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Supplementary material

SUPPLEMENTARY MATERIAL TO

Euler–Euler granular flow model of the combustion of liquid fuels in a fluidized reactor

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TWO-FLUID GRANULAR MODEL OF A FLUIDIZED BED**

The basic and constitutive equations of the two-fluid granular model of a fluidized bed are given in Supplementary material to this paper. could be described by the following set of expressions:[1]

Continuity equation of the gas phase:

$$\frac{\partial}{\partial t}(\alpha_{\rm g}\rho_{\rm g})+\nabla(\alpha_{\rm g}\rho_{\rm g}\vec{u}_{\rm g})=0 \tag{1}$$

Continuity equation of the solid phase:

$$\frac{\partial}{\partial t}(\alpha_{\rm s}\rho_{\rm s})+\nabla(\alpha_{\rm s}\rho_{\rm s}\vec{u}_{\rm s})=0 \tag{2}$$

Momentum conservation equation of the gas phase:

$$\frac{\partial}{\partial t}(\alpha_{\rm g}\rho_{\rm g}\vec{u}_{\rm g})+\nabla(\alpha_{\rm g}\rho_{\rm g}\vec{u}_{\rm g}\vec{u}_{\rm g})=-\alpha_{\rm g}\nabla p+\nabla\cdot\bar{\bar{\tau}}_{\rm g}+\alpha_{\rm g}\rho_{\rm g}\vec{g}+K_{\rm gs}\left(\vec{u}_{\rm g}-\vec{u}_{\rm s}\right) \tag{3}$$

Momentum conservation equation of the solid phase:

$$\begin{aligned}&\frac{\partial}{\partial t}(\alpha_{\rm s}\rho_{\rm s}\vec{u}_{\rm s})+\nabla(\alpha_{\rm s}\rho_{\rm s}\vec{u}_{\rm s}\vec{u}_{\rm s})=\\&=-\alpha_{\rm s}\nabla p+\nabla\bar{\bar{\tau}}_{\rm s}+\alpha_{\rm s}\rho_{\rm s}\vec{g}+K_{\rm gs}\left(\vec{u}_{\rm g}-\vec{u}_{\rm s}\right)\end{aligned} \tag{4}$$

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** Nomenclature is given in the basic paper.

where: $\vec{u}_g$ and $\vec{u}_s$ are the instantaneous velocity vectors for the gas and solid phase, respectively; α_g and α_s are the void fraction of the gas and solid phase, respectively.

The stress tensor of the gas and the granular phases are given by Eqs. (5) and (6), respectively:

$$\bar{\bar{\tau}}_g = 2\mu_g \bar{S}_g + (\lambda_g - \frac{2}{3}\mu_g)\nabla\vec{u}_g \bar{\bar{I}} \tag{5}$$

$$\bar{\bar{\tau}}_s = -p_s \bar{\bar{I}} + 2\alpha_s \mu_s \bar{S}_s + \alpha_s(\lambda_s - \frac{2}{3}\mu_s)\nabla\vec{u}_s \bar{\bar{I}} \tag{6}$$

The strain rate tensor is defined as:

$$\bar{S}_k = \frac{1}{2}\left(\nabla\vec{u}_k + (\nabla\vec{u}_k)^T\right),\ k = g,s \tag{7}$$

The pressure of the granular phase is:[2]

$$p_s = 2\rho_s \Theta_s (1+e_s)\alpha_s^2 g_{0s} \tag{8}$$

The radial distribution function, g_{0s}, for the Syamlal model is equal to:

$$g_0(\alpha_s) = \frac{1}{1-\alpha_s} + \frac{3\alpha_s}{2(1-\alpha_s)^2} \tag{9}$$

where e_s is the restitution coefficient and Θ_s is the granular temperature.

The viscosity of the granular phase consists of the solids shear viscosity μ_s and the bulk viscosity λ_s. The solids bulk viscosity λ_s is a measure of resistance of solid particles to expansion/compression and, according to the Lun *et al*. model,[1] it is defined as:

$$\lambda_s = \frac{4}{3}\alpha_s \rho_s d_s g_{0s}(1+e_s)\left(\frac{\Theta_s}{\pi}\right)^{1/2} \tag{10}$$

The shear viscosity is the result of translator motion (kinetic viscosity, $\mu_{s,kin}$), mutual particle collisions (collision viscosity, $\mu_{s,coll}$) and frictional viscosity ($\mu_{s,fr}$): $\mu_{s,kin} = \mu_{s,kin} + \mu_{s,coll} + \mu_{s,fr}$.

