



Macrosegregation simulation model based on Lattice-Boltzmann method with high computational efficiency

Munekazu Ohno ^{a,*}, Hayato Sato ^b

^a Division of Materials Science and Engineering, Faculty of Engineering, Hokkaido University, Kita 13 Nishi 8, Kita-ku, Sapporo, Hokkaido 060-8628, Japan

^b Graduate School of Engineering, Hokkaido University, Kita 13 Nishi 8, Kita-ku, Sapporo, Hokkaido 060-8628, Japan

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ABSTRACT

A macrosegregation simulation model is developed by coupling solute and energy conservation equations with Lattice-Boltzmann Method (LBM), newly developing technique of computational fluid dynamics. Effect of the solidification shrinkage is taken into account in the present LBM as well as effects of the Darcy's flow and thermos-solutal convection. The present LBM-coupled model is based on modified lattice Bhadnager-Gross-Krook method, the numerical stability of which is better than that of the standard LBM. Accordingly, the present LBM-coupled model can be applied to simulations of macrosegregation behaviors in metallic alloy systems that cannot be handled by the previous LBM-coupled model. The validity of the model was demonstrated by comparing the results for steady-state flows with those of analytical solutions and a conventional model based on the Navier-Stokes equation. In addition, the computational speed of the present model is compared with the one of conventional model in cases of lateral directional solidification of Sn-Bi alloy and continuous casting of a steel slab. It is shown that the present LBM-coupled model enables remarkably faster computation than the conventional model especially in the latter case.

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1. Introduction

Macroseggregation refers to a non-uniform distribution of alloying elements on a scale of ingot. It stems from macroscopic flows of segregated liquids [1–4]. The macroscopic flow occurs in several mechanisms such as thermosolutal convection, a flow due to solidification shrinkage and forced flow and so on. Numerical models have been developed for simulating macrosegregation behaviors. The simulation models have been gradually sophisticated and their usefulness accordingly increases [5–7]. However, the macrosegregation simulations, in general, are computationally demanding and the high computational cost restricts the simulation system to a small size and/or it forces one to employ coarse grid, which often causes inaccurate description of macrosegregation behavior [4]. The numerical models are generally based on momentum, mass, energy and solute conservation equations where the momentum conservation is described by the Navier-Stokes (hereafter abbreviated as NS) equation. The numerical calculation for the NS equation requires a time-consuming calculation for correction of the velocity and pressure, which is a bottleneck restricting

the speed-up of macrosegregation simulation. It is necessary to accelerate the calculation of fluid dynamics.

Lattice-Boltzmann Method (LBM) is a newly developing technique for computational fluid dynamics [8–14]. This is a method based on the lattice-Boltzmann equation that describes the time evolution of particle distribution functions, from which the macroscopic quantities of fluid such as the density, velocity and pressure can be calculated. Importantly, LBM does not require the time-consuming calculation for correction of the velocity and pressure and, hence, it generally enables fast computation of fluid dynamics. Recently, we developed a model for simulating macrosegregation based on LBM in which the NS equation is replaced by the lattice-Boltzmann equation including effects of the thermosolutal flow and Darcy's flow [15]. The accuracy of the LBM-coupled model was investigated by comparing the calculated results for the steady-state flows with the results obtained by analytical solutions and a conventional model based on the NS equation (NS-based model). The results of the LBM-coupled model are almost identical to those of the analytical and the NS-based models. Moreover, we conducted a simulation for solidification in a small ingot of a model alloy where the macrosegregation appears only by natural convection, by means of the LBM-coupled model and the NS-based model. The LBM-coupled model yields almost the same result as the

* Corresponding author.

E-mail address: mohno@eng.hokudai.ac.jp (M. Ohno).

NS-based model. Importantly, the simulation of LBM-coupled model is about five times faster than the one of NS-based model [15].

As described above, the acceleration of macrosegregation simulation was successfully achieved based on LBM. However, the following issues remain to be resolved. Although one cannot neglect effect of the macroscopic flow driven by the solidification shrinkage on the formation of macrosegregation in some cases [1–4], the solidification shrinkage cannot be dealt with in the previous model. More importantly, the LBM-coupled model developed in the previous study cannot be applied to real metallic alloy systems. In this model, the numerical stabilities of LBM and the energy conservation equation limit the Prandtl number to about one order of magnitude larger than typical values in metallic alloys [15]. In other words, when the typical value of thermal diffusivity is employed, the viscosity must be one order of magnitude higher than the typical value in metallic alloys in the light of the numerical stability of LBM. This problem must be resolved. Moreover, it is important to clarify how much acceleration can be achieved in simulations for realistic casting processes. The advantage of parallel computing technique should be investigated because LBM is suitable for parallel computing. These issues are tackled in this paper.

