Supporting Information

Modeling of bubble-structure-dependent drag for bubbling fluidized beds

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Table S1 Governing equations and constitutive correlations used in the model

1. Continuity equations

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}})+\nabla\cdot(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}})=0 \qquad \text{(T1-1)}$$

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}})+\nabla\cdot(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\boldsymbol{u}_{\mathrm{s}})=0 \qquad \text{(T1-2)}$$

2. Momentum conservation equations

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}})+\nabla\cdot(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}}\boldsymbol{u}_{\mathrm{g}})=-\varepsilon_{\mathrm{g}}\nabla p+\varepsilon_{\mathrm{g}}\nabla\cdot\boldsymbol{\tau}_{\mathrm{g}}+\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{g}-\beta(\boldsymbol{u}_{\mathrm{g}}-\boldsymbol{u}_{\mathrm{s}}) \qquad \text{(T1-3)}$$

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\boldsymbol{u}_{\mathrm{s}})+\nabla\cdot(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\boldsymbol{u}_{\mathrm{s}}\boldsymbol{u}_{\mathrm{s}})=-\varepsilon_{\mathrm{s}}\nabla p-\nabla p_{\mathrm{s}}+\varepsilon_{\mathrm{s}}\nabla\cdot\boldsymbol{\tau}_{\mathrm{s}}+\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\mathbf{g}+\beta(\boldsymbol{u}_{\mathrm{g}}-\boldsymbol{u}_{\mathrm{s}}) \qquad \text{(T1-4)}$$

3. Conservation equation of granular temperature

$$\frac{3}{2}[\frac{\partial}{\partial t}(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\theta)+\nabla\cdot(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\theta)\boldsymbol{u}_{\mathrm{s}}]=(-\nabla p_{\mathrm{s}}\mathbf{I}+\boldsymbol{\tau}_{\mathrm{s}}):\nabla\boldsymbol{u}_{\mathrm{s}}+\nabla\cdot(k_{\mathrm{s}}\nabla\theta)-\gamma_{\mathrm{s}}-3\beta\theta+D_{\mathrm{gs}} \qquad \text{(T1-5)}$$

4. Stress tensor

$$\boldsymbol{\tau}_{\mathrm{g}}=\mu_{\mathrm{g}}\{[\nabla\boldsymbol{u}_{\mathrm{g}}+(\nabla\boldsymbol{u}_{\mathrm{g}})^{T}]-\frac{2}{3}(\nabla\cdot\boldsymbol{u}_{\mathrm{g}})\mathbf{I}\} \qquad \text{(T1-6)}$$

$$\boldsymbol{\tau}_{\mathrm{s}}=\mu_{\mathrm{s}}\{[\nabla\boldsymbol{u}_{\mathrm{s}}+(\nabla\boldsymbol{u}_{\mathrm{s}})^{T}]-\frac{2}{3}(\nabla\cdot\boldsymbol{u}_{\mathrm{s}})\mathbf{I}\}+\xi_{\mathrm{s}}\nabla\cdot\boldsymbol{u}_{\mathrm{s}}\mathbf{I} \qquad \text{(T1-7)}$$

5. Solid pressure

$$p_{\mathrm{s}}=(1-\varphi_{1}(\varepsilon_{\mathrm{s}}))p_{\mathrm{s,k}}+\varphi_{1}(\varepsilon_{\mathrm{s}})(p_{\mathrm{s,k}}+p_{\mathrm{s,f}}) \qquad \text{(T1-8)}$$

$$p_{\mathrm{s,k}}=\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\theta+2\rho_{\mathrm{s}}\left(1+e\right)\varepsilon_{\mathrm{s}}^{2}g_{0}\theta \qquad \text{(T1-9)}$$

$$\frac{p_{\mathrm{s,f}}}{p_{c}}=(1-\frac{\nabla\cdot\boldsymbol{u}_{\mathrm{s}}}{n\sqrt{2}\sin(\varphi)\sqrt{\boldsymbol{S}:\boldsymbol{S}+\theta/d_{\mathrm{s}}^{2}}})^{n-1} \qquad \text{(T1-10)}$$

$$p_{c}=\begin{cases}10^{24}(\varepsilon^{*}-\varepsilon_{g})^{10} & \varepsilon_{g}<\varepsilon^{*}\\ 0.05\dfrac{((1-\varepsilon_{g})-\varepsilon_{s}^{\min})^{2}}{(\varepsilon_{g}-\varepsilon^{*})^{5}} & \varepsilon^{*}\le\varepsilon_{g}<(1-\varepsilon_{sf}^{\min})\\ 0 & \varepsilon_{g}>(1-\varepsilon_{sf}^{\min})\end{cases} \qquad \text{(T1-11)}$$

$$\varphi_{1}(\varepsilon_{\mathrm{s}})=\frac{\arctan[25(\varepsilon_{\mathrm{s}}-\varepsilon_{\mathrm{s,min}})(\varepsilon_{\mathrm{s,max}}-\varepsilon_{\mathrm{s,min}})^{-2}]}{\pi}+0.5 \qquad \text{(T1-12)}$$