According to the Syamlal model,[2] the kinetic viscosity is:

$$\mu_{s,kin} = \frac{\alpha_s d_s \rho_s (\Theta_s \pi)^{1/2}}{12(2-\eta)}\left[1 + \frac{8}{5}\eta(3\eta-2)\alpha_s g_{0s}\right] \tag{11}$$

$$\eta = \frac{(1+e_s)}{2}$$

and for the collision viscosity, the following expression is applied:

$$\mu_{\rm s,coll} = \frac{8}{5}\alpha_{\rm s}\rho_{\rm s}d_{\rm s}g_{0\rm s}\eta\left(\frac{\Theta_{\rm s}}{\pi}\right)^{1/2}$$

According to the Schaeffer model,[3] the frictional viscosity is defined as:

$$\mu_{\rm s,fr} = \frac{p_{\rm s}\sin\phi}{2\sqrt{I_{\rm 2D}}}$$

where $p_{\rm s}$ is the granular phase (solids) pressure, ϕ is the angle of internal friction for the particle and $I_{\rm 2D}$ is the second invariant of the deviator of the strain rate tensor.

The last term in Eqs. (3) and (4) is a consequence of the inter-phase interaction drag force, where the coefficient between the fluid and solid (granular) phase, according to the Syamlal–O'Brien model,[4] is:

$$K_{\rm gs} = \frac{3\alpha_{\rm g}\alpha_{\rm s}\rho_{\rm g}}{4u_{\rm r,s}^2 d_{\rm s}} C_{\rm D}\left|\vec{u}_{\rm s} - \vec{u}_{\rm g}\right|,\ C_{\rm D} = \left(0.63 + \frac{4.8}{\sqrt{{\rm Re}_{\rm s}/u_{\rm r,s}}}\right)^2$$

$$\mathrm{Re}_{\rm s} = \frac{\rho_{\rm g}d_{\rm s}\left|\vec{u}_{\rm s} - \vec{u}_{\rm g}\right|}{\mu_{\rm g}} \quad (12)$$

The terminal velocity coefficient for the solid phase, $u_{\rm r,s}$, was determined as:

$$u_{\rm r,s} = 0.5\left(A - 0.06\,\mathrm{Re}_{\rm s} + \sqrt{(0.06\,\mathrm{Re}_{\rm s})^2 + 0.12\,\mathrm{Re}_{\rm s}(2B - A) + A^2}\right)$$

$$A = \alpha_{\rm g}^{4.14},\ B = \begin{cases} = 0.8\alpha_{\rm g}^{1.28} & \alpha_{\rm g} \le 0.85 \\ = \ \ \alpha_{\rm g}^{2.65} & \alpha_{\rm g} > 0.85 \end{cases} \quad (13)$$

The granular temperature, starting from the equations of conservation of fluctuating granular energy, is:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\rho_{\rm s}\alpha_{\rm s}\Theta_{\rm s}) + \nabla(\rho_{\rm s}\alpha_{\rm s}\vec{u}_{\rm s}\Theta_{\rm s})\right] = \left(-\rho_{\rm s}\overline{\overline{I}} + \overline{\overline{\tau}}\right)_{\rm s} : \nabla\vec{u}_{\rm s} + \\ + \nabla(k_{\Theta\rm s}\nabla\Theta_{\rm s}) - \gamma_{\Theta\rm s} + \phi_{\rm gs} \quad (14)$$

The diffusion coefficient or conductivity of the granular temperature, according to Syamlal,[2] is:

$$k_{\Theta_{\rm s}} = \frac{15\alpha_{\rm s}\rho_{\rm s}d_{\rm s}\sqrt{\Theta_{\rm s}\pi}}{4(41 - 33\eta)}\left[1 + \frac{12}{5}\alpha_{\rm s}g_{0\rm s}\eta^2(4\eta - 3)\right] \quad (15)$$

The granular energy dissipation due to the inelastic collisions was defined by Lun *et al.*,[1] as follows:

$$\gamma_{\Theta_s} = \frac{12(1-e_s)g_{0s}}{d_s\sqrt{\pi}}\rho_s\alpha_s\Theta_s^{3/2} \qquad (16)$$

The exchange of kinetic energy between the phases was determined as:

$$\phi_{gs} = -3K_{gs}\Theta_s \qquad (17)$$

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