An explicit scheme for coupling temperature and concentration fields in solidification models

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Abstract

A numerical scheme for coupling temperature and concentration fields in a general solidification model is presented. A key feature of this scheme is an explicit time stepping used in solving the governing thermal and solute conservation equations. This explicit approach results in a local point-by-point coupling scheme for the temperature and concentration and avoids the multi-level iteration required by implicit time stepping schemes. The proposed scheme is validated by predicting the concentration field in a benchmark solidification problem. Results compare well with an available similarity solution. The simplicity of the proposed explicit scheme allows for the incorporation of complex microscale models into a general solidification model. This is demonstrated by investigating the role of dendrite coarsening on the concentration field in the solidification benchmark problem.

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1. Introduction

A general solidification, see Fig. 1, involves a spatial region over which both solid and liquid coexist—a so-called “mushy region.” Often the scale required for the resolution of the solid–liquid interface, in this region, is several orders smaller than the typical cell size used in a discrete numerical solution of the governing macroscopic transport equations. A powerful modeling concept
in this situation is the representative volume element (REV), introduced to the solidification modeling community by Ni and Beckermann [1]. Typically a REV is selected to include a representative and uniform sampling of the mushy region such that local scale solidification processes can be described by variables averaged over the REV.

The combination of the macroscopic transport equations and the specification of the nature of the REV can be used to provide a description of a given solidification system. Fig. 1 illustrates a general alloy system solidifying in a two-dimensional domain. The material in the domain is initially liquid. Solidification is initiated on cooling the left-hand wall. The remaining sides of the domain are insulated. In this system both the solid and liquid phases can flow. The liquid flow can be driven by thermal and solutal buoyancy, shrinkage and forced convection. In the solid phase any columnar structure will move with a prescribed velocity, the casting speed. At low solid fraction, however, equiaxed solid grains can have an independent velocity field that requires the specification of an equation of motion for its resolution [2]. At high solid fractions the equiaxed grains will consolidate and in some systems will move with the prescribed solid phase velocity. An important consequence of the flow in the mushy region is the large-scale transport of the solute components and as a result—in addition to solute variations over the sub-REV (microsegregation)—the solute varies over the domain as a whole (macrosegregation).

A key part in modeling the general system shown in Fig. 1 is the coupling between the temperature and concentration fields [3–10]. The main variables describing these fields are found by solving conservation equations on the macroscale of the REV. A complete resolution, however, requires a coupling between the solid fraction, liquid and solid concentrations, and temperature at the sub-REV scale (local scale) of the dendritic arm spaces. This paper will focus on the development of a general numerical approach for coupling the temperature and concentration fields. In a departure from many of the previous schemes [3–9] the proposed approach uses an explicit time stepping scheme to solve the thermal and concentration conservation equations. The disadvantage of a small time step for stability is offset by a straightforward numerical scheme that can readily incorporate multi-scale behavior. This simplicity is illustrated by the incorporation into the solution algorithm of local scale microsegregation models that can accurately account for both back-diffusion and coarsening effects.

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**Fig. 1.** A general solidification system.
2. Model variables

The essential part of a solidification model is the definition of a set of consistent variables that can describe the state of the solidification. In terms of the general description of solidification systems offered in Fig. 1 four separate types of variable can be identified.

2.1. Microscopic variables

These variables vary at each point in the REV. In many solidification systems heat transport and mass transport in the liquid phase is relatively rapid and it is often reasonable to assume that the solid concentrations of the alloy components, \( C^k_s \), will be the only microscopic variables. Development of macroscopic equations that involve solid concentrations use the intrinsic volume average over the solid phase in the REV, i.e.,

\[
\langle C^k_s \rangle_s = \frac{1}{g} \int_0^g C^k_s \, d\Gamma,
\]

where \( g \) is the solid volume fraction in the REV and the superscript \( k \) is a marker for the \( k \)th component of an \( m \) component system.

