

MODELING OF SOLIDIFICATION

Christoph Beckermann, Ph.D.,
Professor
Department of Mechanical and Industrial Engineering
The University of Iowa
Iowa City, IA 52242

INTRODUCTION

An overview is provided of recent progress in solidification modeling and its application to casting of metal alloys. The overview is structured in the order of increasing length scales: dendrites on a microscopic scale; interactions between dendrites, coarsening, and flow within a unit cell inside the mushy zone; and heat transfer, flow, and species redistribution on a macroscopic scale. It is shown how the transport processes at the different length scales interact to produce certain structures and defects in a casting.

DENDRITES

The most common microstructure formed during solidification of metals and alloys is the dendrite. Figure 1 shows an image of a dendrite of a transparent model substance (succinonitrile) grown in the microgravity environment of space [1]. Such images have enabled the study of the scaling behavior of single dendrites growing freely in an undercooled melt [2, 3]. For example, in the sidebranch plane corresponding to Figure 1, the contour length, U , of the solid-liquid interface as a function of distance Z from the tip is given by

$$U/R = 0.38(Z/R)^{1.5} \quad (1)$$

and the area of the solid, F , by

$$F/R^2 = 0.58(Z/R)^{1.7} \quad (2)$$

where R is the radius of curvature of the dendrite tip. These two scaling relations are valid in the nonlinear sidebranching regime far from the tip, $Z/R > 40$, up to several hundred tip radii back. They apply not only to the dendrite shown in Figure 1, but to different dendrites grown using a variety of undercoolings. The existence of these relations implies that the dendritic structure remains self-similar far from the tip. It is certainly intriguing that the knowledge of the tip radius alone is sufficient to predict structural features of an entire dendrite.

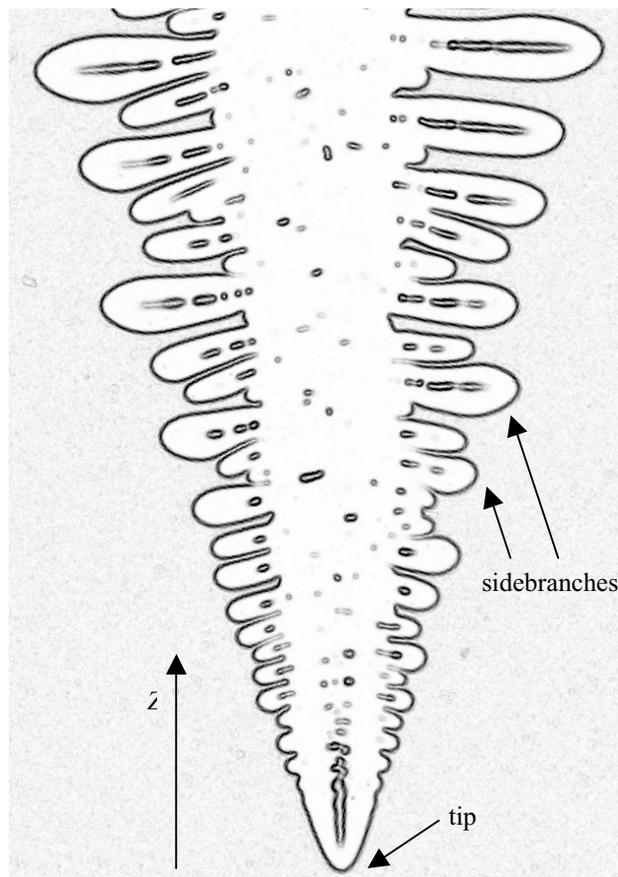


Figure 1: Enlarged image of a succinonitrile dendrite obtained in the Isothermal Dendritic Growth Experiment of Glicksman and coworkers [1] on the space shuttle.

The simulation of dendritic growth and other solidification microstructures has recently experienced much progress due to the availability of novel numerical techniques and increased computational power. In particular, the phase-field method has

been used with great success to model the evolution of complex solidification structures [4]. Figure 2 shows a result from a phase-field simulation of the growth of a single dendrite into an undercooled melt with flow [5]. Such simulations allow the effects of convection in the melt on the growth of the dendrite tips and sidebranches to be quantified and compared to theories and experiments [6-8].

