Modeling of turbulent gas-solid flows.

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Introduction

Recent theories for rapid deformations in gas-solid flow carried out on fluidized bed have attempted to exploit the similarities between the particles of deforming granular mass and the molecules of a disequilibrated gas. Methods from the kinetic theory may then be used to determine, for example, the form of the balance laws for the means of density, velocity and energy and to calculate specific forms for the mean fluxes of momentum and energy and, in these dissipative systems, the mean rate at which energy is lost in collisions.

More ordinary granular flows involve rapid deformations at much higher particle densities. Such flows are common in the industrial transport of cereals, ores, and pharmaceuticals and occur naturally in granular snow avalanches, rock debris slides and underwater sediment slumps. Experiments involving the shear of both dense suspensions of identical, neutrally bouyant, spherical particles particles and dry, denses masses of identical spheres indicate that at sufficiently high rates of shear the dominant mechanism of momentum transfer is collisions between particles.

On this paper a summary is made of the present state of knowlegde of polydispersed gas-solid flow modeling and in particular its application to fluidized beds. Dispersed phase models are based on kinetic theory of granular flow which leads to the transport equations for the velocity moments, closure laws for the stress tensor and energy flux. On the other hand, gas phase is rounded up from the classical ensemble average method and it is not on deep detailed here but is admirably introduced on Enwald et al. (1997).

Three main references was crumbled in order to compare the degree of developing on the polydispersion system modeling: Jenkins-Mancini (1989), Lathouwers-Bellan (2000) and Gourdel-Simonin (1999).

Gas-phase transport equations

The average transport equations for the gas phase arise from multiply the local instantaneous transport equations by the phase indicator χ_g (equal to 1 if the gas phase is present and 0 otherwise) and getting the ensemble averaging. So that the average mass balance equation is:

$$\frac{\partial \alpha_g \overline{\rho}_g}{\partial t} + \nabla \cdot \alpha_g \overline{\rho}_g \mathbf{U}_g = 0 \tag{1}$$

where $\alpha_g = \langle \chi_g \rangle$ is the gas-phase mean fraction rate and $\mathbf{U}_g = \langle \mathbf{u}_g \rangle$ is the gas phase mean velocity.

The averaged momentum balance equation for gas phase is written as:

$$\frac{\partial}{\partial t}\left(\alpha_g \overline{\rho}_g \mathbf{U}_g\right) + \nabla \cdot \left(\alpha_g \overline{\rho}_g \mathbf{U}_g \mathbf{U}_g\right) = \tag{2}$$
$$\nabla \cdot \left(\alpha_g \overline{\boldsymbol{\sigma}}_g - \alpha_g \left\langle \rho_g \mathbf{u}'_g \mathbf{u}'_g \right\rangle_g\right) + \alpha_g \overline{\rho}_g \mathbf{g} - \left\langle \sigma_g \cdot \nabla X_g \right\rangle$$

here the average stress tensor is denoted by $\overline{\boldsymbol{\sigma}}_g$, the "*turbulent*" stress tensor is $\left\langle \rho_g \mathbf{u}'_g \mathbf{u}'_g \right\rangle_g$ which results from fluctuations $\mathbf{u}'_g = \mathbf{u}_g - \mathbf{U}_g$; the average interphase transfer with particles is $-\left\langle \sigma_g \cdot \nabla X_g \right\rangle$. The equation (2) can be rewritten as (decomposing $\overline{\boldsymbol{\sigma}}_g$ on its pressure and viscous parts):

$$\frac{\partial}{\partial t}\left(\alpha_g \overline{\rho}_g \mathbf{U}_g\right) + \nabla \cdot \left(\alpha_g \overline{\rho}_g \mathbf{U}_g \mathbf{U}_g\right) = -\alpha_g \nabla \overline{p}_g \tag{3}$$
$$+\nabla \cdot \left(\alpha_g \overline{\boldsymbol{\tau}}_g - \alpha_g \left\langle \rho_g \mathbf{u}'_g \mathbf{u}'_g \right\rangle_g\right) + \alpha_g \overline{\rho}_g \mathbf{g} + \mathbf{M}'_g$$

where $\overline{\boldsymbol{\tau}}_g$ is the average viscous stress tensor; $\mathbf{M}'_g$ represents exchange of momentum between phases after substraction of the mean gas pressure effect and is due to the combined forces exerted by the fluid on single particle : drag, added mass and lift.