2.2. Messo variables

These variables are uniform in the REV. If heat and liquid mass transport is relatively rapid the messo variables are temperature \( T \), liquid solute concentrations \( C^k_l \), solid phase enthalpy

\[
h_s = c_s T,
\]

where \( c_s \)—which in general can be a function of temperature and concentration—is a specific heat term, and liquid phase enthalpy

\[
h_l = c_l T + \Delta H,
\]

where \( c_l \)—which in general can be a function of temperature and concentration—is a specific heat term and \( \Delta H \) is the latent heat of fusion at a reference temperature.

2.3. Macroscopic-mixture variables

These variables describe the state of the REV. They are the main variables in the mixture macroscopic transport equations. Appropriate definitions are

Mixture enthalpy

\[
[\rho H] = g \rho_s h_s + (1 - g) \rho_l h_l.
\]

Mixture concentration (for a given solute component, \( k = 1, 2, \ldots, m \))

\[
[\rho C]^k = g \rho_s \langle C^k_s \rangle_s + (1 - g) \rho_l C^k_l.
\]
2.4. Flow variables

In this work the solid phases are assumed to be stationary. Although this leads to a limited version of the general system shown in Fig. 1 the columnar dendritic system represented is an appropriate model for a wide range of practical situations. If in addition the liquid flow is uniform over the REV then equations of motion for the liquid phases can be developed in terms of \(U(U,V)\)—the interdendritic volume flow

\[
U = (1-g)u_l, \tag{6}
\]

where \(u_l\) is the actual fluid velocity.

3. Governing equations and solution algorithm

In this section the main equations and steps in a general solution scheme for an alloy solidification are outlined.

3.1. Equations for conservation of heat and solute

Mixture macroscopic conservation equations for heat and solute are derived on adding the two-phase averaged equations presented by Ni and Beckermann [1]. Neglecting dispersive fluxes, using Fourier’s law and expanding the phase enthalpies in terms of temperature (see Eqs. (2) and (3)) the mixture heat equation is

\[
\frac{\partial [\rho H]}{\partial t} + \nabla \cdot (\rho_l U_c_l T + \rho_l U \Delta H) = \nabla \cdot (K \nabla T), \tag{7}
\]

where \(K\) is a phase averaged conductivity (e.g., \(K = gK_s + (1-g)K_l\)).

Neglecting dispersive and macroscopic diffusion fluxes the mixture solute conservation equation is

\[
\frac{\partial [\rho C^k]}{\partial t} + \nabla \cdot (\rho_l U C^k_l) = 0. \tag{8}
\]

There is one conservation for each of the solute components, \(k = 1, 2 \ldots m\), in the alloy.

3.2. Coupling relationships

The full solution of the thermal and solute field requires additional coupling relationships. Two obvious relationships are the definitions of the mixture enthalpy \([\rho H]\), Eq. (4), and the mixture concentration \([\rho C]\), Eq. (5). Two additional relationships are obtained by (1) considering the local scale redistribution of solute in the REV (a process referred to as microsegregation), and (2) enforcing thermodynamic equilibrium at the solid–liquid interface.

A microsegregation relationship is obtained on noting, from the definition in Eq. (1), that the rate of change of a solute species in the solid fraction of the REV can be written as
\[
\frac{dg(C^k_s)}{dt} = k_{\text{par}} C^k_C \frac{dg}{dt} + \int_0^s \frac{\partial C^k_s}{\partial t} d\Gamma.
\] (9)

