Numerical investigation of grid influence on formation of macrosegregation

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The investigation of grid influence on numerical prediction of the formation of macrosegregation is an important issue in the point of view of numerical modelling. The estimation of numerical accuracy for the simulation of complex multiphase phenomena is a difficult modelling process, since the thermophysical properties depend on the temperature and concentration as well. The numerical stability and accuracy of the modelling also depend on the chosen time step and grid size. This paper focuses on the grid influence and modelling questions on macrosegregation in a benchmark ingot using Fe-0·34 wt-%C steel. The FLUENT-ANSYS v6·3 commercial software does not have built-in multiphase solidification and melting module for simulating columnar to equiaxed transition. Therefore, a multiphase model was implemented using User-Defined Functions. The number of grid cells has been increased from 180 to 4300 to define an optimal grid size, to prove the reliability of the model implementation based on solution accuracy. The results show, the macrosegregation pattern does not change significantly above a well-chosen number of grid cells.

Keywords: Multiphase flows, Numerical methods, Grid influence, Macrosegregation

Introduction

The mathematical modelling of metallurgical processes is currently a relevant field related to computational fluid dynamics (CFD) where the flow phenomena have been considered. Gu[1] and Beckermann[1–3] used a model to study the macrosegregation with numerical solution of fully coupled mass, momentum, energy and species conservation in the case of an industrial steel ingot. The present work uses a multiphase model by Ludwig *et al.*[4] and Wu *et al.*[5–6] which is briefly described in this paper. Literature can be readily found in the fields of numerical modelling in material science and engineering (e.g. Rappaz *et al.*,[7] Hattel[8]), in multiphase flows (e.g. Kolev,[9] Brennen[10]), in solidification (e.g. Kurz and Fisher[11]) and in CFD modelling (e.g. Fletcher,[12] Hirsch,[13] Ferziger and Perič[14]). These methods are based on the numerical solution of partial differential equations related to fluid mechanics. Since, the flow phenomena have to be considered in ingot casting, in continuous casting and in electroslag remelting (ESR) processes etc., many more articles, conference papers, books could be suggested, that deal with the numerical stability, accuracy and reliability of the mathematical models in this field.

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Multiphase model description and modelling questions

For modelling solidification and melting phenomena during metallurgical processes using the multiphase approach, the conservation laws are described by integral or partial differential equations. The mass, momentum, energy, species and other problem dependent additional transport equations can be considered exact, but solving them analytically, without taking into account any assumptions, is impossible for most cases of engineering interest. This is the reason for setting up mathematical models of the physical problems and solving the corresponding partial differential equations with numerical methods. Even if the model is nearly exact, some properties of the metallurgical process are not exactly known. For example, all fluid properties depend on temperature, species concentration and pressure, however these dependences are neglected in some special cases.

A multiphase solidification and melting model was developed for the binary system. Three phases were considered, namely liquid phase l, columnar dendrite trunks c and equiaxed grains e. The morphology of the equiaxed grains was approximated by ideal spheres. The growth velocity of equiaxed grain were analytically derived[4–6] as

$$v_{R_e} = \frac{2D_l}{d_e} \cdot \frac{c_l^* - c_l}{c_l^* - c_e^*}, \tag{1}$$

where D_j is the diffusion coefficient, d_e is the diameter of equiaxed grains, c_l^* and c_e^* are the equilibrium species mass fractions at the liquid/solid interface. The

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momentum equation for the columnar phase was not solved, because the dendrite tip was tracked by an explicit type algorithm using the LGK[4–6] model. The distance between two cylinder centres represents the primary dendrite arm spacing λ_1. The growth velocity of columnar dendrite trunks was analytically derived[4–6] as

$$v_{R_c} = \frac{2D_l}{d_c} \cdot \frac{c_l^* - c_l}{c_l^* - c_c^*} \cdot \ln^{-1}\left(\frac{d_{\max}}{d_c}\right), \quad (2)$$

where $d_{\max}$ is the maximal diameter available for cylindrical growth, d_c is the diameter of columnar dendrite trunks, and c_c^* is the equilibrium mass fraction of the columnar phase at the liquid/solid interface. Considering a hexagonal dendrite arrangement with dendrite arm spacing λ_1, the maximal diameter can be chosen as $d_{\max}=1{\cdot}05\lambda_1$. The mass transfer rate from the liquid to the equiaxed phase was defined as

$$M_{le} = v_{R_e} \cdot (n \cdot \pi \cdot d_e^2) \cdot \rho_e \cdot f_{imp}, \quad (3)$$

