Simple metrics for verification and validation of macrosegregation model predictions

I Vušanović[1a] and V R Voller[2]

[1]Faculty of Mechanical Engineering, University of Montenegro, George Washington St. bb 81000 Podgorica, Montenegro
[2]Department of Civil, Environmental, and Geo- Engineering, University of Minnesota, Minneapolis, MN 55455, USA

Email: [a]igor.vusanovic@ac.me

Abstract. While the numerical simulation of macrosegregation is now a common place activity efforts can still be enhanced by developing quantitative measures of the results. Here, on treating the nodal field of concentration predictions from a macrosegregation simulation as a sample from a statistical distribution, we demonstrate how statistical measures can be used in verification and validation. The first set of such measures is simply the central moments of the distribution, i.e., the mean, the standard deviation, and the skewness; measurements that provide quantitative checks of mass balance and grid convergence. In addition, building on recently reported work [1], we also demonstrate how to construct and use a cumulative distribution function (CDF) of the nodal concentration field; a measure that can be used to determine the fraction of the casting volume concentrations less than a specified value. We show how the CDF can be used to compare the influence of various process conditions and phenomena related to domain size, cooling rate, permeability, and micro-segregation.

1. Introduction

Current macrosegregation simulations are advanced and when coupled with sophisticated graphical outputs lead to detailed predictions of the distribution of solute in cast products. Ultimately our objective with these simulations is twofold. In the first place we might like to compare differences in process settings such as cooling conditions, and geometry. Secondly, we may be interested in understanding the basic phenomena underlying the simulations, e.g., microsegregation, and mushy region flow behavior. Clearly, graphical output provides an immediate qualitative evaluation of changing process settings or model phenomena. But this powerful tool is lacking in obvious quantitative measures that can be used in case to case comparisons. One way of obtaining quantitative measures is to treat the predicted nodal values of solute concentrations from a macrosegregation calculation as a statistical distribution. In this way measures of central moments and derived distribution functions [1] can be used as quantitative representations of macrosegregation behavior. The objective of this paper is to introduce these measures and, through a number of example macrosegregation simulations, show how they can be used to evaluate process settings and phenomenological models.

2. Statistical measures

Usually, the output from macrosegregation simulations essentially provides a list, C_i (i=1, 2,..N) of solute concentration values taken from (N) specified discrete points (nodes) in the casting. Often these are more conveniently stored as a set of macrosegregation levels $M_i = C_i / C_0$, where C_0 is the initial solute concentration in the melt. When this data is treated as a sample from a statistical distribution, central moments can be immediately calculated. Each of the first three central moments of such a distribution provides useful quantitative measures.

The first moment is the mean, defined as:

$$\overline{M} = \frac{\sum_{i}^{N} M_i}{N} \tag{1}$$

This will return the average macrosegregation level which can be used as a check on the mass balance of the simulation, i.e., if our simulation is correctly conservative we would expect that $\overline{M} = 1$. The second central moment is the sample standard deviation

$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} \left(M_i - \overline{M} \right)^2} \tag{2}$$

This provides a measure of the spread of the data. Previously introduced as the macrosegregation number [2] it provides a basic measure of the level of macrosegregation. The third moment is the sample skewness, which based on the SKEW function found in spreadsheet software, can be defined as:

$$g = \frac{N}{(N-1)(N-2)} \sum_{i=1}^{N} \left(\frac{M_i - \overline{M}}{s} \right)^3 \tag{3}$$

This measure tells us how much the solute distribution is biased to the positive or negative side of the mean (the initial concentration). For example, a positive value of skewness (g) indicates that positive segregation values have a wider range than negative segregated values.

In addition to measures of central moments we could also construct a distribution function of our data. In recent work Voller and Vušanović [1] have proposed a simple way of constructing a so called Cumulative Distribution Function (CDF). This involves (i) listing the nodal values M_i in descending order, (ii) assigning a rank number j = 1, 2,3, …, N to each item in the list, and then (iii) associating with each entry an inverse Weibul number

$$F_j = \frac{j}{N+1} \tag{4}$$

Essentially the value of F_j is the volume of the solidified casting which has a macrosegregation level greater than or equal to that of $M_j = C_j / C_0$. The method is best suited to cases where the data acquired from experimental or numerical simulations is over a uniform grid. In cases where this is not case, e.g., simulation results obtained with an unstructured or cloud grid, care may need to be taken in constructing and interpreting the CDF.

