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Uncertainty Quantification of Modelling of Equiaxed Solidification

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Abstract. Numerical simulations of metal alloy solidification are used to gain insight into physical phenomena that cannot be observed experimentally. Often validation of such models has been done through comparison to sparse experimental data, to which agreement can be misinterpreted due to both model and experimental uncertainty. Uncertainty quantification (UQ) and sensitivity analysis are performed on a transient model of solidification of Al-4.5 wt.% Cu in a rectangular cavity, with equiaxed (grain refined) solidification morphology. This model solves equations for momentum, temperature, and species conservation; UQ and sensitivity analysis are performed for the degree of macrosegregation. A Smolyak sparse grid algorithm is used to select input values to construct a response surface fit to model outputs. The response surface is then used as a surrogate for the solidification model to determine the sensitivities and probability density functions of the model outputs. Uncertain model inputs of interest include the secondary dendrite arm spacing, equiaxed particle size, and fraction solid at which the rigid mushy zone forms. Similar analysis was also performed on a transient model of direct chill casting of the same alloy.

1. Introduction

Sophisticated numerical models of solidification processes have been developed in which confidence in the results is dependent on how well the input parameters are known and comparison with limited experimental data. Some of the well-established physics in these models include diffusive and convective transport of heat, mass, and momentum, electromagnetics, and solidification thermodynamics. When validating a model with experimental data, the level of agreement is typically discussed qualitatively and frequently the assumption is made that more sophisticated physics would improve agreement. Quantification of model uncertainty will help quantify comparison to experiments and to identify which inputs it would be most profitable to improve.

Monte Carlo uncertainty quantification (UQ) methods consist of repetitive sampling random values of the model inputs or system parameters and evaluating the solution [1]. This process generates probability distribution functions (PDF) for output quantities of interest as a function of input uncertainties. Although Monte Carlo sampling methods are very effective, they quickly become very computationally expensive for complex numerical models. Use of polynomial chaos expansion (PCE) or global polynomial chaos (gPC), which create surrogate models, has significantly reduced computational expense without sacrificing accuracy [2]. The present study aims to quantify the sensitivities and uncertainties in predicting macrosegregation in grain refined, equiaxed solidification...
in a rectangular domain. Insight into uncertainty propagation in that system can be applied to models of more sophisticated processes models, like direct chill casting.

2. Model Description

2.1 Description of Deterministic 2D Solidification Model

Static casting of a simple binary eutectic alloy (Al-4.5wt%Cu) is modeled. The rectangular cavity (Fig. 1) is cooled from the left and an inlet on top allows for feeding due to solidification shrinkage. The momentum equations are from Vreeman et al. [3], who included the effect of free-floating solid grains. This solid forms on grain refiners initially and has increasing interactions among themselves as they solidify. Once a critical volume fraction solid is reached, \(g_{s,\text{pack}}\), the free-floating particles coalesce to form a rigid, stationary (\(u_i = v_i = 0\)), permeable solid structure. This packing fraction is generally treated (as it is here) as a constant and uniform quantity, although it is recognized to be related to the size and morphology of the equiaxed dendrites and the direction and magnitude of the liquid and solid motion relative to the rigid solid [4]. The value of \(g_{s,\text{pack}}\) is taken here to be in the range up to 0.3 [3, 5]. The solid and liquid velocities are found from Stokes law,

\[
\vec{V}_s - \vec{V}_l = \frac{(1 - g_s)}{18 \mu_m} (\rho_s - \rho_l) d^2 \vec{g},
\]

in which \(d\) is the average particle diameter, \(\mu_m\) is the mixture viscosity, and \(g_s\) is the volume fraction solid. This equation treats the equiaxed dendrites as spheres of a uniform, specified diameter. While the unattached solid does not impede the fluid motion, the packed, rigid array of solid dendrites slows the flow in the mushy zone. The mushy zone permeability model used is the Blake-Kozeny formulation:

\[
K = \chi^2 g_s^2 / \rho_l g_s^2.\]

The species and energy conservation equations are shown in equations (2) and (3) in which \(f_s\) is the mass fraction solid. The conservation equations are discretized using the finite volume method and the flow field is solved with the SIMPLER algorithm.

\[
\frac{\partial}{\partial t} (\rho C_i) + \nabla \cdot (\rho f_i \vec{V} C_i) = \nabla \cdot \left( \rho f_i \nabla (C_i) \right) + \nabla \cdot \left( \rho D \nabla (C_i - C) \right) - \nabla \cdot \left( \rho f_i \vec{V} (C_i - C) \right)
\]

\[
\frac{\partial}{\partial t} (\rho C_T) + \nabla \cdot (\rho f_i \vec{V} C_T) = \nabla \cdot \left( \kappa \nabla T \right) - \frac{\partial}{\partial t} (\rho f_i L_f)
\]

\[
- \nabla \cdot \left( \rho f_i L_f \vec{V} \right) - \nabla \cdot \left( \rho f_i \left( c_p_l - c_p_s \right) L_f + L_f \right) \left[ \vec{V} - \vec{V}_s \right]
\]

