Uncertainty Quantification in Solidification Modelling

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Abstract. Numerical models have been used to simulate solidification processes, to gain insight into physical phenomena that cannot be observed experimentally. Often validation of such models has been done through comparison to a few or single experiments, in which agreement is dependent on both model and experimental uncertainty. As a first step to quantifying the uncertainty in the models, sensitivity and uncertainty analysis were performed on a simple steady state 1D solidification model of continuous casting of weld filler rod. This model includes conduction, advection, and release of latent heat was developed for use in uncertainty quantification in the calculation of the position of the liquidus and solidus and the solidification time. Using this model, a Smolyak sparse grid algorithm constructed a response surface that fit model outputs based on the range of uncertainty in the inputs to the model. The response surface was then used to determine the probability density functions (PDF’s) of the model outputs and sensitivities of the inputs. This process was done for a linear fraction solid and temperature relationship, for which there is an analytical solution, and a Scheil relationship. Similar analysis was also performed on a transient 2D model of solidification in a rectangular domain.

1. Introduction
Sophisticated numerical models have been developed to simulate solidification processes and confidence in the results is dependent on how well the input parameters are known and the practicality of comparison with limited experimental data. Some of the well-established physics incorporated into sophisticated solidification models of industrial processes include diffusion and convective transport of heat, mass, and momentum, electromagnetics, and solidification thermodynamics. When validating a model with experimental data, the discussed level of agreement is typically qualitative and frequently the assumption is made that more sophisticated physics would improve numerical results. Sensitivity analysis would be able to evaluate this question and determine which areas need more development.

Monte Carlo uncertainty quantification methods consist of sampling random values of the model inputs or system parameters that govern the model and evaluating the solution [1]. This process generates a probability distribution function (PDF) for output quantities that are of interest as a function of input uncertainties. Although Monte Carlo sampling methods are very effective, they quickly become computationally very expensive for complex numerical models. Use of polynomial chaos expansion (PCE) or global polynomial chaos (gPC), which create surrogate models, have been shown as a vast improvement in terms of computational expense without sacrificing accuracy [2]. The present study aims to quantify the sensitivities and uncertainties in a single, 1D, steady state solidification model as a template to demonstrate a method that can be used in more complex models.
2. Model Description

2.1. Description of 1D Deterministic Model

The solidification process being modeled is for continuous casting of weld filler rod consisting of primary cooling by a copper mold and secondary cooling either by water spray or natural convection. Figure 1 depicts the geometry and boundary conditions for the process.

This model is applied here to the prediction of weld filler rod with a radius of 1 mm. The Biot number (Bi= hR/2k) is assumed to be less than unity, so any radial temperature gradients are assumed to be very small and a one dimensional treatment of the steady state governing equation is valid:

\[
\frac{k}{A_c} \frac{\partial^2 T}{\partial x^2} - \rho c A_c V_{cast} \frac{\partial T}{\partial x} + \rho L_f A_c V_{cast} \frac{\partial f_s}{\partial x} - UP(T - T_m) = 0
\]

where \(A_c\) is the cross-sectional area, \(L_f\) is the latent heat, \(U\) is the heat transfer coefficient, \(c\) is the specific heat, \(k\) is the thermal conductivity, \(f_s\) is the fraction solid and \(P\) is the perimeter. The latent heat advection term requires a relationship between the temperature and the solid fraction. This model will use either a linear dependence for fraction solid or the Scheil model shown in equation 2, where \(T_m\) is the melting temperature of the pure material and \(k_p\) is the partition coefficient. Equation 1 was discretized using the finite volume method and upwind difference advection scheme over a uniform grid. The alloy system used in this study was Ni alloy 625 comprised of 21.5 wt. % Cr, 9.0 wt. % Mo and 3.65 wt. % Nb. The properties of alloy 625 are summarized in Table 1. The model outputs of interest are the liquidus position \((X_L)\), solidus position \((X_S)\), and solidification time \((t_s=|X_S-X_L|/V_{cast})\).

\[
\text{Linear: } f_s = \frac{T_{liq} - T}{T_{liq} - T_{sol}} \quad \text{or Scheil: } f_s = 1 - \left( \frac{T - T_m}{T_{liq} - T_m} \right)^{k_p} \quad (2)
\]

