Simulation of macrosegregation with mesosegregates in binary metallic casts by a meshless method

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**Abstract**

Simulation of macrosegregation with mesosegregates as a consequence of solidification of a binary Sn–10%Pb alloy in a 2-dimensional rectangular cast is tackled in the present paper. Coupled volume averaged governing equations for mass, energy, momentum and species transfer are considered by incorporating Lever solidification rule and incompressible Newtonian fluid with Darcy limit in the mushy zone. Solid phase is assumed stationary. Double diffusive effects in the melt are modeled by the thermal and solutal Boussinesq hypothesis. The physical model is solved by the meshless Local Radial Basis Function Collocation Method (LRBFCM) by using 5-noded influence domains, multiquadrics radial basis functions and explicit time stepping. Pressure–velocity coupling is based on local pressure correction. Adaptive upwinding has to be used for stabilization of the convective terms. The numerical simulations reveal instabilities during solidification process that introduce anomalies in the final segregation map that scale with the typical cast as well as sub-cast dimensions. The main advantages of choosing the represented meshless approach for solving the problem are in its simplicity and similar coding in 2D and 3D, as well as straightforward applicability in non-uniform node arrangements. The locality of the proposed numerical approach is also convenient for parallel execution. It is demonstrated that LRBFCM can be advantageously used in casting simulations where the chemical segregation exhibits industrially relevant multi-scale patterns.

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1. Introduction

Solidification science and engineering represents an interdisciplinary research field of great interest [1–4]. It is founded on thermodynamics and continuum mechanics that has to cope with solids and fluids simultaneously. Its analytical basis can be traced back to Lamé, Clapeyron, Neumann and Stefan [5], while the numerical treatment started by Douglas and Gallie in 1955 [6]. The solidification phenomena include nucleation, dendritic growth, eutectics, peritectics and microstructure selection issues, macrosegregation, homogenization, and macro, meso and microstructures. Many modern industrial processes, in particular, different types of casting [7] rely on findings of solidification science and engineering. Castings are prone to several types of defects, such as porosities, deformation during solidification, including hot tearing, and chemical inhomogeneities also referred to as segregation. The segregation that scales with the whole casting is called macrosegregation, on the other hand, the segregation, much smaller than the size of the casting and much larger than the typical grain size is called mesosegregation. The theoretical description of the chemical segregation in solidification started in the Sixties [8], followed by more precise model studies in the Seventies [8,9]. Recently, this topic has been treated in many applied works, e.g. for static casting [10], continuous casting of steel [11] and direct chill casting of aluminum alloys [12]. Besides the applications, the physical modeling of the problem is also developing [13–16]. Solidification systems are difficult to treat in a closed form and actually only a few analytical solutions exist in connection with the subject [17–19]. Therefore, the use of numerical modeling and simulation is the preferred approach. The performance of numerical methods for solution of the macrosegregation problems remains rather unexplored. Recently, substantial efforts and resources were invested to study the behavior of different numerical methods in the prediction of macrosegregation [4,20], triggered in the framework of the French SMACS project, where a call for contributions to two numerical benchmark test cases was launched [21]. The test is gradually complicated from
natural convection of a low Prandtl fluid \[22\], double diffusive natural convection and to solidification of a binary material. In this work we present a solution of a third part of these benchmark tests by a novel meshless technique. The test deals with the solidification of a Sn–10\%Pb alloy and follows our recent successful application of the same meshless technique for the first part of the benchmark \[22\]. The main complexities in numerical solution of alloy solidification models are moving interfaces with high gradients of physical properties, strong couplings between the conservation equations, different flow regimes in mushy zone and pure liquid, potentially unstable flow patterns in low-Pr liquids such as metals, hyperbolic nature of the solute transport due to almost completely advective transport. The problem of strong coupling between the momentum transport and energy and solute transport via the buoyancy force, and between the thermal field and permeability, makes the solution even more complex and less stable. The complexity of the prediction of macrosegregation is a consequence of the fact that the macrosegregation results from the entire history of the strongly coupled processes of mass, heat, momentum and solute transport from the liquid state up to the end of solidification. The channels (mesosegregates) in segregation profiles have been experimentally observed in different solidified products. In 1988 Sarazin and Hellawell performed analysis of channel formation in the directional solidification of the Pb–Sn alloys \[23\]. The experimental results, similar to the benchmark problem have been reported also in \[24\]. In this paper we focus on a numerical simulation of the phenomena with an emphasis on the meshless numerical technique.