$$\mathbf{M}'_g = -\sum_{\omega}\left[n_\omega \left\langle \mathbf{F}_\omega \right\rangle - n_\omega m_\omega \mathbf{g} + \alpha_\omega \nabla \overline{p}_g\right] \tag{4}$$

The closure relations involve turbulent effects $-\alpha_g \left\langle \rho_g \mathbf{u}'_g \mathbf{u}'_g \right\rangle_g$ which may be predicted using a modified $k-\epsilon$ model accounting for the influence of the particles. The remaining closed relations for the pressure and the average viscous stress tensor in eq. (3) are approximated by their similar behavior to its local instantaneous counterpart

$$\overline{p}_g = \overline{\rho}_g R T_g \tag{5}$$

and in very first approximation the strain rate tensor is

$$\overline{\boldsymbol{\tau}}_g = \mu_g \left[\left[\nabla \mathbf{U}_g + \nabla \mathbf{U}_g^T\right] - \frac{2}{3}\left[\nabla \cdot \mathbf{U}_g\right]\mathbf{I}\right] \tag{6}$$

Particle-phase transport equations.

Microscopic kinetic equations.

Let consider a mixture of spherical particles of several species (A, B, C, ...) characterized by their diameter and density. In collisional dynamics is assuming the participation only of binary species ω and β (being $\omega = A, B, C, \ldots$ and $\beta = A, B, C, \ldots$). The evolution of this system is governed by a set of "Boltzmann" like equations (Chapman and Cowling, 1970):

$$\frac{\partial f_\omega^{(1)}}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\mathbf{c}_\omega f_\omega^{(1)}\right) + \frac{\partial}{\partial \mathbf{c}_\omega} \cdot \left(\frac{\mathbf{F}_\omega}{m_\omega} f_\omega^{(1)}\right) = \sum_\beta \mathbb{J}_{\omega\beta} \tag{7}$$

where $f_\omega^{(1)} = f_\omega^{(1)}(\mathbf{c}_\omega, \mathbf{r}, t)$ is the single ω-particle velocity distribution function; $\mathbf{F}_\omega$ is the external force acting on the particle; m_ω and $\mathbf{c}_\omega$ are the mass and velocity of $\omega-$particle, respectively; $\mathbf{r}$ represents the spatial coordinates and $\sum_\beta \mathbb{J}_{\omega\beta}$ defines the effects of collisions with particles of any species. Average particle properties are derived from $f_\omega^{(1)}$ using the following definition:

$$\langle \psi_\omega \rangle_\omega = \frac{1}{n_\omega} \int \psi_\omega f_\omega^{(1)} d\mathbf{c}_\omega \tag{8}$$

where $\psi_\omega = \psi_\omega(\mathbf{c}_\omega)$ is any particle property, n_ω is the mean number of $\omega-$particle centers per unit volume given by

$$n_\omega = \int f_\omega^{(1)} d\mathbf{c}_\omega \tag{9}$$

we will assume

$$\alpha_\omega \rho_\omega = n_\omega m_\omega \tag{10}$$

where α_ω represents the volumetric fraction of the ω-particles and ρ_ω is the density of a ω-particle. Then

$$\alpha_g = 1 - \alpha_s \tag{11}$$

where the total solid volume fraction is

$$\alpha_s = \sum_\omega \alpha_\omega \tag{12}$$

Employing definition (8) we write the mean translation velocity of $\omega-$particles as

$$\mathbf{U}_\omega = \langle \mathbf{c}_\omega \rangle_\omega \tag{13}$$

Then the fluctuating translation velocity $\mathbf{u}'_\omega$ is

$$\mathbf{u}'_\omega = \mathbf{c}_\omega - \mathbf{U}_\omega \tag{14}$$

Multiplying the equation (7) by property ψ_ω, integrating over the whole velocity domain and using definition (8), the general form of the transport equations governing $\langle \psi_\omega \rangle_\omega$ is written

$$\begin{aligned} \frac{\partial}{\partial t}\left(n_\omega \langle \psi_\omega \rangle_\omega\right) + \nabla \cdot \left(n_\omega \langle \mathbf{c}_\omega \psi_\omega \rangle_\omega\right) = \\ n_\omega \left\langle \frac{\mathbf{F}_\omega}{m_\omega} \cdot \frac{\partial \psi_\omega}{\partial \mathbf{c}_\omega} \right\rangle_\omega + \sum_\beta \mathbb{C}_{\omega\beta}\left(\langle \psi_\omega \rangle_\omega\right) \end{aligned} \tag{15}$$

