Solidification and Shrinkage: Analytical and Numerical Model Development with Case Studies

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Concluding remarks and scope for future work

7.1 CONCLUSIONS

It is observed that the solidification process is associated with the different phenomenons that include the Marangoni effect, equiaxed/columnar grain growth, composition segregation, solidification shrinkage, free surface, etc., occurring at different length scales. The present study thoroughly discusses the effect of shrinkage during eutectic or alloy solidification at a macro-scale. The analytical and numerical models developed are scrutinized and validated either with the experiments performed or with the existing data in the literature. This indicates that the mathematical and numerical model proposed in the present study can precisely anticipate the solidification phenomena. The important conclusions from the above study are brief as follows:

7.1.1 One-dimensional diffusion based solidification model with volumetric expansion and shrinkage effect: semi-analytical approach

- A semi-analytical, 1-D transient heat diffusion model is developed to study the effect of shrinkage or volumetric expansion, eventuating as a result of density difference between solid and liquid phases during solidification of pure substance.

- The model is validated for the finite domain in the absence of volume expansion/shrinkage by comparing the results with those obtained from the existing enthalpy updating based numerical model. Results obtained are within the acceptable error limit

- Case studies are performed with thermo-physical properties of water and paraffin wax to analyse the case corresponding to volume expansion and shrinkage, respectively. The proposed model was applied to predict the temperature, position of the interface, and overall change in domain length during solidification.

- The time duration for complete solidification by proposed model considering volumetric expansion ($\rho_s<\rho_l$) is found out to be more than that without considering volumetric expansion ($\rho_s=\rho_l$), while reverse is found to be true for case study involving shrinkage ($\rho_s>\rho_l$). Both the case studies successfully captured physically consistent results.

7.1.2 Cooling curve prediction for controlled unidirectional solidification under influence of shrinkage: semi-analytical approach

- To predict the cooling curve for desired unidirectional crystal growth, a 1-D semi-analytical transient heat diffusion model is developed for pure/eutectic solidification. The model is validated and scrutinized by undergoing four different case studies.

- The first case study validates the proposed model with the existing enthalpy updating scheme based numerical model, while the second case study is validated by solving inverse and forward problems associated with the constant crystal growth rate.

- The third case study involves the prediction and validation of cooling curve for time-varying crystal growth rate.

- The final and the most crucial validation of the proposed model is presented by comparison between cooling curves obtained from the model prediction and experimentally measured data. Shrinkage during solidification is considered for all the validating case studies except the first one.

- The results obtain from all the case studies are within the permissible error limit of 1.5 % asserting the proposed model to be reliable and robust. The proposed model is beneficial to obtain prior knowledge of cooling curves for controlled crystal growth rate.

7.1.3 Shrinkage induced flow during directional solidification of pure substance in a bottom cooled cavity: A study on flow reversal phenomena

- A numerical model is proposed studying the effect of shrinkage convection over the interface growth during the directional solidification of pure and amorphous materials in a bottom cooled cavity.

- The governing equation were modified incorporating shrinkage effect using volume averaging method.

- A novel volume fraction updating method was implemented to track the interface during eutectic solidification.

- For the bottom cooled configuration, the buoyancy source term is found to play a significant role in defining the convection pattern. The shrinkage induced flow is opposed by the otherwise stably stratified density gradient, leading to a distinct flow reversal phenomenon during the directional solidification in the bottom cooled configuration.

- For low Prandtl number materials such as aluminum and copper, deformation of isotherms adjacent to the undulated solid–liquid interface causes the buoyancy force aided with shrinkage induced inertia to lift the fluid vertically upward along the symmetric center line of the cavity, leading to the sustenance of the flow reversal. Flow reversal does not occur until the central depression of the solid–liquid interface is evolved. On the other hand, for high Prandtl substances such as coconut oil, perturbation of the thermal field due to the shrinkage induced flow field is easily attained. As a result, an early onset of flow reversal can be observed, almost coinciding with the very inception of solid front growth.

- The major outcome of the proposed model in terms of flow reversal phenomena is experimentally validated, considering the directional solidification of coconut oil in a bottom cooled cavity. The experimentally measured flow field and liquid–mushy interface locations are compared with 3D numerical predictions in reasonable agreements.

