SIMULATION IN METALLURGY: PAST ACHIEVEMENTS AND FUTURE CHALLENGES

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Abstract

Metallurgical processes may typically involve many physical phenomena such as fluid flow, heat transfer, solidification, electromagnetism, chemistry, and kinetics in multi-component multi-phase systems. Permanently growing computational power and a massive shift to parallel cloud computing allow us to design multiphysics numerical simulations and thus gain a deeper insight into fundamental and technical issues. This article overviews up-to-date modeling efforts/achievements in the metallurgical discipline and is not afraid to critically assess current drawbacks as well as to show directions for future developments. The topics concerned are local heat treatment of as-cast structures, clogging of submerged entry nozzle, electro-slag rapid remelting, thin slab casting, sedimentation of equiaxed crystals, columnar-to-equiaxed transition due to fragmentation.

Keywords: Local heat treatment, electroslag remelting, electromagnetic stirring, clogging, sedimentation

1. INTRODUCTION

At present days a numerical simulation is without doubt an essential prerequisite for the design optimization of metallurgical processes such as the (semi-)continuous casting, electro-slag remelting [1], thin-slab casting, centrifugal casting [2,3], etc. Permanently growing computational resources (data storage capacity, FLOPS, memory bandwidth), a shift to parallel cloud computing, and last but not least favorable prices for CPU/hour (GB/hour) made the numerical simulation a truly competitive tool compared to traditional approaches such as experiments. Obviously, in order to simulate such processes often involving multiphase and/or multiphysical phenomena, generally an appropriate set of PDEs must be carefully set up taking into account all essential process details. Only then, it makes sense to think about the most suitable method for finding the solution, discretization of the PDEs into a system of linear equations, and eventually an efficient iterative solver. To summarize, the following three points form the crucial ingredients necessary to obtain useful and usable simulation results: hardware, mathematical description of physics appearing in the metallurgical process, and numerical algorithm.

The present work concisely overviews several metallurgical processes looked at from the perspective of state-of-art numerical simulations. For each one of them a brief model description is provided along with the most interesting challenges encountered and yet unresolved issues.

2. LOCAL HEAT TREATMENT OF AS-CAST STRUCTURES

In addition to an excellent cast ability, corrosion resistance, high thermal and electric conductivity, many aluminum alloys can be age hardened by formation of precipitates leading to a significant boost in strength-to-weight ratio. The heat treatment of the whole part can be however a very energy-intensive and costly operation. If only a local strengthening of the alloy is needed, a localized heat treatment e.g. by a laser beam can be

sufficient, leading to significant savings. As it is not clear which process parameters are required to obtain the desired local strengthening, an automatic process optimization via series of subsequent simulations [4,5] was proposed to find optimal laser power, beam diameter, and exposure time so that the overall process energy is minimized and requirements about the local strength are met.

The optimization loop begins with the OpenFOAM® calculation of the energy distribution (**Figure 1b**) and thermal stresses induced by laser beam initial energy insertion, followed by checking maximum von Mises equivalent stress and temperature against the basic yield strength and the solidus temperature of the alloy, respectively. If necessary, when the material yields or remelts, the energy intensity is reduced. Next, a set of Cartesian points is randomly sampled around the location of interest (**Figure 1a**) and fetched into the scientific toolbox MatCalc. There, using temperature curves discrete yield strengths are obtained by running a kinetic calculation at each point. A smooth 3D field of the yield strength is reconstructed by solving the Laplace equation with the discrete yield strengths as source terms (**Figure 1c**). If the yield strength in 3D is as desired, the simulation may proceed to the next time step, otherwise the energy insertion must be readjusted.

Currently, the major modeling drawback is the radius based transformation model used in MatCalc to predict phase transformation of precipitates, which is on the one hand unphysical; on the other hand it is the only available method providing a correct phase dependency. Therefore, setting up a physical model remains a challenge that can be met either through experimental predictions of mechanical/thermodynamic properties or increasingly popular quantum-mechanical calculations [6].

3. CLOGGING OF SUBMERGED ENTRY NOZZLE

In the continuous casting of steel, the melt is supplied through a submerged entry nozzle (SEN) into a copper mold. The SEN clogging is a long lasting problem that may lead to various casting defects or unwanted casting breaks. Several mechanisms of clogging were proposed [7], from which the most widely accepted one assumes non-metallic inclusions (NMIs) such as Al_2O_3, TiN, TiO_2, ZrO_2, etc to be formed by de-oxidation or re-oxidation in the bulk melt and gradually deposited on the SEN wall by adhesive capillary forces and a ssuccessive formation of a sinter bond occuring at high temperatures.