$\mathbb{C}_{\omega\beta}$ represents the mean change rate of ψ_ω transported by $\omega-$particles due to interparticle collision and is written as an integral over all posible binary collisions

$$\begin{aligned} \mathbb{C}_{\omega\beta}(\psi_\omega, \mathbf{r}, t) \quad = \quad & \iiint_{\mathbf{c}_{\beta\omega}\cdot\mathbf{k}>0} (\psi_\omega^* - \psi_\omega) f_{\omega\beta}^{(2)} \\ & \times d_{\omega\beta}^2 (\mathbf{c}_{\beta\omega} \cdot \mathbf{k}) \, d\mathbf{k} \, d\mathbf{c}_\omega \, d\mathbf{c}_\beta \end{aligned} \tag{16}$$

where $d_{\omega\beta}$ is the distance between centres of the spherical particles at collision

$$d_{\omega\beta} = \frac{1}{2}(d_\omega + d_\beta) \tag{17}$$

d_ω and d_β are the diameter of particle ω and β, respectively. After encounter the property is changed to ψ_ω^*. In equation (**??**), a presumed form of the pair distribution function $f_{\omega\beta}^{(2)}$ is nedeed (described in part 4.2) to fully characterize the collision effects. The relative velocity is $\mathbf{c}_{\beta\omega} = \mathbf{c}_\beta - \mathbf{c}_\omega$ and $\mathbf{k}$ is the unit vector directed from the center of the β-particle to that of the ω-particle at collision, stated as

$$\mathbf{k} = \frac{\mathbf{r}_\omega - \mathbf{r}_\beta}{d_{\omega\beta}} \tag{18}$$

The condition $\mathbf{c}_{\beta\omega} \cdot \mathbf{k} > 0$ indicates that integrations are to be taken over all values of $\mathbf{k}$ and $\mathbf{c}_{\beta\omega}$ for which an encounter is impending. The collision point is located at $\mathbf{r} = (d_\beta \mathbf{r}_\omega + d_\omega \mathbf{r}_\beta)/(2d_{\omega\beta})$ while the particle centers are located at $\mathbf{r}_\omega = \mathbf{r} + (d_\omega/2)\mathbf{k}$ and $\mathbf{r}_\beta = \mathbf{r} - (d_\beta/2)\mathbf{k}$ for the ω-particle and β-particle, respectively.

Collision integral expansions.

In order to get a suitable form of $\mathbb{C}_{\omega\beta}$, the pair distribution functions $f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r}, \mathbf{c}_\beta, \mathbf{r} - d_{\omega\beta}\mathbf{k}, t)$ are obtained from an expanded Taylor series. For any function $h(\mathbf{r})$, its expansion on $-\mathbf{a}$ around the point $\mathbf{r}$ is

$$\begin{aligned} h(\mathbf{r} - \mathbf{a}) = h(\mathbf{r}) - \frac{a_i}{1!}\frac{\partial}{\partial r_i} h(\mathbf{r}) + \frac{a_i a_j}{2!}\frac{\partial^2}{\partial r_i \partial r_j} h(\mathbf{r}) \\ - \frac{a_i a_j a_m}{3!}\frac{\partial^3}{\partial r_i \partial r_j \partial r_m} h(\mathbf{r}) + ... \end{aligned} \tag{19}$$

Taking $h(\mathbf{r}) = f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r}_\omega, \mathbf{c}_\beta, \mathbf{r}_\beta)$; $\mathbf{a} = (d_\omega/2)\mathbf{k}$, and expanding in Taylor series around $\mathbf{r}$, the pair distribution function becomes

$$\begin{aligned} f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r}, \mathbf{c}_\beta, \mathbf{r} - d_{\omega\beta}\mathbf{k}) = f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, \mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k}) \\ + \frac{d_\omega}{2} k_i \frac{\partial}{\partial r_i}\left[1 - \frac{d_\omega}{2}\frac{k_j}{2!}\frac{\partial}{\partial r_j} + \left(\frac{d_\omega}{2}\right)^2 \frac{k_j k_m}{3!}\frac{\partial^2}{\partial r_j \partial r_m} - ...\right] \\ \times f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, \mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k}) \end{aligned} \tag{20}$$

