3D CAFE modeling of grain structures: application to primary dendritic and secondary eutectic solidification

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3D CAFE modeling of grain structures: application to primary dendritic and secondary eutectic solidification

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Received 31 May 2011, in final form 1 November 2011
Published 6 December 2011
Online at stacks.iop.org/MSMSE/20/015010

Abstract
A three-dimensional model is presented for the prediction of grain structures formed in casting. It is based on direct tracking of grain boundaries using a cellular automaton (CA) method. The model is fully coupled with a solution of the heat flow computed with a finite element (FE) method. Several unique capabilities are implemented including (i) the possibility to track the development of several types of grain structures, e.g. dendritic and eutectic grains, (ii) a coupling scheme that permits iterations between the FE method and the CA method, and (iii) tabulated enthalpy curves for the solid and liquid phases that offer the possibility to work with multicomponent alloys. The present CAFE model is also fully parallelized and runs on a cluster of computers. Demonstration is provided by direct comparison between simulated and recorded cooling curves for a directionally solidified aluminum–7 wt% silicon alloy.

(Some figures may appear in colour only in the online journal)

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>Volumetric enthalpy</td>
<td>J m$^{-3}$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Thermal conductivity</td>
<td>W m$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Undercooling</td>
<td>K</td>
</tr>
<tr>
<td>$h$</td>
<td>Heat transfer coefficient</td>
<td>W m$^{-2}$ K$^{-1}$</td>
</tr>
<tr>
<td>$g$</td>
<td>Volume fraction</td>
<td>—</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Shape function</td>
<td>—</td>
</tr>
<tr>
<td>$[M]$</td>
<td>Mass matrix</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$[K]$</td>
<td>Conductivity matrix</td>
<td>W K$^{-1}$</td>
</tr>
<tr>
<td>${F}$</td>
<td>Boundary condition vector</td>
<td>W</td>
</tr>
<tr>
<td>$R_E$</td>
<td>Residual</td>
<td>W</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Convergence criterion</td>
<td>—</td>
</tr>
</tbody>
</table>
E  Element  —
I  State index  —
v  Velocity  \( \text{m s}^{-1} \)
a  Kinetic coefficient  \( \text{m s}^{-1} \text{K}^{-m} \)
m  Kinetic coefficient  —
n  Nucleation site density  \( \text{m}^{-3} \)
l_{CA}  Cell size  m
N  Number  —
r  Half diagonal length  m
t  FE time  s
t_m  CA time  s
\( \Delta t \)  FE time step  s
\( \delta t \)  CA time step  s
C  Center  —
V  Volume  \( \text{m}^3 \)
A  Surface  \( \text{m}^2 \)
x  Coordinate  m
l  Length  m

Superscripts
\( X^t \)  Time
\( X^\alpha \)  Phase
\( X^{s_i} \)  Structure \( s_i \)
\( ^{(k)}X \)  Newton–Raphson iteration
\( X^{(i)} \)  Zone

Indices
\( X_i, X_j \)  Nodes
\( X_{\nu}, X_{\mu} \)  Cells
\( X_{\text{ext}} \)  External
\( X_{\text{capt}} \)  Capture
\( X_{\text{mesh}} \)  Mesh
\( X_{\text{eq}} \)  Equilibrium
\( X_L \)  Liquidus
\( X_E \)  Eutectic
\( X_{\text{nucl}} \)  Nucleation
\( X_a \)  Mean deviation
\( X_\sigma \)  Standard deviation
\( X_{\text{max}} \)  Maximum
\( X_0 \)  Initial value
\( X_{\text{end}} \)  Final value

Others
\( \langle X \rangle \)  Volume average quantity
\( \text{min}(X) \)  Minimum
\( |X| \)  Absolute value
\( [X] \)  Matrix
\( \{X\} \)  Vector

2
1. Introduction

Increasing computing facilities have led to a wide development of numerical methods, particularly in the casting area [1]. Three approaches are generally considered for the modeling of structural features in casting. Macrosopic scale methods are based on volume averaging over a representative domain. They can be applied to the entire volume of industrial casting. However, they do not provide direct representation of the structure. Only average grain size and phase fractions can be determined [2]. Microscopic scale methods aim to model the morphology of the solidifying structures. They are yet limited with respect to the number of grains and the domain size. Mesoscopic scale methods, such as the cellular automaton (CA) method, have been developed with the goal to achieve direct simulation of the entire grain structure of ingots or shape casting. The main idea is to represent the envelope of each individual grain over a regular grid of cubic cells. Each CA cell is associated with a state index to indicate whether it is liquid or captured by a growing grain envelope. Starting from all cells in a liquid state, the simplest 3D CA method then consists of an integration of nucleation and growth kinetics to predict the grain structure—referred to as macrostructure—by switching the cell index. The internal morphology of the grains—referred to as microstructure (e.g. network of dendrite trunks and arms)—is not directly described. Because the scales required to model the nucleation and growth kinetics are not tackled, approximate microstructure models are used to describe the internal structure of the grains [3, 4]. For instance, a simple mass balance is integrated into a microsegregation model in order to follow the development of the solidification path.