- 2D numerical studies are performed for the directional solidification of two different pure metals, namely, Al and Cu. Both case studies revealed the onset and sustenance of flow reversal during the solidification process.

- The effect of varying cold boundary temperature, initial temperature of the melt, and cavity height on the onset of flow reversal is studied for bottom cooled directional solidification of pure Al. An increase in all these three parameters is found to promote an early flow reversal when time scale is normalized with respect to the total solidification time.

- The shrinkage induced flow field is found to cause deformation of the planar solid front in the form of a plunge pool. For the square riser, the shape of the plunge pool is found to have a distinct orientation along the length and width of the cavity.

7.1.4 Effect of shrinkage induced flow on solutal instability and macro-segregation during directional solidification of binary alloys

- Effect of grid resolution and time-step resolution on the simulation results are carried out for solidification process involving freckle formation in the presence of shrinkage induced flow. Al-30 wt.% Mg is considered to the model binary system. It is inferred that the phenomena is highly unstable, and achieving complete grid resolution and time-step independence is not possible.

- Model validation is performed with respect to a benchmark problem involving inverse segregation obtained for the bottom-up solidification of Al-4.1 wt.% Cu alloy in the presence of shrinkage induced flow and characterized by heavier solute rejection in the melt during liquid-solid phase transition. Simulation result from the proposed model is compared with existing numerical and experimental data reported in literature, furnishing reasonably good agreement.

- General attributes of shrinkage induced flow on freckle formation is studied for a very high value of cold boundary temperature ($T_c = 720K$) while keeping inlet opening size to be 40 *mm*. The results inferred that the convection field in the melt region at the initial stage of the solidification process is governed solely by the shrinkage induced flow, followed by the advent of the solutal instability adjacent to mushy liquid interface leading to complex flow interactions. One of the major influence of the shrinkage induced flow is manifested by the lateral bending of plumes away from the central plane of symmetry leading to the formation of oblique channels.

- Case study involving the effect of varying inlet opening size is analysed for $T_c = 700K$. It is inferred from the study that the opening size has a substantial impact on the severity of the solute lean region near the opening. The severity of negative segregation adjacent to the opening at the cavity top surface varies from severe to mild entrapment of solute lean composition for small to full opening.

- Next, the effect of cold temperature on the onset of instability and macro-segregation is investigated. A shift of cooling temperature at the bottom surface from high to moderately low range causes the onset of the solutal instability to occur at a comparatively greater height of the mushy-liquid interface. However, further reduction of bottom surface temperature intensifies the strength of shrinkage induced flow, allowing it to perturb the meta-stable solutal field adjacent to the mushy-liquid interface at an early stage of solidification, leading to an early onset of solutal instability. Low cooling temperature also negates the severity of the negative segregation. However, for the entire range of cooling, the thickness of the mushy layer is always found to be greater in the presence of shrinkage induced flow as compared to the predicted mushy layer thickness obtained under the no-shrinkage assumption. The thicker mushy region obtained under the influence of shrinkage induced flow is attributed to the entrainment of fresh melt with nominal composition into the upper bound of the mushy layer, leading to an overall elevation of local liquidus temperature in that region.

- In order to investigate the effect of cooling on the onset of solutal instability, a case study is carried out by varying the cold boundary temperature while considering the central opening sized at the upper surface of the cavity to be 40 *mm*. In terms of onset timing, the results involving shrinkage induced flow consistently predicted early onset of solutal instability as compared to those obtained with no shrinkage assumption. With low cooling temperatures, the onset time difference became substantially large between the studies associated with shrinkage and no-shrinkage assumptions. In terms of the height of the mushy-liquid interface, for high and moderate cold temperatures, solutal instability is found to be triggered at a lower position of this interface in the absence of shrinkage induced flow. However, the gap between the onset locations with and without shrinkage induced flow assumptions in terms of mushy-liquid interface heights diminishes as the cold boundary temperature is lowered, leading to a cross over point below a certain range of T_c. Further lowering of the cold boundary temperature consistently reduces the mushy-liquid interface height corresponding to the onset of solutal instability for shrinkage induced flow assumption, which is completely contrary to the ever-increasing behavior of the same under the no-shrinkage assumption.

