A scaled MP-PIC method for bubbling fluidization

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Abstract

Coarse-grained methods have been widely used in simulations of gas-solid fluidization. However, as a key parameter, the coarse-graining ratio, and its relevant scaling law is still far from reaching a consensus. In this work, a scaling law is developed based on a similarity analysis, and then it is used to scale the multi-phase particle-in-cell (MP-PIC) method, and validated in the simulation of two bubbling fluidized beds. The simulation result shows this scaled MP-PIC can reduce the errors of solids volume fraction and velocity distributions over a wide range of coarse-graining ratios. In future, we expect that a scaling law with consideration of the heterogeneity inside a parcel or numerical particle will further improve the performance of coarse-grained modeling in simulation of fluidized beds.

Keywords: coarse-graining model, coarse-graining ratio, scaling law, MP-PIC method

1. Introduction

In recent decades, various numerical methods have been developed for the research of fluidization and multiphase flow, in which two approaches can be categorized, i.e., the Eulerian-Eulerian method and the Eulerian-Lagrangian method.[1-6]

The Two-Fluid Model (TFM) is a typical Eulerian-Eulerian method, where the gas and particles are viewed as two interpenetrating continua. The conservation equations of the mass, momentum and energy are derived through certain averaging process, and the constitutive relations for the solid phase stress are usually closed using the kinetic theory of granular flow (KTGF).[1,7,8]

In Eulerian-Lagrangian methods, particles are treated as discrete entities. The motion of each particle is tracked with Newton's second law of motion. The particle contact force can be determined through the hard-sphere model[9,10] or soft-sphere model.[2,11] In

the hard-sphere model, collision contact is assumed instantaneous, and only the binary collision is considered. In the soft-sphere model, the linear spring-dashpot model[12] and non-linear Hertz model[13,14] are widely adopted to account for the contact force. An elastic force term and a damping force term are normally used to segregate contacting particles and dissipate energy, respectively. Since less assumptions are introduced, the Eulerian-Lagrangian method enables more accurate prediction compared to TFM. The soft-sphere model is usually applied in the CFD-DEM (computational fluid dynamics-discrete element method), as it is readily compatible with CFD solvers to estimate particle trajectories. However, the computational cost becomes unaffordable for a realistic fluidized bed with huge number of particles to be tracked.

To reduce the number of numerical particles to be tracked, various coarse-grained models have been proposed. According to their difference in the concept of numerical particles, as shown in Fig. 1, those models can be categorized into two types, namely, the coarse-grained-particle (CGP-) based and parcel-based models. In CGP-based models,[15-19] the numerical particle size is coarse-grained, i.e., larger than the original one; the inter-particle force is normally determined with the soft-sphere model and the collision related parameters are determined with the properties of the coarse-grained particles. In parcel-based models, e.g., multi-phase particle-in-cell method (MP-PIC),[20] the numerical particle is a sample particle in a parcel, where a certain number of particles are assumed to behave the same as the sample particle, and the collision related parameters are determined with the properties of the sample particle. The collision between particles is not tracked directly in MP-PIC, instead it is represented with a solid pressure gradient. Compared to CFD-DEM, a bigger time step for updating particles, which is normally the same as that of the fluid phase, can be hence adopted. That makes MP-PIC more suitable for simulation of large-scale fluidized beds.

Fig.1 Two types of coarse-grained particle in coarse-grained method: CGP-based and parcel-based models

2 Scaling laws and coarse-graining ratio

The coarse-graining ratio is a key parameter in coarse-grained models, because it can significantly affect the simulation result.[21,22] In a CGP-based model, the coarse-graining ratio, namely, k, refers to the diameter ratio of CGP to original particles. In a parcel-based model, it refers to the number of particles per parcel, which is usually denoted by n_p. It is obvious that $n_p=k^3$. By scaling the particle size by a factor of k, the number of particles is reduced by k^3. In coarse-grained models, using of numerical particle implies a tradeoff between the efficiency and accuracy in simulation. Smaller coarse-graining

ratio, i.e., less original particles represented by a numerical particle/parcel, means a better and closer to CFD-DEM prediction, but at a higher computational cost.

The dynamics of the numerical particle is described by using Newton's law of motion. Thus, the key issue of a coarse-grained model is to determine its scaling law, which relates the force parameters of the coarse-grained system with those of original particles. The most concerned behavior should be kept unchanged during the coarse-graining. To reproduce with high fidelity the flow field of a fluidized bed, *the most concerned behavior here refers to the time-resolved fields of the gas velocity, particle velocity and solids volume fraction*. Table 1 summarizes the scaling laws in literatures for various coarse-grained models. These scaling laws are presented for different force terms in the solid momentum equation separately, including the gravity, pressure drop, drag and inter-particle forces.

Table.1 Scaling laws for coarse-grained models in literature

In all these models, the kinetic energy of a coarse-grained particle was assumed to equal that of the sum of original particles.[15,18-20,23-28] And the physical properties, like the viscosity and density, were assumed to be unchanged in the coarse-graining. Under this condition, the mass and velocity can be scaled by k^3 and 1, respectively. However, the invariant of the kinetic energy of particles is not sufficient to determine the entire set of force parameters, neither their scaling law. Because it is hard to verify the equivalence between the most concerned behavior and the invariant of the kinetic energy of particles. In practice, the invariant only of the particle kinetic energy is not sufficient to guarantee a determined solution and may lead to multiple solutions of the coarse-grained model. On the other hand, due to the coarse-graining, the velocity difference between original particles in a parcel may be lost. That may require more efforts in the scaling of the particle kinetic energy.