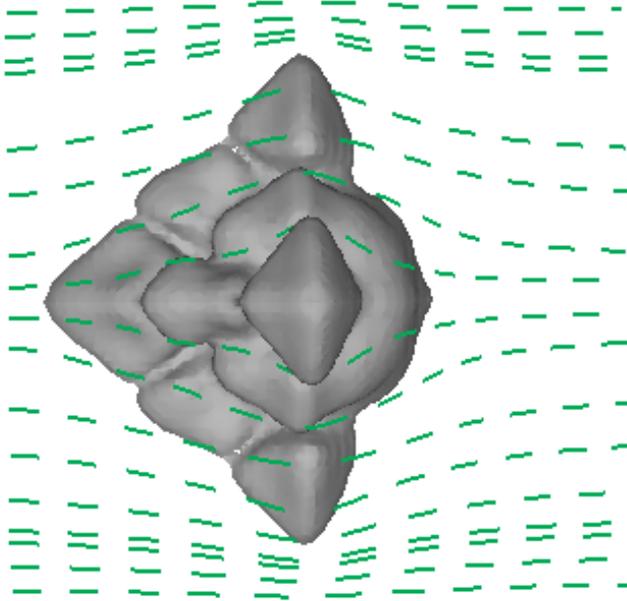


Figure 2: Three-dimensional phase-field simulation of free dendritic growth of a pure substance into an undercooled melt; the melt flows over the dendrite from left to right [5].

MUSHY ZONE

One of the challenges in modeling solidification is how to account for processes occurring on a microscopic scale, such as

dendritic growth and coarsening, in a model for an entire casting. One approach is to use representative elementary volumes (REV) as building blocks in a macroscopic model. By investigating in detail the solidification and transport phenomena in each REV, an averaged description can be obtained. Here it is important to not restrict attention to a single dendrite, but to take into account the presence of and interactions between multiple dendrites inside the mushy zone of solidifying alloys.

Figure 3 shows two-dimensional phase-field simulations of coarsening and flow for a periodic unit cell inside the mushy zone of an Al-4%Cu alloy [9]. The initial circles (left-most panels) represent cuts through dendrite arms of various diameters. As time proceeds, the structure of the solid coarsens. In the simulations with flow (lower panels in Figure 3), the coarser structures offer less flow resistance, resulting in an increase in the melt velocity with time. This in turn implies an increase in the permeability of the mush element. It is important to realize, however, that while the microstructure of the mush affects the flow, the flow also influences the evolution of the microstructure. In the presence of convection, the interfacial area decreases with the square root of time, as opposed to the classical cube-root-of-time coarsening behavior for purely diffusive conditions [9].

CASTINGS

Some of the solidification models developed in the past [10-12] are now being incorporated into commercial software, to enable the casting simulation of complex-shaped, three-dimensional parts.

One important issue in casting simulation is the prediction of macrosegregation (inhomogeneities in the composition on the scale of the casting) [13]. The cause of macrosegregation is the long-range movement of (micro-) segregated liquid and solid in the mushy zone, as shown for a REV in Figure 3. An example of the simulation of macrosegregation formation during solidification of a large steel casting is shown in Figure 4 [14]. It should be noted that due to computer limitations, the prediction of smaller scale macrosegregation features (such as