The components on the right-hand side of this equation depend on the redistribution of solute species during the solidification. The first term on the right of Eq. (9) accounts for the partitioning of a solute species at the solid–liquid interface in the REV. In this case thermodynamic equilibrium has been assumed such that \( C^k_s = k_{\text{par}} C^k_C \) where \( k_{\text{par}} \) is the partition coefficient. In the liquid fraction of the REV the partitioned solute species are rapidly mixed and the liquid concentrations remain uniform. In the solid, however, mass-diffusion is relatively slow and solute gradients will form. Along these gradients solute will back diffuse from the interface, increasing the solute content of the REV solid fraction. The second term on the right side of Eq. (9) accounts for this back-diffusion of solute into the solid. An approximate, more practical, form of Eq. (9) is obtained on noting that the back-diffusion term can be represented as \[11\]

\[
\int_0^s \frac{\partial C^k_s}{\partial t} d\Gamma = \beta g k_{\text{par}} \frac{dC^k_C}{dt},
\] (10)

such that Eq. (9) becomes

\[
\frac{dg\langle C^k_s \rangle}{dt} = k_{\text{par}} C^k_C \frac{dg}{dt} + \beta g k_{\text{par}} \frac{dC^k_C}{dt},
\] (11)

where \( 0 < \beta < 1 \) is a diffusion parameter. In an Appendix A it is shown that the approximation in Eq. (10) is an accurate description of microsegregation processes, consistent with previous models in the literature, and that an appropriate definition of \( \beta \) can be found that accounts for microsegregation phenomena such as back-diffusion and arm coarsening in the REV.

Enforcing thermodynamic equilibrium at the solid–liquid interface provides another coupling relationship. Under this condition, during primary solidification, the temperature and the liquid concentrations are related via the liquidus surface of the phase diagram

\[
T = G(C^1_C, C^2_C, \ldots, C^k_C),
\] (12)

and at the solid–liquid interface the solid concentration of a given species \( (j) \) is

\[
C^j_s = k_{\text{par}} C^j_C.
\] (13)

Solidification of secondary phases will depend on the particular details of the phase diagram and more specific forms of Eqs. (12) and (13) may be required. For example, in a binary-eutectic alloy, during primary solidification the temperature and liquid concentration are related through the liquidus surface (line)

\[
T = T_f - mC_1,
\] (14)

where \( T_f \) is the fusion temperature of the pure solvent and \( m \) is the slope (assumed constant) of the liquidus line. Further the concentration in the primary \( \alpha \) solid, at the solid–liquid interface, is \( C_s = k_{\text{par}} C_1 \). When the eutectic concentration is reached, however, although there is partitioning between the primary \( \alpha \) phase and secondary \( \beta \) phase, there is no net solute partitioning between the combined solid phases and the liquid, and further solidification occurs isothermally at the eutectic temperature, \( T = T_{\text{eut}} \).
3.3. Coupling overview

After a suitable space discretization an explicit time stepping solution of Eqs. (7) and (8) will
directly generate, at each time step, nodal values for the mixture enthalpy $[\rho H]$ and mixture
concentrations $[\rho C]^k$. In order to move the solution forward the following fields

- the liquid concentration, $C^k_l$,
- the intrinsic volume averaged solid concentrations, $\langle C^s \rangle^k$,
- the solid volume fraction, $g$,
- the temperature, $T$,

need to be obtained from these mixture fields.

In a general sense, this solute–thermal coupling requires at each node point in the domain an
iterative solution of the non-linear equation set formed by

- the definition of the mixture enthalpy $[\rho H]$, Eq. (4),
- the definition of the mixture concentration $[\rho C]$, Eq. (5),
- a finite difference approximation of the microsegregation model, Eq. (11),
- a phase diagram relationship, e.g., Eq. (12).

The exact form of these equations and the development of a solver depends on the nature of the
solidification system under study. It is vital to note, however, that by the use of the explicit solver
of the enthalpy and solute conservation equations any solution will be purely local. Thus solution
can be done in a point-by-point fashion with the solution at one node independent of the solution
at any other node. There is no need to recalculate any macroscopic fields as part of the
solution process. The nature of this point-by-point coupling is the key strength of the proposed
explicit time integration scheme. Although there may be a loss in efficiency through the need of a
small time step the approach allows for a great flexibility and generality in dealing with a diverse
range of solidification systems which involve complex coupling relationships in the two-phase
REV.

3.4. Coupling for binary-eutectic alloy

The general coupling method is illustrated on considering a version suitable for a binary-
eutectic alloy.