To derive a full scaling law, various assumptions have been further proposed. For example, Sakai and Koshizuka[15] assumed that each force over a coarse-grained particle is equal to the sum of the forces over the original particles. As these original particles are not fully resolved, the relevant forces are assumed invariant with respect to each original particle. That assumption applies to all the forces in their work, including the gravity, pressure drop and drag force, the scaling law are hence k^3, with the assumption

that the density, viscosity and drag coefficient keep unchanged. In particular, for the inter-particle collision force, Sakai and Koshizuka[15] assumed that, when a pair of coarse-grained particles collide, all the original particles inside the coarse-grained particles take binary collision, inferring a scaling of k^3 for the collision force. In the work of Hilton and Cleary,[29] the spring and damping coefficients are assumed to be k^3 times that of original particles, leading to a k^3 scaling of collision force. Whereas for the drag force, the cross-sectional area of the numerical particle is assumed to be k^2 times that of original particles, hence the scaling of the drag is k^2 therein.

Though the k^3 scaling have been widely applied for the gravity, pressure drop and drag force,[17-20] different strategies have been suggested for scaling the collision force in literature. Lu et al.[18] assumed that the collision dissipation energy should be kept unchanged in the coarse-graining, thereby the restitution coefficient and the damping coefficient are modified for coarse-grained particles. Their scaling for the collision force can be derived thereon but not explicitly presented. According to the momentum and impulse connection, Chu et al.[19] assumed that the acting time of a collision is linearly proportional to the coarse-grained particle diameter, thus following a scaling of k^2. Washino et al.[30] assumed that the momentum flux is unchanged, and the number of original particle pairs across the face of a control volume is k^2 times larger than that of numerical particles, therefore, the scaling of the inter-particle force is also k^2.

Similarity analysis is another useful tool in determining the scaling law. In the work of Liu et al.[17], the Reynolds number, Re, and Archimedes number, Ar, are chosen as the key dimensionless numbers. The gas viscosity, gas density and particle diameter are scaled such that these two dimensionless numbers are kept unchanged in the coarse-graining. In the work of Link et al.[31] and Sutkar et al.[32], Re and Ar are also chosen as the key dimensionless numbers, while the particle density is scaled to keep the dimensionless numbers unchanged. Focusing on binary collisions, Bierwisch et al.[33] proposed several dimensionless numbers to describe the collision force by assuming the energy density is conserved in the coarse-graining. Mu et al.[34] adopted the gravity as a characteristic quantity to normalize the other forces, and the resultant dimensionless forces remain unchanged during the coarse-graining. However, the demand of such an unchanged force ratio is not straightforward. In addition, the

physical properties of the fluid and gravitational acceleration are also adjusted to keep these dimensionless variables unchanged in the work of Mu et al.[34]. The scaling result of Mu et al.[34] is similar to that of Feng and Owen.[35] where based on three basic quantities, i.e., particle density, length and time, and their relevant scale factors, k or 1, the dimension of any other quantities are expressed in terms of these three basic quantities, and then converted into the scale factors.

Beside these works, there are also scaling law studies based on nonlinear collision force models or gas-liquid-particle system.[36-40]

In sum, different understanding exists on certain issues of the coarse-graining, e.g., how the force acting on a coarse-grained particle is determined; whether the physical properties such as the fluid density and viscosity change during the coarse-graining; whether the gravitational acceleration needs to be adjusted. Various scaling laws have been proposed or derived based on different assumptions or dimensionless numbers. However, it is uncertain whether these scaling laws enable *the most concerned behavior* unchanged during the coarse-graining. Furthermore, although various scaling laws have been extensively discussed for CGP-based coarse-grained models in literature, few such efforts were put on the parcel-based MP-PIC method. As summarized in Table 1, the current MP-PIC actually follows a scaling of k^3. It is not clear whether such a scaling is suitable for MP-PIC to capture the most concerned behavior in a bubbling fluidized bed. Indeed, different scaling laws might be expected for different granular or multiphase flow systems if the most concerned behavior for these systems are not the same.

Bearing in mind the disputes in the coarse-graining and its relation with the most concerned behavior, we aim to revisit the scaling relations in MP-PIC in this article, and propose a scaled MP-PIC method to reproduce the flow field with high fidelity during the coarse-graining. This article is organized as follows: first, based on the force balance equations, we develop a scaling law for the gravity, gas pressure gradient, drag and inter-particle force, respectively; then, this scaling law is extended to MP-PIC method, followed by validation with numerical simulations of a bubbling fluidized bed.

Comparison to classic MP-PIC is also presented. The conclusion is presented finally with prospects.

3. A scaling law of coarse-grained method

As discussed in section 2, for a coarse-grained method to reproduce the flow field of a gas-fluidized bed, the coarse-grained particle and original particles are expected to have the same gas velocity, particle velocity and solids volume fraction, i.e.,

$$\boldsymbol{u}_{\mathrm{g,CG}} = \boldsymbol{u}_{\mathrm{g,O}}, \quad \boldsymbol{u}_{\mathrm{p,CG}} = \boldsymbol{u}_{\mathrm{p,O}}, \quad \varepsilon_{\mathrm{s,CG}} = \varepsilon_{\mathrm{s,O}} \tag{1}$$

The Lagrangian method is used to track the motion of numerical particles. As there is no basic difference between the momentum equations of the CGP- and parcel-based methods, in what follows we present the coarse-graining procedure with Newton's equation of motion normally applied in the CGP method, as follows:

$$m_{\mathrm{CG}} \frac{d\boldsymbol{u}_{\mathrm{p,CG}}}{dt} = m_{\mathrm{CG}}\boldsymbol{g} + \boldsymbol{F}_{\mathrm{gp,CG}} + \boldsymbol{F}_{\mathrm{c,CG}} + \boldsymbol{F}_{\mathrm{d,CG}} \tag{2}$$

The right-hand side terms represent the gravity, gas pressure gradient, inter-particle contact force and inter-phase drag force, respectively. As practiced in most of coarse-grained methods, we keep the physical properties (say, viscosity μ, density ρ and Young's modulus Y) and gravitational acceleration unchanged for both the gas and solid phases during the coarse-graining.

