Solution of solidification of a binary alloy by a local meshless technique

Gregor Kosec, Miha Založnik

Abstract—The present paper deals with the numerical simulation of a multiphase system. The solidification of a binary alloy in a rectangular domain is considered. Coupled volume averaged governing equations for mass, energy, momentum and species transfer are introduced as a governing system. The phase properties are resolved from the Lever solidification rule, the fluid dynamics in the porous mushy zone is modeled by a Darcy force and the liquid phase is assumed to behave like an incompressible Newtonian fluid. Double diffusive effects in the melt are modeled by the thermosolutal Boussinesq hypothesis. The governing equations are solved by the novel Local Radial Basis Function Collocation Method (LRBFCM). The fields of all physical quantities are represented on overlapping 5-noded sub-domains through collocation by using multiquadrics Radial Basis Functions (RBF). The involved first and second derivatives of the fields are calculated from the respective derivatives of the RBFs. The equations are solved through explicit temporal discretization and the pressure-velocity coupling is calculated through a local pressure correction scheme. The advantages of the represented meshless approach are its simplicity, accuracy, similar coding in 2D and 3D, and straightforward applicability in non-uniform node arrangements and adaptive node arrangements. The presented spatial discretization technique shows several convenient properties and possibilities for upgrade, whereas stays simple and extremely CPU efficient. On the other hand, the completely local solution procedure makes the implementation and parallelization straightforward (without solving big systems of equations).

Keywords—Meshless, LRBFCM, Local solution procedure, Binary alloy, Solidification, Natural convection, macrosegregation, mesosegregates.

I. INTRODUCTION

The computational modeling of solidification has become an important research subject due to its pronounced influence in better understanding of nature as well as in the development of the advanced technologies. The theoretical description of the chemical macrosegregation in solidification started in the Sixties [1] and more precise model studies in the Seventies [2]. Recently this topic has been treated in many applied works, e.g. for static casting [3], continuous casting of steel [4] and direct chill casting of aluminium alloys [5]. Besides the applications, the physical modeling of the problem is developing [6-10]. The performance of numerical methods for the solution of macrosegregation problems remains rather unexplored, however. Recently, substantial efforts were invested to study the behavior of different numerical methods in the prediction of macrosegregation [11] in the frame of the french SMACS project, where a call for contributions to two numerical benchmark test cases was launched [12]. In this work we present a solution of one of these benchmark tests by a novel meshless technique. It deals with the solidification of a Sn-10%Pb alloy. We show that meshless methods can efficiently tackle this kind of highly nonlinear problems.

The main complexities in solving physical models of alloy solidification are strong nonlinearities and strong couplings. The nonlinearities stem from the hyperbolic nature of the solute transport (completely advective transport) in the potentially unstable natural convection in low-Pr liquids such as metals, in the jump of the enthalpy in the mushy zone and in the two flow regimes in free fluid and in the flow resistant porous mushy zone. On the other hand, 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 less stable. The complexity of the prediction of macrosegregation is a consequence of the fact that the macrosegregation results from the entire transient history of the strongly coupled processes of mass, heat, momentum and solute transfer from the liquid state up to the end of solidification.

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 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, Kansa method [13-23]. However, this work is focused on one of the simplest classes of meshless methods in development today, the local point interpolation [24] Radial Basis Function [25] Collocation Method (RBFCM) [26]. Undoubtedly, these methods can be of great advantage in solving solidification processing problems. In the present paper we use a local variant of RBFCM [26], the Local Radial Basis Collocation Method (LRBFCM). The main advantage of
the local approach is that the spatial discretization problem is simplified to solving small systems instead of large global systems, which might become unstable for increasing number of computational nodes. The LRBFCM approach was recently successfully applied to several problems [27-30].

II. GOVERNING EQUATIONS

The physical model used to describe the macrosegregation in the present paper is based on the continuum Euler description of the conservation laws and on constitutive relations, contributing additional information regarding the diffusion transport, stresses, interfacial forces, buoyancy forces... The original derivation of the volume averaged model can be found in the paper of Ni and Beckerman [6] as well as in the follow-up papers [7, 9, 31] and later developments in the field [10].