Voller and Vušanović have used this CDF approach to investigate the grid dependence of macro-segregation simulations. A result, that when used in conjunction with experimental measurements for a Sn-10%Bi alloy [3] suggests that the positive segregated region may have a power-law tail. Thus indicating that as numerical or measurement resolution is refined one will, up to the formation of a second phase, encounter higher and higher values of solute concentration. Here we will extend the use of the (CDF) recently proposed in [1] and demonstrate how it can also be used to evaluate changes in process and model conditions.

3. A baseline case

As a baseline case, to compare the effects of process and phenomena conditions, we consider the solidification in a side cooled two-dimensional cavity containing an Al-4.5%Cu like alloy, with a fixed columnar microstructure initially at the liquidus temperature. The governing equations are the standard macrosegregation mixture model of heat, solute, and momentum conservation introduced by Bennon and Incropera [4], full details of the equations and solution strategy can be found in [5,6]. We note that our principal intention here is not to detail the model and solution used but rather to illustrate how the statistical measures, introduced above, can be used to systematically study the effects of process and phenomena on macrosegregation, in particular variations in the domain size, cooling conditions, microsegregation treatment, and permeability model. The base case consist of a 20mm x 20mm domain size cooled by applying a constant heat flux $Q=1.0MW/m^2$ on the left vertical side. Key factors in the model include (i) the construction of a microsegregation model to determine the nodal liquid solute concentration field from the predicted mixture concentration C_i, and (ii) a devise to suppress the fluid flow as a nodal solid fraction f_i in the mushy region approaches 1 (full solidification). In the base model we use a lever rule which assumes, within the micro scale of the mushy region (a secondary arm space), complete solute diffusion in both liquid and solid phases. Thus allowing us to determine the liquid concentration from a simple mass balance $C_i = fkC_l + (1-f)C_l$. The standard model to suppress fluid flow, as full solidification is reached, is to add a Darcy like sink term, scaling as ~ (inverse permeability x velocity), to the momentum equation. In the base case, the permeability is modeled as $K=\kappa_0 f^3/(1-f)^2$, where the constant $\kappa_0 = 1.0 \times 10^{-10} m^2$. In this way as we approach full solidification $f \rightarrow 1$ the inverse permeability $K^{-1} \rightarrow \infty$, effectively suppressing the flow velocity in the mush.

The first panel in figure 1 shows the predicted final macrosegregation pattern for the base case using a grid size of 40x40 control volumes and a time step $\Delta t = 2.0 \times 10^{-3}$ sec. The second panel shows the CDF in log – log scale, for four different grid sizes. In support of figure 1, table 1 shows the mean, standard deviation, and skewness change with grid size.
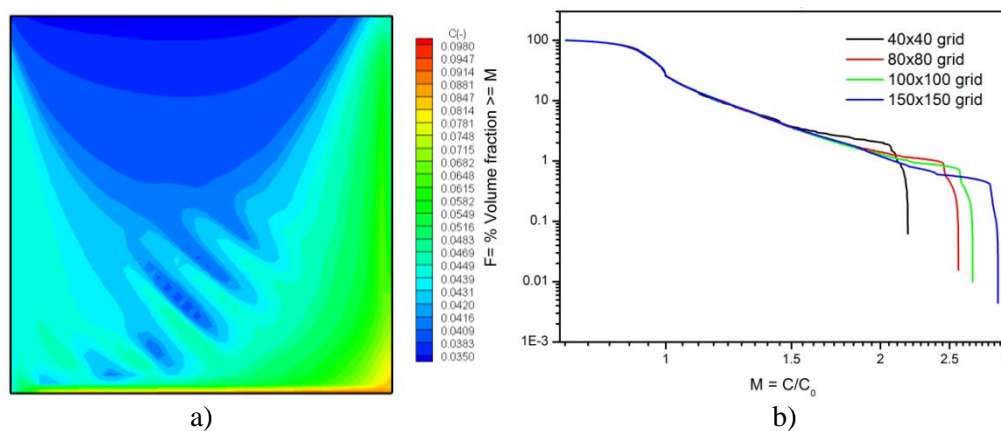

Figure 1. Macrosegregation profile for baseline case (a), and (CDF) for the baseline case with different grid sizes (b).

Matching the findings in Voller and Vušanović [1] the main observation to take from figure 1b), is that as the grid is refined, the positive segregation region extends to the right and the predicted maximum truncation value of (M) increases. Essentially, a finer resolution, be it from simulation or experiments, will continue, up to some physical limit (e.g. the appearance of another solid phase), to uncover additional volumes with higher concentrations. This behavior is also seen in the values of table 1, where both the standard deviation (macrosegregation number) and skewness increase linearly with decreasing grid spacing. This suggests that care needs to be taken when increasing the grid size in computer models, and at the same time indicates why it is often so difficult to economically arrive at grid resolved macro-segregation simulation predictions.

