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On the thermal boundary conditions of particulate-fluid modeling

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ABSTRACT

Sedimentation processes of solid particles in a fluid with heat transfer are simulated using a coupled Lattice Boltzmann Method, Immersed Boundary Method and Discrete Element Method (LBM-IBM-DEM) scheme. In the numerical simulations, solid particles are specified either by a given temperature which is termed Dirichlet boundary condition or by a temperature gradient which is termed Neumann boundary condition. Several cases are examined containing one, two and 504 solid particles settling in a fluid, respectively. All the considered cases could be divided into two groups: Group Dirichlet and Group Neumann according to different styles of boundary conditions employed but under exactly the same initial states. The effects of these two boundary conditions on the particle behavior are quantized.

1. Introduction

A technique that seems simple at first is actually quite intricate and affected by many uncertain factors, just like the Lattice Boltzmann Method (LBM) modeling [1]. People may argue plenty of merits of the LBM to solve various computational fluid dynamics (CFD) problems [2], among which the most attractive one is definitely the ease in programming. Especially when coupling with the immersed boundary method (IBM) [3], the LBM-IBM scheme exhibits great flexibility and potential in handling complicated fluid-structure coupling problems such as the hydrodynamic interaction of elastic filaments [4,5], particulate-fluid interactions [6–8], natural convection of immersed obstacles [9,10] and thermal particulate-fluid interactions [11–13] as focused in this study.

Solid particles moving in a fluid with a different temperature involves complex interaction behaviors leading to a number of non-linear phenomena which is not well understood [14]. Full knowledge of not only the heterogeneous distribution of the solid particles and temperature but also the essential heat transfer mechanisms is highly needed. It was reported by Gan et al. [15] that the thermal convection could play an important role in affecting the solid particle behavior. Gan et al. [15] numerically identified a couple of Grashof-number dependent regimes and the discrepancy of which was supposed to be caused by the formation of microstructures of the trailing vortex or between the particles. In the numerical simulation within an Eulerian-Lagrangian framework [16], the solid particles are either specified by a given temperature which is termed the Dirichlet thermal boundary condition (BC) or specified by a heat flux which is termed the Neumann thermal BC. However, few studies have been conducted to quantize the effects of these two thermal BC on the particle behavior which motivates the present work. The subject does not sound fresh in the conventional heat transfer cases [17] but still deserves a discussion in the context of the LBM-IBM modeling (major difficulty in treating the Neumann type of thermal IBM [18,19] which is detailed later). Comparisons between these two types of BC in the IBM were made by Zhang et al. based on a typical case of flow over a stationary circular cylinder in which significantly different temperature patterns were reported [20]. Therefore, it would be interesting to perform quantitative comparisons of the effects of thermal BC on the particle behavior to characterize the difference.

The Dirichlet thermal BC has been relatively well established in the framework of the LBM-IBM for the thermal particulate-fluid interactions. Hashemi et al. carried out three-dimensional simulations of 1 and 30 particles, respectively, to investigate the settling of hot particles in a cold Newtonian fluid with the effects of Reynolds, Prandtl and Grashof numbers discussed [21]. It was found that the presence of heat transfer can significantly alter the behavior of the settling particles in a fluid. Similar findings were reported in the work of Yang et al. [13] considering 2 particles and the present authors [11,12] considering 504 particles. In our previous works [11,12], a combined LBM-IBM-DEM (DEM: discrete element method [22]) scheme was proposed to investigate the sedimentation of solid particles in a fluid with heat transfer. The DEM calculates the macro behavior of the granular material by monitoring the trajectories of every single particle as well as considering the inter-particle collisions. Therefore, it is quite suitable for capturing the distinctive feature of the solid particles and describing the

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heterogeneous distribution formed [23]. Meanwhile, both conventional LBM and DEM use an explicit scheme to integral which makes the LBM-IBM-DEM scheme favorably achieved. As a natural next step, we enable another function of the LBM-IBM-DEM scheme to treat Neumann thermal BC in this study. It is worthwhile mentioning that the fluid variables on the solid boundary were also evaluated explicitly in the early LBM-IBM schemes [6,24] which may give rise to problems contrary to the physics laws such as the flow penetration into the solid structure. Enhanced treatments to conquer these drawbacks are the multi-direct forcing scheme [25] and implicit correction schemes [26,27]. Numerical investigations on the thermal particulate-fluid interactions via other CFD-DEM modelings have been also reported [28–31], the Dirichlet thermal BC was applied in which the heating process of solid particles by the hot gas was mainly addressed.

There is much less work focusing on the Neumann type of thermal BC in the framework of LBM-IBM. Recent publications are mainly limited by the explicit scheme proposed by Hu et al. [18] and the implicit one proposed by Wang et al. [19]. Hu et al. [18] proposed a direct method to deal with the Neumann thermal BC by distributing the jump of the heat flux on the boundary into the nearby Eulerian points. The basic idea is to find proper weight parameters to construct the solid temperature jump function based on those at the LBM nodes both inside and outside the particle occupied region. The proposed Neumann thermal BC was then used to investigate the natural convection in a horizontal annulus forming multiple steady solutions. Instead, Wang et al. [19] introduced two layers of discrete Lagrangian points on the both sides of the solid physical surface, the temperature correction (related to heat source) on the Lagrangian points were treated as unknowns and thus enabled an implicit calculation. The advantage of the implicit treatment is its capability to guarantee the fit between the calculated temperature gradient at the solid boundary and the specified one. To the best of our knowledge, there is no LBM-IBM-DEM simulation on the thermal particulate-fluid coupling problem via the Neumann thermal BC in the publicly available references. So, the aim of the current paper is two-fold. The first goal is to examine the effect of the Neumann thermal BC on the solid particle behavior in a thermal fluid. The second one is to characterize the difference between the two thermal BCs as mentioned afore.