After solution, at a given time step, for the nodal fields of $[\rho C]$ and $[\rho H]$ each node is called at in
turn and the following steps carried out.

1. The mixture concentration quantity, $C^s$, is estimated from

$$[\rho C] - \rho_l (1 - g^{\text{old}})C^s = [\rho C]^{\text{old}} - \rho_l (1 - g^{\text{old}})C_1^{\text{old}}. \quad (15)$$

An appropriate definition for $C^s$ is the liquid concentration that would result if macrosegrega-
tion, occurred without solidification or back-diffusion into the solid fraction.

2. The equilibrium temperature corresponding to $C^s$ is calculated from the liquidus line in the
phase diagram
\[ T_{\text{equ}} = T_f - mC^s. \] (16)

3. The value of \( T_{\text{equ}} \) is used to determine if solid can form, at the current node, in the given time step. If the condition
\[ \frac{[\rho H] - \rho_i c_l T_{\text{equ}}}{\rho_i \Delta H} > 1, \] (17)
holds solid cannot form and the following settings are made,
\[ g = 0, \quad T = \frac{[\rho H] - \rho_i T}{\rho_i c_l}, \quad \text{and} \quad C_1 = C^s. \]

4. A value of \( g^\text{old} = 1 \) indicates that the phase change is complete at the give node. In this case the only action to complete the solution in the time step is to calculate the nodal temperature, \( T = \frac{[\rho H]}{\rho_c c_p} \).

5. Not meeting the conditions in steps 3 and 4 indicates that a phase change will occur at the node. In this case an iterative loop is required to extract the values of \( T, \, g, \, C_1, \, \text{and} \, \langle C_s \rangle^r \) from the nodal values of \([\rho H]\) and \( C^s\), for use at the next time step.
   - Obtain an initial estimate of \( g^r \)
   \[ (1 - g^r) = 0.5(1 - g^{r-1}) + 0.5 \frac{[\rho H] - [\rho c_p] T^{r-1}}{\rho_i \Delta H}, \] (18)
   where \( r \) is an iteration counter and the iterations are seeded by using old time values. The value 0.5 is an under-relaxation factor.
   - The small part of the liquid \( (g^\text{old} - g) \) that solidifies in the given time step is assumed to solidify according to the lever rule, hence estimates for the liquid concentration \( C_1^r \) can be obtained from the mass balance
   \[ \rho_i (1 - g^\text{old}) C_1^r = \rho_s (g^r - g^\text{old}) k C_1^r + \rho_i (1 - g^r) C_1^r - \rho_s \beta k g^r (C_1^r - C_1^\text{old}). \] (19)
The last term arising from the microsegregation model (11).
   - The current value of \( C_1^r \) will provide updates for the temperature \( T^r \) through the equilibrium relationship (14), viz.
   \[ T^r = T_f - mC_1^r, \] (20)
   where \( C_1^r \) is pegged to be below the eutectic concentration \( C_{\text{eut}} \).
   - The last step in the iteration loop is to update the average concentration in the solid
   \[ \langle C_s \rangle^r = \langle C_s \rangle^\text{old} + (g^r - g^\text{old}) k C_1^r + \rho_s \beta k g^r (C_1^r - C_1^\text{old}). \] (21)

6. The above iterations, usually converge in 3–5 iterations. If during these step the calculated solid fraction rises above 1, indicating a completion of the solidification the settings \( g^r = 1, \, \text{and} \, T_j = \frac{[\rho H]}{\rho_c c_p} \) are made.