Table 1. Statistical measures of macrosegregation results.

Grid spacing (mm)	Mean $\overline{M}$	Standard deviation (s)	Skewness (g)
0.50	1.0	0.05019	3.15733
0.25	1.0	0.05533	3.74400
0.2	1.0	0.05634	3.87929
0.134	1.0	0.05786	4.08245

4. Applications of (CDF) approach for parametric study of macrosegregation

To demonstrate how to use the *C*umulative *D*istribution *F*unction (CDF) in a parametric study we conduct a number of simulation runs where we change a single process or phenomena setting in our base line simulation. The changes are: (1) reductions in the cooling flux Q, (2) an increase in the permeability constant (corresponding to an increase in the assumed secondary arm space), and (3) the use of a Scheil microsegregation model where a zero solid state solute diffusion is assumed. These deviations from the base case are summarized in table 2 and the resulting CDF's (plotted in both linear and log-log scales) are shown in figures 2-4. Note that all runs are done with the relatively coarse grid size of (0.5 mm)

Table 2. Variations of process parameter for CDF analysis of macrosegregation results.

Case	Domain size	Cooling rate	Micro model	Permeability
Baseline case: 20x20mm, $Q=1MW/m^2$, Lever, $\kappa_0=1.0 \times 10^{-10}\,m^2$				
1.1	20x20mm	$Q=0.5\,MW/m^2$	Lever	$\kappa_0=1.0 \times 10^{-10}\,m^2$
1.2	20x20mm	$Q=0.25\,MW/m^2$	Lever	$\kappa_0=1.0 \times 10^{-10}\,m^2$
2.1	20x20mm	$Q=1MW/m^2$	Scheil	$\kappa_0=1.0 \times 10^{-10}\,m^2$
2.2	20x20mm	$Q=1MW/m^2$	Lever	$\kappa_0=1.0 \times 10^{-9}\,m^2$
2.3	20x20mm	$Q=1MW/m^2$	Lever	$\kappa_0=1.0 \times 10^{-11}\,m^2$

With reference to the linear CDF plot (figure 2b) we see that a fast cooling rate, implying a faster solidification rate, leads to less segregation; this is indicated by the reduction in the spread of the CDF as the cooling rate is increased. In contrast, a comparison of the CDF's obtained with a Scheil and lever microsegregation model (figure 3) indicates that for the majority of the casting, the limit microsegregation treatments have little impact on the solute distribution. In the last 5% of the casting, however, as clearly indicated in the log-log plot (figure 3a), there is a pronounced difference. This is driven by the fact that, in the later stages of solidification, the Scheil model leads to significantly higher values of the liquid solute concentration. Finally, as might be expected, changes in the

permeability, figure 4, result in the most dramatic changes in the CDF. With a high value, the flow in the mushy region is more intense and can continue to quite high solid fractions. The result is a much wider solute distribution, terminating with a larger level of macrosegregation *M*. In contrast, a low value effectively cuts the flow in the mushy region providing limited opportunity for macrosegregation and a much tighter CDF.
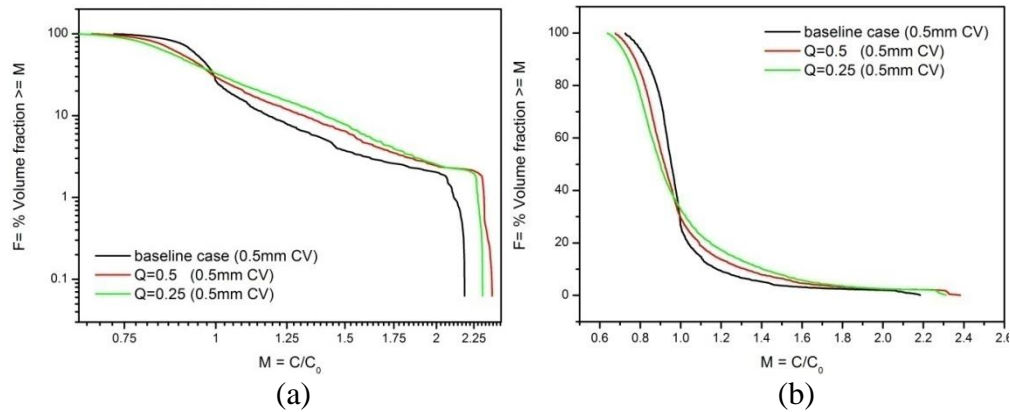