- Effect of shrinkage induced flow on the onset of solutal instability being more prominent for large cooling, the influence of cavity inlet opening size is revisited considering T_c at 523 K while varying the opening size from 40-6 *mm*. Over the range of opening size 40-20 *mm*, both time interval and mushy-liquid interface height corresponding to the onset of solutal instability manifested a monotonically decreasing trend signifying the early onset of solutal instability. The early onset of plume formation for this range of inlet opening size (40-20 *mm*) is attributed to the perturbation of the meta-stable solutal buoyancy field by the shrinkage induced flow within the pure melt region only. However, lowering the opening size below 20 *mm* intensifies the shrinkage induced flow significantly and allows it to penetrate the mushy region itself, leading to the suppression and redistribution of naturally occurring solutal instability of the liquid phase within the mushy layer. The redistribution of the solute rich melt inside the mushy layer eventually leads to plume formation sites along the path of least resistance where primary circulations corresponding to shrinkage induced flow lifts off the fluid from the mushy-liquid interface to the pure melt domain. The entire process of suppression and redistribution of the solutal instability within the mushy region leads to an overall delay of the onset of plume formation, and this effect is evident only when the solidification process is simultaneously subjected to large cooling and small inlet opening size.

- A scaling analysis is attempted to have a criterion that assesses the relative magnitude of shrinkage convection and solutal buoyancy-driven natural convection. A non-dimensional group in the form $Re_{SIF}/(Gr_C.AR)$ is proposed. It was inferred that $Re_{SIF}/(Gr_C.AR) \leq 0.9$ corresponds to no effect of shrinkage induce flow on the onset of solutal instability. Condition $Re_{SIF}/(Gr_C.AR) \geq 0.9$ always corresponds to the early onset of solutal instability with respect to the baseline case involving freckle formation in the absence of shrinkage. For the range $0.9 \leq Re_{SIF}/(Gr_C.AR) \leq 2.0$, larger the value of $Re_{SIF}/(Gr_C.AR)$ earlier the onset of solutal instability. However, for $Re_{SIF}/(Gr_C.AR) > 2.0$ this trend is reversed, *i.e.* larger the value of $Re_{SIF}/(Gr_C.AR)$ later the onset of solutal instability.

7.1.5 Shrinkage defects: Free surface deformation during solidification of Metal Alloys

- A numerical model is developed and proposed to capture the free surface deformation due to shrinkage during the solidification of pure substances and binary alloys. The basic framework of the enthalpy-porosity scheme is modified and coupled with the VOF (volume of fluid) scheme to estimate the void fraction.

- The interface reconstruction is approximated using the donor-acceptor scheme to estimate the flux of volume across the faces. The proposed model is validated by comparing the results obtained from the proposed model with reported observations concerning free surface deformation during the solidification of TNT. Reasonably good agreement between the results obtained from the proposed model and reported data is obtained.

- After validation, three different case studies are performed using the proposed model: (i) solidification of pure aluminium in a bottom cooled mold cavity with a riser at the center, (ii) Solidification of pure aluminium in a top open mold cavity with all cavity surfaces being subjected to Dirichlet or Neumann boundary conditions respectively, and (iii) Solidification of pure Al-4.1 wt.% Cu alloy in a top open mold cavity with side and bottom walls being subjected to Dirichlet and mixed boundary conditions, respectively.

- The analysis involving the first case study successfully captured the shrinkage induced flow field and the gradual lowering of the planner free surface inside the riser. The analysis involving the second case study successfully captured the free surface deformation resembling a funnel shape with an elongated fissure end at the bottom. The analysis pertaining to the second case study also indicated the dependence of free surface deformation depth on the aspect ratio of the mold cavity and heat removal rate. The analysis involving the third case study once more demonstrated the robustness of the proposed model by successfully capturing physically consistent free surface deformation and macro-segregation pattern.

7.2 FUTURE SCOPE

The study investigated in the thesis can be continued in following manner.

- Extension of numerical model for ternary and higher order alloy system.
- Incorporation of void-nucleation schemes to capture internal shrinkage cavities.
- Incorporation of young model in free surface reconstruction algorithm for better representation of free surface.
- Incorporation of surface tension effect for analysing macro-scale surface defect encountered during welding process.

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