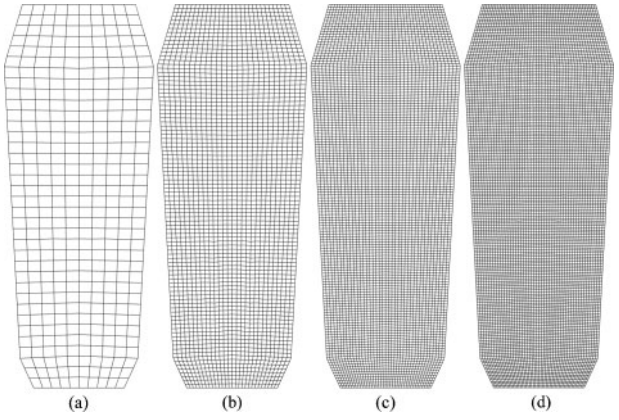
where ρ_e is the density of the equiaxed phase, f_{imp} is the impingement factor.[15] The mass transfer rate from the liquid to columnar phase was defined as

$$M_{lc} = v_{R_c} \cdot \left(\frac{2\sqrt{3} \cdot \pi \cdot d_c}{3\lambda_1^2}\right) \cdot \rho_c \cdot f_{imp}, \quad (4)$$

where ρ_c is the density of the columnar phase, V_{tip} is the tip velocity, and R_{tip} is the tip radius. The impingement factors are different for the spherical and cylindrical growth. An Avrami-type factor was used ($f_{imp}=f_l$) for equiaxed solidification. The impingement factor for columnar solidification was assumed as

$$f_{imp} = \begin{cases} 1{,}0 < d_c \leqslant \lambda_1, \\ 1 - \frac{d_c - \lambda_1}{d_{\max} - \lambda_1}, \lambda_1 < d_c \leqslant d_{\max} \end{cases} \quad (5)$$

After computing the mass transfer rates, the multiphase Eulerian–Eulerian approach is applied to consider the mass, momentum, enthalpy and species conservations. Thermal and solutal buoyancy were modelled by using the Boussinesq approach. The nucleation process was modelled by the Oldfield[4–6] conservation equation which suggests a continuous rather than a discrete distribution of nucleation sites. Since in parallel analytical solutions for describing and modelling complex metallurgical processes do not exist, we have to take into account the errors of the underlying numerical methods as well as the modelling errors based on the assumptions. The conservation equations are reduced to solve linear or non-linear algebraic equations using discretisation methods. On the one hand, the discretisation techniques cause discretisation errors as defined by the difference between the supposed exact solution of the governing equations and the exact solution of the discrete approach. On the other hand, an iterative method is often used, instead of a direct method, for solving the algebraic equation system, which means that we have to take into account the iteration errors. The iteration error is defined as the difference between the exact and the iterative solutions of the discretised algebraic equation system. The direct solution of the algebraic equation system is often uneconomical. Therefore, it is necessary to define a convergence criterion to stop the iterative process of the numerical solution. Even if the solution process is convergent and we iterate long enough, we never obtain the exact solution of the discretised equations.[14]



1 ***a*** **180 grid cells;** ***b*** **1316 grid cells;** ***c*** **2780 grid cells;** ***d*** **4300 grid cells**

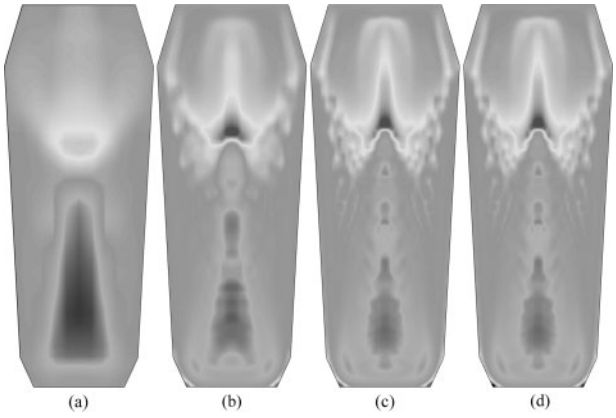
The computer CPUs also have a so-called round-off error due to the finite arithmetic precision, but it does not become significant until the solution error is close to the machine precision. Even if the governing equations are implemented correctly, it is possible to obtain different results with different implementation strategies. The efficiency and accuracy of the numerical methods, implementation strategies and computer codes can be further improved. One of the most significant issues to increase the accuracy of the numerical solution is the grid refinement where it is necessary.