To achieve similitude between the original and coarse-grained systems, we try to first normalize Eq. (2) by identifying the characteristic length and velocity. And these characteristic quantities should be connected with the most concerned behavior in the system. For the collision related force, the characteristic length should be connected with the relative motion between particles, therefore the numerical particle diameter d_{CG} is usually chosen as the characteristic length.[33,41,42] And the characteristic velocity is defined as u_{p0}, which represents the sonic speed in a fluid and is unchanged with the numerical particle dimeter. Whereas for the drag force, several characteristic lengths have been proposed in literature. For example, Glicksman[43] adopted the particle diameter as the characteristic length to scale the drag, and the bed size later on.[44,45] As the drag force reflects the inter-phase interaction, its characteristic length is expected to relate with the spatial distribution of the gas-particle flow fields. Therefore, the bed size L is chosen as the characteristic length for the drag in the following derivation. And it also applies to the gravity and pressure drop. The characteristic velocity for the drag is defined as the superficial gas velocity u_{g0}. And the characteristic time and acceleration

can be derived from the characteristic length and velocity accordingly. In what follows we derive the scaling laws for the gravity, gas pressure gradient, inter-particle contact force and drag force, respectively.

Table. 2 The characteristic quantities adopted in dimensionless equations

3.1 Scaling of gravity and gas pressure gradient

The mass of the numerical particle is assumed to be the sum of that of the original particles. The gravitational acceleration is kept unchanged, so the gravity is dependent on the volume of the numerical particle. Thus, the scaling of the gravity reads

$$m_{\mathrm{CG}}\boldsymbol{g} = k^3 m_{\mathrm{p}}\boldsymbol{g} \tag{3}$$

The gas pressure gradient is also volumetric, thus the coarse-grained pressure gradient should be equal to the sum of that of the original particles, as follows:

$$\boldsymbol{F}_{\mathrm{gp,CG}} = k^3 \boldsymbol{F}_{\mathrm{gp,O}} \tag{4}$$

3.2 Scaling of inter-particle force

To simplify the discussion, this work focuses on a monodisperse system. However, the scaling law of a polydisperse system can be derived likewise as proposed in this article. As an indicative extension, the scaling law for the binary particle collision with different particle diameters is shown in Appendix A. Both the tangential and normal collisions are assumed to follow the same scaling law. For a normal collision between a pair of particles, the motion equation of a particle is given by the spring-dashpot model,[33,46] as follows:

$$m_{\mathrm{eff}}\ddot{\boldsymbol{\delta}}_{\mathrm{n}} = k_n\boldsymbol{\delta}_{\mathrm{n}} + \eta_n\dot{\boldsymbol{\delta}}_{\mathrm{n}} \tag{5}$$

where $\boldsymbol{\delta}_{\mathrm{n}}$ denotes the overlap of a pair of colliding particles, over dot the time derivative and m_{eff} the effective mass determined by

$$m_{\mathrm{eff}} = \frac{m_i m_j}{m_i + m_j} = \frac{1}{2}m_i = \frac{1}{12}\pi d_{\mathrm{p}}^3 \rho_{\mathrm{p}} \tag{6}$$

k_n and η_n denote the spring coefficient and damping coefficient, respectively. Eq. (5) can be normalized by introducing the following dimensionless variables as summarized in Table 2,

$$\boldsymbol{\delta}_{\mathrm{n}}^* = \frac{\boldsymbol{\delta}_{\mathrm{n}}}{d_{\mathrm{p}}}, \quad \dot{\boldsymbol{\delta}}_{\mathrm{n}}^* = \frac{\dot{\boldsymbol{\delta}}_{\mathrm{n}}}{u_{\mathrm{p0}}}, \quad \ddot{\boldsymbol{\delta}}_{\mathrm{n}}^* = \ddot{\boldsymbol{\delta}}_{\mathrm{n}}\frac{d_{\mathrm{p}}}{u_{\mathrm{p0}}^2} \tag{7}$$

Here, the dimensionless overlap $\boldsymbol{\delta}_{\mathrm{n}}^*$ reflects the strain of particle in elastic collision. As the Young's modulus is assumed to be a constant, the unchanged $\boldsymbol{\delta}_{\mathrm{n}}^*$ implies

unchanged solid stress in the coarse-graining. By substituting Eq. (7) into Eq. (5), the dimensionless motion equation reads

$$\frac{1}{12}\pi\ddot{\boldsymbol{\delta}}_{\mathrm{n}}^{*}=\frac{k_{\mathrm{n}}}{d_{\mathrm{p}}\rho_{\mathrm{p}}u_{\mathrm{p0}}^{2}}\boldsymbol{\delta}_{\mathrm{n}}^{*}+\frac{\eta_{\mathrm{n}}}{d_{\mathrm{p}}^{2}\rho_{\mathrm{p}}u_{\mathrm{p0}}}\dot{\boldsymbol{\delta}}_{\mathrm{n}}^{*} \tag{8}$$

where the dimensionless spring and damping coefficients can be defined by

$$\Pi_{1}=\frac{k_{\mathrm{n}}}{d_{\mathrm{p}}\rho_{\mathrm{p}}u_{\mathrm{p0}}^{2}}\,,\qquad \Pi_{2}=\frac{\eta_{\mathrm{n}}}{d_{\mathrm{p}}^{2}\rho_{\mathrm{p}}u_{\mathrm{p0}}} \tag{9}$$

