Appendix

On the fast modeling of species transport in fluidized beds using recurrence CFD

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Two-Fluid model

In this article, we use the TFM approach for the gas-particle flows presenting the involved dynamics in fluidized bed reactors. Therein, both gas phase, \(g\), and solid phase, \(s\), are considered as inter-penetrating continua, and the transport equations of mass and momentum, for a cold fluidization, are given by

\begin{align}
\frac{\partial}{\partial t} \epsilon_g \rho_g + \nabla \cdot (\epsilon_g \rho_g \mathbf{u}_g) &= 0, \\
\frac{\partial}{\partial t} \epsilon_s \rho_s + \nabla \cdot (\epsilon_s \rho_s \mathbf{u}_s) &= 0, \\
\frac{\partial}{\partial t} (\epsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\epsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) &= -\epsilon_g \nabla p + \nabla \cdot (\epsilon_g \mathbf{T}_g - \beta (\mathbf{u}_g - \mathbf{u}_s) + \epsilon_g \rho_g \mathbf{g}), \\
\frac{\partial}{\partial t} (\epsilon_s \rho_s \mathbf{u}_s) + \nabla \cdot (\epsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) &= -\epsilon_s \nabla p - \nabla \cdot (\mathbf{S}_s^{bc} + \mathbf{S}_s^{fr}) + \beta (\mathbf{u}_g - \mathbf{u}_s) + \epsilon_s \rho_s \mathbf{g}. 
\end{align}

(A1)

Inside, \(\epsilon\), \(\rho\) and \(\mathbf{u} = (u, v, w)\) are the volume fraction, density and velocity fields of the corresponding gas (\(g\)) or solid (\(s\)) phase, respectively. \(p\) is the pressure field, while \(t\) and \(\mathbf{g}\), are the time and the gravity acceleration, respectively. The particle-gas interactions are transmitted
by the interface drag forces \( \beta (u_g - u_s) \) where \( \beta \) is predicted following\(^1\), as,

\[
\beta = \frac{3}{4} C_D \epsilon_s \rho_g \frac{\|u_g - u_s\|}{d_s V_r^2}, \quad \text{with} \quad C_D = \left( 0.6 + 4.8 \sqrt{\frac{V_r}{Re_s}} \right)^2, \quad (A2)
\]

and\(^3\) \( V_r = 0.5(a - 0.06 Re_s + \sqrt{(0.06 Re_s)^2 + 0.12 Re_s (2b - a) + a^2}) \)

\[
Re_s = \frac{\rho_g \|u_s - u_g\|d_s}{\mu_g}, \quad a = (1 - \epsilon_s)^{4.14}, \quad b = \begin{cases} 0.8 \epsilon_g^{1.28} & \text{if } \epsilon_s \geq 0.15 \\ \epsilon_g^{2.65} & \text{if } \epsilon_s < 0.15 \end{cases}, \quad (A3)
\]

\( Re_s \) is the relative Reynolds number with a spherical grains diameter \( d_s \) and molecular viscosity of gas phase \( \mu_g \). In the closure of Newtonian interstitial gas, \( T_g = \mu_g (\nabla u_g + (\nabla u_g)^t) \) denotes the gas stress-strain tensor. Whilst the solid stress tensor \( S_{sc}^{kc} \), which arises from collisions between particles (collisional part) and random fluctuations of the transitional motion (kinetic part), is evaluated using the kinetic theory of granular flow (KTGF)\(^4\). Following\(^5\), \( S_{sc}^{kc} \) can be written in a compressible sense to account for the resistance of the granular particles to compression and expansion, as,

\[
S_{sc}^{kc} = (p_{sc}^{kc} - \lambda_{sc}^{kc} \text{tr}(D_s))I - 2 \mu_s^{kc} [D_s - 1/3 \text{tr}(D_s)I], \quad D_s = 1/2 (\nabla u_s + (\nabla u_s)^t); \quad (A4)
\]