Table 1. Thermophysical properties of alloy 625.

| Property                          | Value   |
|----------------------------------|---------|
| Thermal Conductivity [W/mK]      | 25.2    |
| Density [kg/m³]                  | 8440    |
| Specific Heat [J/kgK]            | 670     |
| Latent Heat [J/kg]               | 290,000 |
| Liquidus Temperature [K]         | 1636    |
| Solidus Temperature [K]          | 1430    |
| Pure Ni Melting Temperature [K]   | 1728    |
| Partition Coefficient            | 0.83    |
equation 1 (which can be shown to be valid with a simple scaling analysis for the cases in this study) equation 1 can be solved exactly for the temperature profile in the all-liquid and mushy zones.

\[
\text{Liquid zone: } \frac{T - T_\infty}{T_0 - T_\infty} = \exp\left[-\frac{2U}{\rho CV T_0 R}\right] \tag{3a}
\]

\[
\text{Mushy zone: } \frac{T - T_\infty}{T_{\text{liq}} - T_\infty} = \exp\left[-\frac{St}{St + 1}\left(\frac{2U}{\rho CV T_0 R}\right)(x - X_L)\right] \tag{3b}
\]

2.2. Uncertainty Quantification Model Description

This paper does not introduce new methods of uncertainty quantification, but uses existing methods on computational models, therefore only a brief description of the methodology will be discussed here. The uncertainty quantification model calculates a PDF for each output quantity of interest given the known uncertainty of select inputs (\(\rho, C, L_f, k, \text{ and } U_m\)). This is done by assigning uncertainty to input parameters in the form of a normal distribution and then sampling outputs from the previously described 1-D model to generate a response surface, which then acts as a surrogate to running the full 1-D model. There are various sampling methods including Monte Carlo sampling (MC), Latin Hypercube sampling (LHS), etc. [4], with MC being ideal, but not all models are simplistic enough such that MC is computationally inexpensive. In this work, the Smolyak sparse grid algorithm uses the input PDFs to define the simulation conditions used to construct response surfaces of the model outputs. This algorithm requires far fewer sampling points than either MC or LHS [2,5–7]. Using the response surfaces, the uncertainty of the outputs can be gathered from the deviation of the PDFs and the relative sensitivity of the input parameters is calculated based on the Elementary Effects Method (EEM) [8,9].

The EEM calculates two sensitivity measures to determine the effect on the inputs. The mean sensitivity, \(\mu^*\), assesses the main effects on the output plus all the interaction effects of an input factor. Unlike the analytical sensitivity, which is the derivative of the output function with respect to an input factor, \(\mu^*\) does not carry any sign effects and is always positive. The other parameter is the standard deviation, \(\sigma\), which examines higher order effects. A high value of \(\sigma\) indicates the effects of one input are strongly influenced by other input factors. A low value of \(\sigma\) indicates a linear dependence on the input factor. This model of continuous casting of weld filler rod has been made available to the public through nanohub.org, in which users can perform uncertainty analysis for themselves [10].

3. Results and Discussion

3.1. 1D Model of Continuous Casting of Filler Rod

The numerical casting model was compared to the analytical solution with a linear \(f_c\cdot T\) relationship, only one heat transfer coefficient, and with conduction (Case A). The model was also run with the Scheil solidification model and two heat transfer coefficients; for these conditions there is no analytical solution (Case B). All of the calculations used a rod radius of 0.001 m, a casting speed of 0.2 m/s, a superheat of 20 K, and an ambient temperature of 300 K. Table 2 lists the input uncertainty used in both cases in the form of normal distributions, with a mean, \(\mu\), and standard deviation, \(\sigma\). A level 1 Smolyak run was used to calculate each response surface in Case A for comparison to the analytical solution. Figure 2 shows the PDF of each output from the model for Case A. The uncertainty of the analytical solution (equations 4 and 5) was calculated with equation 6, where \(y\) is an output quantity of interest, \(x\) is an uncertain input, and \(m\) is the number of uncertain inputs. The comparison between the analytical and numerical uncertainties is shown in Table 3, where the analytical mean was calculated using the mean values in Table 2. The analytical and numerical solutions agree very well with each other with the most certain result being \(X_L\) followed by \(X_S\) and the most uncertain calculation being \(t_S\).
\[ X_L = \left( \frac{\rho CRV_{\text{cast}}}{2U} \right) \ln \left( \frac{T_{\text{liq}} - T_w}{T_0 - T_w} \right) \]  \hfill (4) 