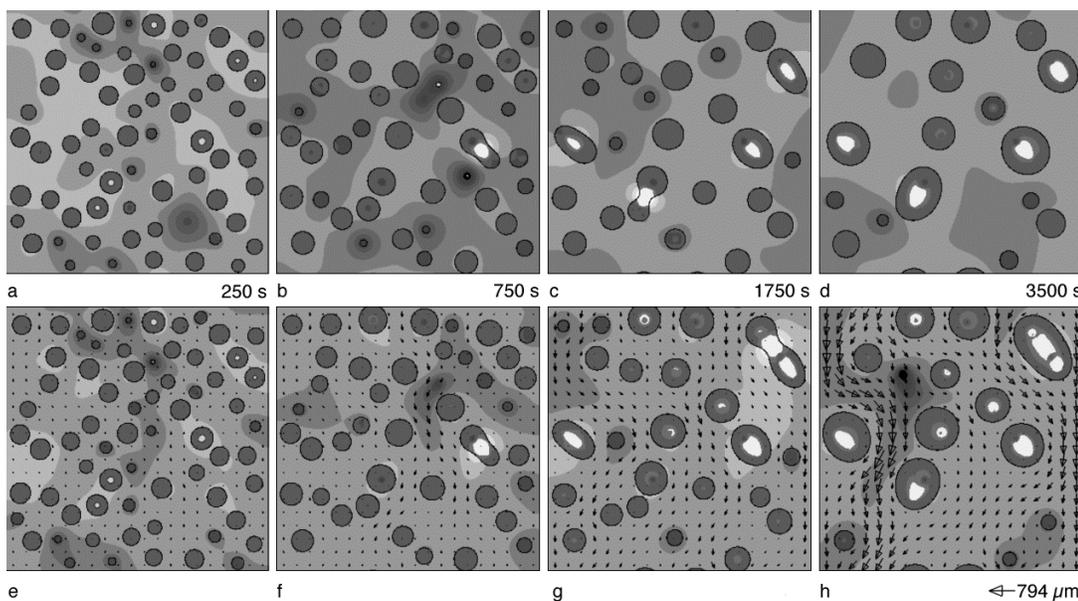


Figure 3: Phase-field simulations of coarsening in and flow through (lower panels only) a periodic unit cell inside the mushy zone of an Al-4 wt.% Cu alloy; the thick black contour lines show the solid-liquid interface; the gray shades indicate Cu concentrations in the liquid and solid [9].

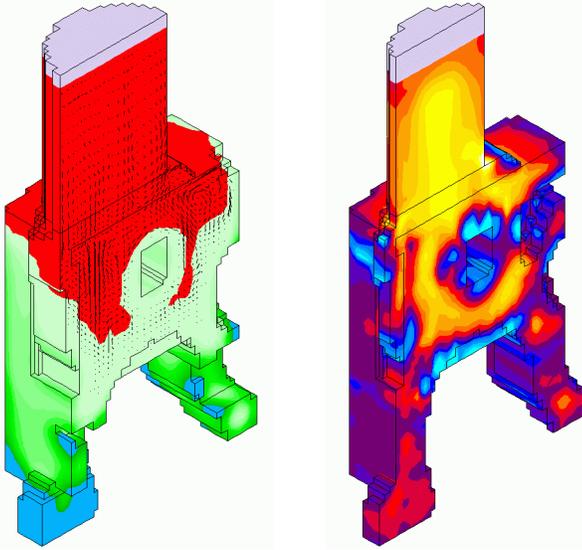


Figure 4: Simulation of macrosegregation formation in a large (2.65 m height) steel casting; left panel: predicted liquid velocities and solid fraction at an intermediate time during solidification; carbon macrosegregation pattern in the fully solidified casting [14].

freckles or A segregates) in large castings is beyond current capabilities.

Another important area that has recently received increased research interest is the prediction of porosity in castings. Porosity significantly reduces the mechanical performance of castings, and porosity-related defects are a major cause of casting rejection and re-work in the casting industry. Porosity ranges in size from microporosity, such as micron-sized gas bubbles, to macroporosity, such as millimeter- to centimeter-sized centerline shrinkage porosity, or even larger shrinkage cavities found in inadequately fed cast sections. Porosity-related defects come about due to the interplay of several phenomena. As the melt cools, the solubility of gases dissolved

in the melt decreases. If the solubility limit is reached, gas will precipitate out of the melt. In addition, gases are much less soluble in solid than in liquid, and hence gas is rejected from the solid to the liquid during solidification, which increases gas levels in the remaining liquid. Finally, the pressure gradient associated with metal flowing through the mushy zone to feed solidification shrinkage decreases the pressure in the casting, which further lowers the solubility. Even in the absence of dissolved gases, pores can form solely due to shrinkage.