And which is closed by a balance of the pseudo-thermal energy (PTE) of particle velocity fluctuations \( i.e. \) granular temperature \( \Theta_s \). Here, \( p_{sc}^{kc} \) identifies the solids pressure\(^6\),

\[
p_s = \rho_s \epsilon_s \Theta_s [1 + 2 (1 + \epsilon_s) g_0 \epsilon_s] \quad \text{with} \quad \epsilon_s = 0.9 \quad \text{and} \quad g_0 = \left( 1 - \frac{\epsilon_s}{\epsilon_{s_{max}}} \right)^{-2.5 \epsilon_{s_{max}}} \quad (A5)
\]

where \( \epsilon_s \) is the coefficient of restitution for particle collisions and \( g_0 \) is the radial distribution function that incorporates the maximum packing limit, \( \epsilon_{s_{max}} \), to the probability of collisions between grains. \( \lambda_{sc}^{kc} \) indicates the granular bulk viscosity\(^6\),

\[
\lambda_{sc}^{kc} = \frac{4}{3} \epsilon_s^2 \rho_s d_s g_0 (1 + \epsilon_s) \sqrt{\frac{\Theta_s}{\pi}}, \quad (A6)
\]
and $\mu^{kc}_s$ the kinetic-collisional granular viscosity, which is given by \(^1\),

$$
\mu^{kc}_s = \frac{4}{5} \varepsilon_s^2 \rho_s d_s g_0 (1 + \varepsilon_s) \sqrt{\frac{\Theta_s}{\pi}} + \frac{\varepsilon_s d_s \rho_s \sqrt{\Theta_s \pi}}{6(3 - \varepsilon_s)} \left[ 1 + \frac{2}{5}(1 + \varepsilon_s)(3\varepsilon_s - 1)\varepsilon_s g_0 \right].
$$

(A7)

Hence, in order to close the system the conservation equation of granular temperature $\Theta_s$ should be solved, and read as,

$$
\frac{3}{2} \frac{\partial}{\partial t} (\varepsilon_s \rho_s \Theta_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \Theta_s) = -S^{kc}_s : \nabla \mathbf{u}_s - \nabla \cdot \mathbf{q} + \Gamma_s - J_v - \sigma_{\Theta_s}.
$$

(A8)

In this equation, $\mathbf{q} = \kappa \nabla \Theta_s$ represents the flux PTE vector where the conductivity of granular energy, $\kappa$, follows \(^1\),

$$
\kappa = \frac{15d_s \rho_s \varepsilon_s \sqrt{\frac{\Theta_s}{\pi}}}{4(41 - 33\eta)} \left[ 1 + \frac{12}{5} \eta^2 (4\eta - 3)\varepsilon_s g_0 + \frac{16}{15\pi} (41 - 33\eta)\eta \varepsilon_s g_0 \right], \text{ with } \eta = \frac{1}{2}(1 + \varepsilon_s).
$$

(A9)

The terms $-S^{kc}_s : \nabla \mathbf{u}_s$ and $-\nabla \cdot \mathbf{q}$, designate the generation and diffusion terms of $\mathbf{q}$, respectively, while $\sigma_{\Theta_s}$ indicates the rate of collisional dissipation of PTE due to inelastic collisions between particles. It can be derived from \(^6\) as,

$$
\sigma_{\Theta_s} = \frac{12(1 - \varepsilon_s^2)g_0}{d_s \sqrt{\pi}} \rho_s \varepsilon_s \Theta_s^{3/2};
$$

(A10)

The transfer of the kinetic energy of random fluctuations in particle velocity, from the solid phase to the gas phase, is represented by the rate of viscous dumping dissipation $J_v$ \(^8\), and the production of gas-particle slip $\Gamma_{s}$ \(^9\). Their relations are given in follow, as,

$$
J_v = 3\beta \Theta_s, \quad \text{and} \quad \Gamma_s = \frac{81 \varepsilon_s \mu^g_s \| \mathbf{u}_g - \mathbf{u}_s \|}{g_0 d_s^3 \rho_s \sqrt{\Theta_s \pi}}.
$$

(A11)

In such cases, when the grains start to endure long in sliding and rubbing contacts, the solid stress is further arising by a frictional contribution $S_{s}^{fr}$ in the dense pockets of the bed. It reads as,

$$
S_{s}^{fr} = p_{s}^{fr} \mathbf{I} - 2\mu_{s}^{fr} [\mathbf{D}_s - 1/3 \text{tr} (\mathbf{D}_s) \mathbf{I}],
$$

(A12)
where $p_f^{fr}$ is the frictional pressure \textit{i.e.} frictional normal stress, and the frictional viscosity $\mu_f^{fr}$ is derived from Coulomb’s law and Shaeffer’s frictional theory\textsuperscript{10} as,

$$
\mu_f^{fr} = \frac{p_f^{fr} \sin \phi}{2\| D_s - 1/3\text{tr}(D_s)I \|} \\
(A13)
$$

Here, $\phi$ is the angle of internal friction of the particle. Using the model\textsuperscript{6}, the radial function in the solid pressure $p_s^{kc}$ formula tends to infinity as the volume fraction tends to the packing limit. Hence, this pressure, resulting from granular kinetic theory, is then directly used in the calculation of Eqs. A13 and A12.