In the coarse-graining, Π_1 and Π_2 are kept unchanged to ensure that the coarse-grained system behaves similarly to the original system, i.e.,

$$\Pi_{1}=\frac{k_{\mathrm{n,O}}}{d_{\mathrm{p}}\rho_{\mathrm{p,O}}u_{\mathrm{p0,O}}^{2}}=\frac{k_{\mathrm{n,CG}}}{d_{\mathrm{CG}}\rho_{\mathrm{p,CG}}u_{\mathrm{p0,CG}}^{2}} \tag{10a}$$

$$\Pi_{2}=\frac{\eta_{\mathrm{n,O}}}{d_{\mathrm{p}}^{2}\rho_{\mathrm{p,O}}u_{\mathrm{p0,O}}}=\frac{\eta_{\mathrm{n,CG}}}{d_{\mathrm{CG}}^{2}\rho_{\mathrm{p,CG}}u_{\mathrm{p0,CG}}} \tag{10b}$$

Since ρ_{s} and u_{p0} are unchanged during the coarse-graining, k_{n} and η_{n} of the numerical particle can be determined by

$$\frac{k_{\mathrm{n,CG}}}{k_{\mathrm{n,O}}}=\frac{d_{\mathrm{CG}}}{d_{\mathrm{p}}}=k,\qquad \frac{\eta_{\mathrm{n,CG}}}{\eta_{\mathrm{n,O}}}=\frac{d_{\mathrm{CG}}^{2}}{d_{\mathrm{p}}^{2}}=k^{2} \tag{11}$$

The overlap of the coarse-grained particle can be determined as $\boldsymbol{\delta}_{\mathrm{n,CG}}=k\boldsymbol{\delta}_{\mathrm{n,O}}$ as the dimensionless overlap also remain unchanged. Thus, the normal collision force $\boldsymbol{F}_{\mathrm{c}}$ of CGP can be determined by

$$\boldsymbol{F}_{\mathrm{c,CG}}=k_{\mathrm{n,CG}}\cdot\boldsymbol{\delta}_{\mathrm{n,CG}}+\eta_{\mathrm{n,CG}}\cdot\dot{\boldsymbol{\delta}}_{\mathrm{n,CG}}=k^{2}\boldsymbol{F}_{\mathrm{c,O}} \tag{12}$$

For further information, the other parameters or flow field information are derived and discussed in Appendix B.

3.3 Scaling of drag force

The scaling of drag force can be derived likewise based on the equation of motion due to the drag, as follows:

$$\frac{1}{6}\pi d_{\mathrm{p}}^{3}\rho_{\mathrm{p}}\boldsymbol{a}_{\mathrm{d}}=\frac{1}{8}\pi C_{d}d_{\mathrm{p}}^{2}\rho_{\mathrm{g}}\left|\boldsymbol{u}_{\mathrm{slip}}\right|\cdot\boldsymbol{u}_{\mathrm{slip}} \tag{13}$$

where $\boldsymbol{a}_{\mathrm{d}}$ is the acceleration induced by the drag and $\boldsymbol{u}_{\mathrm{slip}}$ is the relative velocity between the gas and solid phases, which can be described as $\left(\boldsymbol{u}_{\mathrm{g}}\left(\boldsymbol{x}_{\mathrm{p}}\right)-\boldsymbol{u}_{\mathrm{p}}\right)$.

The following dimensionless variables are then defined by

$$\boldsymbol{u}_{\mathrm{slip}}^{*}=\frac{\boldsymbol{u}_{\mathrm{slip}}}{u_{\mathrm{g0}}},\qquad \boldsymbol{a}_{\mathrm{d}}^{*}=\boldsymbol{a}_{\mathrm{d}}\frac{L}{u_{\mathrm{g0}}^{2}} \tag{14}$$

Substituting the dimensionless variables of Eq. 14 into Eq. 13, we have

$$\boldsymbol{a}_{\mathrm{d}}^{*}=\frac{3}{4}C_d\frac{L}{d_{\mathrm{p}}}\frac{\rho_{\mathrm{g}}}{\rho_{\mathrm{p}}}\left(\boldsymbol{u}_{\mathrm{slip}}^{*}\right)^2 \tag{15}$$

where the only dimensionless parameter for the scaling of the drag coefficient is given by

$$\Pi_3=\frac{3}{4}C_d\frac{L}{d_{\mathrm{p}}}\frac{\rho_{\mathrm{g}}}{\rho_{\mathrm{p}}} \tag{16}$$

During the coarse-graining, Π_3 must be kept constant to make sure that the coarse-grained system is analogous to the original particle system, thus giving

$$C_{d,\mathrm{CG}}=kC_{d,\mathrm{O}} \tag{17}$$

Then the relationship between the drag force of CGP and that of original particle reads

$$\boldsymbol{F}_{\mathrm{d,CG}}=\frac{1}{8}C_{d,\mathrm{CG}}\pi d_{\mathrm{CG}}^2\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{slip,CG}}^2=\frac{1}{8}kC_{d,\mathrm{O}}\pi k^2d_{\mathrm{p}}^2\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{slip,O}}^2=k^3\boldsymbol{F}_{\mathrm{d,O}} \tag{18}$$

By substituting Eq. 3,4,12,18 into Eq. 2, the scaled motion equation for coarse-grained particles is written by

$$m_{\mathrm{CG}}\frac{d\boldsymbol{u}_{\mathrm{p,CG}}}{dt}=k^3m_{\mathrm{p}}\boldsymbol{g}+k^3\boldsymbol{F}_{\mathrm{gp,O}}+k^3\boldsymbol{F}_{\mathrm{d,O}}+k^2\boldsymbol{F}_{\mathrm{c,O}} \tag{19}$$