The remainder of the paper is organized as follows. To make this paper self-contained, the mathematics of the LBM, IBM for the Dirichlet and Neumann types of BC and DEM are briefly introduced in Section 2. For the Neumann thermal BC, the explicit scheme of Hu et al. [18] is inherited in this study. And it is noted that we abandon any iterative or implicit techniques [18] in the IBM mainly to save the computational time. As Yu and Xu pointed out, the expansive part in simulating a particulate-fluid system is mainly related to the solid phase rather than the CFD side [32]. The statement has been proved valid by the development of the state-of-art modeling techniques of the recent decade. A proper simplification on the coupling scheme can be therefore tolerated especially when treating inter-particle collisions dominating systems [33,34] like those focused in this study. Our numerical experiments show that this treatment works well in general. In Section 3, the current code for the Neumann thermal BC is firstly validated through comparing with reference results and then case studies of (1) one cold particle settling in a channel, (2) two particles settling in a channel, and (3) 504 cold particles settling in a cavity are presented. All the considered cases could be divided into two groups: Group Dirichlet and Group Neumann according to different styles of BC employed but under exactly the same initial states. The effects of these BC on the particle behavior are quantized. Finally, conclusions are given in Section 4.

2. Governing equations

In this section, we briefly summarize the governing equations and numerical issues. Since the LBM-IBM treatments on the velocity and thermal BC are in quite similar manners no matter using the Dirichlet or Neumann types, it would be straightforward to introduce them following the same system with the main difference highlighted. For more details, the readers are referred to our previous works in two-dimensional [35,11] and three-dimensional [36,12] cases based on the Dirichlet thermal BC and two-dimensional case [18] based on the Neumann thermal BC.

2.1. Lattice Boltzmann method

In this study, we limit all the discussions in two-dimensional cases where the LBM-D2Q9 model [1] is adopted to simulate the heat and mass transfer behavior of an incompressible Newtonian fluid. The governing equations are the dual distribution models proposed by He et al. [37] as shown below

$$\begin{cases} f_\alpha(\mathbf{r}+\mathbf{e}_\alpha\delta_t, t+\delta_t) = f_\alpha(\mathbf{r},t) - \dfrac{f_\alpha(\mathbf{r},t) - f_\alpha^{eq}(\mathbf{r},t)}{\tau_f} + F_\alpha\delta_t, & \textit{for density} \\ g_\alpha(\mathbf{r}+\mathbf{e}_\alpha\delta_t, t+\delta_t) = g_\alpha(\mathbf{r},t) - \dfrac{g_\alpha(\mathbf{r},t) - g_\alpha^{eq}(\mathbf{r},t)}{\tau_g} + G_\alpha\delta_t, & \textit{for temperature} \end{cases} \tag{1}$$

where $f_\alpha(\mathbf{r},t)$ and $g_\alpha(\mathbf{r},t)$ represent the fluid density and temperature distribution functions, respectively. The superscript eq means equilibrium

$$\begin{cases} f_\alpha^{eq}(\mathbf{r},t) = \rho\omega_\alpha\left[1+3(\mathbf{e}_\alpha\cdot\mathbf{u}) + \dfrac{9}{2}(\mathbf{e}_\alpha\cdot\mathbf{u})^2 - \dfrac{3}{2}|\mathbf{u}^2|\right], & \textit{for density} \\ g_\alpha^{eq}(\mathbf{r},t) = T\omega_\alpha\left[1+3(\mathbf{e}_\alpha\cdot\mathbf{u}) + \dfrac{9}{2}(\mathbf{e}_\alpha\cdot\mathbf{u})^2 - \dfrac{3}{2}|\mathbf{u}^2|\right], & \textit{for temperature} \end{cases} \tag{2}$$

where $\mathbf{r}$ is the space position vector, $\mathbf{e}_\alpha$ is the fluid velocity, δ_t is the discrete time step, the index α runs from 0 to 8 standing for different fluid moving directions which is the unique feature of the LBM-DNQN model [1], the values of the weights are: $\omega_0 = 4/9$, $\omega_\alpha = 1/9$ for $\alpha = 1-4$ and $\omega_\alpha = 1/36$ for $\alpha = 5-8$, $\mathbf{u}$, ρ and T are the macro fluid velocity, density and temperature, respectively. t denotes time, τ_f and τ_g denote the non-dimensional relaxation times of the density and temperature evolutions, respectively, which can be expressed as

$$\begin{cases} \tau_f = \dfrac{L_c u_c}{Re c_s^2 \delta_t} + 0.5, & \textit{for density} \\ \tau_g = \dfrac{L_c u_c}{Re Pr c_s^2 \delta_t} + 0.5, & \textit{for temperature} \end{cases} \tag{3}$$

where c is the lattice speed and c_s is the lattice speed of sound, L_c and u_c are the characteristic length and velocity, respectively, and Re, Pr and Ra are the Reynolds, Prandtl and Rayleigh numbers, respectively

$$Ra = \begin{cases} \dfrac{c_p\rho\beta L_c^3\Delta T}{k\mu}, & \textit{for Dirichletthermal BC} \\ \dfrac{c_p\rho^2 g\beta L_c^4 Q}{k^2\mu}, & \textit{for Neumannthermal BC} \end{cases} \tag{4}$$

where c_p, k, β, μ, ΔT and Q are the specific heat capacity, thermal conductivity coefficient, thermal expansion coefficient, kinetic viscosity, temperature difference and heat flux, respectively. $\mathrm{Pr} = c_p\mu/k$ and the Grashof number is $Gr = Ra/\mathrm{Pr}$. At last, F_α and G_α in Eq. (1) are the source terms which are evaluated via the IBM in Section 2.2.