A decent coupling between the CA method and the finite element (FE) method was proposed to solve the heat flow problem [5]. This was necessary as the growth kinetics of the grains depends on the temperature, and the temperature depends on the fraction of solid formed due to the latent heat released upon the phase change, as recognized from the first developments of the CAFE model [4, 6]. For that purpose, a FE mesh much coarser than the CA grid could be used since the scale characterizing heat flow is usually orders of magnitude larger than the scale describing microstructures. However, limitations to this CAFE coupling scheme exist, and are listed as follows:

(i) enthalpy computed at FE nodes was interpolated at CA cells and conversion of enthalpy into temperature and fraction of solid was achieved for each cell, requiring large memory resources,

(ii) summation over CA cells for redistribution at FE nodes was done for temperature and solid fraction, leading to possible incoherency with the enthalpy at the FE nodes,

(iii) although all previous works supposed that the time step was small enough to avoid an iterative solution of the energy equation, the error induced could not be estimated,

(iv) only the development of the primary dendritic structure was modeled, an isothermal transformation at the eutectic temperature being achieved when later converting the remaining interdendritic liquid into solid,

(v) implementation in 3D was not achieved, mainly because of (i).

This work proposes solutions to remove all the above listed limitations.

2. Modeling

The energy conservation is reduced to heat diffusion for a material with a constant density:

\[
\frac{\partial \langle H \rangle}{\partial t} - \nabla \cdot (\kappa \nabla T) = h(T - T_{\text{ext}})
\]  

(1)
where $T$ is the temperature, $t$ is the time and $\kappa$ is the thermal conductivity. The average volumetric enthalpy, $\langle H \rangle$, is defined by the volume fraction of the phases $\alpha$, $g^{\alpha}$, and the corresponding volumetric phase enthalpy, $(H^{\alpha})^{\alpha}$:

$$
\langle H \rangle = \sum_{\alpha} g^{\alpha} (H^{\alpha})^{\alpha}.
$$

Heat exchange takes place at the boundaries of the simulation domain. It is defined by the heat transfer coefficient, $h$, and the external temperature, $T_{ext}$. A flow chart is presented in figure 1 to illustrate the sequence of the models described hereafter together with their interplays.

2.1. FE model

The heat diffusion problem is solved with a FE method. The enthalpy at time $t + \Delta t$, $\langle H \rangle^{t+\Delta t}$, is deduced from the enthalpy at time $t$, $\langle H \rangle^t$, from a weak formulation using a general Newton–Raphson implementation. The enthalpy variation over iteration $(k + 1)$, $d(H) = (k+1)\langle H \rangle - (k)\langle H \rangle$, is computed from values at iteration $(k)$ of the enthalpy, $(k)\langle H \rangle$, the temperature, $(k)T$, and the estimated derivative $(k)(dT/d(H))$ [7]:

$$
[[M] + [K](k)(dT/d(H))][d(H)] = -[M](k)\langle H \rangle - \langle H \rangle^t - [K](k)T + \{F\}.
$$

Matrices $[M]$, $[K]$ and the boundary condition vector $\{F\}$ are defined as

$$
[M] = \int_{\Omega} \frac{1}{\Delta t} \phi_i \phi_j \ d\Omega
$$

$$
[K] = \int_{\Omega} \kappa \nabla \phi_i \nabla \phi_j \ d\Omega + \int_{\partial \Omega} h \phi_i \phi_j \ dS
$$

$$
\{F\} = \int_{\partial \Omega} h \phi_i T_{ext} \ dS
$$

where $\phi_i$ and $\phi_j$ are the interpolation and weighting functions. The residual of the solution at iteration $(k + 1)$, $(k+1)R_E$, is defined by

$$
(k+1)R_E = -[M](k+1)\langle H \rangle - \langle H \rangle^t - [K](k+1)T + \{F\}.
$$

At the beginning of the iteration procedure, vectors $(k)\langle H \rangle$, $(k)T$ and $(k)(dT/d(H))$ are initialized using the converged values at the previous time step, $(\langle H \rangle^t)$, $(T^t)$ and $(dT/d(H))^t$. Convergence is achieved after $(k + 1)$ iterations if $(k+1)R_E$ becomes smaller than a chosen value $\varepsilon$:

$$
(k+1)R_E/\varepsilon < \varepsilon
$$

where $(0)R_E$ is the residual of the first iteration of the first macroscopic time step, introduced because of non-preconditioning in residual calculations. The last known vectors $(k+1)\langle H \rangle$ and $(k+1)T$ become the solution vectors $(k)\langle H \rangle^{t+\Delta t}$ and $(k)T^{t+\Delta t}$. If convergence is not achieved, another iteration is performed. The new $(k+1)(dT/d(H))$ used for the next iteration $(k + 1)$ is set for every node as the last numerical variation of $T$ versus $H$, i.e. $(k+1)T - (k)T)/((k+1)\langle H \rangle - (k)\langle H \rangle)$. Sub-increments may occur if the system has diverged, i.e. $(k+1)R_E > (k)R_E$. In this case, the solution is supposed to be contained between the last two calculated enthalpies $(k+1)\langle H \rangle$ and $(k)\langle H \rangle$. Several intermediate solutions $(c)\langle H \rangle = (k)\langle H \rangle + c((k+1)\langle H \rangle - (k)\langle H \rangle)$ are tried, with $0 < c < 1$. The residual is estimated for all these values, and the best $(c)\langle H \rangle$ is used for the next iteration. Convergence usually requires several iterations. In the common approach [5], however, the equation was solved only once per time step, meaning that the
number of iterations was forced to be one. This situation corresponds to imposing $k = 1$ in the above procedure. As a consequence, convergence was not necessarily achieved.

The use of $\left(\frac{dT}{d\langle H\rangle}\right)$ is necessary as well as a general method to convert enthalpy into temperature. Explanations are now given on how the CA approach together with a microsegregation model permits such a conversion.
2.2. CA model

Nucleation and growth kinetics are integrated on the cell lattice defined by the CA grid. The goal is to change the state indices of the cells \( v, I(i) \), so as to mimic the development of grain structures defining zone \( (i) \) defined by structure \( s_i \); \( i = [1, N^v] \) with \( N^v \) the number of structures. Because nucleation and growth are temperature dependent, this is done using the temperature deduced at the FE nodes.