3.5. Equations of motion

The last the solution step is to solve for the velocity field. Due to the explicit time integration of the thermal and solutal fields this step can be carried out independently and global iteration that involves the concentration and temperature fields is not required.
Under the assumption of a fixed columnar microstructure the equation of motion for the liquid interdendritic velocity \( \mathbf{U} = (U, V) \) can be written in the general form

**U-momentum:**

\[
\frac{\partial}{\partial t} (\rho U) + \nabla \cdot (\rho U U) = -(1 - g) \frac{\partial p}{\partial x} + \nabla \cdot [(1 - g) \mu \nabla U] - M_x,
\]

(22)

**V-momentum:**

\[
\frac{\partial}{\partial t} (\rho V) + \nabla \cdot (\rho U V) = -(1 - g) \frac{\partial p}{\partial y} + \nabla \cdot [(1 - g) \mu \nabla V] - \rho_l (1 - g) g_{\text{rav}} - M_y,
\]

(23)

**Continuity:**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0.
\]

(24)

**Note:**

The vector term \( \mathbf{M} = (M_x, M_y) \) accounts for additional terms, in particular terms arising from the two-phase nature of the mushy region. Beckermann and Wang [2] provide a detailed accounting of the exact nature of these terms for a wide range of solidification systems. The leading role of the term is to account for the friction between the solid and liquid fractions and reduce the velocity \( \mathbf{U} \) to zero as the solid fraction \( g \) approaches 1. In this way a somewhat ad hoc but often used model for \( \mathbf{M} \) is to treat the two-phase region as a porous media and use the Carman–Kozeny relationship

\[
\mathbf{M} = K_0 \frac{g^2}{(1 - g)^3} \mathbf{U}.
\]

(25)

If the Boussinesq assumption is invoked the body force term in the \( y \)-momentum equation is modeled as

\[
\rho_l g_{\text{rav}} = \rho_l^{\text{ref}} g_{\text{rav}} \left( \beta_T (T - T^{\text{ref}}) + \sum \beta_C^{\text{ref}} (C^{\text{ref}} - C^{\text{ref}}) \right),
\]

(26)

where \( \rho_l^{\text{ref}} \) is a constant reference density, \( \beta_T \) is thermal expansion coefficient, and \( \beta_C^{\text{ref}} \) are the solutal expansion coefficients.

### 4. Testing

#### 4.1. Testing overview

Testing of algorithms for investigation of heat and mass transfer systems require two steps. (1) A test to confirm that the proposed solution algorithm accurately solves the model equations, and (2) a comparison with experimental data to confirm that the underlying model is a reasonable representation of the physical situation. The focus of this paper is the establishment of an explicit coupling scheme for the thermal solutal part of a general solidification model. In this circumstance the principle interest will be to confirm that the proposed solution approach is accurate. Towards this end a test system involving the “inverse” segregation in a binary-eutectic alloy cooled from
below will be investigated. This system has been used extensively in the literature in both experimental and numerical studies [12–15]. In particular the current author has proposed a benchmark problem that admits a similarity solution for testing the accuracy of a given numerical scheme [16]. Even though this problem has been previously solved in the literature [6,17], it is valid to use here to test the newly proposed explicit scheme for thermal solute coupling.

4.2. The benchmark problem

Consider a binary-eutectic alloy cooled by a fixed temperature, \( T_{\text{chill}} < T_{\text{eut}} \), at its base \( z = 0 \). Fig. 2 shows a schematic of the system, note that in this system the vertical distance from the chill is given in terms of the similarity variable \( \xi \). As solidification moves upwards, due to the shrinkage, a liquid flow is induced down towards the chill. The effect of this down-flow is to increase the solute content in the solidification region, creating, on final solidification, a positively segregated \((C > C_0)\) solid. Appropriate values for the benchmark are given in Table 1. Note these are close to an aluminum–copper alloy but the solid–liquid density ratio has been increased to fully illustrate the effect of flow on the final concentration field. Further, a fixed chill temperature and a small superheat \((T_{\text{sup}} = 1)\) has been imposed a requirement if the system is to admit a similarity solution [16].

For the limit microsegregation cases of zero solid diffusion \((\beta = 0 \text{ in Eqs. (19) and (21)})\) and complete solid diffusion \((\beta = 1 \text{ in Eqs. (19) and (21)})\) Voller provides predicted concentration \((\frac{[C]}{[C]_0} = \frac{q}{[C]_0})\) profiles from the similarity solution (Table 2 in Ref. [16]). These values will be used for comparisons purposes in this paper.

