification front would significantly reduce the growth rate of the solidification front, or cause remelting locally. The predicted shell thickness is validated against the experimental data from literature [50].

2.2 Calculation of Floatation of Particles in Tundish

A discrete phase model (DPM) coupled with the turbulent flow was applied to track the motion of particles in liquid melt. The solver includes two-way coupling between

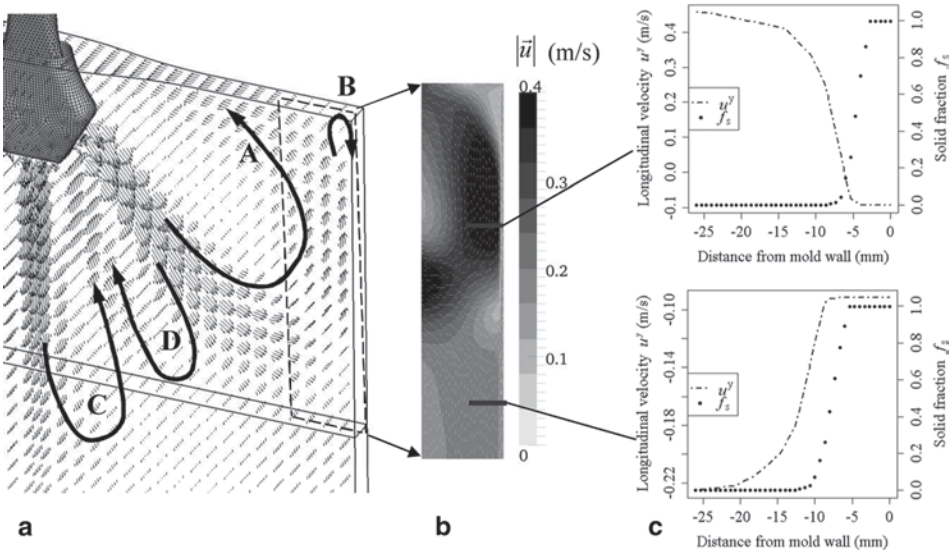


Fig. 2: Simulation result of a TSC [48]. **a** 3D distribution of the velocity field; **b** zoomed velocity field in the central plane near the narrow face; **c** detailed velocity profile and solid volume fraction along two paths across the mushy zone at the narrow face

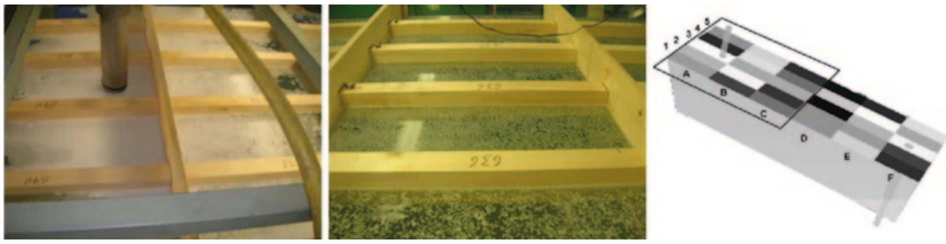


Fig. 3: Wooden frames were mounted on the tundish top surface of the water model to capture the float particles (*left*). The top surface of the calculation domain is also divided into the same number of patches, conforming the areas of the grid of the wooden frame (*right*)

continuous and discrete phases, particle/wall interaction, influence of turbulence on the particles, and a wide range of the injection sub-models.

To verify the DPM solver, a water modeling experiment on a model tundish (voestalpine Stahl, Linz) was carried out. Plastic particles (ϕ3.5 mm) were injected through the nozzle. As particles are lighter (density: 950 kg/m^3) than water, they tend to rise and finally reach the water/air surface. Transparent walls of the tundish permitted to capture the particle motion during the experiment with the speed camera. Wooden frames (Fig. 3) were mounted on the top water surface to capture the rest particles at the end of experiment. The captured particles by each frame were dried and weighted. In the meantime a numerical simulation was performed. The top surface (boundary) was also divided into the corresponding number of patches, conforming the locations and areas of the grid of the wooden frame. The comparison between experiment and simulation is shown in Fig. 4. The model prediction showed good agreement with the experiment along the tundish walls.