**Nucleation.** Nucleation sites are attributed to the cells for each type of structure. A single cell can possibly contain more than one nucleation site for each type of structure. For instance, in the case of an Al-7 wt\% Si alloy, nucleation of a primary dendritic microstructure can first take place below the liquidus temperature, followed by the nucleation of a eutectic microstructure below the eutectic temperature after further cooling [8], thus corresponding to \( N^v = 2 \). Each nucleation site is associated with a critical undercooling for the microstructure \( s_i, \Delta T^v_{nucl} \). For the attribution of a nucleation site, a cell is randomly picked along with a critical undercooling assuming a Gaussian distribution. Its parameters are the mean deviation for the critical undercooling, \( \Delta T^v_{nucl} \), the standard deviation, \( \sigma^v_{nucl} \), and the nucleation side density, \( n^v_{max} \). Note that Gaussian parameters for nucleation on mold surfaces and in the melt may differ.

All the cells \( v \) are initialized with values of the state index corresponding to a fully liquid state. When the local temperature of a cell \( T_v \) becomes lower than the critical temperature for the nucleation site associated with structure \( s_i \) contained in cell \( v, T^v_{nucl} = T^v_{eq} - \Delta T^v_{nucl} \), a new grain is created. In the case of the dendritic structure for the Al-7 wt\% Si alloy, \( i = 1 \), and the equilibrium temperature for the grain structure \( s_1 \), \( T^v_{eq} \), is nothing but the liquidus temperature, \( T_L \). For the eutectic structure, \( i = 2 \) and \( T^v_{eq} = T_E \), i.e. the eutectic temperature defined by the binary phase diagram. A unique grain number is attributed to cell \( v \) for each nucleation event and its state index is switched to a value corresponding to a non-liquid state.

**Growth.** Every cell is associated with an expanding geometrical shape that locally fits the grain shape. Its nature depends on the solidifying structure of the material. For instance, the Al-7 wt\% Si alloy solidifies with primary fcc crystals that adopt a dendritic growth morphology with trunks and arms aligned along the \( \langle 100 \rangle \) crystallographic directions. The corresponding growing shape associated with the cells is then a square in 2D and an octahedron in 3D with main half diagonals defined by the \( \langle 100 \rangle \) crystallographic directions, as illustrated in figure 2 [3, 9]. Apices correspond to the leading dendrite tips of the crystal. The positions of apices defined by half diagonals \( r(i) \) are updated using the local temperature \( T_v \), to compute the growth velocity of microstructure \( s_i \) in cell \( v, v^v_i \):

\[
v^v_i = a^v (\Delta T^v_{nucl})^{m^v}
\]

where \( \Delta T^v_{nucl} = T^v_{eq} - T_v \) is the local undercooling, \( a^v \) and \( m^v \) are parameters deduced from fitting growth kinetics models established for the microstructure \( s_i \) [10, 11].

The shape associated with cell \( v \) can eventually become large enough to encompass the center of a neighboring cell. The neighboring cell is then ‘captured’ and its state index is switched to a value that corresponds to the growing structure, with the same grain number as the capturing cell. A new smaller shape is associated with the captured cell, in a way that one of the apices is at the same position as the capturing apex. The objective is to preserve the local microstructure–liquid growth front. For more details on capture geometry considerations, see [3]. In the present algorithm, all liquid cells are successively scanned for capture by their direct neighbors, i.e. 8 neighbors in 2D and 26 neighbors in 3D. In case a liquid cell can be...
Figure 2. (a) 2D and (b) 3D computation of the fraction of a grain structure \( j \) developing in the central cell \( \nu \). The present shape associated with cell \( \nu \) in 2D (3D) is a square (an octahedron) with surface (volume) \( A^{(j)}_\nu \) \( (V^{(j)}_\nu) \). At the time when cell \( \nu \) switched from liquid to a mushy state, surface (volume) \( A^{(j)}_{\nu_{\text{capt}}} \) \( (V^{(j)}_{\nu_{\text{capt}}}) \) was recorded. The maximum size of the square (octahedron) corresponding to surface (volume) \( A^{(j)}_{\nu_{\text{max}}} \) \( (V^{(j)}_{\nu_{\text{max}}}) \) is reached when the square (octahedron) encompasses the center of cell \( \mu \), as \( \mu \) is the most distant neighbor for cell \( \nu \).

captured by several neighboring cells during the same time step, the cell with the most grown structure is favored.

Note that in past implementations, only the dendritic grain structure was represented. The present developments offer the advantage of a generalization for the tracking of additional structures such as the eutectic in the binary Al-7 wt% Si alloy. As for the primary mushy zone for which the internal dendritic microstructure is not represented, the detailed morphology of the two-phase lamella of the intragranular eutectic microstructure is not directly simulated. Interaction between the structures is yet to be provided: eutectic nucleation can occur in both mushy cells or liquid cells whereas dendritic nucleation can only happen in liquid cells.
Similarly, the eutectic grains can propagate in liquid cells as well as in mushy cells while the dendritic grains can only grow in liquid cells. In principle, the CAFE model could thus be extended to additional grain structures.

