nanomaterials

Supplementary Materials

Flow behavior of nanoparticle agglomerates in a fluidized bed simulated with porous-structure-based drag laws

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Section S1. Governing equations for gas/solid flows.

Mass conservation for phase i (i = *g* for gas and *s* for solid):

$$\frac{\partial(\varepsilon_i\rho_i)}{\partial t}+\nabla\cdot(\varepsilon_i\rho_i\vec{v}_i)=0$$

Linear momentum balance for gas and solid phases:

$$\frac{\partial\left(\varepsilon_g\rho_g\vec{v}_g\right)}{\partial t}+\nabla\cdot\left(\varepsilon_g\rho_g\vec{v}_g\right)=-\varepsilon_g\nabla p_g+\nabla\cdot\bar{\bar{\tau}}_g+\beta_{gs}\left|\vec{v}_s-\vec{v}_g\right|+\varepsilon_g\rho_g\vec{g}$$

$$\frac{\partial(\varepsilon_s\rho_s\vec{v}_s)}{\partial t}+\nabla\cdot(\varepsilon_s\rho_s\vec{v}_s)=-\varepsilon_s\nabla p_s+\nabla\cdot\bar{\bar{\tau}}_s+\beta_{gs}\left|\vec{v}_s-\vec{v}_g\right|+\varepsilon_s\rho_s\vec{g}$$

Transport equation for the solid phase granular temperature:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s\rho_s\Theta_s)+\nabla\cdot(\varepsilon_s\rho_s\vec{v}_s\Theta_s)\right]=\left(-p_s\bar{\bar{I}}+\bar{\bar{\tau}}_s\right)\cdot\nabla\vec{v}_s+\nabla\left(k_{\Theta_s}\nabla\Theta_s\right)-\gamma_{\Theta_s}+\Phi_{gs}$$

Section S2. Constitutive equations of gas-solid flow.

Gas stress tensor:

$$\bar{\bar{\tau}}_g = \varepsilon_g \mu_g \left[\nabla v_g + \nabla v_g^T\right] - \frac{2}{3}\varepsilon_g \mu_g \nabla \cdot v_g \vec{I}$$

Solid stress tensor:

$$\bar{\bar{\tau}}_s = \mu_s \left[\nabla v_s + \nabla v_g^T\right] - \frac{2}{3}\mu_s \nabla \cdot v_s \vec{I}$$

where solid shear viscosity is:

$$\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fr}$$

The collisional contribution to shear viscosity is:

$$\mu_{s,col} = \frac{4}{5}\varepsilon_s \rho_s g_{0,ss}(1 + e_{ss})\sqrt{\frac{\Theta_s}{\pi}}$$

The kinetic contribution to shear viscosity:

$$\mu_{s,kin} = \frac{10 d_s \rho_s \sqrt{\Theta_s \pi}}{96 \varepsilon_s g_{0,ss}(1 + e_{ss})}[1 + \frac{4}{5}\varepsilon_s g_{0,ss}(1 + e_{ss})]^2$$

The frictional contribution to shear viscosity [1]:

$$\mu_{s,fr} = p_f \sin(\varphi)/2\sqrt{I_{2D}}$$

Solid phase bulk viscosity:

$$\lambda_s = \frac{4}{3}\varepsilon_s d_s^2 \rho_s g_{0,ss}(1 + e_{ss})\sqrt{\frac{\Theta_s}{\pi}}$$

Collision dissipation energy [2]:

$$\gamma_\Theta = \frac{12(1 - e_{ss}^2) g_{0,ss}}{d_s \sqrt{\pi}} \rho_s \varepsilon_s^2 \Theta_s^{3/2}$$

Solids pressure:

$$p_s = \varepsilon_s \rho_s \Theta_s + 2\rho_s(1 + e_{ss})\varepsilon_s^2 g_{0,ss}$$

Thermal energy diffusion coefficient:

$$k_\Theta = \frac{25 d_s \rho_s \sqrt{\Theta_s \pi}}{64 g_{0,ss}(1 + e_{ss})}[1 + \frac{6}{5}\varepsilon_s g_{0,ss}(1 + e_{ss})]^2 + 2\rho_s \varepsilon_s^2 d_s g_{0,ss}(1 + e_{ss})\sqrt{\frac{\Theta_s}{\pi}}$$

Radial distribution function:

$$g_{0,ss} = [1 - (\frac{\varepsilon_s}{\varepsilon_{s,max}})^{1/3}]^{-1}$$

Dissipation of granular temperature by gas damping:

$$\Phi_{gs} = -3\beta\Theta_s$$

Section S3. The drag model used in this work.

Huilin-gidaspow drag model [3]:

Huilin-gidaspow drag model is a combination of the previous drag models proposed by Wen and Yu [4] and Ergun [5]. It introduces a transition function to smoothly switch the drag coefficients at the bed porosity of 0.8. The pressure drop due to friction between gas and particles is described by the Ergun equation [5] as the bed porosity is less than 0.8 and Wen and Yu equation as the bed porosity is larger than 0.8.

$$\beta_1 = 150\frac{\varepsilon_s(1-\varepsilon_g)\mu_g}{\varepsilon_g d_a^2} + 1.75\frac{\rho_g\varepsilon_s|\vec{v}_s-\vec{v}_g|}{d_a} \quad (\varepsilon_g \leq 0.8)$$

$$\beta_2 = \frac{3}{4}C_d\frac{\varepsilon_s\varepsilon_g\rho_g|\vec{v}_s-\vec{v}_g|}{d_a}\varepsilon_g^{-2.65} \quad (\varepsilon_g > 0.8)$$

$$\beta_{gs} = \beta_1 \quad (\varepsilon_g < 0.8)$$

$$\beta_{gs} = \varphi\beta_1 + (1-\varphi)\beta_2 \quad (\varepsilon_g > 0.8)$$

$$\varphi = \frac{1}{2} + \frac{\arctan\big(262.5(\varepsilon_s - 0.2)\big)}{\pi}$$

where drag coefficient is:

$$C_d = \frac{24}{Re_s}[1 + 0.15(Re_s)^{0.687}] \quad (Re_s < 1000)$$

$$Re_s = \frac{\rho_g d_a|\vec{v}_s - \vec{v}_g|}{\mu_g}$$

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