2.3 Modelling the Transient Slag/Melt/Air Interfaces

A volume of fluid (VOF) model is applied to track the moving interfaces. Typically for the continuous casting, three fluid phases are involved: liquid melt, covering slag, and air. A demonstrative simulation result of the VOF model is shown in Fig. 5, presenting the transient behavior of the moving interfaces between the melt, slag and air, and the flow pattern in the meniscus region around SEN. The risk of entrapment of torn slag (in form of droplet) by the bulk melt, one of the concerns of the industry process, is found to be highly dependent on the flow pattern at the meniscus. Therefore, it is necessary to perform such kind of calculations to investigate the flow pattern and the possible slag entrapment. Additionally, the flow results provide valuable information to analyze the chemical erosion of the SEN. Industry practice has indicated that the chemical erosion by the molten slag at the SEN-slag-melt triple junction point is strongly influenced by the flow around the SEN.

To verify the VOF model a water-oil-air modelling experiment is performed. The water represents the liquid steel, and the natural oil is used to mimic the slag layer. The experimental set-up represents an under-scaled (1/3) conventional slab casting system. A series of experiment conditions was investigated for two different SEN designs and six casting speeds in the range from the lowest to the highest possible one. Figure 6 shows a preliminary simulation result with the default VOF settings typically used for solidification modelling, and a comparison with an experimental result. It shows a promising agreement. Although most physical properties of the water and oil are available, there are still some properties which need to be determined experimentally: contact angles with the SEN wall, surface tensions (interface energies between phases).

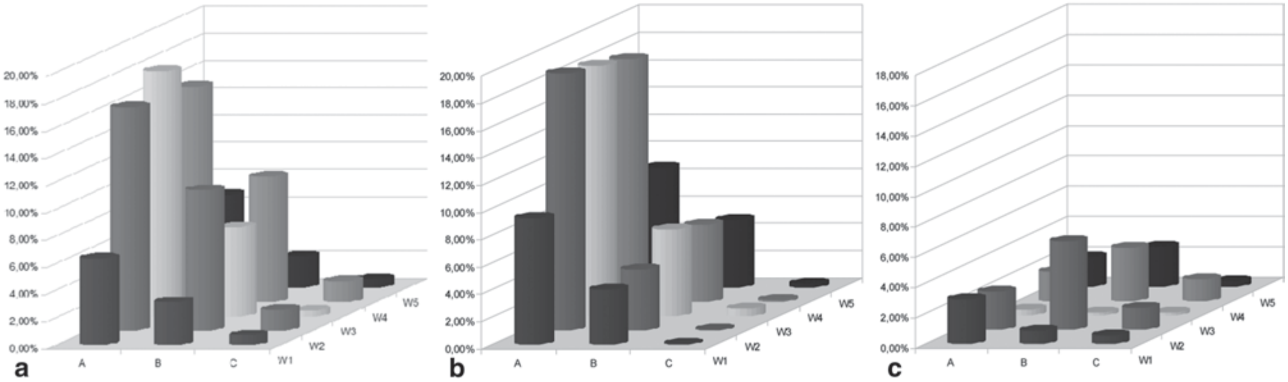


Fig. 4: Comparison of the particle distribution (wt% of particles being captured by each frame) between experiment and simulation: **a** experimentally captured particles; **b** numerically predicted; **c** deviation of the predicted result from the experiment

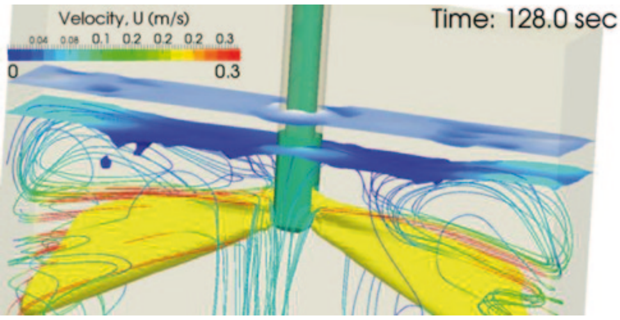


Fig. 5: A VOF simulation shows the flow pattern and dynamics of melt-slag-air interfaces