\[ X_S = X_L - \frac{St + 1}{St} \frac{\rho CRV_{\text{cast}}}{2U} \ln \left( \frac{T_{\text{sol}} - T_w}{T_{\text{liq}} - T_w} \right) \]  \hfill (5) 

\[ \sigma_y = \sqrt{\sum_{i=1}^{q} \left( \frac{\partial y}{\partial x_i} \right)^2} \]  \hfill (6)

**Table 2.** Uncertainty of input parameters in the form of a normal distribution.

| Input Parameter                      | Case A          | Case B          |
|--------------------------------------|-----------------|-----------------|
| Thermal Conductivity [W/mK]          | - \( \mu: 25 \) \( \sigma: 0.63 \) |                 |
| Density [kg/m³]                      | \( \mu: 8440 \) \( \sigma: 42.2 \) | \( \mu: 8440 \) \( \sigma: 211 \) |
| Specific Heat [J/kgK]                | \( \mu: 670 \) \( \sigma: 3.35 \) | \( \mu: 670 \) \( \sigma: 16.5 \) |
| Latent Heat [J/kg]                   | \( \mu: 290,000 \) \( \sigma: 1450 \) | \( \mu: 290,000 \) \( \sigma: 7250 \) |
| Primary Heat Transfer Coefficient [W/m²K] | \( \mu: 5,000 \) \( \sigma: 25 \) | \( \mu: 5,000 \) \( \sigma: 750 \) |
| Secondary Heat Transfer Coefficient [W/m²K] | - \( \mu: 10,000 \) \( \sigma: 1,500 \) |                 |
| Partition Coefficient                | - \( \mu: 0.83 \) \( \sigma: 0.02075 \) |                 |

**Figure 2.** Probability density functions of the model outputs for Case A.

**Table 3.** Comparison between the analytical and model uncertainties for Case A.

| Output | Analytical Solution | Case A          |
|--------|---------------------|-----------------|
| \( X_L \) (m) | \( \mu: 0.00168 \) \( \sigma: 1.48\times10^{-5} \) | \( \mu: 0.00169 \) \( \sigma: 1.40\times10^{-5} \) |
| \( X_S \) (m) | \( \mu: 0.0431 \) \( \sigma: 3.59\times10^{-4} \) | \( \mu: 0.0431 \) \( \sigma: 3.58\times10^{-4} \) |
| \( t_S \) (s)  | \( \mu: 0.207 \) \( \sigma: 1.74\times10^{-3} \) | \( \mu: 0.207 \) \( \sigma: 1.74\times10^{-3} \) |
A more complicated case (Case B) was run for which there is no analytical solution and which uses a Scheil model and has two different heat transfer coefficients. The alloy was simplified to a Ni-9 wt. % Mo binary in which the partition coefficient was assumed to be constant. A level 3 Smolyak sparse grid algorithm was used because of the better fit over levels 1 and 2 according to the root mean square error (RMSE). The output uncertainties are given in Table 4 and the sensitivities are given in Table 5. The most uncertain output is the solidification time and the most certain is the location of the liquidus temperature. All outputs are most sensitive to the mold heat transfer coefficient, followed by material properties such as $\rho$, $c$, or $L_f$. To produce physically accurate results the uncertainty of the measured mold heat transfer coefficient needs to be much less than the 30% assumed here. Even though the partition coefficient determines the freezing range of the alloy, other material properties have a larger influence on the outputs.