Consequently the collisional term $\mathbb{C}_{\omega\beta}$ can be expressed as the sum of two contributions: the collisional source and the collisional flux (Dahler and Sather, 1963):

$$\mathbb{C}_{\omega\beta} = \chi_{\omega\beta} - \nabla \cdot \boldsymbol{\theta}_{\omega\beta} \tag{21}$$

where the collisional source term, $\chi_{\omega\beta}$, is

$$\begin{aligned} \chi_{\omega\beta}(\psi_\omega) = d_{\omega\beta}^2 \iiint_{\mathbf{c}_{\beta\omega}\cdot\mathbf{k}>0} [\psi_\omega^* - \psi_\omega] f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r}_\omega, \mathbf{c}_\beta, \mathbf{r}_\beta) \\ \times [\mathbf{c}_{\beta\omega} \cdot \mathbf{k}] \, d\mathbf{k} \, d\mathbf{c}_\omega \, d\mathbf{c}_\beta \end{aligned} \tag{22}$$

and the collisional flux, $\boldsymbol{\theta}_{\omega\beta}$, is given by

$$\begin{aligned} \boldsymbol{\theta}_{\omega\beta}(\psi_\omega) = -\frac{d_{\omega\beta}^3}{2} \iiint_{\mathbf{c}_{\beta\omega}\cdot\mathbf{k}>0} [\psi_\omega^* - \psi_\omega] \mathbf{k} \\ \times \left[1 - \frac{d_\omega}{2}\frac{k_j}{2!}\frac{\partial}{\partial r_j} + \left(\frac{d_\omega}{2}\right)^2 \frac{k_j k_m}{3!}\frac{\partial^2}{\partial r_j \partial r_m} - ...\right] \\ \times f_{\omega\beta}^{(2)}(\mathbf{c}_\omega, \mathbf{r}_\omega, \mathbf{c}_\beta, \mathbf{r}_\beta) [\mathbf{c}_{\beta\omega} \cdot \mathbf{k}] \, d\mathbf{k} \, d\mathbf{c}_\omega \, d\mathbf{c}_\beta \end{aligned} \tag{23}$$

According to Jenkins and Richman (1985) only the lowest orders terms in Taylor series expansions are retained; this is justified when the spatial gradients of the mean fields remain small with respect to the particle size. The kinetic theory of dilute gases corresponds to the limit case when all expansion terms are negligible, so that the collisional term reduces to the collisional source term.

Particle moment balance equations

Balance of Mass : Substituting $\psi_\omega = m_\omega$ in eq. (15), we obtain the transport equation of mass of the ω-particles.

$$\frac{\partial}{\partial t}(n_\omega m_\omega) + \nabla \cdot (n_\omega m_\omega \mathbf{U}_\omega) = 0 \tag{24}$$

Balance of linear Momentum: Substituting $\psi_\omega = m_\omega \mathbf{c}_\omega$ in eq. (15) we obtain:

$$\frac{\partial}{\partial t}\left(n_\omega m_\omega \mathbf{U}_\omega\right) + \nabla\cdot\left(n_\omega m_\omega \mathbf{U}_\omega \mathbf{U}_\omega\right) = \tag{25}$$
$$-\nabla\cdot\left[n_\omega m_\omega \left\langle \mathbf{u}'_\omega \mathbf{u}'_\omega\right\rangle_\omega + \sum_\beta \boldsymbol{\theta}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right)\right]$$
$$+\sum_\beta \boldsymbol{\chi}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right) + n_\omega \left\langle \mathbf{F}_\omega\right\rangle_\omega$$

where $n_\omega m_\omega \left\langle \mathbf{u}'_\omega \mathbf{u}'_\omega\right\rangle_\omega$ is the kinetic contribution and $\sum_\beta \boldsymbol{\theta}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right)$ are the collisional contributions to the effective particulate stress tensor. The collisional source term is written as $\sum_\beta \boldsymbol{\chi}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right)$, and the final term on the right hand side of eq. (25) represents the average force excerted on the particles by the fluid. From (23), the collisional contributions forms are

$$\boldsymbol{\theta}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right) = -\frac{m_\omega d_\omega^3}{2}\iiint_{\mathbf{c}_{\beta\omega}\cdot\mathbf{k}>0}\left(\mathbf{c}^*_\omega - \mathbf{c}_\omega\right)\mathbf{k}$$
$$\times\left[1 - \frac{d_\omega}{2}\frac{k_j}{2!}\frac{\partial}{\partial r_j}\right] f^{(2)}_{\omega\beta}(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, \mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k}) \tag{26}$$
$$\times\ \left[\mathbf{c}_{\beta\omega}\cdot\mathbf{k}\right] d\mathbf{k}\ d\mathbf{c}_\omega\ d\mathbf{c}_\beta$$

the expression for the change $\mathbf{c}^*_\omega - \mathbf{c}_\omega$ is given by the microscopic collision model (see section).