In this paper the solidification of a binary alloy in a two-dimensional rectangular domain $\Omega$ with boundary $\Gamma$ is considered. A so-called “minimal” (simplified to the largest possible degree) solidification model is adopted. At the macroscopic scale it accounts for heat transfer, solute transport and for incompressible Newtonian flow (with additional Darcy drag in the mushy region), driven by thermosolutal natural convection. The Boussinesq hypothesis is used to describe the buoyancy force. The phase change is modeled assuming local thermodynamic equilibrium (Lever rule) at the scale of the solidification structures and is fully coupled with the macroscopic transport. The problem is formulated by the following system of partial differential equations, identical as proposed in [12].

$$\nabla \cdot \mathbf{v} = 0, \quad \rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{f}_L \cdot \nabla \mathbf{v} = -f_L \nabla P + \mu \nabla^2 \mathbf{v} - f_L \frac{\mu}{K} \mathbf{v} + f_L \mathbf{b},$$

(1)

$$\rho \frac{\partial h}{\partial t} + \rho \mathbf{v} \cdot \nabla h = \Delta \nabla^2 T,$$

(2)

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = 0; \quad C = f_L C_L;$$

(3)

$$\mathbf{v} = f_L \mathbf{v}_L, \quad K = K_0 \left(\frac{f_L}{1 - f_L}\right)^2,$$

(4)

$$\mathbf{b} = \rho_{\text{sat}} \left[1 - \beta_l (T - T_{\text{sat}}) - \beta_c (C - C_{\text{sat}})\right] \mathbf{g},$$

(5)

$$h = c_r T + f_L L,$$

(6)

$$C = \left[ f_L + \left(1 - f_L\right) k_p \right] C_L,$$

(7)

$$T = T_r + m C_L.$$

(8)

The transport equations describe the temporal evolution of the leading quantities, $\mathbf{v}, h, C$: superficial liquid velocity, enthalpy, and average concentration, respectively, as well as the pressure $P$. $\mathbf{v}_L$ stands for the intrinsic liquid velocity. The permeability $K$ is linked to a permeability constant $K_0$ and to the liquid fraction $f_L$ by the Kozeny-Carman relation (6). The thermal conductivity $\lambda$, specific heat $c_p$ and density $\rho$ of the solid and the liquid phase are assumed to be equal and constant. The liquid density varies only in the buoyancy term $\mathbf{b}$ (Boussinesq hypothesis), where it depends on the temperature $T$, the liquid concentration $C_L$, the thermal expansion coefficient $\beta_l$, the concentration expansion coefficient $\beta_c$, as well as on the reference density $\rho_{\text{ref}}$ given at reference temperature $T_{\text{ref}}$ and reference concentration $C_{\text{ref}}$. The viscosity $\mu$, the liquidus slope $m_L$ and the binary equilibrium partition coefficient $k_p$, are constant as well. The symbols $I, \mathbf{g}, T_r$ stand for time, gravity acceleration and the fusion temperature of the pure solvent, respectively. The solute diffusion is neglected at the macroscopic scale.

III. NUMERICAL SOLUTION PROCEDURE

The introduced physical model does not have a closed form solution and in order to solve it, an efficient numerical approach has to be employed. In this paper we use a novel local meshless approach with local pressure velocity coupling. Such an approach has already been successfully applied to several thermo-fluid problems [30, 32-35]. A general idea behind the local meshless methods is the use of local sub clusters of domain nodes, named local support domains, for the approximation of a field. With the selected support domain, an approximation function is introduced as a sum of weighted basis functions

$$\theta(p) = \sum_{n=1}^{N_{\text{basis}}} \alpha_n \Psi_n(p),$$

(9)

where $\theta$, $N_{\text{basis}}$, $\alpha_n$ and $\Psi_n$ stand for the approximation function, the number of basis functions, the approximation coefficients and the basis functions, respectively. The basis could be selected arbitrarily, however in this paper Hardy’s Multiquadrics (MQs)