**Microscopic time step calculation.** The CA model requires having a time step small enough to prevent the propagation of the growth front over a distance larger than the cell size. The FE time step, $\Delta t$, called macroscopic time step, is usually very large. It is divided into microscopic time steps, $\delta t$, defined as

$$
\delta t = \min \left( \frac{l_{CA}}{v_{max}^v}, \Delta t \right)
$$

where $l_{CA}$ is the cell size of the CA grid and $v_{max}^v$ is the maximum velocity of the growth fronts considering all possible growing microstructures $s_i$ in cell $v$. The CA model is thus solved over the microscopic time step $\delta t$ from an initial microscopic time $t_m = t$ to the final time $t_m = t + \Delta t$. Update of the microscopic time step $t_m$ is achieved up to reaching the macroscopic time step $t_m = t + \Delta t$ at the end of the loop on microscopic time steps (figure 1).

For a cell $v$ belonging to the element $E_v$ of the FE mesh, the temperature $T_{m}^{in}$ is linearly interpolated at the center of the cell, $x_v$, using the relation

$$
T_{m}^{in} = \sum_{n \in E_v} \phi(x_n) T_{m}^{in}
$$

where, for each node $n$ belonging to element $E_v$, $T_{m}^{in}$ is the temperature at the beginning of the microscopic time step and $\phi(x_n)$ is the shape function estimated at position $x_n$. Temperature $T_{m}^{in}$ is used for the nucleation and growth procedures of the CA calculations. Thus, the CA algorithms correspond to an explicit resolution scheme. Temperatures $T_{m}^{in}$ and $T_{m}$ are still updated at each microscopic time step, i.e. several times per macroscopic time step, as will be explained in the next section. This update limits the error introduced by the explicit scheme but slows down the resolution time.

2.3. Coupling schemes

**Fraction of grain structures.** A volume fraction of the envelope of the structure $s_i$ is defined for each cell $v$ by the corresponding zone $(i)$, $g_{v}^{(i)}$. This is illustrated in figures 2 and 3. The phases contained in the envelope of the grain depend on the nature of the structure. In the case of primary solidification for an Al-7 wt% Si alloy, a dendritic solid forms. Its envelope defines a mushy zone $(1)$ growing into a free zone of liquid $(0)$. The mushy zone is made of a mixture of solid $s_1$ in zone $(1)$, $s_1^{(1)}$, plus a liquid in zone $(1)$, $l^{(1)}$, while the free zone of liquid is only made of liquid $l^{(0)}$ (figure 3(a)). The latter notation is the same as that used in the most recent segregation models [12–14], permitting to deal with multiple microstructures, including dendritic, peritectic and eutectic transformations.

For the grain structure $s_i$ present in zone $(i)$ in a given cell $v$, three cases may happen:

- $g_{v}^{(i)} = 0$, no zone $(i)$ is formed and the associated structure $s_i$ is absent,
- $0 < g_{v}^{(i)} < 1$, the structure $s_i$ is the developing zone $(i)$ in cell $v$,
- $g_{v}^{(i)} = 1$, structure $s_i$ has fully filled cell $v$.

The intermediate situation corresponds to the growth of structure $s_i$ in cell $v$ upon development of zone $(i)$, thus defining the new structure $s_i^{(i)}$. At the time $t_{v}^{\text{cap}}$, when the center of cell $v$ is reached by one of its neighbors or when nucleation takes place in cell $v$, the initial shape associated with cell $v$ is centered in $C_v^{(0)}$ (only equal to the cell center $C_v$ of coordinates $x_v$ in
Figure 3. Calculation of fractions of phases for the central cell ν containing (a) a growing dendritic structure only or (b) a dendritic and a eutectic structure growing in liquid. All the structures are supposed to grow from the same center and with the same orientation. Interrupted lines delimit the structure zones. Dashed zone corresponds to g(0), i.e. the extradendritic liquid. Dotted zone is the dendritic mush g(1). Plain color zone is the eutectic region g(2). Each structure fraction within every zone is given by a tabulated solidification path.

Later on, upon cooling, a new structure may form in cell ν so s(i) remains with j ≠ i. This is typically the case when the interdendritic eutectic reaction takes place as illustrated in figure 3(b). Upon growth of the eutectic structure s(2), the dendritic structure s(1) inherited from the development of the mushy zone with the dendritic structure s(1) is still present in the envelope defined by the eutectic grain envelope. In the absence of a solid phase transformation, the volume fraction of the dendritic structure s(1) does not evolve anymore. It is frozen by the development of the interdendritic eutectic structure s(2).
Conversion of enthalpy. As explained in the description of the FE model, conversion of enthalpy into temperature is required. Considering the coexistence of several zones \((j)\) in which microstructures \(s(j)^i\) and liquids \(l(j)^i\) develop, this is done using the following relations:

\[
g^j = g^j \sum_{i=1}^{N^j} g^j_i \tag{13}
\]

\[
g^j = g^j \left( 1 - \sum_{i=1}^{N^j} g^j_i \right) \tag{14}
\]

\[
\langle H \rangle = \sum_{j=0}^{\infty} \left[ \sum_{i=1}^{N^j} (g^j_i \langle H^s(j)^i \rangle^j + g^j_i \langle H^l(j)^i \rangle^j) \right] \tag{15}
\]

\[
g^j_i = g^j(T) \tag{16}
\]

\[
\langle H^s(j)^i \rangle^j = H^s(T) \tag{17}
\]

\[
\langle H^l(j)^i \rangle^j = H^l(T) \tag{18}
\]

where \(g^j(T), H^s(T)\) and \(H^l(T)\) are the temperature tabulations of the volume fraction of solid \(s\), the enthalpy for solid \(s\) and the enthalpy of liquid \(l\), respectively. The tabulations are explicitly assumed independent of the zone \((j)\) in which phase \(s\) is located. Consequences of this approximation are discussed elsewhere [14]. Figure 4 provides the tabulated values for the Al–7 wt% Si alloy. In practice, the volume fraction of solid \(s_1\) in zone \((1)\), \(s_1^1\), can be deduced from a classical microsegregation model. In figure 4, the Gulliver–Scheil approximation was used [5].