The purpose of this study is to construct a model for macrosegregation simulations with high computational efficiency based on LBM that can be applied to the simulations for realistic solidification processes in metallic alloy systems. To this end, the effect of solidification shrinkage is introduced in LBM. Moreover, the model is constructed based on the recently-developed Modified Lattice Bhadrnager-Gross-Krook (MLBGK) method [16], the numerical stability of which is much higher than that of the standard LBM. Then, the model is applied to the simulations for lateral directional solidification of Sn-Bi alloy and continuous casting of steel. The computational speeds are investigated in comparison with the results of the conventional NS-based model. The paper is organized as follows. The LBM-coupled model and the NS-based model are explained in the next section. The results of steady-state flow, lateral directional solidification and continuous casting are described in Sections 3, 4 and 5, respectively. The conclusions are given in the last section.

2. Numerical methods

2.1. Conventional model based on the Navier-Stokes equation

In this study, the LBM-coupled model is constructed by coupling the MLBGK method with the solute and energy conservation equations. As is similar to the previous work, the present modeling rests on a NS-based model developed in early studies [17–19], which was chosen because the numerical implementation is relatively straightforward and the simulation results for lateral directional solidification of Sn-Bi alloy and continuous casting of steel were already reported [17–19].

In the NS-based model, the incompressible fluid flow is calculated by the following equations [19],

$$\nabla \cdot \mathbf{u} = -\beta \frac{\partial f_s}{\partial t} \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho_0} + \nu \nabla^2 \mathbf{u} + \frac{\rho_0 + \delta \rho}{\rho_0} \mathbf{g} - \frac{\nu}{K} \mathbf{u} \quad (2)$$

where $\mathbf{u}$ is the velocity vector of fluid, β is the solidification shrinkage rate, f_s is the volume fraction of solid, p is the pressure, ρ_0 is the density at a reference state, ν is the kinematic viscosity, $\delta \rho$ represents the density change due to the variation of temperature and concentration, $\mathbf{g}$ is the gravitational acceleration and K is the

permeability. In contrast to the previous work, the continuity Eq. (1) includes the effect of solidification shrinkage. In the NS equation (Eq. (2)), the third and fourth terms on the right-hand side represent effects of thermosolutal convection and the Darcy's flow, respectively. In this study, the permeability K is given by $K = K_0(1 - f_s)^3 / f_s^2$, where K_0 is the permeability coefficient.

Eqs. (1) and (2) are coupled with the following energy conservation and solute conservation equations [17–19],

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = a_T \nabla^2 T + \frac{\Delta H}{c_h} \frac{\partial f_s}{\partial t} \quad (3)$$

$$\frac{\partial C_L}{\partial t} + \mathbf{u} \cdot \nabla C_L = \frac{\partial f_s}{\partial t} \frac{(1 - k_e)C_L}{1 - f_s} \quad (4)$$

where T is the temperature, a_T is the thermal diffusivity, ΔH is the latent heat and c_h is the specific heat capacity, C_L is the solute concentration in the liquid and k_e is the equilibrium partition coefficient. In the solute conservation Eq. (4), the diffusion term is omitted and the reaction term on the right-hand side is based on the Scheil model.

Although several numerical methods were developed for solving the NS equation such as MAC [20] and SIMPLE methods [21], a time-consuming calculation is required for correction of the velocity and pressure in these methods. Hence, the computational burden for solving NS equation is generally high and it occupies a large part of the computational cost of macrosegregation simulations. Hence, a key to acceleration of the macrosegregation simulations lies in the calculation of fluid flow. In this study, the continuity Eq. (1) and NS Eq. (2) are replaced by LBM.

We carried out simulations of the above-mentioned NS-based model to compare its results with those of the LBM-coupled model. In the present study, Eqs. (1) and (2) were solved based on the SIMPLE method in all simulations. The energy and solute conservation Eqs. (3) and (4) were discretized based on a finite difference method with a second order accuracy in space and they were solved using a first order Euler scheme. One must pay attention to numerical accuracy of advection term because it affects the stability and accuracy of macrosegregation simulations. In this study, the advection terms were calculated based on the third-order upwind scheme. The total variation diminishing scheme [22] was employed to stabilize the numerical simulation only in the case of continuous casting of a steel slab.

2.2. LBM-coupled model

LBM has attracted a great deal of attention as an effective computational method for fluid dynamics [8–14]. LBM can be viewed as a discrete version of the Boltzmann equation. In the previous study, influence of solid fraction, Darcy's flow and thermosolutal convection were taken into account in LBM and it was coupled with the energy and solute conservation equations [15]. This LBM-coupled model developed in the previous work is first described in this sub-section. In this study, the model including the effect of solidification shrinkage is first developed based on the previous model, and then, it is reformulated based on the MLBGK model [16].

In LBM, the fluid consists of fictive and microscopic particles moving at discrete velocities in discrete directions on a lattice. Their collective behavior determines the macroscopic quantities of fluids such as the density, velocity and pressure. The lattice-Boltzmann equation is written as [14],

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}, t) = -\frac{1}{\tau} [f_\alpha(\mathbf{x}, t) - f_\alpha^{(eq)}(\mathbf{x}, t)] + F_\alpha \delta t \quad (5)$$

where f_α represents the distribution function for the particle moving at a discrete velocity $\mathbf{e}_\alpha$ in a discrete direction specified by α .

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