Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Material for

Structured Bubbling in Vibrated Gas–Fluidized Beds of Binary Granular Particles: Experiments and Simulations

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CFD-DEM Model Equations

DEM is a Lagrangian approach in which all particles are tracked by explicitly solving for their trajectories using Newton's laws[1]. For a particle with an index i, the linear and angular momenta balance equations are as given in Eqs. 1 and 2, respectively.

$$m_i \frac{d^2\vec{x}_i}{dt^2} = \vec{F}_{i,n} + \vec{F}_{i,t} + \vec{F}_{i,f} + \vec{F}_{i,b} \tag{1}$$

$$I_i \frac{d\vec{\omega}_i}{dt} = \vec{r}_{i,c} \times \vec{F}_{i,t} \tag{2}$$

Here, $\vec{F}_{i,n}$ is the normal particle–particle contact force, $\vec{F}_{i,t}$ is the tangential particle–particle contact force. $\vec{F}_{i,f}$ is the force exerted by the surrounding fluid on the particle. The body force from gravity is $\vec{F}_{i,b}$. The particle's mass, its position and angular velocity are given by m_i, $\vec{x}_i$ and $\vec{\omega}_i$, respectively. The contact forces are obtained from the linear–spring-dashpot model comprising a linear spring and dashpot in the normal direction as well as a slider and dashpot in the tangential direction. The particle–particle friction and restitution coefficients as well as normal and tangential spring and damping coefficients are the input model parameters for calculating contact forces.

The flow of an incompressible gas phase in the presence of dispersed particulate phase is governed by volume–averaged continuity and Navier–Stokes equations, which are as given in Eqs. 3 and 4, respectively.

$$\frac{\partial(\rho_g \alpha_g)}{\partial t} + \vec{\nabla} \cdot (\rho_g \alpha_g \vec{u}_g) = 0 \tag{3}$$

$$\frac{\partial(\rho_g \alpha_g \vec{u}_g)}{\partial t} + \vec{\nabla} \cdot (\rho_g \alpha_g \vec{u}_g \vec{u}_g) = -\alpha_g \vec{\nabla} p + \rho_g \alpha_g \vec{g} - \vec{R}_{pg} + \vec{\nabla} \cdot \bar{\bar{\tau}} \tag{4}$$

Here, $\vec{g}$ is the acceleration due to gravity, $\alpha_g$is the gas phase volume fraction in the cell, $\vec{u}_g$ is the gas velocity and ρ_g is the gas density. $\bar{\bar{\tau}}$ is the Newtonian stress tensor for the gas phase, p is the gas pressure and $\vec{R}_{pg}$ is the net momentum exchange between particulate and gas phases per unit

volume of the computational cell. This momentum exchange term is based on particle–based drag forces:

$$\vec{R}_{pg} = \kappa_{pg}\left(\vec{u}_g - \langle\vec{u}_p\rangle\right) \tag{5}$$

$$\kappa_{pg} = \frac{1}{V_{cell}}\left(\frac{\sum_{i=1}^{i=N_{cell}} \vec{F}_{drag,i}}{\left|\vec{u}_g - \langle\vec{u}_p\rangle\right|}\right) \tag{6}$$

Here, κ_{pg} is the gas cell drag coefficient, $\vec{u}_g$ is the gas cell velocity, $\langle\vec{u}_p\rangle$ is the average particle velocity in the cell, V_{cell} is the volume of the cell, N_{cell} is the number of particles in the cell and $\vec{F}_{drag,i}$ is the drag force on individual particle i. κ_{pg} is calculated using the model proposed by Ding and Gidaspow[2], which is a combination of the Wen and Yu[3] and Ergun[4] correlations, shown below:

For $\alpha_g > 0.8$,

$$\kappa_{pg} = \frac{3}{4}C_d\left(\frac{\alpha_g(1-\alpha_g)\left|\vec{u}_g - \vec{u}_p\right|}{d_p}\right)\alpha_g^{-2.65} \tag{7}$$

$$C_d = \frac{24}{\alpha_g Re_p}\left(1 + 0.15(\alpha_g Re_p)^{0.687}\right) \tag{8}$$

$$Re_p = \frac{\left|\vec{u}_g - \vec{u}_p\right| d_p}{\nu_g} \tag{9}$$

whereas for $\alpha_g \leq 0.8$:

$$\kappa_{pg} = 150\left(\frac{(1-\alpha_g)^2\nu_g}{\alpha_g d_p^2}\right) + 1.75\left(\frac{(1-\alpha_g)\left|\vec{u}_g - \vec{u}_p\right|}{d_p}\right) \tag{10}$$

Here, ν_g is the kinematic viscosity of the gas phase.

2.3.1 MFM Model Equations

The gas phase continuity and momentum equations are given by[5]:

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \vec{\nabla} \cdot \left(\alpha_g \rho_g \vec{u}_g\right) = 0 \tag{12}$$

$$\frac{\partial(\alpha_g \rho_g \vec{u}_g)}{\partial t} + \vec{\nabla} \cdot \left(\varepsilon_g \alpha_g \vec{u}_g \vec{u}_g\right) = -\alpha_g \vec{\nabla} p + \vec{\nabla} \cdot \bar{\bar{\tau}} + \alpha_g \rho_g \vec{g} + \sum_{m=1}^{M=2} \kappa_{sg,m}(\vec{u}_{s,m} - \vec{u}_g) \tag{13}$$

Here, s refers to a solids phase, and m acts as a counter for the two solids phases.