4. Application of the scaling law to MP-PIC

4.1 MP-PIC method

MP-PIC is a parcel-based coarse-grained method developed to simulate dense particulate flows or gas-particle flows.[20,47-52] The gas-phase continuity and momentum equations in MP-PIC is analogous to Navier-Stokes equations, as follows:

$$\frac{\partial}{\partial t}\left(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\right)+\boldsymbol{\nabla}\cdot\left(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}}\right)=0 \tag{20}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}}\right)+\boldsymbol{\nabla}\cdot\left(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}}\right)=$$

$$-\varepsilon_{\mathrm{g}}\boldsymbol{\nabla}p+\boldsymbol{\nabla}\cdot\bar{\bar{\tau}}_{\mathrm{g}}+\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{g}-\frac{1}{V_{\mathrm{cell}}}\sum_{i=1}^{n_T}n_{\mathrm{p}}\boldsymbol{F}_{\mathrm{d},i}\frac{1}{6}\pi d_{\mathrm{p}}^3\rho_{\mathrm{p}} \tag{21}$$

where ε_{g} denotes the void fraction, V_{cell} the volume of cell, n_T the total parcel number in a fluid cell, i the ith parcel/sample particle in the cell, n_{p} the number of particles per parcel, or, the coarse-graining ratio. $\bar{\bar{\boldsymbol{\tau}}}_{\mathrm{g}}$ is the gas-phase stress tensor,

$$\bar{\bar{\boldsymbol{\tau}}}_{\mathrm{g}}=2\mu_{\mathrm{g}}\bar{\bar{S}}_{\mathrm{g}} \tag{22}$$

$$\bar{\bar{\boldsymbol{S}}}_{\mathrm{g}}=\frac{1}{2}\left[\boldsymbol{\nabla}\boldsymbol{u}_{\mathrm{g}}+\left(\boldsymbol{\nabla}\boldsymbol{u}_{\mathrm{g}}\right)^{\mathrm{T}}\right]-\frac{1}{3}\boldsymbol{\nabla}\cdot\boldsymbol{u}_{\mathrm{g}}\bar{\bar{\boldsymbol{I}}} \tag{23}$$

For the solid phase, a number of particles are lumped into one parcel, and the motion of this parcel could be represented by one sample particle, which is tracked with

Newton's law of motion. The contact force in MP-PIC takes effect through a solid pressure.[16,47,53] The particle motion equations read

$$\frac{d\boldsymbol{x}_\mathrm{p}}{dt} = \boldsymbol{u}_\mathrm{p} \tag{24}$$

$$\frac{d\boldsymbol{u}_\mathrm{p}}{dt} = -\frac{\boldsymbol{\nabla} p}{\rho_\mathrm{p}} - \frac{\boldsymbol{\nabla} p_\mathrm{s}}{\varepsilon_\mathrm{s}\rho_\mathrm{p}} + \frac{\beta}{\varepsilon_\mathrm{s}\rho_\mathrm{p}}\left(\boldsymbol{u}_\mathrm{g}(\boldsymbol{x}_\mathrm{p}) - \boldsymbol{u}_\mathrm{p}\right) + \boldsymbol{g} \tag{25}$$

where the third term in the right side is the $\boldsymbol{F}_{\mathrm{d},i}$ in Eq. (21). p_s is the solid pressure,[47,54]

$$p_\mathrm{s} = p_\mathrm{s}^* \frac{\varepsilon_\mathrm{s}^\alpha}{\varepsilon_{\mathrm{s},max} - \varepsilon_\mathrm{s}} \tag{26}$$

here, $\varepsilon_{\mathrm{s},max}$ is the solid volume fraction at close packing; p_s^* and α are empirical constants. The current scaling relation is realized through modifying the classic formulation of the interparticle stress.[20,55] Its applicability with respect to the interparticle friction, however, needs more efforts in future. The drag model is of great importance to fluidization simulation.[56-62] In this work, the EMMS-bubbling drag[22,63] is adopted, as follows:

$$\beta_\mathrm{G} = \begin{cases} 150\dfrac{\varepsilon_\mathrm{s}\mu_\mathrm{g}}{\varepsilon_\mathrm{g} d_\mathrm{p}^2} + 1.75\dfrac{\rho_\mathrm{g}\left|\left(\boldsymbol{u}_\mathrm{g}(\boldsymbol{x}_\mathrm{p}) - \boldsymbol{u}_\mathrm{p}\right)\right|}{d_\mathrm{p}}, & \varepsilon_\mathrm{g} < 0.8 \\ \dfrac{3}{4}\dfrac{\rho_\mathrm{g}\varepsilon_\mathrm{s}\varepsilon_\mathrm{g}\left|\left(\boldsymbol{u}_\mathrm{g}(\boldsymbol{x}_\mathrm{p}) - \boldsymbol{u}_\mathrm{p}\right)\right|}{d_\mathrm{p}} C_{d0}\varepsilon_\mathrm{g}^{-2.7}, & \varepsilon_\mathrm{g} \geq 0.8 \end{cases} \tag{27}$$

$$C_{d0} = \begin{cases} 0.44, & \mathrm{Re} \geq 1000 \\ \dfrac{24(1 + 0.15\mathrm{Re}^{0.687})}{\mathrm{Re}}, & \mathrm{Re} < 1000 \end{cases} \tag{28}$$

$$\mathrm{Re} = \frac{\varepsilon_\mathrm{s}\rho_\mathrm{g}\left|\left(\boldsymbol{u}_\mathrm{g}(\boldsymbol{x}_\mathrm{p}) - \boldsymbol{u}_\mathrm{p}\right)\right| d_\mathrm{p}}{\mu_\mathrm{g}} \tag{29}$$

$$\beta = \beta_\mathrm{G} \cdot H_d \tag{30}$$

where β_G is the drag coefficient adopted in Ding and Gidaspow[64], and H_d is the heterogeneity index.

4.2 Scaling laws for MP-PIC

MP-PIC is a parcel-based coarse-graining method, in which only the sample particle is tracked, and the motion of the other particles is assumed the same as the sample particle. As summarized in Table 1, its scaling is actually k^3 for all the terms. By applying the scaling laws derived in section 2 to the motion equation of MP-PIC, we can get the new scaled equations, which is referred to as the scaled MP-PIC hereinafter.