![Fig. 2. An inverse segregation system.](image-url)
4.3. Explicit scheme compared with the benchmark

The key simplification in the inverse segregation system, Fig. 2, is that the flow field (the shrinkage-induced flow towards the chill) is one-dimensional and can be effectively determined with the mass continuity equation alone. Under this observation the steps, in a given time step, of the proposed explicit scheme are as follows:

1. Solve for the mixture concentration, use an explicit finite difference scheme of Eq. (8), viz.

$$[\rho C]_I = \frac{\Delta t}{\Delta x} [\rho]_I (U_{I+1}C_{I+1} - U_I C_I),$$

(27)

where all terms on the right are determined at the old time level, $I$ is the nodal position, node $I$ is nearer the chill than node $I + 1$, $U_I$ is the interdendritic fluid velocity at the interface between node $I - 1$ and node $I$, and an upwinding treatment that assumes that flow is always towards the chill has been employed.

2. Solve for the enthalpy, also using an explicit scheme, i.e., from Eq. (7)

$$[\rho H]_I = \frac{\Delta t}{\Delta x^2} K(T_{I-1} - 2T_I + T_{I+1}) - \frac{\Delta t}{\Delta x} [\rho]_I (U_{I+1}C_{I+1} - U_I C_I) - \frac{\Delta t}{\Delta x} \rho I H(U_{I+1} - U_I).$$

(28)

3. Invoke the coupling scheme, Eq. (15)–(21) to obtain the current nodal values for the liquid concentration, $C_L^k$, the solid concentrations, $\langle C_s^k \rangle$, the solid volume fraction, $g$, and the temperature, $T$.

4. Solve for the flow, use the continuity equation, viz.

$$U_I = U_{I+1} + \frac{\Delta x (|\rho|_{I+1} - |\rho|_I)}{\rho I \Delta t},$$

(29)

where all terms are at the current time level.

Solution is carried on a grid of 401 nodes in a domain of length 0.4 m. Results, predictions of concentration, are compared with the similarity values tabulated by Voller [16]. Fig. 3 shows results for the case of no back-diffusion, $\beta = 0$, and complete solid state diffusion $\beta = 1$. These results clearly show that the proposed method can provide results of sufficient accuracy. The calculations are taken out to 250 s of solidification. A time step of $\delta t = 0.01$ s is used. Despite this

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Table 1

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<thead>
<tr>
<th>Data for inverse segregation problem</th>
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<tbody>
<tr>
<td>$c$</td>
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<tr>
<td>$K$</td>
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<td>$\Delta H$</td>
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<td>$T_{\text{out}}$</td>
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<tr>
<td>$T_I$</td>
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<td>$T_{\text{chill}}$</td>
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relatively small time step the CPU time on a Pentium III processor is \( \sim 20 \) s. Although this is \( \sim 5 \) times slower than a previous semi-implicit scheme [6]—working on the same space grid with time step of \( \delta t = 1 \), the performance is not prohibitive. Further the local nature of the thermal solute coupling in the explicit scheme could offers distinct advantages of simplicity and flexibility in moving towards more complex systems. Systems that could greatly tax the iterative operation of an implicit time stepping scheme.

5. The effect of coarsening

The above explicit scheme can be used to make a quantitative assessment of the effect of coarsening on macrosegregation predictions. Consider the inverse segregation system in Fig. 2. With reference to Appendix A, the situation when the solid state diffusion is characterized by a Fourier number (see Eq. (A.5)) \( \alpha = 0.2 \) can be modeled in the proposed method on using Eq. (A.7) to set \( \beta = 0.2857 \). This value assumes no coarsening of the arm spaces. If coarsening of the microstructure occurs, with the typical time scale of \( t^{1/3} \), then \( \beta = 0.4792 \), Eq. (A.10). Predictions using these two values of \( \beta \) are shown in Fig. 4. Comparison with the cases of no back-diffusion \( \beta = 0 \) and complete solid state diffusion \( \beta = 1 \) are also shown to provide a reference. There is a clear effect of coarsening, reflected in the almost doubling in the value of the diffusion parameter \( \beta \) when coarsening is accounted for. Further information on the effect of coarsening is provided in