The meshless or sometimes also named meshfree or mesh reduction methods represent a class of numerical methods where an arbitrarily distributed set of nodes, without any additional topological relations between them, is used. Such meshless methods represent a promising technique to avoid problems with polygonisation. There exist several meshless methods such as the Element free Galerkin method, the Meshless Petrov–Galerkin method, the point interpolation method, the point assembly method, the finite point method, smoothed particle hydrodynamics method, reproducing kernel particle method, and Kansa method \[25–35\]. This work is focused on one of the simplest classes of meshless methods in development today, the local point interpolation \[36\] Radial Basis Function \[37\] Collocation Method (RBFCM) \[38\]. In the present paper we use a local variant of RBFCM \[38\], the Local Radial Basis Function Collocation Method (LRBFCM). The main advantage of the local approach is that the spatial discretization of the problem is simplified to solving only small systems of algebraic equations instead of a large global system as in Kansa method \[25,31\] that might become unstable for increased number of computational nodes. The LRBFCM approach was already successfully applied to several thermo-fluid situations, ranging from laminar to turbulent as well as from single to two phase situations \[39–44\]. The LRBFCM has been recently also compared with GRBFCM and extended to the three dimensional problems \[45–47\].

2. Governing equations

The minimal solidification model, i.e. solidification model, simplified to the largest possible degree, is addressed in the present paper. The set of governing equations is based on continuum conservation laws and related constitutive relations. The model comprises energy transport, solute transport, incompressible Newtonian and porous Darcy fluid flow, and Eutectic phase diagram coupled with the solute transport over the phase front for consideration of the microscopic level. The model originates in the paper of Ni and Beckerman \[13\] and was later employed in many works \[14–16\]. In this paper we address the solidification in a two dimensional rectangular domain \(\Omega\) with boundary \(\Gamma\). The identical problem has been proposed in \[21\] within a call for a benchmark solutions. The problem is formulated as a system of four coupled Partial Differential Equations (PDE), Kozeny–Carman relation, Boussinesq approximation, and transport over the phase front on the macroscopic scale, coupled with a phase diagram.

\[
\mathbf{v} \cdot \nabla \mathbf{v} = 0, \quad \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\nabla P + \rho \mathbf{v}^2}{\rho} - \nabla \left( \frac{\partial T}{\partial T} \mathbf{v} - \frac{\partial T}{\partial \mathbf{v}} \right),
\]

\[
\frac{\partial h}{\partial t} + \rho \mathbf{v} \cdot \nabla h = g, \quad \frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C_L = 0,
\]

\[
\mathbf{v} = f_1 v_t, \quad \mathbf{v} = \mathbf{v}_C, \quad \mathbf{v} = \mathbf{v}_L,
\]

\[
K = K_0 \left( 1 - f_1^3 \right),
\]

\[
b = \rho ref \left( 1 - \beta_T (T - T_{ref}) - \beta_C (C_L - C_{ref}) \right),
\]

\[
h = c_0 T + f_1 L,
\]

\[
C = \left[ f_1 + \left( 1 - f_1 \right) k_0 \right] C_L,
\]

\[
T = T_T + m_t C_L.
\]

The following quantities are involved in the PDE: liquid velocity \(\mathbf{v}\), intrinsic liquid velocity \(\mathbf{v}_t\), enthalpy \(h\), average concentration \(C\), and the pressure \(P\). The permeability \(K\) is defined through a permeability constant \(K_0\) and the liquid fraction \(f_1\). The thermophysical properties, i.e. viscosity \(\mu\), thermal conductivity \(\lambda\), specific heat \(c_p\) and density \(\rho\) are assumed to be equal and constant in both phases. The buoyancy term \(b\) depends on the temperature \(T\), the liquid concentration \(C_L\), the thermal expansion coefficient \(\beta_T\), the concentration expansion coefficient \(\beta_C\), the reference density \(\rho_{ref}\) given at the reference temperature \(T_{ref}\) and the reference concentration \(C_{ref}\). The binary phase diagram is defined by the liquidus slope \(m_t\), the equilibrium partition coefficient \(k_p\) and fusion temperature of the pure solvent \(T_T\). Symbols \(t\) and \(g\) stand for time and gravity acceleration, respectively. We seek the solution of the temperature, velocity, pressure and concentration fields at time \(t = t_0 + \Delta t\), where \(t_0\) represents initial time and \(\Delta t\) a positive time increment. The problem is schematically presented in Fig. 1. In \[48\] it was shown that the presented “minimal” solidification model can be solved with the presented local meshless based solution procedure for cases without mesosegregate anomalies. In the present paper we present a solution of the SMACS benchmark solidification exercise for the alloy Sn–10\%Pb (see Table 1 for thermo-physical properties). This case is from the numerical point of view considerably more difficult to solve due to the presence of mesosegregates. The case is defined for a rectangular domain with dimensions \(10 \times 6\) cm. However, computational domain can be reduced to \(5 \times 6\) cm due to the symmetry (Fig. 1).