Balance of fluctuating kinetic energy: Taking $\psi_\omega = \frac{1}{2} m_\omega c^2_\omega$ in eq. (15), using (24) and (25) we can derive the transport equation for fluctuating kinetic energy of ω-particles, q^2_ω

$$\frac{\partial}{\partial t}\left(n_\omega m_\omega q^2_\omega\right) + \nabla\cdot\left(n_\omega m_\omega \mathbf{U}_\omega q^2_\omega\right) = \tag{27}$$
$$-\left(n_\omega m_\omega \left\langle \mathbf{u}'_\omega \mathbf{u}'_\omega\right\rangle_\omega + \sum_\beta \boldsymbol{\theta}_{\omega\beta}\left(m_\omega \mathbf{U}_\omega\right)\right)\cdot\nabla\mathbf{U}_\omega$$
$$-\nabla\cdot\left(n_\omega m_\omega \frac{1}{2}\left\langle\left[\mathbf{u}'_\omega\cdot\mathbf{u}'_\omega\right]\mathbf{u}'_\omega\right\rangle_\omega + \sum_\beta \boldsymbol{\theta}_{\omega\beta}\left(m_\omega q^2_\omega\right)\right)$$
$$+\sum_\beta \chi_{\omega\beta}\left(m_\omega q^2_\omega\right) + n_\omega\left\langle \mathbf{F}_\omega\cdot\mathbf{u}'_\omega\right\rangle_\omega$$

where $q^2_\omega = \frac{1}{2}\left\langle \mathbf{u}'_\omega\cdot\mathbf{u}'_\omega\right\rangle_\omega = \frac{1}{2}\left\langle u'^2_\omega\right\rangle_\omega$.

Mixture balance equations.

Following Jenkins and Mancini (1989), the balance laws for the mixture are obtained by summing the corresponding balance laws for the single species. The mixture mass density is

$$\alpha_s \rho_s = \sum_\omega n_\omega m_\omega \tag{28}$$

where α_s is given by eq. (12). The mixture mass average velocity is

$$\alpha_s \rho_s \mathbf{U}_s = \sum_\omega n_\omega m_\omega \mathbf{U}_\omega \tag{29}$$

then the fluctuating velocity with respect to the mixture average velocity is written

$$\mathbf{u}''_\omega = \mathbf{c}_\omega - \mathbf{U}_s \tag{30}$$

while the $\omega-$diffusion velocity is the mean of the fluctuating velocity:

$$\mathbf{v}_\omega = \left\langle \mathbf{u}''_\omega\right\rangle_\omega = \mathbf{U}_\omega - \mathbf{U}_s \tag{31}$$

The variance of the fluctuation $\mathbf{u}''_\omega$ is written

$$\left\langle \mathbf{u}''_\omega\cdot\mathbf{u}''_\omega\right\rangle_\omega = \left\langle \mathbf{u}'_\omega\cdot\mathbf{u}'_\omega\right\rangle_\omega + \mathbf{v}_\omega\cdot\mathbf{v}_\omega \tag{32}$$

The mixture temperature is defined as

$$n_s T_s = \sum_\omega \frac{1}{3} n_\omega m_\omega \left\langle \mathbf{u}''_\omega\cdot\mathbf{u}''_\omega\right\rangle_\omega = \tag{33}$$
$$\sum_\omega n_\omega m_\omega\left[\frac{2}{3}q^2_\omega + \frac{1}{3}\mathbf{v}_\omega\cdot\mathbf{v}_\omega\right]$$

with $n_s = \sum_\omega n_\omega$.

The equation of mass balance for the mixture is obtained by summing the ones of the species:

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\right) + \nabla\cdot\left(\alpha_s\rho_s\mathbf{U}_s\right) = 0 \tag{34}$$

The equation of linear momentum balance for the mixture is obtained in the same way