The simulations begin with quiescent liquid with a superheat of 21.8K (940K). The inlet to the domain feeds the solidification shrinkage with liquid at the nominal composition and superheated temperature. Alloy properties are in (Table 1) and further details of the model are in [3].
Table 1. Thermophysical properties of Al-4.5 wt.% Cu.

| Property                        | Value          |
|---------------------------------|----------------|
| Liquid Density [kg/m³]          | 2460           |
| Solid Density [kg/m³]           | 2750           |
| Specific Heat [J/kg K]          | 1006           |
| Latent Heat [J/kg]              | 3.9x10⁵        |
| Thermal Conductivity [W/m K]    | 137.5          |
| Liquid Viscosity [kg/m s]       | 0.0023         |
| Eutectic Temperature [K]        | 821            |
| Solid Thermal Expansion [1/K]   | 2.25x10⁻⁵      |
| Liquid Solutal Expansion [1/K]  | -0.73          |
| Solid Solutal Expansion [1/K]   | -0.87          |
| Partition Coefficient           | 0.17           |

2.2 Description of Uncertainty Quantification Model

This work uses existing UQ techniques, so only a brief description of the methodology will be given here. The UQ model calculates a PDF for each of the output quantities of interest given the known uncertainty of select inputs. Here, the outputs of interest are measures of the levels of macrosegregation, the first of which is the macrosegregation number, \( M = \sqrt{\frac{1}{V} \iiint (C/C_o - 1)^2 \, dV} \), which is a normalized standard deviation and has been used to quantify the overall level of segregation for castings starting with Prescott [6] and Schneider and Beckermann [7]. Another metric, similar to one recently developed by Voller and Vušanović for quantifying positive segregation [8], is the standard deviation of the Weibull distribution, \( W \). The last macrosegregation metric is the volume fraction of ingot outside the compositional specification, \( V_{spec} \).

For this study, the Cu compositional specification of Al alloy 2014 (ASTM B209) is used, which has a range of 3.9 – 5.0 wt.% Cu. These three measures of macrosegregation can be seen in Figure 2, in which the shaded region is the specification range. Uncertainty is assigned to input parameters in the form of normal or uniform distributions. Outputs are then sampled from the full numerical model to generate a response surface, which then acts as a surrogate to running the full solidification model. In this work, the computationally efficient Smolyak sparse grid algorithm [2,9–11] is used to sample the numerical model. Different polynomial functions can be fitted to model outputs of interest to form response surfaces based on the level of the Smolyak algorithm. The fit of the response surface to the sampled points is quantified by using the root mean square error (RMSE). Each input parameter is randomly sampled 10,000 times and the response surface is used to calculate the output PDFs, which are characterized by their normal standard deviation and their actual shapes are shown below. The resulting output PDFs can aid in evaluating the validity of numerical models by comparing the uncertainty of the experimental measurement to that of the numerical model.

The relative sensitivities of the outputs to changes in the input parameters are calculated using the sampled points from the model and the Elementary Effects Method (EEM) [12,13]. The EEM calculates two sensitivity measures to determine whether the inputs have negligible, linear, or nonlinear effects on the outputs. A distribution of elementary effects is calculated for each input parameter by varying them independently with a constant step change across all levels of the other parameters, and calculating the result with the response surface for the array of inputs. The mean sensitivity, \( \mu^* \), is the estimate of the mean of the distribution of the absolute value of the elementary effects. Unlike the analytical sensitivity, \( \mu^* \) is always positive. For \( \mu^* \) values near zero, the input has a small or negligible effect on the output, values much greater indicate the input plays a significant role in determining the output. The second parameter, \( \sigma^* \), is a measure of the standard deviation of the output sensitivity distribution. A high value of \( \sigma^* \) (a wide distribution), indicates the effects are strongly influenced by other inputs. A low value of \( \sigma^* \) indicates a linear dependence on the input. The algorithms and methods described in this section have been compiled into a single publically available framework along with a graphical user interface, the PRISM Uncertainty Quantification (PUQ) tool [14,15]. This tool assumes the chosen numerical model incorporates the basic physics to adequately predict the output of interest.