$$\Psi_n(p) = \sqrt{\left|p - p^*\right|^2 / \sigma_c^2 + 1},$$

(10)

with $\sigma_c$ standing for the free shape parameter of the basis function, are used. By taking into account all support domain nodes and equation (11), the approximation system is obtained. In this paper we use collocation (the number of support nodes is the same as the number of basis functions). With the constructed collocation function an arbitrary spatial differential operator ($L$) can be computed

$$L \theta(p) = \sum_{n=1}^{N_{\text{basis}}} \alpha_n L \Psi_n(p).$$

(11)

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
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$$\theta_{sc} = \sum_{\alpha} \alpha \left( a \frac{\partial}{\partial n} \Psi_{\alpha}(p) + b \Psi_{\alpha}(p) \right).$$ (14)

For the temporal discretization we use two-level explicit time stepping

$$\rho_b \frac{\theta - \theta_0}{\Delta t} = \nabla \cdot (D \nabla \theta_b) - \nabla \cdot (\rho_b v_0 \theta_b) + S_b,$$ (15)

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 $\Delta t$. Pressure-velocity coupling is performed through the correction of the intermediate velocity

$$\tilde{v} = v_0 + \Delta t \left( -\nabla p_b + \nabla \cdot (\mu \nabla v_0) + b_v - \nabla \cdot (\rho \nu_0 v_0) \right).$$ (16)

The equation (16) did not take into account the mass continuity and so corrections are added

$$\tilde{v}^{n+1} = \tilde{v} + \xi \Delta t \frac{\rho}{\Delta t} \tilde{P}^{n+1} + \tilde{P},$$ (17)

where $m, \xi$ and $\tilde{P}$ stand for pressure velocity iteration index, velocity correction and pressure correction, respectively. By combining the momentum and the mass continuity equations the pressure correction Poisson equation emerges

$$\nabla \tilde{v} = \frac{\Delta t}{\rho} \nabla^2 \tilde{P}.$$ (18)

Instead of solving the global Poisson equation exactly, the pressure correction is guessed from the divergence of the intermediate velocity.

$$\tilde{P} = \frac{\ell^3}{\Delta t} \nabla \tilde{v}.$$ (19)

The proposed assumption makes solving of the pressure velocity coupling iteration local. Such an approach is very CPU efficient, as it needs only one computation for each pressure correction. With the computed pressure correction the pressure and the velocity can be corrected as

$$\tilde{v}^{n+1} = \tilde{v}^{n} - \zeta \Delta t \frac{\rho}{\Delta t} \tilde{P}^{n+1} + \zeta \tilde{P},$$ (20)

where $\zeta$ stands for the relaxation parameter. The iteration is performed until the criterion $\nabla \cdot \tilde{v} < \varepsilon_v$ is met in all computational nodes. The approach is similar to the artificial compressibility method, which has been recently under intense research [36-38] and in the framework of the Finite Differences Method to the SOLA approach [39]. Proposed numerical solution has been implemented in a C++ language and parallelized through an OpenMP protocol.

The coupling between micro and macro scales (conservation equations and phase change) is determined locally for each computational node. It can be computed analytically since the lever rule is used to describe phase change.

$$a \varepsilon_v^2 + b \varepsilon_v + c = 0,$$

$$a = (k_p - 1) L,$$

$$b = (k_p - 1)(c_p T_f - h) - k_p L,$$

$$c = k_p (h - c_p T_f) - c_p m_C L.$$ (21)

The details about the equation (21) coupling can be found in [5, 40].

Solutal transport in metallic materials is commonly advection dominated and under the proposed model assumption of zero diffusion on the macroscopic scale it is completely advective. Thus it can produce numerical instabilities from its hyperbolic nature. To alleviate this problem, the adaptive upwind technique [41] is used to solve the advection term in such transport equations.