The above formulation permits us to verify that a given zone \((j)\) is fully filled with solid plus liquid phases, \(g^j = g^j + g^p\). The volume fraction of a zone \((j)\) is defined for a given cell \(v\) of the CA grid with equation (12). However, it has not yet been defined for a FE node \(n\), \(g^j\). This is done for each zone \((j)\) using a summation over the cells:

\[
\left( g^j \right) = \frac{\sum_v \phi(x_v) g^j_v}{\sum_v \phi(x_v)} \tag{18}
\]

The conversion of enthalpy into temperature is conducted at the end of each microscopic time step \(t_m + \delta t\). For that purpose, the enthalpy is linearly interpolated at each node over time within the macroscopic time step \(\Delta t\):

\[
\langle H \rangle^j_{t_m + \delta t} = \langle H \rangle^j_t + \left( \langle H \rangle^j - \langle H \rangle^j_t \right) (t_m + \delta t - t) / \Delta t \tag{19}
\]

where \(\langle H \rangle^j_t\) is the last known enthalpy as explained in the FE section. Thus, also evaluating the volume fraction of each zone \((j)\) at the end of the microscopic time step, \(g^j_{(j)_{t_m + \delta t}}\), with equation (18) and using equations (13)–(17), values of the node temperature, \(T^j_{t_m + \delta t}\), and of the fraction of all phases \(s^j\), \(g^{j}_{t_m + \delta t}\), can be deduced. This is performed with a standard Brent algorithm [15].

The above conversion is schematized in figure 1. It offers several progresses with respect to the previous method proposed by Guillemot et al [5]. In addition to the fact that conversion is not conducted at the cells of the CA grid but at the FE nodes, corresponding to several orders of magnitude less computational resources, it also permits full coherency between variables \(T, \langle H \rangle\) and \(g^{j}_{t_m + \delta t}\). This was not the case previously since the latter quantities were summed up at the nodes from values computed at the cells. While coherency was satisfied at the cells, it was not the case at the nodes.
Figure 4. Tabulated properties for the Al–7 wt% Si alloy (thin black curves) assuming Gulliver–Scheil approximation with (a) average enthalpy for $l$ = liquid, $s_1$ = dendritic structure, $s_2$ = eutectic structure, and (b) volume fraction of structures $s_1$ and $s_2$. The solidification path including undercooling of structures extracted for a single mesh node of a simulation is drawn as thick curves for (a) the average enthalpy of the system $\langle H \rangle$ and (b) the volume fraction of structures $s_1$ and $s_2$.

Iterative scheme. Several Newton–Raphson iterations have to be performed to ensure convergence, as the system is not linear. This is also schematized in figure 1. However, iterative resolution has never been applied when coupling with the solidification path predicted by the CAFE model. Resolution was limited to a single iteration by imposing $k = 1$. The main reason is that the whole information at the cell grid has to be copied at the beginning of the macroscopic time step for use as the starting state of all upcoming iterations. This implies to save all cells’ information (state, $I_i^{(t)}$, and growth shape, $r_i^{(t)}$), almost doubling the total memory used. This was implemented in this work, mostly because the new conversion of enthalpy takes place at the FE node and no longer at the CA cells, thus permitting to decrease the amount of allocated memory. Indeed, variables at the cells, $\langle H \rangle_i$, $g_i^{(j)}$, $g_i^s$ and $T_i$, are no longer needed compared with the previous coupling scheme [5]. The second reason is the current parallel version of the model that runs on a cluster of computers. Access to a larger amount of memory is thus possible.
Table 1. Material parameters for the Al–7 wt% Si alloy as well as boundary conditions [5] (simulations displayed in figures 5 and 6).

<table>
<thead>
<tr>
<th>Alloy property</th>
<th>Symbol</th>
<th>Unit</th>
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<tr>
<td>Thermal conductivity</td>
<td>κ</td>
<td>W m(^{-1}) K(^{-1})</td>
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<tr>
<td>Growth kinetics s(_{1}) = Dendritic</td>
<td>a(_{s1})</td>
<td>2.9 \times 10^{-6} m s(^{-1}) K(^{-1}) m(^{-1})</td>
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<tr>
<td>s(_{2}) = Eutectic</td>
<td>m(_{s2})</td>
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<td>Nucleation parameters</td>
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<td>At chill: single crystals</td>
<td>ΔT(_{0})</td>
<td>0.0 °C</td>
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<tr>
<td>In volume: no nucleation</td>
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<td>Boundary conditions</td>
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<td></td>
</tr>
<tr>
<td>Heat transfer coefficient</td>
<td>H</td>
<td>500.0 W m(^{-2}) K(^{-1})</td>
</tr>
<tr>
<td>External temperature</td>
<td>T(_{ext})</td>
<td>100.0 °C</td>
</tr>
<tr>
<td>Initial temperature</td>
<td>T(_{0})</td>
<td>800.0 °C</td>
</tr>
<tr>
<td>Ingot length</td>
<td>L</td>
<td>0.1 m</td>
</tr>
</tbody>
</table>

3. Numerical tests

The CAFE model is first tested in order to check its ability to model solidification with melt undercooling for both dendritic and eutectic structures. This is done based on the solution provided by a one-dimensional (1D) front-tracking (FT) model [17]. It provides the solution for unidirectional solidification of an Al–7 wt% Si ingot. The FT model allows us to track the dendritic and eutectic fronts in 1D, and to retrieve temperature and solid fractions along the ingot. The geometry used is 100 mm long. Heat is extracted through one face of the ingot (position 0 mm), with a boundary condition defined by a heat transfer coefficient, h, and an external temperature, T\(_{ext}\). The other boundary of the 1D ingot is adiabatic. Details on simulation parameters are given in table 1. Further description of the case is given in [5]. As the current CAFE implementation runs only in 2D and 3D, a 1 mm width is set in 2D, and a 1 mm × 1 mm section in 3D, the length being unchanged.