2.4 Magneto Hydrodynamics (MHD) in Electric Current Induced Flow

Electric current induced flows are present in many industrial processes, such as electro slag remelting, vacuum arc remelting, electrolyzes, DC arc furnaces, smelting, aluminum reduction cells, and more. Studying the mechanism of generation and development of the flows within a current carrying fluid due to the interaction of an electric current with a self-magnetic field is important in order to improve understanding of these engineering processes. In spite of the practical significance, some essential features of these flows have not yet been explored.

A VOF approach is coupled with MHD to study the formation and departure of a droplet beneath the melting electrode during ESR process [51]. As shown in Fig. 7, the electric current is strongly influenced by the phase distribution (shape of the departure droplet). In turn, the induced Lorentz force and Joule heat will influence the remelting and the motion of the droplet which will further adjust the electric current. With these interactions, two phenomena can be anticipated: one is the fluctuation of the electric resistance (voltage swing), and the other is the horizontal motion of the droplet. Actually both phenomena have been observed indirectly during operation of industry processes.

2.5 Importance of Interdendritic Flow in the Formation of ESR Melt Pool

Industry practise indicates that the crystal morphology during solidification of the big ESR ingot is dominantly columnar and dendritic. Here an enthalpy-based mixture solidification model [8–14] is used for modelling the solidification of the big ESR ingot. The two-phase mushy zone is treated as a porous media, within which the interdendritic flow is calculated according to the permeability. The permeability of the solidifying mushy zone has been the topic of many researchers. A literature survey of the mush permeability suitable for solidification of steel was made [52]. Some representative models are summarized in Fig. 8a. The models can be categorized in two different groups. Isotropic models (e.g. Blake-Kozeny model) assume that the permeability is independent of flow direction. In contrast, anisotropic models (e.g. Schneider-Beckermann and Heinrich-Poirier models) take into account anisotropy of the permeability.

Recently, we have refined the ESR solidification model to consider the anisotropic behavior of the flow in the mushy zone using Heinrich-Poirier model. It is observed that the newly implemented model can significantly improve the prediction of the distribution of mushy zone and pool depth, as shown in Fig. 8b.

2.6 Influence of Electric Conductivity of Slag on the Solidification of ESR Ingot

The literature survey has raised a question about the uncertainty of the electric conductivity of the molten slag and solidified slag skin. The reported electric conductivity of molten slag (σ_{molten}) varies from 100 to 300 $\Omega^{-1}m^{-1}$; the exact variation range of the electric conductivity of solid slag skin (σ_{solid}) is not clear. Some people believe that the solid slag skin behaves as isolation material, and some evidence does show a significant portion of electric current across the slag skin entering into mold. The question above cannot be answered by the numerical model itself, but we can address the importance of these properties in

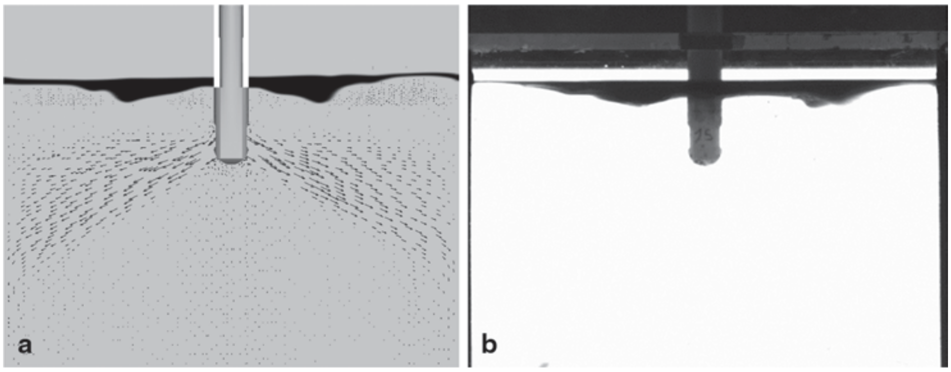


Fig. 6: A preliminary simulation result of the water-oil-air interfaces (**a**) and comparison with the experiment (**b**)