IV. NUMERICAL EXAMPLE

In [40] it was shown that the presented “minimal” solidification model can be solved with the present meshless method for a case, where no mesosegregates (sharp banded “mesoscopic” instabilities in the concentration field) are present. The case was computed with two completely different numerical codes. The extensive comparisons showed good agreement. However, in the present paper we are presenting a solution of the SMACS benchmark solidification exercise [11] for the alloy Sn-10%Pb (see Table I for thermophysical properties). This case is numerically considerably more difficult to solve due to the presence of mesosegregates. As we explained later on, these present a challenge to the method of spatial resolution and equation coupling. A rectangular domain with dimensions 10x6 cm is considered. The initial and boundary conditions are set to

$$v(p, t) = 0,$$

$$\frac{\partial v}{\partial p}(p = 0, t) = \frac{\partial v}{\partial p}(p = 1, t) = \frac{\partial v}{\partial p}(p = l, t) = 0.$$ (22)

$$\frac{\partial}{\partial t} T(p, t) = \frac{\partial}{\partial t} T(p = 0, t) = \frac{\partial}{\partial t} T(p = l, t) = 0.$$ (23)

$$\frac{\partial}{\partial t} C(p, t) = 0,$$ (24)

$$\frac{\partial}{\partial p} C(p = 0, t) = 0,$$ (25)

$$C(p, t) = C(p = 0, t) = C(p = l, t) = C_0.$$ (26)

The case is schematically presented in Figure 1.

A case originates from call for benchmark solution under the SMACS project [12] and it is similar to the Hebditch and Hunt experiment [2]. The simulation starts with $T_0 = 220^\circ C$, $f_{eb} = 1$, $v_0 = 0 \text{ m/s}$, $C_0 = 10\%$, heat transfer coefficient is set to
The solidification process starts with cooling of the right wall through the Robin boundary. As the initial liquid cools, the thermo-solutal natural convection is set up. After about \( t \approx 40 \) s (Figure 2) the principal characteristics can be recognized: a positive segregation patch at the bottom of the enclosure and a negative segregation zone in the central upper part. This pattern is easily explained by combining eq. (3) and eq. (10)

\[
d\frac{C}{dt} = -\frac{1}{m_L} \cdot \mathbf{v} \cdot \nabla T, \tag{29}
\]

which shows that the segregation tendency depends on the direction of the flow with respect to the isotherms (note that \( m_L < 0 \)). The solidification, and thus the advancement of the mushy zone, is retarded at the bottom due to local enrichment, and accelerated at the top due to local depletion in solute.

Furthermore, we can already see the development of channel mesosegregates in the lower half of the enclosure. These banded segregation structures occur due to instabilities in the porous mushy zone in the form of “channels”. The solidification in the channels is retarded; the solid fraction in the channels is thus lower and the hydrodynamic permeability higher. Due to the lower drag in the channels, the flow through the mushy zone passes preferentially along the channels. The higher flow rate induces stronger segregation along the channels as can be explained by eq. (29). After 600 s the system reaches the final solidified state (Figure 3). In Figure 3 the final macrosegregation map is presented, where one can clearly see the “channels” in concentration field at the bottom of the domain. The mechanisms of the destabilization of the mushy zone are still unknown. Right now it is not yet clear what triggers the first perturbation and in which field. However, such mesosegregates have been observed experimentally \[42\] and it is clear that such behavior is present in nature and that it is not induced by numerical instability. After a first perturbation of the mushy zone, the strong couplings in the system amplify the effect, which grows until the material completely solidifies. The instabilities are captured in the cross-section of the concentration profile (Figure 4) at \( p_y = 1.0 \) cm.

Recently, the identical physical model was solved with the present meshless method for an Al-4.5% Cu alloy \[40\] in order to assess the dynamics and behavior of such problems. While the basic phenomena in that case were the same, mesosegregates were not present. The fields were therefore smoother and the system dynamics less sensitive due to the absence of instabilities. The analysis showed good convergence behavior of the meshless method and comparisons with a finite-volume method showed very good agreement of the solutions in all aspects. The present paper extends the problem to a much more complex situation. The solidification of Sn-10%Pb produces instabilities in the macrosegregation map, which are hard to resolve due to steep local gradients of velocity, pressure and concentration. Furthermore they are sensitive to the spatial resolution \[43\]; a sufficient resolution is necessary to resolve them. Currently, the topic is under extensive research under the French project SMACS \[11, 12, 43, 44\]. Results from different numerical codes are compared in order to understand the behavior and to see if reasonable agreement between different numerical methods and computational codes can be found. In order to confirm the benchmark solution there is an ongoing experiment, as well.