The volume of a parcel equals the sum of the volume of the original particles represented by the parcel, thus the equivalent diameter of the parcel is given by

$$d_{\mathrm{CG}} = \sqrt[3]{n_{\mathrm{p}}} d_{\mathrm{p}} = k d_{\mathrm{p}} \tag{31}$$

The CGP-based numerical particle is used during the derivation of scaling law for particle collision force. While in MP-PIC, collision induced forces are described by the interparticle stress, where the parcel-based numerical particle is used. Unlike the CGP-based model, the collision process is not tracked in the parcel-based MP-PIC model, so are the duration of collision and collision frequency. It should be noted that the interparticle stress in MP-PIC is not equivalent to the solid stress in KTGF. In the scenario of KTGF, particles experience frequent collisions with each other, thus there exists a velocity distribution for a group of particles (say, nearly the Maxwellian distribution). As a result, the solid stress in KTGF includes two parts, one is kinetic due to velocity fluctuation, and the other is collisional due to particle collisions. In MP-PIC, the particles inside a parcel or numerical particle have exactly the same velocity, and hence there is no particle collision between them. So, it is not suitable to incorporate the solid stress of KTGF into the MP-PIC method directly. Instead, for MP-PIC, the interparticle stress only accounts for the interaction between numerical particles. Thus, in a given space, the collision-induced forces described by the interparticle stress can be correlated by the particle collision force at any instant, as follows:

$$\boldsymbol{\nabla} p_{\mathrm{s}} \cdot V \propto \boldsymbol{F}_{\mathrm{c}} \cdot N_{\mathrm{c}} \tag{32}$$

where V is the volume of the space; N_{c} is the number of collisions in the volume, F_{c} the mean collision force.

In the current work, the scaling law of the imaginary number of collisions, N_{c}, in MP-PIC framework is assumed as follows:

$$N_{\mathrm{c,CG}} = \frac{1}{k^3} N_{\mathrm{c,O}} \tag{33}$$

This assumption is actually the same as what has been widely used in CGP-based models, i.e., when a pair of coarse-grained particles collide, all the original particles inside the coarse-grained particles take binary collision.[15] An additional discussion about N_{c} is shown in Appendix C.

In original MP-PIC, the scaling law of collision force is k^3, and it can be derived that $(\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathrm{CG}} = (\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathrm{O}}$. While when applying Eqs. 32, 33 and the novel scaling of Eq.12, we have

$$\frac{(\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathbf{CG}} \cdot V}{(\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathbf{O}} \cdot V} = \frac{\boldsymbol{F}_{\mathrm{c,CG}} \cdot N_{\mathrm{c,CG}}}{\boldsymbol{F}_{\mathrm{c,O}} \cdot N_{\mathrm{c,O}}} = \frac{k^2 \boldsymbol{F}_{\mathrm{c,O}} \cdot \frac{1}{k^3} N_{\mathrm{c,O}}}{\boldsymbol{F}_{\mathrm{c,O}} \cdot N_{\mathrm{c,O}}} = \frac{1}{k} \tag{34}$$

Thus, the solid pressure of a parcel reads

$$(\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathrm{CG}} = \frac{(\boldsymbol{\nabla} p_{\mathrm{s}})_{\mathrm{O}}}{k} \tag{35}$$

The drag force of a particle is

$$\boldsymbol{F}_{\mathrm{d,O}} = \beta_{\mathrm{O}}\left(\boldsymbol{u}_{\mathrm{g,O}}\left(\boldsymbol{x}_{\mathrm{p,O}}\right) - \boldsymbol{u}_{\mathrm{p,O}}\right)\frac{1}{6}\pi d_{\mathrm{p}}^{3}\frac{1}{\varepsilon_{\mathrm{s,O}}} \tag{36}$$

and the drag force of a parcel is

$$\boldsymbol{F}_{\mathrm{d,CG}} = \beta_{\mathrm{CG}}\left(\boldsymbol{u}_{\mathrm{g,CG}}\left(\boldsymbol{x}_{\mathrm{p,CG}}\right) - \boldsymbol{u}_{\mathrm{p,CG}}\right)\frac{1}{6}\pi d_{\mathrm{CG}}^{3}\frac{1}{\varepsilon_{\mathrm{s,CG}}} \tag{37}$$

According to the basic requirement of a coarse-grained model as shown in Eq. 1,

$$\boldsymbol{u}_{\mathrm{g,CG}} - \boldsymbol{u}_{\mathrm{p,CG}} = \boldsymbol{u}_{\mathrm{g,O}} - \boldsymbol{u}_{\mathrm{p,O}} \tag{38}$$

and the scaling law of Eq. 18,

$$\frac{\boldsymbol{F}_{\mathrm{d,CG}}}{\boldsymbol{F}_{\mathrm{d,O}}} = \frac{\beta_{\mathrm{CG}}\left(\boldsymbol{u}_{\mathrm{g,CG}}\left(\boldsymbol{x}_{\mathrm{p,CG}}\right) - \boldsymbol{u}_{\mathrm{p,CG}}\right)\frac{1}{6}\pi d_{\mathrm{CG}}^{2}\frac{1}{\varepsilon_{\mathrm{s,CG}}}}{\beta_{\mathrm{O}}\left(\boldsymbol{u}_{\mathrm{g,O}}\left(\boldsymbol{x}_{\mathrm{p,O}}\right) - \boldsymbol{u}_{\mathrm{p,O}}\right)\frac{1}{6}\pi d_{\mathrm{p}}^{3}\frac{1}{\varepsilon_{\mathrm{s,O}}}} = k^{3} \tag{49}$$

the drag coefficient is kept the same during the coarse-graining,

$$\beta_{\mathrm{CG}} = \beta_{\mathrm{O}} \tag{40}$$

Likewise, we can derive the gravity and gas pressure gradient for a parcel as follows:

$$\boldsymbol{g}_{\mathrm{CG}} = \boldsymbol{g}_{\mathrm{O}} \tag{41}$$

$$\boldsymbol{\nabla} p_{\mathrm{CG}} = \boldsymbol{\nabla} p_{\mathrm{O}} \tag{42}$$