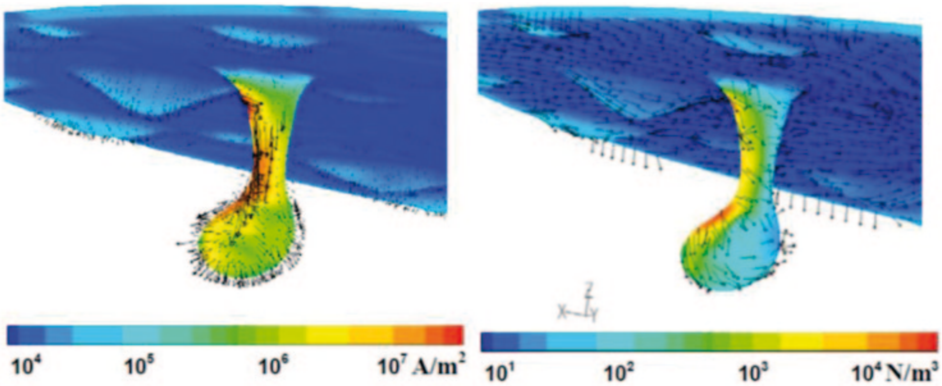


Fig. 7: Calculated electric current (*left*) and Lorentz force (*right*) distribution on the surface of a departure droplet beneath the melting electrode during ESR process

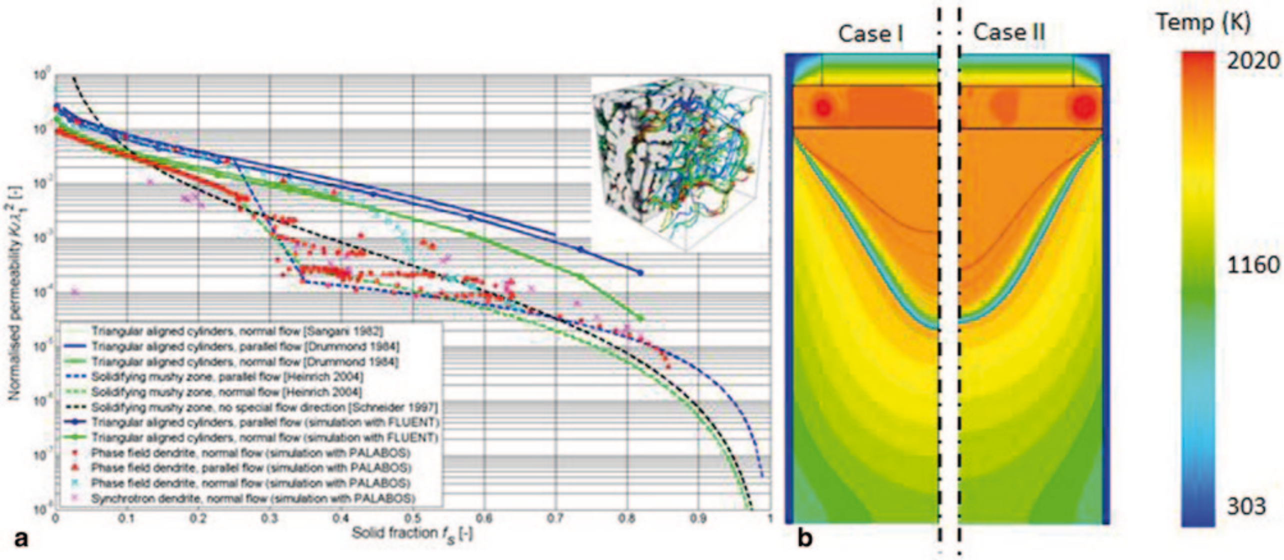


Fig. 8: Numerical study of the influence of the permeability models on the predicted melt pool. **a** A literature survey of the mushy permeability [52]. **b** Comparison of the predicted melt pools by using two different models of permeability: Case I—Blake-Kozeny isotropic permeability model (*left half*), Case II—Heinrich-Poirier anisotropic permeability model (*right half*)

the operation of the ESR process, hence to draw attention to this issue for future study.