3. Results and Discussion

Macrosegregation begins with solute partitioning during solidification and is affected by subsequent liquid motion relative to the solid. In grain refined alloys, there are two different
mechanisms by which this occurs, settling of free-floating solid grains and flow in the rigid mushy zone. For Al-4.5 wt.% Cu the flow in the rigid mushy zone is driven primarily by shrinkage induced flow. The settling of particles is dependent on their size, the flow in the mushy zone is dependent on the dendrite arm spacing, and both phenomena depend on the formation of the rigid mushy zone and relative size of the slurry.

Figure 2. Composition distribution of a grain refined Al-4.5 wt% Cu alloy showing the ingot volume fraction occupied at each composition, normal distribution of the data, and the Weibull distribution of the data. The shaded area is the specified range of alloy 2014.

3.1 2D Model of Solidification in a Rectangular Domain
The uncertain model parameters used for this study that influence macrosegregation are shown in Table 2. The inputs are given either as a normal distribution with a mean, $\mu$, and deviation, $\sigma$, or a uniform distribution with a minimum and maximum. The packing fraction, $g_{\text{pack}}$, uncertainty distribution is treated as uniform because no one value in the range is more probable than the rest.

| Input Parameter       | Case A              | Case B              | Case C              |
|-----------------------|---------------------|---------------------|---------------------|
| Particle size ($d$) [m] | $\mu = 30 \times 10^{-6}$  
$\sigma = 7.5 \times 10^{-6}$ | $\mu = 3 \times 10^{-5}$  
$\sigma = 7.5 \times 10^{-6}$ | $\mu = 30 \times 10^{-6}$  
$\sigma = 7.5 \times 10^{-6}$ |
| Dendrite arm spacing ($\lambda$) [m] | $91 \times 10^{-6}$  
$\mu = 91 \times 10^{-6}$  
$\sigma = 9.5 \times 10^{-6}$ | $91 \times 10^{-6}$  
$\mu = 91 \times 10^{-6}$  
$\sigma = 9.5 \times 10^{-6}$ |
| $g_{\text{pack}}$ [-] | 0.15                | 0.15                | Min = 0.0          
Max = 0.3                   |

Figure 3. Output PDFs for Case A, where $d$ has a standard deviation of 25%.

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The output PDFs from Case A are shown in Figure 3, which were produced with a level 3 Smolyak run resulting in a cubic polynomial response surface. The response surface for $W$ and $V_{\text{spec}}$ are shown in Figure 4 along with the model outputs, in which $W$ and $M$ have similar response surfaces. The settling velocity increases with $d$, causing the free-floating solid to form a rigid mushy more easily and changing the shape of the rigid mushy zone as more particles settle along the bottom of the cavity. This increased settling rate leads to less segregation because the rigid zone grows more rapidly from the bottom of the domain. There is also less horizontal shrinkage flow leading to segregation and more vertical shrinkage flow. The macrosegregation metrics all decrease with increasing $d$, but the function for $V_{\text{spec}}$ behaves differently at extreme values of $d$ leading to a different PDF. The resulting PDFs for $W$, $M$, and $V_{\text{spec}}$ are not very sensitive to $d$, as their PDFs vary over small ranges.

The dendrite arm spacing, $\lambda$, affects the permeability of the rigid mushy zone as dictated by the Blake-Kozeny model and is assigned a standard deviation of 10% for its uncertainty distribution. The output PDFs from Case B are shown in Figure 5, where the response surfaces were produced with a level 3 Smolyak. The response surfaces for $W$, $M$, and $V_{\text{spec}}$ are in Figure 6. The relationship between $\lambda$ and $W$ and $M$ is almost linear, so the resulting PDFs are normal distributions. However, the relationship between $\lambda$ and $V_{\text{spec}}$ is highly nonlinear and, for small $\lambda$, the casting is entirely within the specification limits. These different $\lambda$ relationships demonstrate differences between the macrosegregation metrics. $W$ and $M$ show a more or less normal distribution, while the $V_{\text{spec}}$ metric shows a high probability (in this range of $\lambda$) that the input will be in spec and a very low probability that any more than 3% of the ingot volume will be out of the composition range.

The critical packing fraction, $g_{s,\text{pack}}$, controls the location of the rigid mushy zone formation and indirectly controls the pattern of particle settling. Because $g_{s,\text{pack}}$ is the lowest $g_s$ value in the rigid mushy zone, it also determines the highest permeability and so the strongest flow in that region. Figure 7 shows the PDFs for the Case C macrosegregation, based on the same uncertainties in $d$ and $\lambda$ as in Cases A and B and a uniform input PDF for $g_{s,\text{pack}}$. The output sensitivities produced with a level 1 Smolyak are shown in Table 3. The distributions of each metric are dominated by the uniform

