International Journal of Heat and Mass Transfer 116 (2018) 940–950

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Cellular automaton modeling of dendritic growth of Fe-C binary alloy with thermosolutal convection

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A R T I C L E I N F O

Article history:
Received 26 May 2017
Received in revised form 6 September 2017
Accepted 19 September 2017

Keywords:
Cellular automaton
Dendritic growth
Thermosolutal convection
Numerical simulation

A B S T R A C T

Embedded the thermal and solutal buoyancy into the momentum conservation equation as an additional force term using the Boussinesq approximation, a 2D CA-FVM model is extended to simulate the dendritic growth with thermosolutal convection. The model is firstly validated by comparison of numerical predictions with the benchmark test of Rayleigh – Bénard convection and the analytical solutions of the stagnant film model for the free dendritic growth with thermosolutal convection, and good agreements between the numerical results with analytical solutions are obtained. Later, numerical simulations for both the equiaxed and columnar dendritic growth of Fe-0.82wt%C binary alloy with thermosolutal convection are performed. The results show that, for the equiaxed dendritic growth in an undercooled melt, the dendrite tip growth rapidly decreases from the high velocity to a relative low steady-state value. With the further growth of dendrite, the thermosolutal convection induced by the solute rejection and latent heat release is enhanced and four vortexes are developed between the dendrite arms. Thus, the asymmetries of the dendrite morphology, temperature and solute profiles are intensified. For the columnar dendritic growth with thermosolutal convection under the unidirectional solidification process, the thermosolutal convection transports the rejected solute downward and makes the solute enrich at the interdendritic region. The thermosolutal convection facilitates the upstream dendritic growth, but inhibits the downstream dendritic growth. Moreover, with the increase of deflection angle of gravity, the advection on the top region and the clock-wise vortex flow at the interdendritic region intensified, and finally the columnar dendrite morphology becomes more asymmetrical.

1. Introduction

Dendritic structure is widely observed in the metallic alloys and has a great influence on the alloy properties [1,2]. During the solidification of metallic alloys, the dendritic growth is usually accompanied with the latent heat release and solute redistribution, and thus natural convection is inevitably developed under the gravity due to the density variations in the liquid caused by thermal and solutal gradient. Conversely, the natural convection induced by the thermosolutal buoyancy would change the thermal and solutal profile and finally affects the dendritic growth. Meanwhile, the natural convection affects not only the dendrite morphology but also the solute distribution, resulting in the semi- and macrosegregation formation. Such as: the preferential interdendritic flow is in favor of channel segregation formation [3–5] and the long distance flow is tend to facilitate macrosegregation formation [6–8]. Such uneven solute distribution has detrimental effects on the alloy properties and should be avoided during the solidification of metallic alloys. Therefore, the effect of the thermosolutal convection on the dendritic growth should be elucidated in order to control the structural and chemical homogeneities of cast products and achieve the desired mechanical properties of final products.

Numerical simulation, as a powerful method, has attracted a lot of interests of researchers in the field of the natural convection effects on the dendritic growth in recent decades. Tönhardt and Amberg [9] were the pioneers in the numerical simulation of natural convection effects on the dendritic growth. They firstly incorporated the thermal buoyancy term into the momentum conservation equations to develop a two-dimensional (2D) phase field (PF) model for the dendritic growth in the presence of thermal convection using an adaptive finite element method and preliminarily investigated the effect of natural convection on the growth of pure succinonitrile (SCN) crystals. The asymmetric dendrite morphology was well predicted and quantitatively consistent with results of terrestrial experiments. Bänsch and Schmidt [10] presented a 2D sharp-interface (SI) model to investigate the effect of

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https://doi.org/10.1016/j.ijheatmasstransfer.2017.09.074
0017-9310/