3.1. Single grain structure and no iterations

Figure 5 shows the predicted temperature and solid fraction at equidistant points along the ingot, beginning at the chill–metal interface (0 mm) and ending at the metal–air interface (100 mm). Thick gray curves correspond to the predictions of the FT model. Thin black curves correspond to the predictions of the CAFE model with the solidification path computed at the nodes. The most striking difference is shown at the eutectic transformation (T\(_{E}\) = 577 °C) in figure 5(a). In the FT model, the eutectic front is tracked using its own growth kinetics, leading to an undercooling of about 3 °C. This is observable on the 100 mm temperature curve. The eutectic plateau is clearly below T\(_{E}\). In this CAFE simulation, only the primary dendritic structure is considered and no iterations are performed, as was the case in [5]. Because the eutectic structure is not modeled, the conversion of enthalpy is conducted assuming an isothermal transformation at the eutectic temperature. There is consequently no undercooling below the eutectic temperature so that a plateau is predicted at T\(_{E}\). However, the top part of the temperature curves show reasonable agreement between the CAFE and FT predictions as was the case in [5] when the enthalpy conversion was still applied at the cells. The plateaus around 613 °C correspond to the formation of the dendritic structure, i.e. with an undercooling of
about 5 °C. Dendritic undercooling is also shown on solid fraction curves in figure 5(b), where solid fraction suddenly rises from 0 to 0.13. Two types of oscillations are observed on the temperature curves. The first ones happen during the first stage of solidification at around 613 °C. They are due to slope changes in the $H$ to $T$ conversion, and can be avoided with simulation refinement (e.g. by diminishing the time step). A few other oscillations appear around the eutectic transformation, as big steps. They are also caused by slope change, but they are mostly due to the mesh size which is very coarse. When a node is reached by the eutectic front, its temperature is set to $T_E$ until its solid fraction is equal to one. This blockage of the temperature has an impact on connected elements. Each ‘oscillation step’ corresponds to a node reached by eutectic.

3.2. Multiple grain structures and iterations

Figure 6 shows the comparison between the FT and CAFE simulations when considering all new developments, i.e. node conversion, dendritic and eutectic grain structures together with the iteration procedure activated. The improvement is clear, as the eutectic undercooling
Figure 6. Predicted time evolution of (a) temperature and (b) fraction of solid using the 1D FT model (thick gray curves) [17] and the CAFE model (thin black curves) with two structures and the coupling scheme at nodes with iterations.

is represented well and no more oscillations are visible. The agreement between predicted temperatures is clearly improved. There is still a small difference on solid fraction curves, especially at 0 mm. This is due to the eutectic transformation which is very fast in that area. It is the point where eutectic and dendritic structures appear first, so latent heat can be released quickly in the ingot, which is still mostly liquid. Solid fraction can increase abruptly. In fact, these phenomena can be better simulated with the CAFE model by reducing the mesh size and the time step.

3.3. Numerical parameters

Table 2 gives a summary of the quantitative comparison between the FT and the CAFE temperature predictions, with and without iterations, for different simulation parameters. The mean deviation, $|\Delta T|$, the standard deviation, $|\Delta T|_\sigma$, and the maximum deviation, $|\Delta T|_{\text{max}}$, between the two models are given. All CAFE simulations are run in 2D, unless specified. A reference case, Ref.a, is chosen, so that the influence of each model parameter is independently shown.
Table 2. Deviations of the predicted cooling curves for the 1D Al–7 wt% Si ingot using the CAFE model with and without iterations for different simulation parameters: cell size, $l_{CA}$, macro time step, $\Delta t$, convergence criterion, $\epsilon$, and number of nodes along the direction of solidification, $N_{\text{mesh}}$. Quantitative comparisons are provided for the mean deviation, $|\Delta T|_m$, the standard deviation, $|\Delta T|_\sigma$, the maximum deviation, $|\Delta T|_{\text{max}}$, and the calculation (CPU) time.

<table>
<thead>
<tr>
<th>Case</th>
<th>Ref.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l_{CA}$ (µm)</td>
<td>100</td>
<td>10</td>
<td>500</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>$\Delta t$ (s)</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.01</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>$\epsilon$ (—)</td>
<td>$4 \times 10^{-2}$</td>
<td>$4 \times 10^{-2}$</td>
<td>$4 \times 10^{-2}$</td>
<td>$4 \times 10^{-4}$</td>
<td>1</td>
<td>$4 \times 10^{-2}$</td>
<td>$4 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td>$N_{\text{mesh}}$ (—)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>200</td>
<td>100</td>
</tr>
</tbody>
</table>