The Eulerian-Lagrangian approach was adapted to study the SEN clogging (**Figure 2**). NMIs are treated as spherical Lagrangian particles (2-10 μm) draged by the turbulent flow solved with the shear-stress transport (SST) k-ω model available in the commercial CFD code ANSYS-FLUENT 14.5. In the turbulent boundary layer a stochastic near-wall model was employed to trace status of each particle. Once a particles hits the wall, it is irreversibly transformed into a clog porous material with a porosity determined from the post-mortem analysis of experimental clog samples. The clog front is tracked by an algorithm developed earlier originally for tracking the solidification front of columnar dendrites [8].

The model offers general features of clogging/fouling and therefore could be also applied in other fields or applications such as pharmaceutical industries, HVAC applications, automotive industry, food production, etc. Although the model has been verified against a laboratory experiment and a reasonable agreement was found between the calculated and measured data, several model uncertainities exists and further refinements are therefore necessary such as a more accurate estimation of the clog permeability, taking into account non-spherical particles, considering solidification inside the clog, and last but not least revising the theory on evolution of the turbulent boundary layer around a porous material.

4. ELECTRO-SLAG RAPID REMELTING (ESRR)

The electro-slag remelting (ESR) process is used to purify super-alloys by remelting as-cast consumable electrode into a high-grade ingot. Recently, the electroslag rapid remelting (ESRR) process has emerged offering roughly up to 10 times higher melt rates compared to the conventional ESR process, which is achieved by utilizing a T-shape mold with an embedded graphite ring for collecting the current in the slag.

As an experimental analysis and measurements of the ESRR process are hard to design especially due to materials' opacity and very high temperatures (~1900°C), a numerical simulation apparently seems to be the only viable way of shedding light on invisible phenomena inside a large industrial size ingot. A numerical model was set up [9] in the commercial CFD code ANSYS-FLUENT 14.5 considering governing equations for turbulent flow (shear-stress transport k-ω model), solidification/melting (the lever rule), electromagnetic field ($A-\phi$ method). The coupled PDEs of Multiphysics with a large number of DoFs on the industrial scale would however require enormous computational resources. Hence, several assumptions must be necessarily adopted such as solving the electromagnetic field only once beforehand, freezing the motion of any fluid-fluid interface, prescribing explicitly the air gap thickness between the ingot and the mold, approximating falling melt droplets through the slag by mass/momentum/energy source terms in the melt pool (**Figure 4**).

Despite quite a few simplifications, the proposed model yet offers a realistic insight into unexplored casting process and thus, opens the possibility to optimize operational parameters such as the power supply, the melt rate, the immersion depth, the slag type/weight, the current ratio, and the fill ratio.

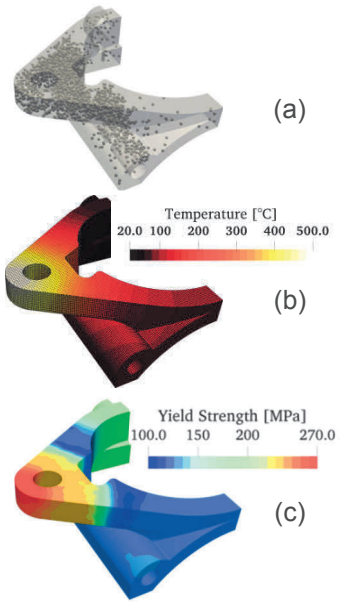

Figure 1 Random Cell Distribution (a), Temp field (b), Yield strength (c) [4]

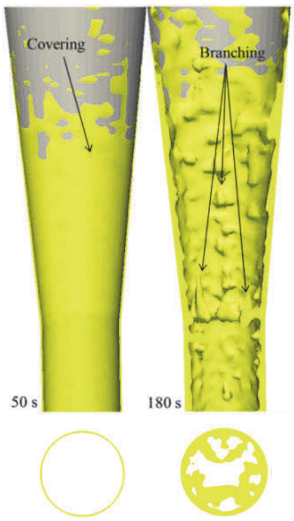

Figure 2 Progress of SEN clogging (covering → bulging → branching) [7]