the thermal convection on dendritic crystal growth using a finite element method, and the results showed that the thermal convection had a strong effect on the dendritic morphology, side branching and growth rate. Miller et al. [11,12] coupled the Lattice Boltzmann method (LBM) with the PF method to develop a 2D LBM-PF model for the dendritic growth with thermal convection, and firstly performed calculations of the microstructure evolution during the Czochralski growth of GeSi single crystals. Zhao et al. [13] developed a 2D SI model for the dendritic growth with convection using an adaptive finite element method. The distinct advantages of the model were that the natural convections generated by contraction, thermal and solutal buoyancy and forced convections were all included with primitive parameters, and extensive model validation and application were illustrated. The predicted results for the SCN crystals growth with thermal convection and the equiaxed dendritic growth into an undercooled pure melt with forced convection were in excellent agreement with the results of Tönhardt and Amberg [9], and the results of Beckermann et al. [14], respectively. Moreover, some new findings were concluded that convection induced by the contraction promoted the solidification rate and destabilized the solid/liquid (S/L) interface and the thermosolutal convection developed ahead of the S/L interface. Steinbach and co-workers [15–17] proposed a 2D PF model for the dendritic growth with thermosolutal convection and predicted the constrained dendritic growth of Al-4wt% Cu alloy with thermosolutal natural convection during the unidirectional solidification process. The results demonstrated that the interdendritic convection crucially depended on the gravity direction and had a significant effect on the dendrite arm spacing and dendrite morphology. Chen and Lan [18] firstly developed an adaptive 3D PF method to investigate the effect of natural convection on free dendritic growth and the results demonstrated that at the low supercooling, the dendritic growth was more sensitive to the gravity level and orientation, and the results were consistent with previous experimental observations. Yuan and Lee [19] incorporated the energy, mass and momentum conservation equations with the kinetic equations of dendritic growth to develop a cellular automaton (CA) model, where the modified decentered square/octahedron algorithm [20] was implemented to explicitly track the S/L interface, and investigated the effects of both forced and natural convection on the dendritic growth of Ni-Nb alloy. Later, they [4,21] adopted the 3D CA model to investigate the complex phenomena of solute segregation, interdendritic thermosolutal convection and dendritic growth, and clarify the mechanisms of freckle initiation and growth in the unidirectional solidified Pb-Sn alloy and Ga-In alloy. Shi et al. [22] proposed a modified CA model to simulate the dendritic growth in the presence of natural convection during unidirectional solidification of NH_4Cl-H_2O solution and a good agreement was obtained between the numerical results and experiment measurements. Zhu and co-workers [23–26] incorporated LBM with CA method to develop a 2D CA-LBM model for the dendritic growth with convection and simulated the single and multi-dendritic growth of binary alloy in the presence of natural convection. The results showed that the dendrite morphology was significantly influenced by the natural convection and the predicted steady-state growth parameters were in good agreement with the theoretical solutions.

According to the above mentioned literatures, numerous methods, such as PF method [9,11,12,15–18], SI method [10,13] and CA method [4,19,21–26], have been successfully adopted to investigate the dendritic growth in the presence of natural convection and numerical studies have contributed a lot to reveal the complex interaction of solute segregation, natural convection and dendritic growth. Whereas, additional work remains to be performed, especially for the quantitative characterization of interdendritic flow, which is a key factor for the formation of freckle defect and macrosegregation.

In the present study, the previous developed 2D CA-FVM model [27] is extended to reveal the dendritic growth with thermosolutal convection by including the effect of thermal and solutal buoyancy. The model is firstly validated against the benchmark test of Rayleigh – Bénard convection and analytical solution of the stagnant film model for the free dendritic growth with thermosolutal convection. Subsequently, the model is adopted to simulate the equiaxed dendritic growth and columnar dendritic growth with thermosolutal convection.

2. Model description

The previous developed 2D CA-FVM model [27] has fully coupled the energy, mass and momentum conservation equations with the kinetic equations of dendritic growth, and has been proved that it was capable of predicting the dendritic growth in the presence of forced convection [28]. Whereas, the thermosolutal convection induced by the thermal and solutal buoyancy, which is usually accompanied with the dendritic growth and has great effects on the dendritic growth, is ignored. Here, the thermal and solutal buoyancy is incorporated into the momentum conservation equations using the primitive additional term to take the thermosolutal convection effects into consideration.

2.1. Momentum, mass and energy transport equations

Assuming the fluid flow is incompressible, the fluid flow is governed by the Navier-Stokes equations and described in the following forms:

Continuity equation:

$$\nabla \cdot \mathbf{U} = 0 \tag{1}$$

Momentum conservation equation:

$$\rho \frac{\partial \mathbf{U}}{\partial t} + \rho \mathbf{U} \cdot \nabla \mathbf{U} = -\nabla p + \nabla(\mu \nabla \mathbf{U}) + F \tag{2}$$

where $\mathbf{U}$ is the velocity vector, ρ is the density, μ is the viscosity, p is the hydrostatic pressure, t is the time, and F is the total force of thermal and solutal buoyancy.

According to the Boussinesq approximation [29], the density is linearly dependent of temperature and only appears in the buoyancy term of the momentum equation. Thus, the total buoyance force can be determined by

$$F = -\rho_{ref} g (\beta_t (T - T_{ref}) + \beta_c (C_l - C_{ref})) \tag{3}$$

where g is the gravitational acceleration, ρ_{ref}, T_{ref} and C_{ref} are respectively the reference density, temperature and composition, β_t and β_c are respectively the thermal and solutal expansion coefficients, T and C_l are respectively the local temperature and solute concentration of melt.

The solute diffusion in the presence of fluid flow is given by Fick's law with convection effect, as shown below:

$$\frac{\partial C_e}{\partial t} + \xi \mathrm{U} \cdot \nabla C_e = D_e \cdot \nabla^2 C_e \tag{4}$$

where ξ is the state parameter of CA cell (if the cell state is liquid or interface, ξ is 1; if the cell state is solid, ξ is 0), C_e and D_e are respectively the equivalent solute concentration and solute diffusion coefficient, and defined as followings:

$$C_e = C_s f_s + C_l f_l = C_l (1 - (1 - k_0) f_s) \tag{5}$$

$$D_e = D_s f_s + D_l f_l \tag{6}$$