An example of the simulation of porosity formation in a steel casting is shown in Figure 5 [15]. To validate the predictions, two types of casting trials were conducted: one without applied pressure and one where the solidifying steel was subjected to a higher than atmospheric pressure. Pressurization was accomplished through the top riser. The trials were performed with 3”T x 6”W x 50”L plates, cast with the rigging shown in Figure 5a. The predicted final pore volume percentages for the non-pressurized and pressurized riser cases are shown in Figure 5b. The scale for these results is given at the far right of Figure 5. As expected, pressurizing the riser significantly reduces the amount of porosity that forms in the castings. Figures 5c and 5d provide a comparison between the casting trial radiographs and the simulation results for the non-pressurized and pressurized cases, respectively. Good qualitative agreement is seen. In particular, the simulation nicely reproduces the narrow band of centerline porosity in the plate. However, the visible porosity on the non-pressurized casting radiograph in Figure 5c extends closer to the riser than in the simulation result, and the porosity region in the pressurized casting radiograph in Figure 5d is shorter than seen in the simulation result. The differences in the simulation results and the casting trials are likely due to several factors, including unknown gas levels in the casting trials, uncertainties in the permeability, and the fact that the simulations did not include filling. Still, the simulation results qualitatively capture the phenomena seen in the casting trials. Additional studies are currently underway to validate the porosity model. In addition, the model is being applied to predict microporosity formation in aluminum alloy castings.

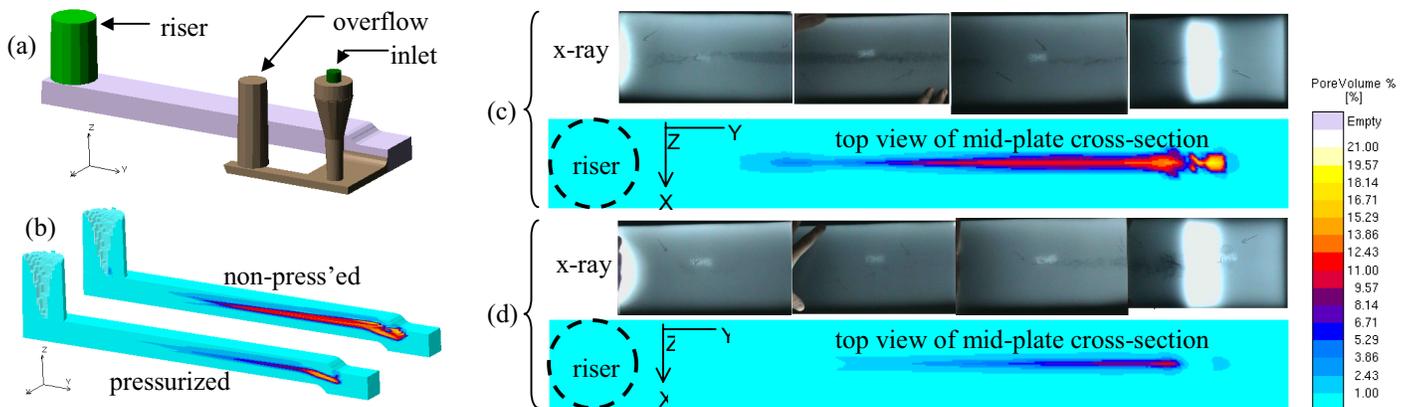


Figure 5: Simulation of porosity formation in a steel casting with and without a pressurized riser, and comparison with casting trials: (a) rigging for trial castings; (b) pore volume percentages with and without pressurization; and comparison between radiographs of castings and simulations for (c) a non-pressurized casting, and (d) a pressurized casting [15].

CONCLUSIONS

While much progress has been made in solidification modeling during the last two decades, there are several issues that require increased research attention. These include modeling of:

- solidification of multicomponent alloys, taking into account the formation of multiple phases
- grain structure transitions (e.g., columnar to equiaxed)
- deformation of the solid in the mush
- segregation in the presence of moving solid and undercooled liquid
- fragmentation of dendrites
- flow effects on the growth rates and structures of dendrites, eutectics, etc.