(a) Without iterations

<table>
<thead>
<tr>
<th>Case</th>
<th>Ref.a</th>
<th>1a</th>
<th>2a</th>
<th>3a</th>
<th>4a</th>
<th>5a</th>
<th>6a</th>
<th>3Da</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_m$ (°C)</td>
<td>0.1652</td>
<td>0.1601</td>
<td>0.1580</td>
<td>0.0393</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_\sigma$ (°C)</td>
<td>0.0831</td>
<td>0.3228</td>
<td>0.3474</td>
<td>0.0515</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_{\text{max}}$ (°C)</td>
<td>14.8</td>
<td>11.3</td>
<td>12.2</td>
<td>0.840</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>CPU time</td>
<td>24min02s</td>
<td>5h27s</td>
<td>25min47s</td>
<td>4h28s</td>
<td>—</td>
<td>—</td>
<td>2h56s</td>
<td>3h36s</td>
</tr>
</tbody>
</table>

(b) With iterations

<table>
<thead>
<tr>
<th>Case</th>
<th>Ref.b</th>
<th>1b</th>
<th>2b</th>
<th>3b</th>
<th>4b</th>
<th>5b</th>
<th>6b</th>
<th>3Db</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_m$ (°C)</td>
<td>0.0438</td>
<td>—</td>
<td>0.0557</td>
<td>0.0397</td>
<td>0.0435</td>
<td>0.0836</td>
</tr>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_\sigma$ (°C)</td>
<td>0.0568</td>
<td>—</td>
<td>0.0820</td>
<td>0.0551</td>
<td>0.0585</td>
<td>0.1425</td>
</tr>
<tr>
<td>$</td>
<td>\Delta T</td>
<td>_{\text{max}}$ (°C)</td>
<td>0.681</td>
<td>—</td>
<td>0.901</td>
<td>0.804</td>
<td>0.766</td>
<td>4.527</td>
</tr>
<tr>
<td>CPU time</td>
<td>1h24s</td>
<td>—</td>
<td>1h10s</td>
<td>5h27s</td>
<td>5h01s</td>
<td>47min44s</td>
<td>7h11s</td>
<td>11h29s</td>
</tr>
</tbody>
</table>

Without iterations, the macro time step has the strongest impact on the results. Replacing the $10^{-1}$ s reference time step with a $10^{-2}$ s time step (case 3a) gives a mean deviation four times lower, a standard deviation seven times lower and the maximum deviation falls below 1 °C. More interestingly, the deviations observed are about the same as the converged reference case using $10^{-1}$ s time step, Ref.b. This result justifies the initial hypothesis that a sufficiently small time step permits us to avoid iterative resolution [5]. The $10^{-1}$ s time step here is too large to reach good agreement between FT and CAFE without iterations, since the maximum deviation for Ref.a reaches 14.8 °C.

For converged solutions performed with iterations, the time step has almost no influence. This is also coherent. It is noticeable that iterative coupling makes the resolution time four times longer for the reference case. However, if we compare case 3a and Ref.b, the iterative resolution is three times faster for the same deviation induced. An ideal time step between $10^{-1}$ and $10^{-2}$ s could have been faster for the same precision without iteration.

Concerning iterative convergence, it is clear that a smaller criterion on the residual gives better results. However, a reasonable limit has to be taken as over-precision does not improve deviations significantly, while substantially increasing the resolution time. Case 5b ($\epsilon = 1$) corresponds to no convergence, the system computing at least two iterations to get the residual. That is why divergences are lower than in the reference case without iterations, Ref.a, and computation time is doubled.

When no iterations are performed, the cell size has a very limited impact although visible on the predicted cooling curves (cases 1a and 2a). As expected, diminishing the cell size lowers the deviation. The most obvious change is on the maximum error, but with 10 µm cells it remains very high (> 10 °C). Note also that this value is not very representative of the deviations, because it only happens at the very end of solidification. As soon as there is no more liquid, no more heat is released and the temperature suddenly falls. The effect of the cell...
size is more visible on converged simulations (case 2b with respect to Ref. 1b), but it is still quite limited and the computation time is not significantly changed.

Finally, the mesh definition has also an impact on the cooling curves. The difference on non-converged results (case 6a) is not the one expected: the finest mesh gives larger deviations. As there is no correction, cumulative errors are bigger. To retrieve the same results, it is usually necessary to divide the time step by two if the mesh is twice finer. In this case, the time step was already too large with a 100 node mesh. It is then logical that a 200 node mesh leads to worse results. On the other hand, convergence (case 6b) allows reaching an even better fit with the FT model than any other case. It thus clearly reveals the limitation induced by the mesh size. Resolution time is still significantly increased.

The reference case is finally computed in 3D, for both non-iterative (3Da) and iterative (3Db) coupling algorithms. Deviations are globally smaller than in 2D, because of value averaging. As the FT model is only applicable in 1D, probes are set at the center of the ingot section in the CAFE simulations. Resolution time is again dramatically longer.

It results from the previous considerations that iterative coupling, if used correctly, allows a serious precision improvement, without substantially increasing the resolution time. However, the non-iterative algorithm gives mean and standard deviations that are acceptable in most cases (<0.5 °C). If care is taken when choosing the time step, results are close to the solution.

4. Application

The new multiple structure CAFE model is tested on an Al–7 wt% Si cylindrical ingot for which an experiment is available with a detailed description in [16]. The ingot is a vertical cylinder of diameter 70 mm. The measured length at the end of the solidification is 170 mm. The bottom of the ingot is in contact with a copper chill. Temperature probes are localized at 20, 40, 60, 80, 100, 120 and 140 mm from the bottom of the ingot.