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\mathbf{U}_s\right) + \nabla\left(\alpha_s\rho_s\mathbf{U}_s\mathbf{U}_s\right) = -\nabla\cdot\mathbf{P}_s + \tag{35}$$
$$\sum_\omega n_\omega\left\langle\mathbf{F}_\omega\right\rangle_\omega + \sum_\omega\left[\sum_\beta \boldsymbol{\chi}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right)\right]$$

by definition (22)

$$\boldsymbol{\chi}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right) + \boldsymbol{\chi}_{\beta\omega}\left(m_\beta\mathbf{U}_\beta\right) = \frac{1}{4}\iiint_{\mathbf{c}_{\beta\omega}\cdot\mathbf{k}>0}\left[\boldsymbol{\psi}^*_{\omega\beta} - \boldsymbol{\psi}_{\omega\beta}\right] \tag{36}$$
$$\times f^{(2)}_{\omega\beta}\left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, \mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k}\right) d^2_{\omega\beta}$$
$$\times\left[\mathbf{c}_{\beta\omega}\cdot\mathbf{k}\right] d\mathbf{k}\ d\mathbf{c}_\omega\ d\mathbf{c}_\beta$$

where $\boldsymbol{\psi}_{\omega\beta} = m_\omega\mathbf{c}_\omega + m_\beta\mathbf{c}_\beta$. By neglecting the effect of external forces during collisions, the linear momentum of any binary system is conserved during collision, this is $\boldsymbol{\psi}^*_{\omega\beta} = \boldsymbol{\psi}_{\omega\beta}$,

$$\forall\ \omega,\beta \qquad \boldsymbol{\chi}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right) + \boldsymbol{\chi}_{\beta\omega}\left(m_\beta\mathbf{U}_\beta\right) = 0 \tag{37}$$

and we obtain

$$\sum_\omega\sum_\beta \boldsymbol{\chi}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right) = 0 \tag{38}$$

The effective mixture stress tensor is written

$$\mathbf{P}_s = \sum_\omega\left[n_\omega m_\omega\left\langle\mathbf{u}'_\omega\mathbf{u}'_\omega\right\rangle_\omega + n_\omega m_\omega\mathbf{v}_\omega\mathbf{v}_\omega + \sum_\beta\boldsymbol{\theta}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right)\right] \tag{39}$$

or, using (32),

$$\mathbf{P}_s = \sum_\omega\left(n_\omega m_\omega\left\langle\mathbf{u}''_\omega\mathbf{u}''_\omega\right\rangle_\omega + \sum_\beta\boldsymbol{\theta}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right)\right) \tag{40}$$

According to Jenkins and Mancini, the mixture balance of temperature is given by

$$\frac{\partial}{\partial t}\left(n_s T_s\right) + \nabla\cdot\left(n_s\mathbf{U}_s T_s\right) = -\nabla\cdot\mathbf{Q}_s - \mathbf{P}_s\cdot\nabla\mathbf{U}_s \tag{41}$$
$$-\sum_\omega\sum_\beta\left[\frac{2}{3}\chi_{\omega\beta}\left(m_\omega q^2_\omega\right) + \mathbf{v}_\omega\cdot\boldsymbol{\chi}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right)\right]$$
$$+\sum_\omega n_\omega\mathbf{v}_\omega\cdot\left\langle\mathbf{F}_\omega\right\rangle_\omega$$

and the mixture energy flux $\mathbf{Q}_s$ is

$$\mathbf{Q}_s = \sum_\omega \left(n_\omega m_\omega \frac{1}{3} \left\langle \left[\mathbf{u}^{''}_\omega \cdot \mathbf{u}^{''}_\omega \right] \mathbf{u}^{''}_\omega \right\rangle_\omega + \sum_\beta \frac{2}{3} \boldsymbol{\theta}_{\omega\beta} \left(m_\omega q^2_\omega \right) \right) \tag{42}$$

Modelling approaches.

Jenkins and Mancini (1989)

- Model is developed for binary mixture of particles in vacuum
- Transport equations of momentum and temperature are solved for mixture.
- Transport equations of mass are solved for each particle species with a diffusion model.

Lathouwers and Bellan (2000)

- Model is developed for dense binary mixture of particles in gas.
- Transport equations of mass, momentum and energy are solved for each particle species.
- The turbulent effects of gas-phase are neglected.
- The kinetic contribution in the effective stress tensor is neglected and only the collisional part is taken into account.

Gourdel and Simonin (1999)

- Model is developed for dilute binary mixture of settling particles in homogeneous isotropic gas turbulent flow.
- Transport equations of mass, momentum and energy are solved for each particle species.
- The model accounts simultaneously for dragging along the fluid turbulence and intersticial drag effect.
- The collisional flux in the effective stress tensor is neglected and then only the kinetic part is taken into account.

Closure models for collisional terms

Microscopic collision modelling.