4.3 Scaled MP-PIC equation

By substituting Eqs. 35, 40, 41 and 42 into Eq. 25, we have the parcel motion equation as follows:

$$\frac{d\boldsymbol{u}_{\mathrm{p}}}{dt} = -\frac{\boldsymbol{\nabla} p}{\rho_{\mathrm{p}}} - \frac{1}{k}\frac{\boldsymbol{\nabla} p_{\mathrm{s}}}{\varepsilon_{\mathrm{s}}\rho_{\mathrm{p}}} + \frac{\beta}{\varepsilon_{s}\rho_{\mathrm{p}}}\left(\boldsymbol{u}_{\mathrm{g}}\left(\boldsymbol{x}_{\mathrm{p}}\right) - \boldsymbol{u}_{\mathrm{p}}\right) + \boldsymbol{g} \tag{43}$$

In principle, the drag force represents the inter-phase interaction and hence its scaling law should also apply to the gas-phase motion equation. As the drag coefficient does not change during coarse-graining, the gas-phase equation remains unchanged. Table 3 summarizes the difference between the original and scaled MP-PIC methods.

Table. 3 Sample particle parameters in original and scaled MP-PIC

5. Validation and analysis

5.1 Simulation settings

We performed simulation of two bubbling fluidized beds to validate the scaled MP-PIC. The open source CFD software OpenFOAM was used. As the simulation accuracy is highly dependent on the closure relations such as the inter-phase and inter-particle

forces model, the validation mainly relates with the reproducibility of simulation when using different coarse-graining ratios.

Fig. 2 shows the schematic diagram of 2D domain of bubbling bed 1[65] with a height of 1.0 m and inner width of 0.14 m, and bubbling bed 2[66] with a height of 2.464 m and inner width of 0.267 m. Spherical particles are initially packed with a height of 0.5 m and void fraction of 0.45 ($\varepsilon_s = 0.55$) for bubbling bed 1, and a height of 1.2 m and void fraction of 0.44 ($\varepsilon_s = 0.56$) for bubbling bed 2. The gas flows into the bed from the bottom inlet with a speed of 0.1 m/s and 0.06 m/s, respectively, and out of the pressure outlet at the top. The non-slip boundary conditions is applied for gas phase at the walls. For particles, the particle-wall interaction is determined based on the restitution coefficient as listed in Table 4. The Cartesian grid with a resolution of 70×500 is adopted for bed 1, and a resolution of 100×1000 for bed 2. Both have been tested to allow a mesh-independent prediction.

For both two bubbling beds, the simulations last for 25 s, and the durations of the last 15 s are used for statistical analysis. The EMMS/bubbling drag models are employed for both cases. The heterogeneity index, H_d, which characterizes the drag difference between a realistic system and a homogeneous one, are summarized in Appendix D. The numerical settings are summarized in Table 4.

Fig.2 Schematic diagram of two bubbling beds

Table.4 Numerical settings for bubbling bed 1[65] and bed 2[66]

5.2 Bubbling fluidized bed 1

Fig.3 shows instantaneous snapshots of the void fraction distribution in the bubbling bed 1. Generally, the original MP-PIC and the scaled MP-PIC give similar flow fields, both with dynamic bubbles and almost the same bed expansion. Small bubbles form near the bottom of the bed and gradually merge into larger ones. These bubbles are irregular in shape, and rise mainly in the middle of the bed. Both approaches predict a breakup of large bubble at the surface of the bed at about t=1.5 s. The snapshots are found to be insensitive to the value of n_p, thus only those with n_p=10 are shown here.

Fig. 3 Void fraction distribution in bubbling bed 1 at different instants (n_p=10)

Figs. 4 and 5 show the time-average axial profile of solid volume fraction, and the lateral profiles of solid volume fraction and axial velocity. For both the original and scaled MP-PIC, the simulated expansion height increases with the coarse-graining ratio. While the increase is more significant in the original MP-PIC. It should be noted that, when n_p>400, the parcel size is as large as the grid size, leading to a divergence of simulation. Thus, no bigger n_p is considered for the original MP-PIC.

The lateral profiles at h=0.5 m are also shown in Figs.4 and 5. With the original MP-PIC, the lateral profiles of the solids volume fraction distribution are similar to each other when n_p≤200, whereas for the case of n_p=400, the solids volume fraction is obviously higher. By comparison, the lateral profiles of the solids volume fraction predicted by using the scaled MP-PIC show similar trend with all values of n_p.

Both the original and scaled MP-PIC predict the so-called core-annular distribution of the axial particle velocity, with particles flowing upward in the center, and downward near the wall. By comparison, with the original MP-PIC, the axial velocity shows greater discrepancy with different n_p. With the increase of the coarse-graining ratio, the axial velocity is higher in the middle of the bubbling bed. For the results of the scaled MP-PIC, the axial velocity changes slightly.

Fig. 4 Axial profiles of the time–average solids volume fraction and lateral profiles of the time-average solids volume fraction and axial velocity at h=0.5 m in bubbling bed 1 with various n_p (original MP-PIC)

Fig. 5 Axial profiles of the time–average solids volume fraction and lateral profile of the time-average solids volume fraction and axial velocity at h=0.5 m in bubbling bed 1 with various n_p (scaled MP-PIC)

To quantitatively analyze the effect of the scaled MP-PIC, we calculate the deviations of the simulation results with different n_p. Here, we take the simulation result with the smallest n_p as the reference case to determine the deviation as follows:

$$\sigma = \sqrt{\frac{\sum(x - x_1)}{n - 1}} \tag{44}$$

Where x is the simulation result with different n_p, x_1 denotes the simulation result with the smallest n_p, i.e., 10, and n is the sample size of different n_p.