As there is no mechanical resolution in the present CAFE model, no shrinkage can be predicted. In order to account for shrinkage, a 173 mm length simulation domain is used, slightly larger than the final measured length of the ingot. This was shown to be necessary in order to retrieve simulation curves [17]. Recorded temperature at 0 mm is deduced from a second-order extrapolation of the 20, 40, 60 and 80 mm probes. That temperature is used for the bottom boundary condition of the CAFE simulation. As in [17], a small heat flux, \( Q = 3000 \text{ W m}^{-2} \), is also imposed on the top face of the ingot in the first part of the simulation, while \( t < 900 \text{ s} \). Growth kinetics of dendritic and eutectic structures, specific heat, conductivity and other material properties are the same as in [17].

The parameters of the CAFE simulation are given in table 3. Time step is 0.1 s. The cell size is 250 \( \mu \text{m} \), meaning about 43 \( \times \) 10⁶ cells are necessary over the whole volume. Due to the heavily demanding computer resources, this simulation was run on 12 processors using parallel computing.

Figure 7 provides with 3D representation of the predicted time sequence of the dendritic grain structure. The eutectic structure forms only within the dendritic grains. It is not displayed in this figure. As can be seen, predicted grain shapes are columnar in the bottom part of the ingot and equiaxed in the top part. A columnar-to-equiaxed transition (CET) is modeled. However, the CET appears to happen sooner in the simulation, as the height of the transition is predicted at 108.3 mm while it was measured at 118 mm in the experiment. Moreover, the size of the equiaxed grain structure could not be predicted as small as it was measured. These differences can be explained by several causes. First the simulation does not include grain sedimentation, which may play an important role in the average grain size. It was also suggested that the CET was caused in this experiment by dendrite fragmentation taking part
Table 3. Simulation parameters for the 3D Al–7 wt% Si cylindrical ingot (figures 7 and 8).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step</td>
<td>$\Delta t$</td>
<td>0.1 s</td>
</tr>
<tr>
<td>Cell size</td>
<td>$l_{CA}$</td>
<td>$250 \times 10^{-6}$ m</td>
</tr>
<tr>
<td>Nucleation parameters (chill)</td>
<td>$s_1 = \text{dendritic}$</td>
<td>$\Delta T_i^{s_1} = 0.0$ °C</td>
</tr>
<tr>
<td></td>
<td>$n_{i \text{max}}$</td>
<td>$5 \times 10^5$ m$^{-2}$</td>
</tr>
<tr>
<td>Nucleation parameters (chill)</td>
<td>$s_2 = \text{eutectic}$</td>
<td>$\Delta T_i^{s_2} = 0.0$ °C</td>
</tr>
<tr>
<td></td>
<td>$n_{i \text{max}}$</td>
<td>$5 \times 10^5$ m$^{-2}$</td>
</tr>
<tr>
<td>Nucleation parameters (volume)</td>
<td>$s_1 = \text{dendritic}$</td>
<td>$\Delta T_i^{s_1} = 0.5$ °C</td>
</tr>
<tr>
<td></td>
<td>$n_{j \text{max}}$</td>
<td>$10^9$ m$^{-3}$</td>
</tr>
<tr>
<td>Nucleation parameters (volume)</td>
<td>$s_2 = \text{eutectic}$</td>
<td>$n_{j \text{max}} = 0$ m$^{-3}$</td>
</tr>
<tr>
<td>Ingot height</td>
<td>$l$</td>
<td>0.173 m</td>
</tr>
<tr>
<td>Number of FE nodes</td>
<td>$N_{\text{mech}}$</td>
<td>$43 \times 10^3$ —</td>
</tr>
</tbody>
</table>

Figure 7. External view of the modeled 3D Al–7 wt% Si cylindrical ingot during the CET transition, at different times of the CAFE simulation.
at the columnar growth front when the temperature gradient in the liquid becomes sufficiently low [17]. That phenomenon is not considered by the present CAFE simulation. Instead, we presume that nucleation of equiaxed grains happen on nucleation sites that are already present in the liquid volume. Other physical phenomena, such as shrinkage and macrosegregation, may also have an influence on the CET.

Figure 8 shows the comparison of experimental and predicted cooling curves. The agreement is overall very good. Differences are due to the above-mentioned facts, in addition to the fact that the imposed temperature is actually only an interpolation of the measured temperatures. Shrinkage plays an especially important role in the curves’ evolution. The CET clearly appears on the results through a recalescence on the 140 mm probe, i.e. 5 °C below the liquidus temperature. This prediction cannot be retrieved without structure representation (i.e. using only a FE solver without accounting for grain structures), and did not reach this agreement in 2D. The eutectic plateau is also visible below the eutectic temperature on the 140 mm predicted curve, with some undercooling corresponding to eutectic growth.
5. Conclusion

The different conversion scheme tested showed considerable improvements of the CAFE model. The node coupling scheme allows significant reduction of the resolution time. The implementation of multiple structures led to better results on the predicted cooling curves, taking into account nucleation and growth undercooling of secondary structures such as eutectic. Finally, the iterative developments proved that although an error is induced by skipping convergence, it is mostly negligible if care is taken with the choice of the macroscopic time step.

These developments in 3D led to the prediction of columnar-to-equiaxed transition in an Al–7 wt% Si ingot. The time evolution of the grains and the cooling curves are simulated, showing good agreement with the experiment. In particular, the recrystallization due to the growth of equiaxed grains is well predicted.

Several phenomena still have to be modeled, the most important being macrosegregation. Previous works have only been done in 2D [18–21], which now needs to be extended in 3D.

Acknowledgment

This work was partly funded by the Agence Nationale de la Recherche (Paris, F) under reference ANR-08-HABISOL-012-01.

References

[16] Gandin Ch-A 2000 ISIJ Int. 40 971–9