The initial and boundary conditions are set to

\[
\mathbf{v}(p_x = \Omega_0, t) = \mathbf{v}(p_y = \Omega_0, t) = \mathbf{v}(p_x = 0, t) = 0, \quad \frac{\partial}{\partial p_x} \mathbf{v}(p_x = 0, t) = 0, \quad \frac{\partial}{\partial p_y} \mathbf{v}(p_y = 0, t) = 0, \quad \frac{\partial}{\partial p_y} \mathbf{v}(p_y = \Omega_0, t) = 0
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modern computer architectures through different parallel computing strategies [34]. It is important to point out that the typical solidification simulations require vast amount of computational resources; hence the efficiency of computer implementation is of major importance. The details of LRBFCM can be perceived from [39,48,49]. We elaborate the important basics of the method, particularly the adaptive upwinding and pressure–velocity coupling in the continuation of the present paper. The LRBFCM spatial discretization is based on an approximation of a considered field over the support domain with trial functions. The radial basis functions are used for trial functions and their coefficients are determined by collocation. The locality of the method is introduced in the selection of a local support domain, i.e. only local sub-clusters of nodes are considered in support domain. An approximated function \( \theta(p) \), where \( p \) represents a position vector, is introduced as a sum of weighted basis functions

\[
\theta(p) = \sum_{n=1}^{N_{basis}} a_n \psi_n(p),
\]

where \( N_{basis}, a_n \) and \( \psi_n \) stand for the number of trial functions, the approximation coefficients and the trial functions, respectively. The approximation coefficients are obtained from collocation of Eq. (18) in points \( p_n; n = 1, 2, ..., N_{basis} \) where the values of \( \theta(p_n) \) are known. In this paper we use Hardy’s Multiquadratics (MQs) as trial functions

\[
\psi_n(p) = \sqrt{(p-p_n)^2 + C^2} + 1.
\]

where \( C \) stands for the free shape parameter. With the constructed collocation function, action of an arbitrary spatial differential operator \( L \) can be computed

\[
L[(p) = \sum_{n=1}^{N_{basis}} a_n L \psi_n(p).
\]

The implementation of the Dirichlet boundary condition is straightforward. In order to implement Neumann and Robin boundary conditions a special case of interpolation is needed. In these boundary nodes the function directional derivative instead of the function value is known and therefore the equation in the interpolation system changes to

\[
\theta_{bc} = \sum_{n=1}^{N_{basis}} a_n \left( \frac{\partial \psi_n}{\partial n} \right)(p) + b \psi_n(p).
\]

where \( a \) and \( b \) define considered boundary condition.

The well-known upwind stabilization technique, originally developed in connection with FDM by Courant [50], is being used to treat the completely advective solute transport. To minimize the numerical dissipation, the upwind offset is derived from the local field values and configuration of the influence domain. The proposed adaptive upwind scheme [51] uses local Péclet number to evaluate magnitude and direction of the upwind offset (6) (Fig. 2).

\[
\delta = \frac{v}{|v|} \left[ \text{cosh}(Pe) - \frac{1}{Pe} \right] p^\text{Birk} \sigma_{ij} W.
\]

where \( \delta_{ij} W \) is a parameter determining the maximum offset normalized to the characteristic influence domain \( p^\text{Birk} \). In the present case \( p^\text{Birk} \) is set to the maximal distance between the support domain nodes. The \( \delta_{ij} W \) is used to control the magnitude of upwind used. The described upwind has been already used in the context of LRBFCM in simulation of turbulent fluid flow [49]. In this work upwind is used for alleviating the instabilities of advection term in solute transport equation (4).
The temporal discretization is done through the use of two-level explicit time stepping

$$\rho_0 - \theta_0 = \nabla \cdot (D_0 \nabla \theta_0) - \nabla \cdot (\rho_0 \nu_0 \theta_0) + S_0,$$

where zero-indexed quantities stand for the values at the initial time, and $D$, $S$ for general diffusion coefficient, and source term, respectively. The time step is denoted with $\Delta t$. The pressure–velocity coupling is performed through the correction of the pressure, based on the divergence on the intermediate velocity ($\nabla \cdot \overline{\mathbf{v}}$), computed from discrete variant of Eq. (2).