The time evolution of the simulation is presented through the normalized values in the mid-point (\( p_x = 2.5 \) cm and \( p_y = 3.0 \) cm) (Figure 5), where the quantities are normalized as

\[
\tilde{\theta} = \frac{\theta(t) - \theta(t = 600)}{\theta(t = 0) - \theta(t = 600)} . \tag{30}
\]

The results presented in present paper were computed with the local explicit LRBFCM on 26996 uniformly distributed nodes. Support domains were constructed by selecting the central node and closest four nodes. For temporal discretization a time step of \( 1e^{-5} \) s has been used and the pressure-velocity coupling relaxation parameter has been set to \( 1e^{-7} \).
TABLE I
THERMOPHYSICAL AND PROCESS PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (ρ)</td>
<td>7.00e+03  kg/m³</td>
</tr>
<tr>
<td>Specific heat (cₚ)</td>
<td>2.60e+02  J/kgK</td>
</tr>
<tr>
<td>Thermal conductivity (λ)</td>
<td>0.55e+02 W/mK</td>
</tr>
<tr>
<td>Latent heat of pure Al (L)</td>
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</tr>
<tr>
<td>Liquid dynamic viscosity (μ)</td>
<td>1.00e-03 Pa s</td>
</tr>
<tr>
<td>Thermal expansion coefficient (βₜ)</td>
<td>6.00e-05 K⁻¹</td>
</tr>
<tr>
<td>Solutal expansion coefficient (βₜ)</td>
<td>-5.30e-03 %⁻¹</td>
</tr>
<tr>
<td>Reference temperature (Tᵣ)</td>
<td>2.20e+02 °C</td>
</tr>
<tr>
<td>Reference concentration (Cᵣ)</td>
<td>1.00e+01 %</td>
</tr>
<tr>
<td>Reference density (ρᵣ)</td>
<td>7.00e+03 kg/m³</td>
</tr>
<tr>
<td>Gravity acceleration (g)</td>
<td>g = 9.80e+00 m/s²</td>
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<tr>
<td>Permeability constant (Kₚ)</td>
<td>2.34e-11 m⁻¹</td>
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<tr>
<td>Pure Sn melting temperature (Tₛ)</td>
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<tr>
<td>Sn-Pb eutectic temperature (Tₑ)</td>
<td>1.83e+02 °C</td>
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<tr>
<td>Eutectic concentration (Cₑ)</td>
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</tr>
<tr>
<td>Cu solubility in Al at eutectic temperature (Cₑ)</td>
<td>2.49e+00 %</td>
</tr>
<tr>
<td>Liquidus slope (mₑ)</td>
<td>-1.28e+00 °C/%</td>
</tr>
</tbody>
</table>

V. CONCLUSIONS AND PERSPECTIVES

The present paper is focused on the numerical simulation of a multiphase system, more precisely on the coupled heat and mass transport during solidification of a binary Sn-10%Pb alloy. In addition to the complex couplings of the solidification model, the solution of this specific problem is a particular challenge due to the presence of channel mesosegregates. These structures develop as a consequence of instabilities of the coupled heat and mass transport and develop sharp gradients of concentration, velocity and pressure. Their resolution requires a proper full coupling of the governing equations and an ability of the numerical method to deal with the localized high gradients.

It has been shown that even the simplest possible local meshless method 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.

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 flexible point adaptivity strategy [45] makes it a promising alternative for such complex problems. The focus of our future work is on implementation of more sophisticated meshless technique, including the adaptive node distribution strategy, in order to capture more details about the mesosegregates formation.

REFERENCES