The m^{th} solids phase continuity and momentum equations are given by:

$$\frac{\partial(\alpha_{s,m} \rho_{s,m})}{\partial t} + \vec{\nabla} \cdot \left(\alpha_{s,m} \rho_{s,m} \vec{u}_{s,m}\right) = 0 \tag{14}$$

$$\begin{aligned} &\frac{\partial(\alpha_{s,m} \rho_{s,m} \vec{u}_{s,m})}{\partial t} + \vec{\nabla} \cdot \left(\alpha_{s,m} \rho_{s,m} \vec{u}_{s,m} \vec{u}_{s,m}\right) \\ &\quad = -\alpha_{s,m} \vec{\nabla} p - \vec{\nabla} p_{s,m} + \vec{\nabla} \cdot \bar{\bar{\tau}}_{s,m} + \alpha_{s,m} \rho_{s,m} \vec{g} + \kappa_{sf,m}\left(\vec{u}_g - \vec{u}_{s,m}\right) - \kappa_{ss,k,m} \end{aligned} \tag{15}$$

Here, $\alpha_{s,m}$ and $\rho_{s,m}$ are the volume fraction and density of the m^{th} solids phase. The solids-fluid momentum exchange is calculated using the Gidaspow drag law[6], as described in the CFD-DEM section. The solids-solids momentum exchange of Gera et al.[7] is given by:

$$\begin{aligned} \kappa_{ss,k,m} &= 3\frac{\pi}{2}(1+e)\frac{\left(d_{s,k} + d_{s,m}\right)^2}{2\pi\left(\rho_{s,k} d_{s,k}^3 + \rho_{s,m} d_{s,m}^3\right)} \rho_{s,k} \rho_{s,m} \\ &\quad \rho_{s,k} \rho_{s,m} g_{0,km} \left|\vec{u}_{s,k} - \vec{u}_{s,m}\right| + S_{coef} p_c \end{aligned} \tag{16}$$

Here, the subscripts k and m reference solids phases, and d_s is the diameter of the particles in a solids phase. Further, e is the restitution coefficient, c_{fkm} is the coefficient of friction between the kth solids phase and the mth solids phase, S_{coef} is the segregation slope coefficient, $g_{0,km}$ is the radial distribution function at contact between the k^{th} and m^{th} solids phases. p_c is the solids pressure at a critical state, in which the granular assembly deforms without volume change.

The m^{th} solids phase stress tensor is given by:

$$\bar{\bar{\tau}}_{s,m} = \mu_{s,m}\left(\nabla\vec{u}_{s,m} + \nabla\vec{u}_{s,m}^{\,T}\right) - \frac{2}{3}\mu_{s,m}\left(\nabla\cdot\vec{u}_{s,m}\right)\bar{\bar{I}} \tag{17}$$

The solids pressure and solids viscosity for the m^{th} phase are given by:

$$p_{s,m} = p_{s,m}^{k} + p_{s,m}^{f} \tag{18}$$

$$\mu_{s,m} = \mu_{s,m}^{k} + \mu_{s,m}^{f} \tag{19}$$

Here, the superscripts k and f refer to kinetic and frictional contributions, respectively.

The Guo-Boyce frictional stress model is given by[8]:

$$p_c = \begin{cases} \dfrac{\left((\alpha_{s,max} - \alpha_{s,minf})\dot{\gamma}d_{s,m}\right)^2\rho_{s,m}}{\delta^2} + A_{pc}\left(\alpha_s + \delta - \alpha_{s,max}\right)^{n_{pc}} & \alpha_s > (\alpha_{s,ma} \\ t_1\dfrac{\left((\alpha_{s,max} - \alpha_{s,minf})\dot{\gamma}d_{s,m}\right)^2\rho_{s,m}}{\left(\alpha_{s,max} - \alpha_s\right)^2} & \alpha_{s,minf} \le \alpha_s \le (\alpha_{s,ma} \\ 0 & \alpha_s < \end{cases} \tag{20}$$

$$t_1 = \frac{2\times arctan[10^4\times(\alpha_s - \alpha_{s,minf})]}{\pi} \tag{21}$$

$$\frac{p_{s,m}^{f}}{p_c} = \left(1 - \frac{\vec{\nabla}\cdot\vec{u}_{s,m}}{n\sqrt{2}\sin(\phi)\sqrt{S_m{:}S_m + \dfrac{\Theta}{d_p^2}}}\right)^{n-1}\frac{\alpha_{s,m}}{\sum_{m=1}^{M=2}\alpha_{s,m}} \tag{22}$$

$$\mu_{s,m}^{f} = \frac{\sqrt{2}p_s^f sin(\phi)}{\sqrt{S_m{:}S_m + \dfrac{\Theta}{d_p^2}}}\left\{n - (n-1)\left(\frac{p_s^f}{p_c}\right)^{\frac{1}{n-1}}\right\}\frac{\alpha_{s,m}}{\sum_{m=1}^{M=2}\varepsilon_{s,m}} \tag{23}$$

$$n = \begin{cases} \dfrac{\sqrt{3}}{2\sin(\phi)} & \vec{\nabla}\cdot\vec{u}_{s,m} \ge 0 \\ 1.03 & \vec{\nabla}\cdot\vec{u}_{s,m} < 0 \end{cases} \tag{24}$$

$$\mu_{bulk}^{f} = -\frac{2}{3}\mu_{s,m}^{f} \tag{25}$$

Here, $\dot{\gamma}$ is the shear rate, ϕ is the angle of internal friction, $\boldsymbol{S}$ is the deviatoric rate-of-strain tensor, and Θ_s is the granular temperature. Further, A_{pc} and n_{pc} are two constants used in the Schaeffer granular stress model[9].

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