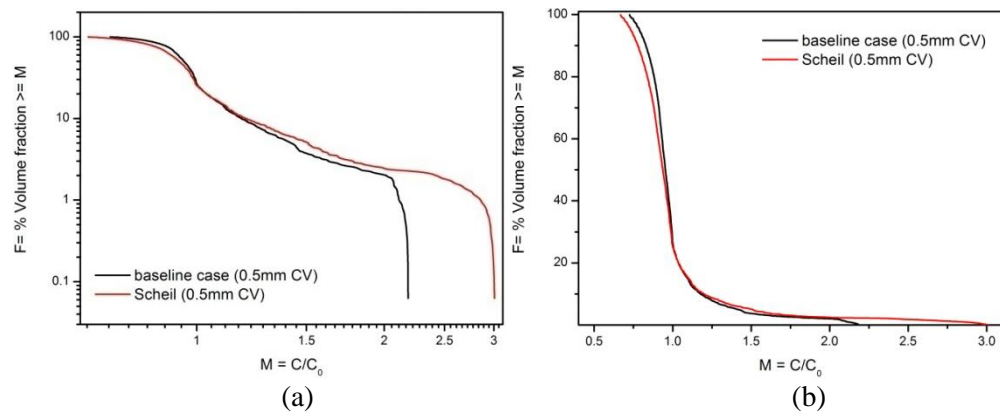**Figure 2.** Influence of cooling rate (a) log-log scale, (b) linear scale.

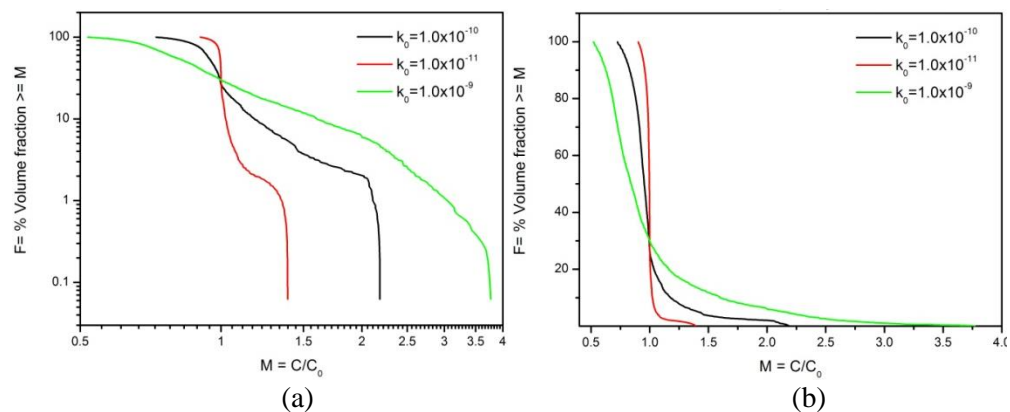**Figure 3.** Influence of microsegregation model (a) log-log scale, (b) linear scale.

Figure 4. Influence of different permeability in Darcy law (a) log-log scale, (b) linear scale.

5. Remarks and conclusions

Here we have demonstrated how simple statistical measures can be used to guide us in constructing reliable macrosegregation simulations. Even given the accuracy limitations of the grid size and the physical shortcomings in the mixture model, these statistical measures, in particular the Cumulative Distribution Function (CDF), provide two important insights. The first, supporting the initial work presented in Voller and Vušanović [1], is that the power-law tail in the CDF indicates why it is often so difficult to grid converge macrosegregation simulation. The second, is that the shape and spread of the CDF is extremely sensitive to change in the parameters that control the fluid flow in the mushy region. In practice there are many factors that can control the fluid flow in the mushy region, in particular coarsening of the arm spaces (leading to a transient permeability) and the movement of solid grains (non-fixed microstructure). As a result, although it may be obvious to state, we believe that it is in the modeling treatment of the mushy region flow that drives the observed divergence between macrosegregation code predictions observed in benchmark studies [2]. Therefore, in moving towards simulations that can consistently and faithfully match those seen in experiment or plant, it is key to focus on the development of robust physical models of the flow in the mushy region. Use of the statistical approaches demonstrated here, in particular the Cumulative Distribution Function [1], will be a useful tool in developing and tuning such models.

References
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