$$p^{m+1} = p^m + \frac{1}{\Delta t} \nabla \cdot \overline{\mathbf{v}}^m,$$

with index $m$ bookkeeping the iteration. The corrected pressure is used to re-compute new intermediate velocity. The iterations take place until a reasonably solenoidal velocity field is achieved. The approach has been extensively tested in [22,42]. The represented coupling is similar to the artificial compressibility method (ACM) [52,53] or the SOLA approach [54]. However, the ACM and SOLA do not use internal iteration for velocity correction and as such do not assure precise transient solution.

The coupling between the conservation equations and the phase change is also determined locally. The use of Level rule for determination of the phase change simplifies the coupling to the

![Fig. 2. Scheme of the upwind technique in the meshless context. The function value is calculated instead of in the considered node in the upwind offset position.](image)

![Fig. 3. Definition of benchmark control points and cross-section lines. $P$ stands for control points, $V$ for vertical and $H$ for horizontal cross-section lines.](image)

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following closed form solution \[48\]

\[
af^2 + bf + c = 0, \\
a = (k_p - 1)L, \\
b = (k_p - 1)(c_p T_F - h) - k_p L, \\
c = k_p (h - c_p T_F) - c_p m_L C. \\
\]

\[25\]

4. Numerical implementation

The presented numerical methodology is implemented in C++ programming language and compiled with Intel compiler 13. The numerical method, including the pressure velocity coupling, is completely local, therefore the bulk of the computationally demanding part of the code is parallelized through the OpenMP.

Fig. 4. Concentration and velocity at different stages of solidification. Last (bottom right) plot stands for fully solidified state.
API. All computations are done on CPU Intel(R) Xeon(R) E5520 @ 2.27 GHz based computers. A detailed execution performance of the presented numerical methodology, i.e. speedup analyses, cache utilization, etc, has been recently presented for a shared memory parallelization \[55\] and for multiple Graphics Processing Units \[56\].

In all computations five nodded support domains are used and the meshless shape parameter is set to $c = 90$. All computations are done with time step $\Delta t = 10^{-5}$ and pressure–velocity relaxation parameter is set to $\zeta = 10^{-8}$.

\section{5. Results and discussion}

The solidification of Sn–10\%Pb alloy is considered with the process parameters defined in Table 1. The solidification transient starts with a well-mixed ($C_0 = 10\%$), stationary over-heated liquid ($T_0 = 220\,^\circ$C). The heat is extracted from the right side of the domain, described by the Robin boundary conditions. As the initial liquid cools, the thermo-solutal natural convection is set up.

The thermal and solutal natural convection (7) drives the flow clockwise. The solidification process starts when the liquid temperature reaches the Liquidus temperature (Table 2). The main characteristics of the segregation are visible soon after the beginning of the solidification. The only mechanism for solute transport is the advection (4) thus the segregation characteristics, at least on a global scale, depends only on the main flow behavior. A positive segregation patch at the bottom of the enclosure and a negative segregation patch in the upper part is clearly visible. The pattern can be explained by combining Eq. (3) and Eq. (10) into

\begin{equation}
\frac{\partial C}{\partial t} = -\frac{1}{m_L} \mathbf{v} \cdot \nabla T
\end{equation}

Eq. (26) shows the dependence of segregation tendency on the direction of the flow and the isotherms (note that $m_L < 0$). The isotherms are in both cases similar, therefore the macrosegregation

- Fig. 5. Concentration horizontal (left) and vertical (right) cross-sections of the steady state concentration profile.
- Fig. 6. Temporal development of temperature in control points.
- Fig. 7. Temporal development of liquid fraction in control points.
- Fig. 8. Temporal development of concentration in control points.
profile is governed by the flow only. Besides the macrosegregation, the formation of mesosegregates starts in the mushy zone as the solidification front advances. The channel-like anomalies in concentration field occur as a consequence of instabilities in the porous mushy zone. The solidification in the channels is slowed down, i.e. the solid fraction in the channels is lower and consequently the hydrodynamic permeability is higher. The lower drag in the channels makes the flow through the channels stronger, and the stronger flow induces stronger segregation (26). The mechanisms of the initial destabilization are still unknown. It is not yet clear what generates the first perturbation. However, phenomenon has been observed experimentally [57], which confirms that such behavior is not a product of numerical instabilities but of a not yet explained natural phenomenon. After a first perturbation the strong couplings between transport mechanics and phase change amplify the effect until the material is completely solidified.