### Table 4. Output uncertainties for Case B.

| Parameter       | Mean $\mu$ | Standard Deviation $\sigma$ |
|-----------------|------------|-----------------------------|
| $X_L$ (m)       | 0.00184    | 2.94 x 10^{-4}              |
| $X_S$ (m)       | 0.054      | 4.31 x 10^{-3}              |
| $t_S$ (s)       | 0.261      | 1.93 x 10^{-2}              |

### Table 5. Sensitivity of the uncertain inputs on the outputs for Case B.

| Sensitivity Parameter | Sensitivity Parameter | $X_L$ (m) | $X_S$ (m) | $t_S$ (s) |
|-----------------------|-----------------------|-----------|-----------|-----------|
| Density (kg/m$^3$)    |                       | $\mu$: 2.66 x 10^{-4} | $\mu$: 4.94 x 10^{-3} | $\mu$: 2.33 x 10^{-1} |
|                       |                       | $\sigma$: 9.38 x 10^{-5} | $\sigma$: 1.42 x 10^{-3} | $\sigma$: 7.17 x 10^{-3} |
| Specific Heat (J/kgK) |                       | $\mu$: 2.66 x 10^{-4} | $\mu$: 1.78 x 10^{-3} | $\mu$: 7.57 x 10^{-3} |
|                       |                       | $\sigma$: 9.39 x 10^{-5} | $\sigma$: 5.11 x 10^{-4} | $\sigma$: 2.66 x 10^{-3} |
| Latent Heat (J/kg)    |                       | $\mu$: 5 x 10^{-7} | $\mu$: 3.16 x 10^{-3} | $\mu$: 1.58 x 10^{-2} |
|                       |                       | $\sigma$: 4.97 x 10^{-6} | $\sigma$: 9.09 x 10^{-4} | $\sigma$: 4.55 x 10^{-3} |
| Thermal Conductivity (W/mK) |   | $\mu$: 3.85 x 10^{-6} | $\mu$: 5 x 10^{-7} | $\mu$: 2.18 x 10^{-5} |
|                       |                       | $\sigma$: 1.68 x 10^{-5} | $\sigma$: 4.97 x 10^{-6} | $\sigma$: 9.04 x 10^{-5} |
| Partition Coefficient |                       | $\mu$: 1.25 x 10^{-6} | $\mu$: 1.35 x 10^{-4} | $\mu$: 6.81 x 10^{-4} |
|                       |                       | $\sigma$: 7.81 x 10^{-6} | $\sigma$: 4.77 x 10^{-5} | $\sigma$: 2.41 x 10^{-4} |
| Mold Heat Transfer Coefficient (W/m$^2$K) | | $\mu$: 2.02 x 10^{-3} | $\mu$: 2.69 x 10^{-2} | $\mu$: 1.24 x 10^{-1} |
|                       |                       | $\sigma$: 1.09 x 10^{-3} | $\sigma$: 5.96 x 10^{-3} | $\sigma$: 3.21 x 10^{-2} |
| Secondary Heat Transfer Coefficient (W/m$^2$K) | | $\mu$: 0 | $\mu$: 5.74 x 10^{-3} | $\mu$: 2.87 x 10^{-2} |
|                       |                       | $\sigma$: 0 | $\sigma$: 6.54 x 10^{-3} | $\sigma$: 3.27 x 10^{-2} |

Figure 3. $X_L$, $X_S$, and $t_S$ for Case B as a function of Pe where the black dots are the mean values and the white dots are 2$\sigma$ away from the mean.
Case B was run for various Peclet numbers ($Pe = L_c V_{cast}/\alpha$) in which $L_c$ is the characteristic length taken from the classical fin theory ($L_c = \sqrt{k A_c / U_m P}$) where $A_c$ is the cross-sectional area [11]. Figure 3 shows the results from these simulations. Both the mean and deviation of $X_L$ and $X_S$ increase with $Pe$ but at different rates. As all the heat being extracted from the liquid is through the mold, the change in $X_L$ with $Pe$ is linear. At low $Pe$, $X_S$ has a relatively large slope as the majority of the heat extraction is through the mold and the advection of $L_f$ is minimal. As $Pe$ increases, the advection of $L_f$ and the secondary heat transfer coefficient become more important causing the slope of $X_S$ to decrease. The uncertainty in $t_S$ is large at low $Pe$ but decreases substantially for large $Pe$. At low $Pe$, $X_L$ and $X_S$ are similar in order of magnitude making small differences result in large uncertainties in $t_S$, while, for large $Pe$, $X_S$ is orders larger than $X_L$ so small fluctuations do not impact $t_S$.