The benchmark ingot

Integral or partial differential equations, which describe the physical phenomena of metallurgical processes, require accurate initial and boundary conditions. These are often difficult to specify exactly as well, which means that we need further assumptions. Although, the governing equations can be exact in certain cases, but the approximations at the boundary can also have an effect on the solution. The geometry can also be difficult to represent exactly, therefore it is necessary further assumptions about that details which make difficult to generate an appropriate grid.

The solidification of a binary 'steel' ingot (Fe–0·34 wt-%C) with a relatively small size (diameter: 66 mm, height: 170 mm) was set up for multiphase solidification simulations.[5,6] The heat transfer coefficient between the ingot and the die is $h=700$ W m^{-2} K^{-1}, and air flow has been taken into account at the top, where the heat transfer coefficient is $h=100$ W m^{-2} K^{-1}. The number of grid cells has been increased from 180 to 4300 in half of the symmetrical domain (see Fig. 1). The systematic grid refinement is a very important part of the verifying process, because it helps to reduce the discretisation errors and to define an optimal grid size starting from which the results do not change significantly.

The finite volume method (FVM) based FLUENT-ANSYS v6·3 CFD code was used for solving the conservation equations of the Eulerian–Eulerian multiphase model. The FLUENT-ANSYS v6·3 commercial software does not have built-in multiphase solidification and melting module for simulating columnar to equiaxed transition. Therefore, the equations (1)–(5)



2 Predicted macrosegregation patterns using different size of grid; the results show, the pattern does not change significantly above a well-chosen number of grid cells; the middle value of the grey scale is the initial concentration

were implemented to set up the partial differential equation system for numerical solution.

Results and discussion

The physical phenomena of the multiphase solidification and melting related metallurgical processes are always grid independent, because of their invariant nature. For modelling, a grid is required to solve the governing equations on a finite domain. Therefore, the numerical solution and the implementation can be grid dependent. The influence of the grid size on numerical integration accuracy was investigated by Runge[16] at the beginning of the 20th century. Recently, Roache[17] (1994) and Ferziger and Perič[18] (1996) have given more details about the estimation of discretisation errors. The simplest way is the Richardson extrapolation which assumes that computation can be done on grids sufficiently fine that monotone convergence is obtained. The order of discretisation error $\tilde{p}$ can be computed from the results on three or more consecutive grids when all grids are fine enough

$$\tilde{p}=\log\left(\frac{\varphi^i_{2\tilde{h}}-\varphi^i_{4\tilde{h}}}{\varphi^i_{\tilde{h}}-\varphi^i_{2\tilde{h}}}\right)\cdot\log^{-1}\tilde{r}, \tag{6}$$

where $\tilde{r}$ is a grid density factor, $\varphi^i_{\tilde{h}}$ is the solution in the ith cell (e.g. volume fraction, liquid velocity, macrosegregation etc.) on a grid with an average spacing $\tilde{h}$. The $\varphi^i_{\tilde{h}}$ is chosen to be mixture concentration, $\varphi^i_{\tilde{h}}=c^i_{mix}$. The mixture concentration represents the formation of macrosegregation at the end of the solidification. The discretisation error can approximately be estimated as follows[14]

$$\breve{\varepsilon}^i_{\tilde{h}}\cong\frac{\varphi^i_{\tilde{h}}-\varphi^i_{2\tilde{h}}}{\tilde{r}^{\tilde{p}}-1}, \tag{7}$$

and in order to quantify the overall error, the maximum norm of the discretisation error is

$$\left\|\breve{\varepsilon}_{\tilde{h}}\right\|_\infty:=\max_{1\le i\le n}\left|\breve{\varepsilon}^i_{\tilde{h}}\right|\cdot \tag{8}$$

