Joint Proposal for Diploma Project

Lattice Boltzmann simulation of fluid flow through dendrites in the mushy zone

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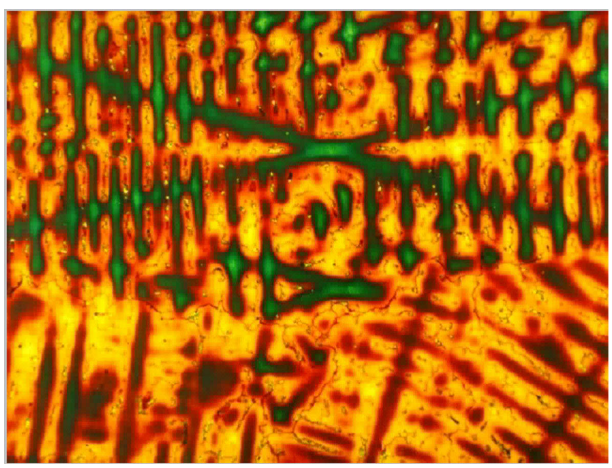

Figure 1: Micrograph of dendrites.

Motivation

Why are we interested in fluid flow in the "mushy zone" of a steel melt, where solidification [1] has progressed to a point where we have a mixture of dendrites and liquid steel?

- porosity: The liquid steel cannot flow fast enough since the flow is hindered (sometimes even blocked) by the dense network of dendrites to compensate for solidification shrinkage. These could lead to the formation of pores.

- hot tearing in continuous casting: Similar phenomena as the formation of pores, but in presence of tensile stress (possible channels for feeding flow?)
- macrosegregation phenomena strongly depend on the fluid flow on a microscale between the dendrites
- shear thinning: decrease of the viscosity of the semi-solid metal when a shear rate is applied (it is assumed that due to the shearing, solid bridges between grains are broken).
- ductility of mushy zone, brittle temperature range: for high solid fractions $f_s \simeq 0.95$ formation of liquid films. In this situation any openings of the mushy zone along these films cannot be compensated by liquid flow since the permeability is too low. This leads to very low ductility, regardless of the strain rate.
- Multiscaling: microsegregation between the dendrite ⇒ derive boundary model for a large scale flow simulation of the whole strand (macrosegregation)

Method

Computational fluid flow simulations of the incompressible Navier-Stokes equation will be performed with the Lattice Boltzmann method (LBM). A simple implementation of LBM allows to investigate flow resistance through dendrites without temperature effects (possibility to parameterize Darcy's law for the mushy zone); taking into account temperature gradients LBM can describe convection effects.

The advantages of LBM are ease of implementation of boundary conditions for flow in structures with high tortuosity (references [2, 3, 4], and ease of parallelization. Parallelization is necessary for the size and complexity of systems that need to be considered for a realistic modeling of the mushy zone. The LBM method can easily be combined with other models, for example a model to account for diffusion, or for solidification (phase transition). To our knowledge there is no commercial LBM code available. A great advantages of this in house code compared to commercial CFD codes is its transparency of the model and the great flexibility. The simulation can easily and in a controlled way be altered and extended.

What is needed

In order to perform LBM calculation of flow through dendrites, dendrite structures are needed. As a first step, a parameter study of the influence of primary, secondary, ternary,… arm spacing on the flow can be carried out with simple geometrically generated structures.
In a second step more realistic structures can either be generated with cellular automata methods [5, 6], which could be carried out in cooperation with another group; or, if available, dendrite structures can be taken from computer tomograph investigations or X-ray microtomography [7, 8] of real steel samples. according to The Book tomography is used to study solidification structures.

Feasibility of diploma thesis

- R. E. Zillich and S. Hahn both have experience with the LBM method; both have implemented LBM code which can be used for introducing a student to LBM (learning by reading a simple example implementation)
- application side: Siemens VAI has the expertise in continuous casting technologies and metallurgy
- no "fluid-structure interaction" is to be considered (such as breaking off of dendrites; growth of dendrites)
- optionally, and depending on the progress made in the course of the thesis, thermal gradients can be simulated with LBM

Outlook

After a successful diploma thesis there is the opportunity for more extensive work within the scope of a PhD thesis. For example, the simulation could be combined with a solidification model and microsegragation model (mass transfer equation at the solidification interface, diffusion equation, phase transformation) to account for the resulting concentration gradients of the components and the liquid solid phase transformation during the flow simulation. Another option is to derive boundary models from the microstructure simulation which could be used in large scale simulation of flow phenomena in continuous casting like, for example, macrosegregation.
It is also possible to allow for breaking off of dendrites to address questions related to shear thinning and hot tearing.

References

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