Fig. 6 Axial deviation profile of solid volume fraction and lateral deviation profile of solid volume fraction and axial velocity in bubbling bed 2

The axial and lateral profiles of deviation are calculated and shown in Fig. 6. For axial deviation profile, the deviation of the scaled MP-PIC is smaller than that of the original MP-PIC. Probably due to the strong oscillation near the bed surface, the deviations of both methods are much higher at $h \approx 0.75$ m than at the other elevations. For the lateral deviation profiles of the solid volume fraction and axial velocity, the scaled MP-PIC also outperforms the original one by showing much lower deviations at most of positions. However, the discrepancy near the wall is still obvious. That may be explained by that the scaling law in this study is proposed to scale the inter-particle forces, therefore, for the interaction between particles and the wall, the scaling law may deserve more efforts.

5.3 Bubbling fluidized bed 2

Fig. 7 shows instantaneous snapshots of void fraction distribution of bubbling bed 2 with n_p=10. Again, we found that the snapshots are insensitive to the value of n_p. Compared to the bubbling bed 1, the bubbles in bubbling bed 2 is smaller and more dispersive. Both approaches predict a breakup of large bubble at the surface of the bed at about t=3.0 s.

Fig. 7 Void fraction distribution in bubbling bed 2 at different instants (n_p=10)

Figs. 8 and 9 show the time-average axial profile of solid volume fraction, and the lateral profiles of solid volume fraction and axial velocity. The expansion increases with coarse-graining ratio for both the original and scaled MP-PIC, whereas the discrepancy of the scaled MP-PIC is smaller. The maximal n_p reaches 1200 in bubbling bed 2, as smaller original particles and larger cells are applied. The lateral profiles at h=0.75 m are also shown in Figs. 8 and 9. Both the original and scaled MP-PIC predict similar trend of solids volume fraction with lateral position at various n_p. For the axial velocity, the core-annular distribution is predicted in both approaches. Whereas with the increase of the coarse-graining ratio, the predicted axial velocity is higher in the middle range of lateral position.

Fig. 8 Axial profiles of time–average solid volume fraction and lateral profile of time-average solid volume fraction and axial velocity at h=0.75m in bubbling bed 2 with various n_p (original MP-PIC)

Fig. 9 Axial profiles of time–average solid volume fraction and lateral profile of time-average solid volume fraction and axial velocity at h=0.75 m in bubbling bed 2 with various n_p (scaled MP-PIC)

The axial and lateral profiles of deviation are shown in Fig. 10. For the axial profile of the deviation of solid volume fraction, the scaled MP-PIC outperforms again the original MP-PIC by showing smaller deviation over most range of elevation. For the lateral deviation profile of solid volume fraction, the scaled MP-PIC shows obvious improvement, while the deviation near the wall is still higher than at the other positions. For axial velocity, the generally both methods show comparable deviation.

Fig. 10 Axial deviation profile of solid volume fraction and lateral deviation profile of solid volume fraction and axial velocity in bubbling bed 2

It is worth noting that, in a bubbling fluidized bed, the gas and particles are heterogeneously distributed over a wide range of scales. The existence of meso-scale bubble structure is the critical characteristics of such a fluidized bed, and can significantly affect the drag force and inter-particle forces.[67,68] In this preliminary work, although the EMMS drag model is applied, the effect of meso-structure is not considered during the derivation of the scaling law for the coarse-graining. We expect that a scaling law based on the heterogeneity inside a parcel or numerical particle will help improve the performance of coarse-grained modeling. It should be noted that, the effect of the coarse-graining ratio and grid size on the drag as well as the simulation result, as investigated in the literature,[61,69] may deserve more efforts in future study

6. Conclusion

The coarse-graining ratio is a key parameter in coarse-grained methods. To consider its effect, the relationship between the forces of a numerical particle and those of a real particle is established based on a similarity analysis of the coarse-graining, and then applied in MP-PIC. Two bubbling beds are simulated with this scaled MP-PIC at different coarse-graining ratios. The following conclusions can be drawn:

(1) The inter-particle contact force of a numerical particle follows a scaling of k^2.
(2) The drag force of a numerical particle follows a scaling of k^3.
(3) The scaled MP-PIC method reduces the errors of solids volume fraction and particle velocity distribution in simulation of bubbling fluidized beds.
(4) We expect that a scaling law with consideration of the heterogeneity inside a parcel or numerical particle will help improve the performance of coarse-grained modeling in simulation of fluidized beds.

Notation

a_{d}	acceleration induced by drag force (m/s^2)
C_d	drag coefficient
d	particle diameter (m)
e	restitution coefficient
g	gravitational acceleration (m/s^2)
H_d	heterogeneity index
k	coarse-graining ratio
L	bed size (m)
m	mass (kg)
n	sample size
n_{p}	coarse-graining ratio
n_{T}	parcel number in one cell
N	particle number density
N_{C}	number of collisions
p	pressure (Pa)
p_{s}^*	solid pressure parameter (Pa)
$\boldsymbol{u}$	velocity (m/s)
$\boldsymbol{x}$	location (m)
Y	Young's module (Pa)
α	solid pressure parameter
β	drag coefficient (kg/m^3 s)
ε	volume fraction
$\boldsymbol{\delta}_{\mathrm{n}}$	particle overlap (m)
σ	deviation
k_{n}	spring coefficient (N/m)
η_{n}	damping coefficient (kg/s)
$\bar{\bar{\boldsymbol{\tau}}}$	stress tensor (Pa)
ρ	density (kg/m^3)
μ	viscosity (Pa s)

Subscript

0	characteristic

eff	effective
g	gas phase
p	particle
s	solid phase
O	original particle system
CG	numerical particle/numerical particle system

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