By altering the electric conductivity of the molten slag and solid slag skin, the electric current will choose different current paths. On the one hand, it modifies the distribution of Joule heat release in the slag layer, hence influences the temperature field and solidification of the ingot. On the other hand, the distribution of Lorentz force is strongly dependent on the electric current path, which will modify the flow pattern in both slag layer and melt pool, and consequently influence the solidification of the ingot. As an example, two extreme cases are compared in Fig. 9. Obviously, the shape of the final melt pool and solidifying mushy zone depend strongly on whether the

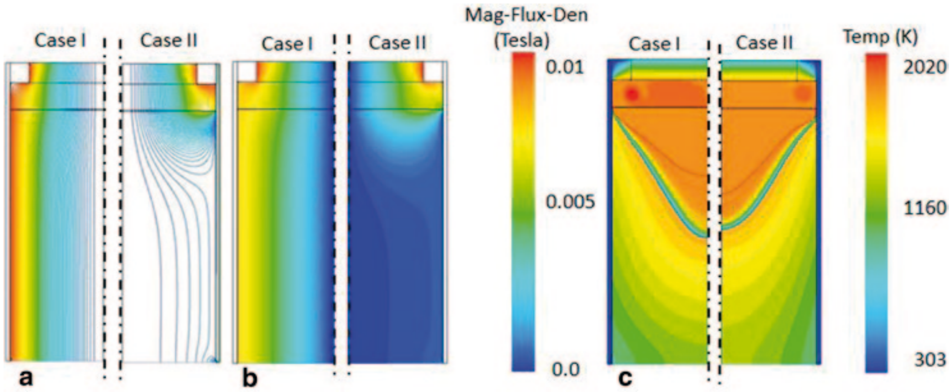


Fig. 9: Influence of the electric conductivities of the molten and solid slags on the electric current distribution (**a**), magnetic field (**b**) and temperature field and mushy zone (**c**). Here the electric conductivity of the molten slag is assumed to be constant ($\sigma_{molten} = 100\ \Omega^{-1}m^{-1}$), but two extreme cases for the solid slag skin are compared: Case I (*left half*) with $\sigma_{solid} = 0.001\ \Omega^{-1}m^{-1}$; Case II (*right half*) with $\sigma_{solid} = 48\ \Omega^{-1}m^{-1}$

electric current is 'allowed' to enter into the mold across the solid slag skin.

2.7 Influence of Frequency of the Applied AC Current

Not only the electric conductivity but also the power supply, the frequency of the applied AC current, can affect the electric current path. At high frequency, due to the so-called skin effect, the electric current tends to go near the extremity of the electrode and along the ingot surface. Figure 10 illustrates the effect of the frequency of the applied AC current on the current path and the final melt pool shape and mushy zone of the ingot. The most significant difference is the pool depth and the standing height (distance from the slag-pool interface to the start of solidification at the ingot surface). Part of this study was published elsewhere [53].

2.8 Modelling of Macrostructure and Macrosegregation

One ambitious goal of applying the solidification models (Table 1) is to analyse or predict the macrostructure and macrosegregation of engineering castings, but this still relies on future enhancement of the hardware resource. The computational expense increases relative to the increasing number of phases. On the other hand, the newly developed models need sufficient laboratory validations before they are implemented for applications in engineering processes. Here two examples are shown to illustrate some potential of those models.