In case that the cold fluidization is accompanied with non-reactive chemical species conversions, the evolution of this last can be determined by resolving the transport equation of $j^{th}$ specie mass fraction, $\gamma_j$. Considering that the species are non-interacted and propagated on the gas or solid phase, such homogeneous species in a mixture of no additional source, then its convection-diffusion equations follow,

$$
\frac{\partial}{\partial t}(\epsilon_g \rho_g \gamma_j) + \nabla \cdot (\epsilon_g \rho_g u_g \gamma_j) = -\nabla \cdot (\epsilon_g \chi_j), \\
\frac{\partial}{\partial t}(\epsilon_s \rho_s \gamma_j) + \nabla \cdot (\epsilon_s \rho_s u_s \gamma_j) = -\nabla \cdot (\epsilon_s \chi_j) \\
(A14)
$$

Therein, $\chi_j = -\rho_j D_j \nabla \gamma_j$ designates the diffusion flux of $j^{th}$ specie that arises due to the gradients of concentration, and the dilute approximation (Fick’s law) is used for the diffusion coefficient $D_j$. In this work, we roughly consider an identical constant value of $D_j$ mixture for the solid and gas phase. However, the evaluation of $\rho_j$ is set as an incompressible ideal gas on the gas phase and following the volume weighted mixing law on the solid phase.

In another situation, when the heat transfer phenomenon is of a major interest, the mathematical modeling of dynamics in fluidized bed is basically controlled by Eqs. A1 and A8, where the buoyancy forces returned to density variation, are rigorously neglected. However, additional equations of the enthalpy (energy) transport appear to calculate the temperature of the gas $T_g$.
and solid $T_s$ phase, as follows,

$$\frac{\partial}{\partial t}(\epsilon_g \rho_g h_g) + \nabla \cdot (\epsilon_g \rho_g u_g h_g) = \nabla \cdot (\epsilon_g \kappa_g \nabla T_g) + \alpha(T_s - T_g) + T_g : \nabla u_g + \epsilon_g \frac{\partial p}{\partial t} + \nabla \cdot \epsilon_g p u_g,$$

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s h_s) + \nabla \cdot (\epsilon_s \rho_s u_s h_s) = \nabla \cdot (\epsilon_s \kappa_s \nabla T_s) + \alpha(T_g - T_s) - (S^{kc}_s + S^{kr}_s) : \nabla u_s + \epsilon_s \frac{\partial p}{\partial t} + \nabla \cdot \epsilon_s p u_s.$$ (A15)

Therein, $h_i = c^i_p T_i$, is the specific enthalpy of the corresponding $i$ phase, assuming constant specific heats $c^i_p$. The quantity $\alpha(T_s - T_g)$ defines the heat exchange between the gas and solid phases, where,

$$\alpha = \frac{6 \kappa_g \epsilon_s N u}{d_s^2},$$ (A16)

is the volumetric interphase heat transfer coefficient. Basically, it designates the product of the specific interfacial exchange area and the gas-solid heat transfer coefficient, $\alpha_{sg} = \kappa_g N u/d_s$.

Here, $N u$ is the Nusselt number that measures the convective heat transferred between a single sphere and the surrounding fluid. It’s value is approached following, as,

$$N u = 2 + 0.6 Re_s^{1/2} Pr^{1/3},$$ (A17)

where $Pr = c^g_p \mu_g / \kappa_g$ is the Prandtl number. In this work, and for sake of simplicity, we consider roughly, in Eqs. A15, that the solid thermal conductivity $\kappa_s$ has an equivalent constant value to the gas phase one $\kappa_g$.

For more details about transport equations, constitutive relations and closure models, adopted in the framework of TFM, the reader is referred to.

References