**Figure 4.** Response surfaces of $W$, $M$, and $V_{\text{spec}}$ for Case A.

**Figure 5.** Output PDFs for Case B, where $\lambda$ has a 10% standard deviation.
uncertainty of $g_{s,pack}$, and each metric is also most sensitive to this parameter (followed closely by $\lambda$). Small $g_{s,pack}$ values form the rigid mushy zone with still enough permeability to allow significant macrosegregation-causing buoyancy induced flow, while larger values of $g_{s,pack}$ form the rigid solid with much less permeability. Also, the settling velocity of the free-floating solid is a function of the slurry fraction solid, therefore the larger $g_{s,pack}$ the stronger the settling velocity. The uncertainty of $g_{s,pack}$ is large and overwhelms the uncertainty of the other two parameters, so more information is needed about particle packing to get more certain macrosegregation predictions, also the value selected for $\lambda$ should be chosen carefully.

3.2 Direct Chill Casting Model

The UQ approach shown here for static casting is also applied to a transient model of direct chill casting of Al-4.5 wt. % Cu with a 50 cm diameter [16]; Figure 8 is a schematic of that process. The uncertain input parameters are the particle size and heat transfer boundary conditions. The value of the boundary heat transfer coefficients from [17] are complex and are multiplied by an uncertainty factor with a mean value of 1 and a standard deviation of 0.15. The particle size has the same uncertainty as in the previous study. The simulations were run until the solid metal height was 1.5 m and then the macrosegregation level was measured in the steady state region using the metrics described previously. Along with the macrosegregation metrics, the steady state sump depth and height above the bottom block at which the composition reaches steady state are also outputs of interest.
The resulting PDFs from the DC casting simulations are shown in Figure 9, which were produced with a level 1 Smolyak, and the sensitivities are shown in Table 4. The macrosegregation metrics are more sensitive to the thermal boundary conditions than the free-floating particle size, while the sump depth and height to steady state is equally sensitive to both uncertain inputs. A large portion of the macrosegregation in DC casting is due to negative centreline segregation caused by shrinkage driven flow. The depth of the sump does not change much even for large variations in the heat transfer, indicating that the formation of the rigid mushy zone is independent of the thermal characteristics in the range considered. The deviations of the output PDFs are relatively small; therefore the particle size and heat transfer coefficient measurements can be known within 20 and 30% respectively and still have a small influence on the results. Based on the static casting results, the critical packing fraction will likely have more of an effect on the segregation levels than the other parameters.

Table 4. Output sensitivities for the DC casting model.

| Inputs   | $W$       | $M$        | $V_{\text{spec}}$ | S.S. Height (m) | Sump Depth (m) |
|----------|-----------|------------|-------------------|-----------------|----------------|
| H.T.C. (W/mK) | $\mu = 1.42 \times 10^{-3}$ | $\mu = 4.91 \times 10^{-3}$ | $\mu = 9.43 \times 10^{-4}$ | $\mu = 9.00 \times 10^{-2}$ | $\mu = 3.16 \times 10^{-2}$ |
| $\sigma$    | $1.42 \times 10^{-3}$  | $4.91 \times 10^{-3}$  | $9.43 \times 10^{-4}$  | $9.00 \times 10^{-2}$  | $3.16 \times 10^{-2}$  |
| $d$ (m)     | $\mu = 8.74 \times 10^{-5}$ | $\mu = 1.71 \times 10^{-3}$ | $\mu = 0.00$ | $\mu = 8.00 \times 10^{-2}$ | $\mu = 2.03 \times 10^{-2}$ |
| $\sigma$    | $3.05 \times 10^{-5}$  | $1.20 \times 10^{-3}$  | $0.00$  | $8.00 \times 10^{-2}$  | $2.03 \times 10^{-2}$  |

Figure 8. Schematic of DC casting process.

Figure 9. Probability distribution functions of the model outputs for DC casting.
4. Conclusions
Uncertain model input parameters that govern transport phenomena in grain refined alloy solidification were examined for their effect on macrosegregation using the publically available PUQ framework. Using a model of solidification in a rectangular domain, the critical packing fraction and dendrite arm spacing had more of an effect on the segregation than the free-floating particle size. More information is needed on the mechanisms of particle attachment and formation of the rigid mushy zone to lower the effects of $g_{s,\text{pack}}$ on the uncertainty of the macrosegregation model predictions. In modelling of grain refined alloys using DC casting, the thermal boundary conditions of the process and free-floating particle size do not significantly impact the depth of the sump. Also, the uncertainty of the predicted macrosegregation level was small using input parameters with 20-30% uncertainty. It is expected, as in static casting of grain refined alloys, that $g_{s,\text{pack}}$ will have the largest effect on the uncertainty of the macrosegregation predictions in DC casting.

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