Future research on any of the above issues will increasingly rely on first principles, direct numerical simulation of solidification on a microscopic scale using, for example, the phase-field method. However, the use of direct numerical simulation for an entire casting will not be an option until at least the year 2050 [16].

ACKNOWLEDGMENTS

Writing of this article was made possible, in part, through funding of the author by NASA, NSF, DOE, and DOD. The help of the author's present and former graduate students, research engineers, and collaborators is gratefully acknowledged.

REFERENCES

1. Glicksman, M.E., Koss, M.B., and Winsa, E.A., Physical Review Letters, Vol. 73, p. 573, 1993.
2. Li, Q., and Beckermann, C., "Scaling Behavior of Three-Dimensional Dendrites," Physical Review E, Vol. 57, pp. 3176-3188, 1998.
3. Li, Q., and Beckermann, C., "Evolution of the Sidebranch Structure in Free Dendritic Growth," Acta Materialia, Vol. 47, pp. 2345-2356, 1999.
4. Boettinger, W.J., Warren, J.A., Beckermann, C., and Karma, A., "Phase-Field Simulation of Solidification," Annual Review of Materials Research, Vol. 32, pp. 163-194, 2002.
5. Lu, Y., Beckermann, C., and Karma, A., "Convection Effects in Three-Dimensional Dendritic Growth," in Proceedings of ASME IMECE2002, Paper No. IMECE2002-32838, Nov. 2002.
6. Beckermann, C., Diepers, H.J., Steinbach, I., Karma, A., and Tong, X., "Modeling Melt Convection in Phase-Field Simulations of Solidification," J. Computational Physics, Vol. 154, pp. 468-496, 1999.
7. Tong, X., Beckermann, C., and Karma, A., "Velocity and Shape Selection of Dendritic Crystals in a Forced Flow," Physical Review E, Vol. 61, pp. R49-R52, 2000.
8. Tong, X., Beckermann, C., Karma, A., and Li, Q., "Phase-Field Simulations of Dendritic Crystal Growth in a Forced Flow," Physical Review E, Vol. 63, 061601 (16 pages), 2001.
9. Diepers, H.J., Beckermann, C., and Steinbach, I., "Simulation of Convection and Ripening in a Binary Alloy Mush Using the Phase-Field Method," Acta Materialia, Vol. 47, pp. 3663-3678, 1999.
10. Beckermann, C., and Viskanta, R., "Double-Diffusive Convection during Dendritic Solidification of a Binary Mixture," PhysicoChemical Hydrodynamics, Vol.10, pp. 195-213, 1988.
11. Ni, J., and Beckermann, C., "A Volume-Averaged Two-Phase Model for Solidification Transport Phenomena," Metallurgical Transactions B, Vol. 22B, pp. 349-361, 1991.
12. Wang, C.Y., and Beckermann, C., "Equiaxed Dendritic Solidification with Convection: Part 1. Multi-Scale /-Phase Modeling," Metall. and Mater. Transactions A, Vol. 27A, pp. 2754-2764, 1996.
13. Beckermann, C., "Modelling of Macrosegregation: Applications and Future Needs," International Materials Reviews, Vol. 47, pp. 243-261, 2002.
14. Schneider, M.C., Beckermann, C., Lipinski, D.M., and Schaefer, W., "Macrosegregation Formation During Solidification of Complex Steel Castings: 3-D Numerical Simulation and Experimental Comparison," in Modeling of Casting, Welding and Advanced Solidification Processes VIII, eds. B.G. Thomas and C. Beckermann, TMS, Warrendale, PA, pp. 257-264, 1998.
15. Carlson, K.D., Lin, Z., Hardin, R.A., Beckermann, C., Mazurkevich, G., and Schneider, M.C., "Modeling of Porosity Formation and Feeding Flow in Steel Casting," in Modeling of Casting, Welding and Advanced Solidification Processes X, TMS, Warrendale, PA, 2003 (in press).
16. Voller, V.R., and Porte-Agel, F., "Moore's Law and Numerical Modeling," J. Computational Physics, Vol. 179, pp. 698-703, 2002.