Assuming exclusively binary collisions without friction effects, perfectly spherical, smooth particles in translation motion, the relation between velocities of the particles right before and after an encounter is developed below. Considering a collision between two spherical species ω and β of diameters d_ω , d_β and mass m_ω , m_β , then the relative velocity before and after collision $\mathbf{c}_{\beta\omega} = \mathbf{c}_\beta - \mathbf{c}_\omega$ and $\mathbf{c}^*_{\beta\omega} = \mathbf{c}^*_\beta - \mathbf{c}^*_\omega$, are related by

$$\mathbf{k} \cdot \mathbf{c}^*_{\beta\omega} = -e_{\omega\beta} \left(\mathbf{k} \cdot \mathbf{c}_{\beta\omega} \right) \tag{43}$$

where $e_{\omega\beta}$ is the coefficient of restitution ($e_{\omega\beta} = e_{\beta\omega}$). The mass-centre velocity $\mathbf{G}_{\omega\beta}$ of the two particles will move uniformly throughout the encounter; this constant velocity is given by,

$$\mathbf{G}_{\omega\beta} = \frac{m_\omega \mathbf{c}_\omega + m_\beta \mathbf{c}_\beta}{m_\omega + m_\beta} \tag{44}$$

consequently

$$\begin{aligned} m_\omega \left(\mathbf{c}^*_\omega - \mathbf{c}_\omega \right) &= -m_\beta \left(\mathbf{c}^*_\beta - \mathbf{c}_\beta \right) \\ &= \frac{m_\omega m_\beta}{m_\omega + m_\beta} \left(1 + e_{\omega\beta} \right) \left(\mathbf{k} \cdot \mathbf{c}_{\beta\omega} \right) \mathbf{k} \end{aligned} \tag{45}$$

For a given particle property $\psi_\omega = \psi_\omega \left(\mathbf{c}_\omega \right)$ we may use this last expression to calculate its change $\psi^*_\omega - \psi_\omega$ in a collision.

Presumed pair distribution function (Enskog's Theory):

In order to calculate the terms appearing in collisional source and collisional flux, $\boldsymbol{\chi}_{\omega\beta}$ and $\boldsymbol{\theta}_{\omega\beta}$, presumed forms of the pair distribution functions $f^{(2)}_{\omega\beta}$ are needed in order to perform the integrations (22) and (23). With the assumption of molecular chaos, which implies no correlations between neighbouring particles induced by interaction with the fluid turbulence, the pair distribution functions are written on terms of the single velocity distribution functions $f^{(1)}_\omega$ and $f^{(1)}_\beta$:

$$\begin{aligned} & f^{(2)}_{\omega\beta} \left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, \mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k} \right) = \\ & g_{\omega\beta}\left(\mathbf{r}\right) \; f^{(1)}_\omega \left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k} \right) f^{(1)}_\beta \left(\mathbf{c}_\beta, \mathbf{r} - \frac{d_\beta}{2}\mathbf{k} \right) \end{aligned} \tag{46}$$

where $g_{\omega\beta}\left(\mathbf{r}\right)$ is the radial distribution function given in the next section.

Radial distribution function

The radial distribution functions at contact $g_{\omega\beta}\left(\mathbf{r}\right)$ account for the increase of probability of collision when the system becomes dense in the frame of the Enskog's theory. They are equal to unity if the system is very dilute and they tend to infinity when the system tend to random packed particle system. The position vector $\mathbf{r}$ at contact point in collision is

$$\mathbf{r} = \frac{d_\beta \mathbf{r}_\omega + d_\omega \mathbf{r}_\beta}{2 d_{\omega\beta}} \tag{47}$$

where $d_{\omega\beta}$ is given by (17).

Jenkins and Mancini:

The radial distribution functions at contact for binary mixtures are taken from that reported by Masoori (1971), which are in best agreement with numerical simulations.

$$\begin{aligned} g_{\omega\beta} &= \frac{1}{1-\alpha_s} + \frac{3}{2}\frac{d_\omega d_\beta}{d_\omega + d_\beta}\frac{\xi_\omega}{\left(1-\alpha_s\right)^2} \\ &+ \frac{1}{2}\left(\frac{d_\omega d_\beta}{d_\omega + d_\beta}\right)^2 \frac{\xi^2_\omega}{\left(1-\alpha_s\right)^3} \end{aligned} \tag{48}$$

where $\xi_\omega = \frac{1}{3}\pi\left(\sum_\omega n_\omega d^2_\omega\right)$ and $\alpha_s = \sum_\omega \alpha_\omega$ is the total solid volume fraction.