The solidification process is presented in Fig. 4, where the concentration profiles, together with the velocity fields, are plotted for different stages of the solidification. The results are computed with 27,000 uniformly distributed nodes and upwind magnitude \( \sigma_{UW} = 0.5 \). The results are further analyzed on cross-sections and control points defined in Fig. 3. In Fig. 5 horizontal and vertical cross-sections of steady-state concentration are presented. Furthermore, temporal developments of temperature (Fig. 6), liquid fraction (Fig. 7), and concentration (Fig. 8) are presented in nine control points. (P1-9). The adaptive upwind stabilization of the advection term is used to solve the problem. The magnitude of the stabilization should be minimal, since the upwind introduces artificial numerical diffusion. The analysis of the influence of the upwind magnitude is presented in Fig. 9. It can be clearly seen that a

**Fig. 9.** Effect of the upwind magnitude on the simulation results. The concentration cross-sections at \( V_1 \) for different upwind magnitudes.

![Concentration cross-sections at V1 for different upwind magnitudes.](image1)

**Fig. 10.** Convergence plots as a function of the density of spatial discretization in terms of mean (top left), maximum (top right), and minimum (bottom left) value, and standard deviation (bottom right) of the steady state concentration.

![Convergence plots as a function of the density of spatial discretization.](image2)

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stronger upwind diminishes the mesosegregation patterns, but when using too low upwind, the results diverge. Respectively, we use a reasonably small upwind magnitude ($\sigma_{uw} = 0.5$).

Finally, we present the convergence plot in terms of mean, max and min value, and standard deviation of steady state concentration profile in Fig. 10.

Five computer codes have been recently used to simulate a similar (Exercise 2 from in [4]) with mesosegregates, as tackled in the present paper. Four computer codes were based on the finite volume formulation and one code was based on the finite element method with unstructured triangular mesh. We can observe that even though the qualitative macrosegregation pattern with mesosegregates of the different solutions is the same, notable differences exist in the evolutions and local behavior. The main differences are located in the channels and in their vicinity. The number of channels and the intensity of segregation inside the channels vary from one computer code to another. Even with fine meshes, it has not been possible to find a unique solution, mesh independent and similar to all the contributions. See the details in [4]. Respectively, also the contribution in the present paper cannot be considered as fully converged, however we believe the best on the involved node density. The present paper shows that LRBFCM is capable of solving such complex problems. Furthermore, the local pressure-velocity coupling is successfully employed for computations of fluid-flow through the mushy zone in the presence of instabilities.

6. Conclusions

A physical model for calculating the macrosegregation with mesosegregates in the cast has been numerically solved in the present paper. The conditions correspond to the numerical Exercise 1 in [21]. By the best knowledge of the present authors no other published references exist with respect to the tackled case. Extensive tabulation of the results has been done respectively, in order to facilitate comparisons with alternative numerical approaches. The problem is highly nonlinear, since it includes

- completely advective transport of species that is unstable by its nature,
- potential unstable natural convection in the low-Prandtl liquids such as metals,
- the high jump in the enthalpy near the phase change,
- and the presence of two flow regimes; free fluid and Darcy porous media flow in the mushy zone.

The nonlinearities are combined with the following strong couplings:

- between the mass and momentum conservation,
- between the momentum transport and energy and solute transport via buoyancy force,
- between the thermal field, concentration field and permeability,
- between the permeability and fluid flow.

The LRBFCM is for the first time used to solve macrosegregation problems that exhibits mesosegregation as a consequence of the above listed physical features. We demonstrate that such complex problems can be tackled with the represented extremely straightforward and intuitive meshless numerical approach that needs to include adaptive upwind. We measure the effect of this stabilization tool on the results and show high sensitivity of the results on the selection of the upwind magnitude. The proposed novel meshless method shows several convenient properties like straightforward implementation and parallelization suitability, CPU effectiveness and several degrees of freedom for optimization, which makes the method flexible. The dynamic point adaptivity strategy [58,59] makes it a promising alternative even for complex problems of the same kind. This might replace the need for adaptive upwind. Related attempts are in the focus of our future research, together with coupling of the macro-mesoscopic predictions with the cellular automata based grain structure evolution. A compatible meshless strategy, relying on points instead of polygons has been developed recently [60].

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