![Fig. 3. Comparison of explicit scheme and similarity [16] predictions of solute concentration in the mushy region of an inverse segregation. The continuous lines are the benchmark similarity solution, the symbols are the explicit scheme predictions.](image-url)
Fig. 4. The effect of coarsening on solute concentration predictions in the mushy region.

Fig. 5. Variation of non-coarsening ($\beta$) and coarsening ($\beta^+$) diffusion parameters with Fourier number.

Fig. 5. This figure compares the values of the non-coarsening $\beta$ (Eq. (A.7)) with the coarsening $\beta$ (Eq. (A.10)) across the range of Fourier numbers. This figure indicates that the maximum difference of coarsening will occur at small Fourier numbers. In the Scheil limit, zero back-diffusion with $x = 0$, the effect of coarsening is equivalent to a finite back-diffusion characterized by a Fourier number of $x = 0.1667$. 
6. Conclusions

A general scheme for modeling complex solidification systems has been proposed. The key feature in this scheme is that the heat and concentration conservation equations are solved using explicit time integration. In this scheme the disadvantage of a small time step for stability is countered by a local coupling of the thermal and solutal fields that does not involve outer iteration of the macroscopic equations. This local coupling allows for a high degree of ease and efficiency in the modeling of complex microscale phenomena such as coarsening. This is demonstrated by successfully applying the proposed scheme to a benchmark problem [16].

The developed model coupled to a recent microscale models [21,23] is used to study the effect of coarsening on macrosegregation predictions for the benchmark problem. The results indicate that there can be a noticeable difference in the solute concentration in the mushy region when coarsening is accounted for. In a general setting the exact level of any effect due to coarsening will be problem dependent and more noticeable in problems with a low back-diffusion Fourier number. Note, however, in the proposed explicit coupling there is a zero cost involved in adding coarsening, the only requirement is appropriate modeling of the diffusion parameter, see (A.10) in Appendix A.

Appendix A

A central part of the proposed scheme is the modeling of the back-diffusion in the REV by the approximation (see Eq. (10))

\[ \int_0^\infty \frac{\partial C_s}{\partial t} \, d\Gamma = \beta gk_{\text{par}} \frac{\partial C_1}{\partial t}. \]

The object of this Appendix is to show how this model is arrived at and to demonstrate its accuracy in modeling microsegregation.

In the first place consider microsegregation (local scale redistribution of solute) in the REV in which no macrosegregation occurs, i.e., the mixture concentration of solute \( [\rho C] = [\rho]C_0 \) is constant (a so-called “closed system”). A suitable domain for this problem is a representative half secondary arm spacing \( X_0 \), see Fig. 6. In this arm spacing, assuming a constant density and a fixed microstructure, \( X_0 = \text{constant} \) (no coarsening), the mixture concentration is

\[ C_0 = g\langle C_s^k \rangle_s + (1-g)C_1^k, \]  
(A.1)