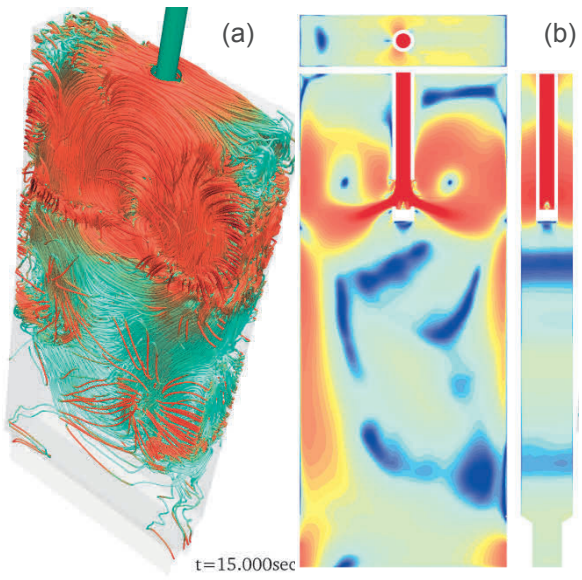

Figure 3 Meniscus of continuous casting - current paths (a), time-averaged velocity field around SEN (b)

5. THIN-SLAB CASTING

An emergence of thin slab casters delivered a reduction in the number of process steps involved in the production of hot rolled coils especially by avoiding the slab reheating furnace before the hot rolling. Increasing casting speeds to around 5 m/min and allowing for casting medium and high carbon steels naturally promotes sensitivity to e.g. edge/surface cracking, breakouts. Significant energy savings and accelerated production rates are conditioned upon carefully addressing the mold and SEN design, hydraulic oscillations of mold, use of electromagnetic brakes, high pressure descaling nozzles, quality of mold powder, optimal water spray cooling, etc.

Once again, also here a numerical model comes handy [10]. Using OpenFOAM®, a solidification model is developed taking into account a turbulent flow of a liquid melt, formation of the solid shell and its deformation in the funnel shape of the mold, and not least of all three phase system namely melt, slag, and air. In addition, tracking of non-metallic inclusions was implemented by means of Lagrangian particles in order to monitor

another source of defects. Recently, a new MHD feature has been added to study the electromagnetic stirring (**Figure 3**).

After a successful verification against the water model, the numerical model proved to be useful in explaining the mechanism of slag entrapment and the SEN refractory erosion region. Further, it helped a lot during testing new SEN designs, although along the way to victory few troubles related to turbulence modeling and mesh size were encountered.

6. SEDIMENTATION OF EQUIAXED CRYSTALS

Coming to more fundamental topics, unlike immobile columnar crystals, equiaxed crystals may float or sediment. Depending on the solid fraction the crystals exhibit different rheological behavior below and above the packing limit (**Figure 5**). At low solid fractions the crystals resembles a Newtonian fluid with a viscosity determined according to the power-law viscosity model for a solid-particle system. At high solid fraction however the crystals reveal viscoplastic behavior i.e. the stress tensor depends on the strain rate. Therefore, the deformation of metallic alloys in the semi-solid state is a complex process especially when investigating the entire spectrum of the solid fraction range. Our numerical endeavors (OpenFOAM®) relies on a two-phase Eulerian-Eulerian volume-averaging model for the liquid and the solid phase. Interactions are controlled by isotropic and deviatoric part of the momentum exchange term. The former triggers the sedimentation process, the latter represents the drag between the moving crystals and the surrounding liquid. Most importantly, the deviatoric part of the stress tensor is constructed carefully to ensure a smooth transition between the submerged object and the viscoplastic regime.

Although several numerical tests were performed on a small scale geometry (10 x 10 mm) showing encouraging and physically intelligible results, the complete validation of the model is still needed. Next, at the current stage the model is ready to be extended to account for the nucleation and the growth of equiaxed crystals, which is a next step to be taken.

7. COLUMNAR-TO-EQUIAXED TRANSITION DUE TO FRAGMENTATION

Here, a solidification model of a binary alloy (Sn-10wt%Pb) was developed in the Eulerian frame, taking into account three phases such as rigid/stationary columnar crystals growing from the wall, equiaxed crystals and the liquid phase as moving phases [11,12]. This numerical model was proposed to reproduce the as-cast structure and macrosegregation observed in experiments [13] designed according to the fine configuration of Hebditch and Hunt. As it is believed the formation of equiaxed crystals is dominated by remelting secondary arms of columnar dendrites, fragmentation is incorporated into a three-phase mixed columnar-equiaxed solidification model.

The precise benchmark experiment and the simulation results are in a satisfactorily good agreement and the main features of the final as-cast structure are captured such as the concentration maps and the columnar-to-equiaxed transition (**Figure 6**). Nevertheless, using a constant parameter referred to as a fragmentation coefficient is doubtful and must be improved as many contributing factors such as the curvature effect of the dendrites, the latent heat induced thermal fluctuation, the diffusion in the interdendritic melt are merged into a single number. It is worth noting that although the current model is able of capturing channel segregates, their size and distribution are typically mesh-size-dependent especially on a large-scale grid.