6. Solid shear viscosity

$$\mu_{\mathrm{s}}=(1-\varphi_{2}(\varepsilon_{\mathrm{s}}))\mu_{\mathrm{s,k}}+\varphi_{2}(\varepsilon_{\mathrm{s}})(\mu_{\mathrm{s,k}}+\mu_{\mathrm{s,f}}) \qquad \text{(T1-13)}$$

$$\mu_{\mathrm{s,k}} = \frac{4}{5}\varepsilon_{\mathrm{s}}^{2}\rho_{\mathrm{s}}d_{\mathrm{s}}g_{0}(1+e)\sqrt{\frac{\theta}{\pi}} + \frac{10\rho_{\mathrm{s}}d_{\mathrm{s}}\sqrt{\pi\theta}}{96(1+e)\varepsilon_{\mathrm{s}}g_{0}}[1+\frac{4}{5}g_{0}\varepsilon_{\mathrm{s}}(1+e)]^{2} \tag{T1-14}$$

$$\mu_{\mathrm{s,f}} = \frac{\sqrt{2}p_{\mathrm{s,f}}\sin(\psi)}{\sqrt{\boldsymbol{S}:\boldsymbol{S}+\theta/\mathrm{d}_{\mathrm{s}}^{2}}}\{n-(n-1)(\frac{p_{\mathrm{s,f}}}{p_{\mathrm{c}}})^{1/(n-1)}\} \tag{T1-15}$$

$$n = \begin{cases} \dfrac{\sqrt{3}}{2\sin(\varphi)} & \nabla\boldsymbol{u}_{s} \geq 0 \\ 1.03 & \nabla\boldsymbol{u}_{s} < 0 \end{cases} \tag{T1-16}$$

$$\varphi_{2}(\varepsilon_{\mathrm{s}}) = \frac{\arctan[96(\varepsilon_{\mathrm{s}} - \varepsilon_{\mathrm{s,min}})]}{\pi} + 0.5 \tag{T1-17}$$

7. Bulk viscosity

$$\xi_{\mathrm{s,k}} = \frac{4}{3}\varepsilon_{\mathrm{s}}^{2}\rho_{\mathrm{s}}d_{\mathrm{s}}g_{0}\left(1+e\right)\left(\frac{\theta}{\pi}\right)^{1/2} \tag{T1-18}$$

$$\xi_{\mathrm{s,f}} = -\frac{2}{3}\mu_{\mathrm{s,f}} \tag{T1-19}$$

8. Thermal conductivity of particles

$$k_{\mathrm{s}} = \frac{25\rho_{\mathrm{s}}d_{\mathrm{s}}\sqrt{\pi\theta}}{64(1+e)g_{0}}[1+\frac{6}{5}(1+e)g_{0}\varepsilon_{\mathrm{s}}]^{2} + 2\varepsilon_{\mathrm{s}}^{2}\rho_{\mathrm{s}}d_{\mathrm{s}}g_{0}\left(1+e\right)\left(\frac{\theta}{\pi}\right)^{1/2} \tag{T1-20}$$

9. Dissipation of fluctuation kinetic energy

$$\gamma_{\mathrm{s}} = 3(1-e^{2})\varepsilon_{\mathrm{s}}^{2}\rho_{\mathrm{s}}g_{0}\theta(\frac{4}{d_{\mathrm{s}}}\sqrt{\frac{\theta}{\pi}} - \nabla\cdot\boldsymbol{u}_{\mathrm{s}}) \tag{T1-21}$$

10. Rate of energy dissipation per unit volume

$$D_{\mathrm{gs}} = \frac{d_{\mathrm{s}}\rho_{\mathrm{s}}}{4\sqrt{\pi\theta}g_{0}}(\frac{18\mu_{\mathrm{g}}}{d_{\mathrm{s}}^{2}\rho_{\mathrm{s}}})^{2}\left|\boldsymbol{u}_{\mathrm{g}} - \boldsymbol{u}_{\mathrm{s}}\right|^{2} \tag{T1-22}$$

Table S2 Correlations and parameters used in the model

1. Number density of particles in the emulsion phase and bubbles

$$n_{\mathrm{e}}=\frac{(1-\delta_{\mathrm{b}})(1-\varepsilon_{\mathrm{e}})}{\pi d_{\mathrm{s}}^{3}/6} \quad \text{(T2-1)}$$

$$n_{\mathrm{b}}=\frac{\delta_{\mathrm{b}}}{\pi d_{\mathrm{b}}^{3}/6} \quad \text{(T2-2)}$$