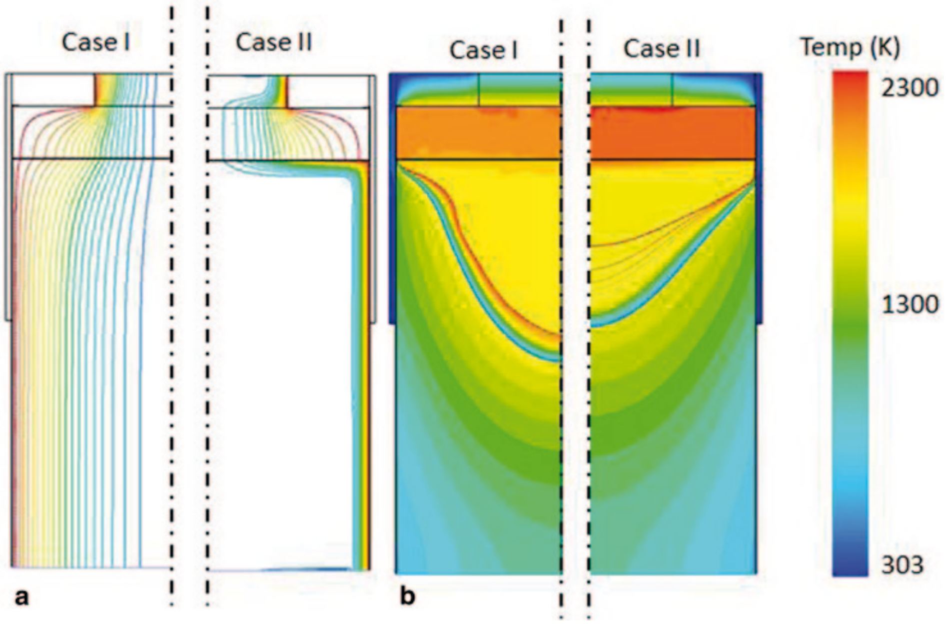
A 5-phase mixed columnar-equiaxed solidification model [35, 36] was proposed. Evaluations [38] were performed by comparison with laboratory castings. Some classical experiments of the Al-Cu ingots were conducted and the as-cast structural information including distinct columnar and equiaxed zones, macrosegregation, and grain size distribution were analyzed. The final simulation results exhibited good agreement with experiments in the case of high pouring temperature, as shown in Fig. 11. It was also found that the predicted as-cast structure for the casting poured at low temperature was somehow different from the experimental one. The casting is small ($\phi 75 \times 135$). The premature solidification during mold filling plays significant role in the subsequent solidification. The ignorance of this premature solidification during mold filling is believed to be mainly responsible for the disagreement between prediction and experiment for the casting poured at low temperature.

A three-phase mixed columnar-equiaxed solidification model [28–30] was used to calculate the macrosegregation in an engineering ingot (2.45 ton), as shown in Fig. 12. The main features of mixed columnar-equiaxed solidification in such an ingot were quantitatively modelled: growth of columnar dendrite trunks; nucleation, growth, and sedimentation of equiaxed crystals; thermosolutal convection of the melt; solute transport by both convection and crystal sedimentation; and the columnar-to-equiaxed transition (CET). The predicted as-cast macrostructure and the segregation pattern were in qualitative agreement with the reported experimental results. Some segregation mechanisms were numerically analyzed. Discontinued positive-negative segregation just below the hot top was predicted because of the formation of a local mini-ingot and the subsequent sedimentation of equiaxed grain within the mini-ingot. Quasi A-segregates in the middle radius region between the casting outer surface and the centerline were also found. The quasi A-segregates were predicted to originate from the flow instability, but both the appearance of equiaxed crystals and their interaction with the growing columnar dendrite tips significantly strengthened the segregates.

3. Summary Discussions

A trend for the process modelling of solidification/melting is to incorporate the interfacial phenomena occurring locally below the micro-structural scale into the macroscopic transport system with a volume averaging approach. In the last decades, a series of volume-averaging solidification/melting models has been developed by different researchers including significant contributions of the authors. This article reported briefly on the current activities in the CD-Lab—"Advanced Process Simulation of Solidification and Melting." The main goal of this CD-lab is to apply the previous models with necessary extensions/modifications to address engineering problems being raised from (Austrian) metallurgy industry.