Fig. 6. Testing of approximate microsegregation model.
where
\[ g(C_k^s) = \int_0^g C_k^s d\xi, \]  
(A.2)
and \( \xi = x/X_0 \). Differentiating with respect to the normalized time \( \tau = t/t_f \) (\( t_f \) = the time to complete solidification), leads to
\[ \frac{dg}{d\tau} (k_{par} - 1) C_k^s + \int_0^g \frac{\partial C_k^s}{\partial \tau} d\xi + (1 - g) \frac{dC_k^s}{d\tau}. \]  
(A.3)
The back-diffusion term can be written as
\[ \int_0^g \frac{\partial C_k^s}{\partial \tau} d\xi = \beta g k_{par} \frac{\partial C_k^s}{\partial \tau}. \]  
(A.4)
The first term on the right of (A.4) is an exact representation where
\[ \alpha = \frac{D t_f}{X_0^2}, \]  
(A.5)
is the Fourier number and \( D \) is the mass diffusivity. The last term on the right of (A.4) is the approximate model used in the paper. If \( \beta \) is a constant then Eq. (A.3) can be integrated to give [11]
\[ g = \frac{1}{1 - \beta k_{par}} \left( 1 - \left[ \frac{C_k^s}{C_0} \right]^{(1-\beta k_{par})/(k_{par}-1)} \right), \]  
(A.6)
which has the well known form of the Brody–Flemings microsegregation model [18]. Voller [11] shows that under the conditions of a prescribed cooling rate it is reasonable to assume a constant value of \( \beta \), viz
\[ \beta = \frac{2\tau}{1 + 2\tau}, \]  
(A.7)
which matches a form previously suggested by Ohnaka [19] for the case of parabolic growth of solid. Note that in the limit of zero mass diffusion in the solid (\( D = 0 \) \( \beta = 0 \), and as the mass diffusion increases, \( D \to \infty, \beta \to 1 \).

In the model presented above a fixed microstructure has been assumed. In reality this is not often the case and one would expect the arm to coarsen (increase in size) as the solidification proceeds. A typical time scale for the coarsening process is \( X_0(\tau) \sim \tau^{1/3} \) [20]. Voller and Beckermann [21] have shown that across a wide range of solidification conditions that coarsening can be modeled by replacing the Fourier number in a basic microsegregation model that does not account for coarsening with a diffusion parameter defined by
\[ \alpha^+ = \frac{X_f^2}{X_0^2} \alpha + 0.1, \]  
(A.8)
where \( X_f \) is the final half arm spacing on full solidification. If this form is to be used in Eq. (A.4) to model microsegregation with coarsening the value \( \beta \) resulting from Eq. (A.7) needs to be constant. This requires that an average value, \( \gamma \), for the time varying term \( (X_f/X_0)^2 \). A definition for the value of \( \gamma \) is obtained by averaging the back-diffusion over the time step, i.e.,
If the growth of the solid is (or close to) parabolic, it can be shown, by the chain rule, that $M C \zeta / M \zeta$, evaluated at the solid–liquid interface, scales as $C_{24}^s$. Then, on noting that, if $a_{\zeta} = 3$ coarsening model holds, $(X_f / X_0)^2 \sim \tau^{-2/3}$, integration of Eq. (A.9) will give $\gamma = 1.8$. The bottom line is that in the absence of coarsening the $\beta$ term in the approximate back-diffusion treatment is given by Eq. (A.7). If a $\tau^{1/3}$ coarsening is present then this term is calculated as

$$\beta = \frac{2(1.8x + 0.1)}{1 + 2(1.8x + 0.1)}.$$  (A.10)

The performance of the microsegregation model in Eq. (A.6) when applied to a coarsening situation can be checked by comparing its predictive performance against a full numerical solution of the diffusion and coarsening in the half arm space. Consider the case of the binary-eutectic alloy with $C_0 = 4.9$, $C_{cut} = 33.2$, and $k_{par} = 0.16$. Eq. (A.6) with $\beta$ given by Eq. (A.10) can be used to predict the fraction of eutectic for a range of Fourier numbers (for a given Fourier number simply substitute $C_{cut} = 33.2$ for $C_0$ in Eq. (A.6)). Comparison with full numerical predictions and experimental data [22] is shown in Fig. 7. This result clearly shows the accurate performance of the model Eqs. (A.6) and (A.10) in comparison with full numerical and experimental results. Note as a point of comparison the model results when coarsening is not accounted for is also shown in Fig. 7 (evaluate $\beta$ with Eq. (A.7)). A complete discussion of the numerical method and details of the experimental data can be found in a recent paper by Voller [23].

References