Note that other norms can be used as well. The estimation of the numerical errors is required to obtain numerically reliable macrosegregation patterns and to know the difference between numerically predicted and measured results. The systematic grid refinement is necessary by factor of $\tilde{r}$ to reduce the discretisation errors in each cells. It helps to define an optimal grid size starting from which the results do not change significantly. An average grid size $\tilde{h}$ and the mixture concentration $\varphi^i_{\tilde{h}}=c^i_{mix}$ in each grid cell are required to compute the order of discretisation error $\tilde{p}$ based on the equation (6). After knowing the $\tilde{p}$ values, the discretisation error can be estimated by equation (7) in each grid cell. In order to quantify the overall error, hereby the maximum norm of the discretisation error $\left\|\breve{\varepsilon}_{\tilde{h}}\right\|_\infty$ was taken into account in equation (8). An example of how to compute the discretisaton error based on the final macrosegregation pattern can be seen in Table 1. This example considers the $\varphi^{\max}_{cmix}$ maximum values of the macrosegration pattern to show how to use equation (6)–(8), however the $\left\|\breve{\varepsilon}_{\tilde{h}}\right\|_\infty$ values of maximum norm are valid for the computational domain in Table 1. The number of grid cells has been increased from 180 to 4300 to define an optimal grid size, to prove the reliability of model implementation. When we have a coarse grid with 180 cells, one can see that the numerically predicted bottom zone of negative segregation, which is caused by the sedimentation of equiaxed grains, is different from the other simulations when the number of grid cells was increased by a factor of $\tilde{r}$ (see Fig. 1). The coarse grid also can cause different positive segregation patterns at the ingot top. This positive segregation is explained by convection of segregated melt from the ingot center, but when we do not have a sufficient number of grid cells, the flow simulation and the numerical accuracy can be unreliable. With increasing the number of grid cells, the 'A' and 'V' type segregation patterns have been appeared which were observed in the classical experiments[19,20] as well. The results show in Fig. 1 that the macrosegregation pattern does not change significantly above a well-chosen number of grid cells, at least from 2780 cells in our case. Therefore, the simulation can predict grid independent numerical solution, which means that the final macrosegregation pattern is numerically reliable based on the model assumptions and solution

Table 1 Estimation of the discretisation error based on the final macrosegregation patterns

a_j [cells]	$\tilde{h}$ [m]	$\varphi^{\max}_{cmix}$ [kg/kg]	$\tilde{r}_j$ [1]	$\tilde{p}_j$ [1]	$\left\|\breve{\varepsilon}_{\tilde{h}}\right\|_\infty$ [1]
$a_1=180$	0·0065933	0·004066002	$\tilde{r}_1=2$	$\tilde{p}_1\cong9{\cdot}693486$	$\approx1{\cdot}002\times10^{-6}$
$a_2=1316$	0·0023547	0·004894002	$\tilde{r}_2=a_2/a_1\cong7{\cdot}31$	$\tilde{p}_2\cong3{\cdot}377414$	$\approx1{\cdot}209\times10^{-9}$
$a_3=2780$	0·0016483	0·004894010	$\tilde{r}_3=a_3/a_1\cong15{\cdot}4$	$\tilde{p}_3\cong2{\cdot}454658$	$\approx1{\cdot}209\times10^{-9}$
$a_4=4300$	0·0013186	0·004895000	$\tilde{r}_4=a_4/a_1\cong23{\cdot}8$	$\tilde{p}_4\cong2{\cdot}117282$	$\approx1{\cdot}209\times10^{-9}$

accuracy. The numerical solutions are always approximate solutions, therefore the error estimations play an important role in the explanation of the simulation results. According to Ferziger and Perič, the best measure of the efficiency of a solution method is the computational effort required to achieve the desired accuracy.[14]

Summary

A multiphase model was developed by Ludwig *et al.*[4] and Wu *et al.*[5,6] which was briefly described in this paper. The model implementation provides a good opportunity to perform a grid study for macrosegregation in ingot casting. The number of grid cells has been increased from 180 to 4300 to define an optimal grid size, to prove the reliability of model implementation. The results show, the macrosegregation pattern does not change significantly above a well-chosen number of grid cells, at least from 2780 cells in our case. Therefore, the proposed model can predict grid independent numerical solution, which means that the final macrosegregation pattern is numerically reliable based on the model assumptions and solution accuracy.

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