Fig. 10: Influence of the AC current frequency on the electric current distribution (**a**), and the temperature field and mushy zone (**b**). Two cases are compared: Case I with frequency of 0.1 Hz: Case II with frequency of 50 Hz



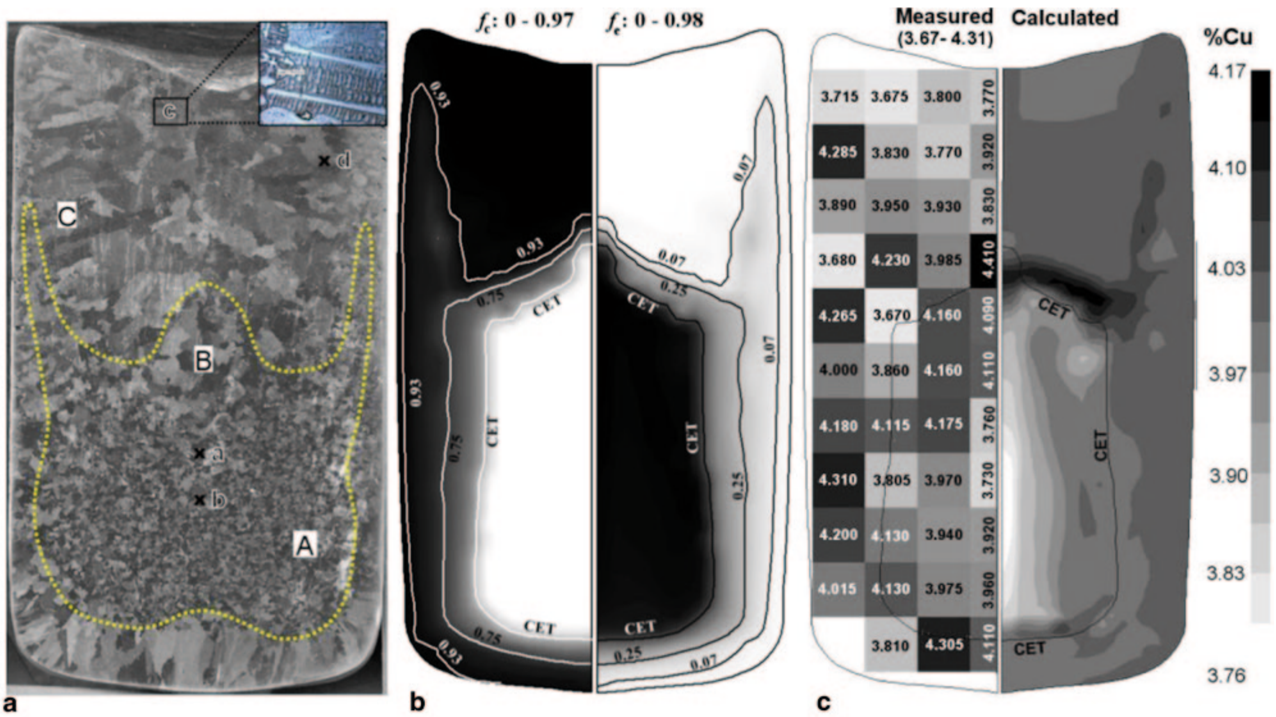
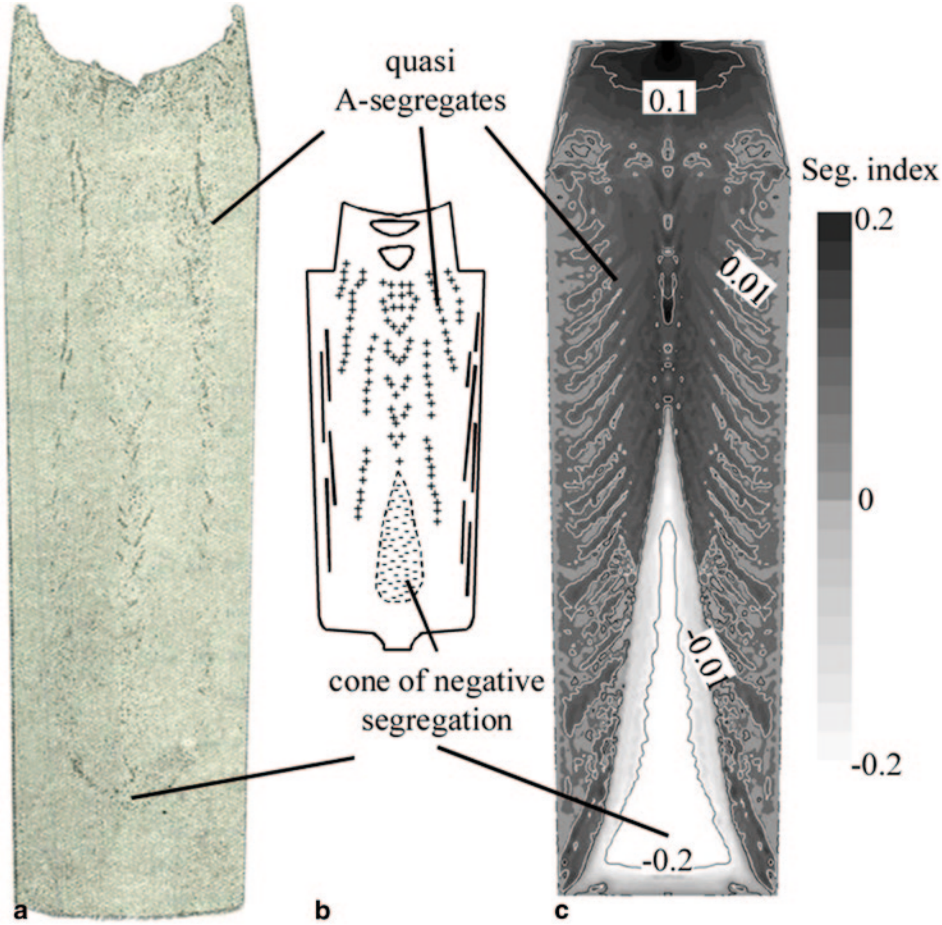