2. Drag force of emulsion phase and inter-phase[28-30]

$$F_{\mathrm{de}}=\frac{1}{8}\pi d_{\mathrm{s}}^{2}\rho_{\mathrm{g}}[200\frac{(1-\varepsilon_{\mathrm{e}})\mu_{\mathrm{g}}}{\varepsilon_{\mathrm{e}}{}^{3}d_{\mathrm{s}}\rho_{\mathrm{g}}}\frac{1}{U_{\mathrm{slip,e}}}+\frac{7}{3}\frac{1}{\varepsilon_{\mathrm{e}}{}^{3}}]U_{\mathrm{slip,e}}^{2} \quad \text{(T2-3)}$$

$$F_{\mathrm{db}}=\begin{cases}0.125\pi d_{\mathrm{b}}^{2}\rho_{\mathrm{e}}(1-\delta_{\mathrm{b}})^{-0.5}38Re_{\mathrm{int}}^{-1.5}U_{\mathrm{slip,int}}{}^{2} & Re_{\mathrm{int}}\le 1.8\\ 0.125\pi d_{\mathrm{b}}^{2}\rho_{\mathrm{e}}(1-\delta_{\mathrm{b}})^{-0.5}[2.7+24Re_{\mathrm{int}}^{-1}]U_{\mathrm{slip,int}}{}^{2} & Re_{\mathrm{int}}>1.8\end{cases} \quad \text{(T2-4)}$$

3. Mean density in the emulsion phase

$$\rho_{\mathrm{e}}=\rho_{\mathrm{g}}\varepsilon_{\mathrm{e}}+\rho_{\mathrm{s}}(1-\varepsilon_{\mathrm{e}}) \quad \text{(T2-5)}$$

4. Viscosity in the emulsion phase[31]

$$\mu_{\mathrm{e}}=\mu_{\mathrm{g}}[1+2.5(1-\varepsilon_{\mathrm{e}})+10.05(1-\varepsilon_{\mathrm{e}})^{2}+0.00273\exp(16.6(1-\varepsilon_{\mathrm{e}}))] \quad \text{(T2-6)}$$

5. Superficial velocity in the emulsion phase

$$U_{\mathrm{e}}=\frac{\rho_{\mathrm{g}}U_{\mathrm{g,e}}+\rho_{\mathrm{s}}U_{\mathrm{s,e}}}{\rho_{\mathrm{g}}\varepsilon_{\mathrm{e}}+\rho_{\mathrm{s}}(1-\varepsilon_{\mathrm{e}})} \quad \text{(T2-7)}$$

6. Superficial slip velocity of emulsion phase and inter-phase

$$U_{\mathrm{slip,e}}=U_{\mathrm{g,e}}-\frac{\varepsilon_{\mathrm{e}}U_{\mathrm{s,e}}}{1-\varepsilon_{\mathrm{e}}} \quad \text{(T2-8)}$$

$$U_{\mathrm{slip,int}}=(1-\delta_{\mathrm{b}})(U_{\mathrm{b}}-U_{\mathrm{e}}) \quad \text{(T2-9)}$$

Nomenclature

a acceleration [m s^{-2}]

C particle fluctuating velocity [m s^{-1}]

C_D drag coefficient of a single particle

d particle diameter [m]

d_b bubble diameter [m]

e restitution coefficient

F_{de} drag force in the emulsion phase per unit volume[N]

F_{db} drag force acting on the bubble per unit volume[N]

g_0 radial distribution function

g gravity [m s^{-2}]

k_s conductivity of fluctuating energy [kg m^{-1} s^{-1}]

N_{df} energy dissipation [W kg^{-1}]

p fluid pressure [Pa]

p_s particle pressure [Pa]

Re Reynolds number

u velocity [m s^{-1}]

U superficial velocity [m s^{-1}]

U_{mf} minimum fluidizing gas velocity [m s^{-1}]

$U_{slip,e}$ superficial slip velocity in emulsion phase [m s^{-1}]

$U_{slip,int}$ superficial slip velocity between bubble and emulsion [m s^{-1}]

Greek letters

β drag coefficient [kg m^{-3} s^{-1}]

γ collisional energy dissipation [kg m^{-3} s^{-1}]

ε volume fration

θ granular temperature [m^2 s^{-2}]

λ thermal conductivity [m^2 s^{-2}]

μ viscosity [Pa s]

ξ bulk viscosity [Pa s]

ρ density [kg m^{-3}]

τ stress tensor [Pa]

δ bubble holdup

Subscripts

b bubble phase

e emulsion phase

g gas phase

int inter-phase

s solids phase

w wall