8. CONCLUSIONS

Nowadays, thanks to computational resources growing larger every day and much tireless effort of other scientists spent in developing multiphysical models and efficient algorithms of solving various PDEs, there is

no doubt about the relevancy and usefulness of a numerical simulation also in the modeling of solidification fundamentals and metallurgical processes.

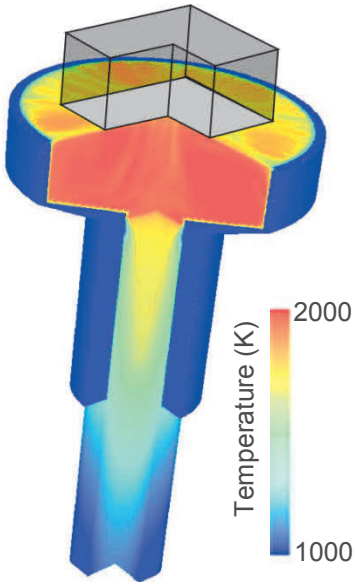

Figure 4 Thermal field in slag, mold and ingot [9]

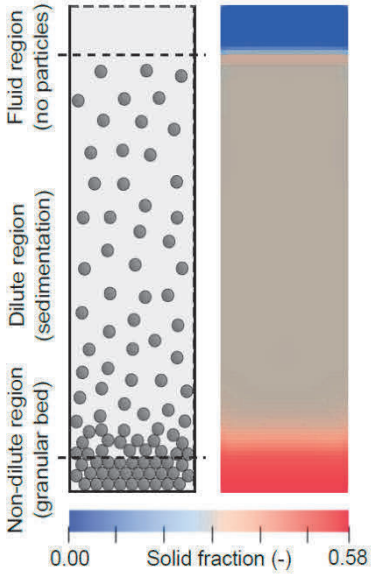

Figure 5 Sedimentation and granular bed of equiaxed crystals

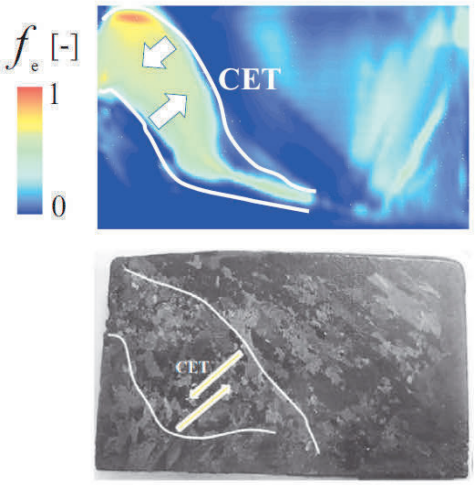

Figure 6 As-cast structure: volume fraction of equiaxed phase [12]

In the present article, several ongoing activities related to the modeling of solidification are briefly described along with current drawbacks and challenges. Among more fundamental topics, we have pointed out a complex rheological behavior of equiaxed crystals floating/sedimenting inside the liquid melt, depending on the actual solid fraction. Further, it was shown that the fragmentation of columnar dendrites by remelting may be sometimes the only source of nucleation. In addition, we have in short commented on modeling of several industrial applications, typically relying on commercial and open-source CFD codes such as ANSYS-FLUENT and more flexible OpenFOAM®. Recently, for instance, a full 3D numerical model has been extensively used to optimize a T-shape mold of an electro-slag rapid remelting unit. Also, since many years a continuous casting simulation, at present concentrated on the thin-slab casting, has been uninterruptedly developed and improved by including more accurate turbulence models (LES), the deformation of a solidifying shell, and the electromagnetic stirring. Apart from investigating solidification phenomena, a clogging mechanism of a submerged entry nozzle (SEN) by non-metallic inclusions was thoroughly explored via a numerical simulation. Despite a good agreement with a laboratory experiment, it is not yet clear how to mathematically describe the turbulent motion of a suspended particle around a complex structure of the clog simplified by the volume-averaged porous media approach. Last, an example of an automatic process optimization via simulation (APOS), namely a local heat treatment of as-cast structures by a LASER beam, was presented. Thermal and stress calculations were performed in OpenFOAM®, followed by 0D kinetic calculations at selected points in MatCalc. The optimization loop was based on the multiple objective genetic algorithm available in DAKOTA. Phase transformations of precipitates in aluminum alloys (A356) still lack a physical model and that could be considered the main drawback of the otherwise elegant simulation.

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