3.2. 2D Model of Static Casting with Fluid Flow

The uncertainty quantification approach in Section 2.2 is now applied to a 2D continuum mixture model of transient transport phenomena during solidification of an Al-4.5 wt. % Cu alloy [12]. For this study, the permeability model of the Darcy drag in the mushy zone is adjusted to examine the effect of the uncertainty of each permeability model on average macrosegregation levels and solidification time. The 20 cm by 20 cm mold is cooled from one side using a constant heat transfer coefficient of 1000 W/m²K. The permeability models are given in equations (7-9), where $\lambda$ is the secondary dendrite arm spacing, $g_l$ is the liquid volume fraction, and $g_s$ is the solid volume fraction [4].

$$KI: \quad K = \frac{\lambda^2 g_l^3}{180 g_s^2}$$ (7)

$$KII: \quad K = \frac{\lambda^2 g_l^3}{180 g_s^{4/3}}$$ (8)

$$KIII: \quad K = \frac{\lambda^2 g_l^3}{80 g_s}$$ (9)

These models were chosen based on their behavior in the low $g_s$ region of the mushy zone, shown in Figure 4, which is where there is flow in the mushy zone strong enough to affect heat and solute transport [5]. Table 6 gives the properties used as inputs to the model, where the mean and standard deviation are given for the secondary dendrite arm spacing, $g_l$ is the liquid volume fraction, and $g_s$ is the solid volume fraction [4].

$$M^{Cu} = \left[ \frac{1}{V_{casting}} \int V_{solid} \left( \frac{C_{Cu}}{C_{Cu}^o} - 1 \right)^2 dV \right]^{1/2}$$ (10)

Table 6. Property values for Al-4.5 wt. % Cu alloy.

| Property                      | Value 1 | Value 2 | Value 3 |
|-------------------------------|---------|---------|---------|
| Density (kg/m³)               | 2605    |         |         |
| Specific Heat (J/kgK)         | 1006    |         |         |
| Latent Heat (J/kg)            | 390,000 |         |         |
| Thermal Conductivity (W/mK)   | 137.5   |         |         |
| Dynamic Viscosity (kg/ms)     | 0.0014  |         |         |
| Thermal Expansion (1/K)       | 1.17x10⁴|         |         |
| Melting Temperature of Pure Al (K) | 933.5  |         |         |
| Eutectic Temperature (K)      | 821.2   |         |         |
| Eutectic Composition (wt. fr. Cu) | 0.33    |         |         |
| Maximum solubility of Cu in Al (wt. fr. Cu) | 0.0565 |         |         |
| Secondary dendrite arm spacing (μm) | μ=100 σ=10.5 |         |         |
Figure 4. Normalized permeability as a function of solid fraction [4].

Figure 5. Macrosegregation number and solidification time probability density functions showing the effect of the permeability model chosen.

The permeability model KI has the largest amount of segregation on average and the largest uncertainty in the model prediction (Figure 5a), as expected from its larger K values at low $g_s$ (Figure 4). The uncertainty in $M^{cw}$ due to KI has some overlap with KIII and even less with KII. Model KII has the narrowest range of probabilities for segregation and, while KII has a much lower mean segregation level than KI, its range is roughly the same. The mean values of solidification times for KII and KIII are the same, whereas KI has a slightly longer $t_S$. The higher interdendritic flow with KI causes more segregation and the enriched bulk fluid slows the overall time to freeze. Still, the mean values are within 2% of each other, indicating that the uncertainties in the $K$ models have only a small effect on solidification time, which is expected because the flow is a secondary effect on $t_S$.

4. Conclusions
The procedure we used here was able to quantify uncertainties in a simplified 1D steady state solidification model of weld filler rod that agreed well with the analytical solution. A more realistic and complicated model (Case B) showed the inputs to which the model is most sensitive are the heat transfer coefficients. Material properties that had the most influence on the outputs are the specific heat, density, and, for $X_S$ and $t_S$, the latent heat. In order to produce accurate results, these inputs parameters need to be measured to lesser uncertainty than the 5% assumed here. The uncertainty in $t_S$ decreased with increasing Peclet number, while the uncertainty increased with $X_L$ and $X_S$. The 2D casting models quantified the large uncertainty in segregation levels and small effect on freezing times due to uncertainty in dendritic arm spacings in three mushy zone permeability models.
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