Fig. 11: As-cast macrostructure and macrosegregation of an Al-4 wt.% Cu casting (ϕ75×135), poured at 800 °C in a graphite mold. **a** Macrostructure, mixed columnar, and equiaxed regions separated by CET; **b** Predicted macrostructure, distribution of volume fraction of columnar crystals (*left-half*) and volume fraction of equiaxed crystals (*right-half*). **c** Measured (*left-half*) and calculated (*right-half*) Cu-segregation

Significant progresses were made as demonstrated by the selected simulation examples:

- Full 3D flow-solidification simulation of thin slab casting (TSC), targeted at optimization of the submerged entry nozzle (SEN) design.
- 2D axisymmetric calculation of electro-slag remelting (ESR) process, targeted at the optimization of the ESR operation parameters.
- Analysis of the coupled MHD-CFD phenomena (3D) to gain knowledge about the complicated physics embedded in engineering processes.

Fig. 12: Macrosegregation pattern in an engineering steel ingot (2.45 ton). **a** Sulphur print of the as-cast ingot, **b** schematic of the typical macrosegregation pattern in steel ingots, and **c** predicted macrosegregation pattern (black for the positive segregation and white for the negative segregation) overlapped with isolines. The segregation is quantified by a segregation index: $(c_{\text{mix}} - c_0)/c_0$



- Laboratory evaluations of some advanced modelling features for calculation of the particle motion in tundish, dynamics of air/slag/melt interfaces of continuous casting of slab, macrostructure and macrosegregation in ingot casting.

In the meanwhile we still face challenges:

- Numerical models intended for engineering application need further validations, preferably against engineering processes directly. The pilot or plant trials, in addition to laboratory experiments, for both TSC and ESR with available operation parameters and intermediate or final casting results are desired.
- Computational expenses increase with the process scale (size) and the complexity (number of phases involved) of the model. A suitable model for a certain engineering process is often chosen (Table 1) by making a compromise between the model complexity and the calculation cost. Ongoing efforts are (i) the enhancement of the hardware capacity and parallel computing efficiency, (ii) the optimization of algorithms, (iii) the simplification of the numerical model.

4. Acknowledgments

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