Lathouwers and Bellan:

The radial distribution functions at contact $g_{\omega\beta}\left(\mathbf{r}\right)$ are taken from Jenkins-Mancini (1989), eq. (48), but corrected with the maximum value of solid fraction for a random packing of spheres (Campbell, 1989) to prevent overpacking:

$$g_{\omega\beta} = \frac{1}{1-\alpha_s/\alpha_m} + \frac{3}{2}\frac{d_\omega d_\beta}{d_\omega + d_\beta}\frac{\xi_\omega}{\left(1-\alpha_s/\alpha_m\right)^2} + \frac{1}{2}\left(\frac{d_\omega d_\beta}{d_\omega + d_\beta}\right)^2 \frac{\xi_\omega^2}{\left(1-\alpha_s/\alpha_m\right)^3} \qquad (49)$$

where $\alpha_m = 0.64$. One model proposed by Lun and Savage (1986) is believed to give good results for shearing of small finite systems at high concentrations:

$$g_\omega = \left(1 - \frac{\alpha_\omega}{\alpha_m}\right)^{-2.5\alpha_m} \qquad (50)$$

In order to compare this models, Fig. 1 shows the behavior of radial distribution functions in a monodisperse system

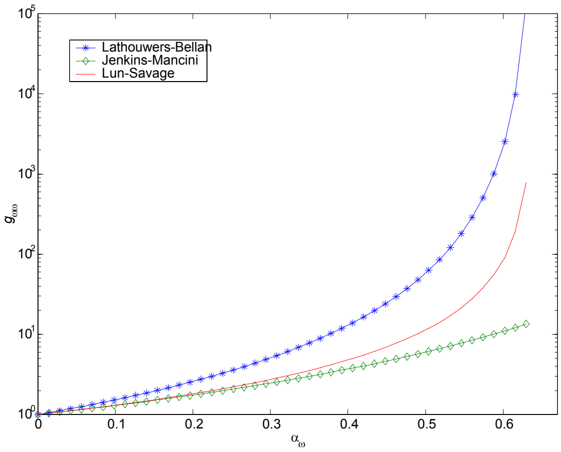

Fig. 1 Comparison of radial distribution function g_ω in a monodisperse system.

Gourdel and Simonin:

The radial distribution function $g_{\omega\beta}$ is taken equal to the limited value for dilute flows ($\alpha_s \ll 1$)

$$g_{\omega\beta} = 1 \qquad (51)$$

SINGLE PARTICLE VELOCITY DISTRIBUTION FUNCTIONS.

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Jenkins and Mancini:

The single particle distribution function in (46) is evaluated at contact point during collision by Taylor expansion:

$$f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}\right) = \left[1 + \frac{d_\omega}{2}k_i\frac{\partial}{\partial r_i} + \left(\frac{d_\omega}{2}\right)^2 \frac{k_i k_j}{2!}\frac{\partial^2}{\partial r_i \partial r_j}\right] f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r}\right) \qquad (52)$$

Chapman-Enskog's procedure is employed to derive the suitable single particle velocity distribution function. The solution for nearly elastic spheres is obtained by perturbating the uniform state of a system of elastic particles:

$$f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r}, t\right) = \left(1 + \phi_\omega\right)\ f_\omega^{(0)}\left(\mathbf{c}_\omega, \mathbf{r}, t\right) \qquad (53)$$

where $f_\omega^{(0)}$is written

$$f_\omega^{(0)} = n_\omega\left(\frac{m_\omega}{2\pi T_s}\right)^{3/2} \exp\left(-\left(\frac{m_\omega}{2T_s}\right)\left(\mathbf{c}_\omega - \mathbf{U}_s\right)^2\right) \qquad (54)$$

here $\mathbf{U}_s$ is the mixture mean velocity and T_s is the mixture temperature given by eq.(29) and eq.(33). The expansion parameter ϕ_ω is the relative change of the hydrodynamical variables over a mean free path and following Jenkins-Mancini (1989), it has the form

$$\phi_\omega = -\mathbf{A}_\omega \cdot \nabla \ln T_s - \mathbf{B}_\omega : \nabla \mathbf{U}_s + \mathbf{H}_\omega \nabla \cdot \mathbf{U}_s - n_s \mathbf{Z}_\omega \cdot \mathbf{d}_\omega + \sum_\omega \mathbf{L}_{\omega\beta}\left(1 - e_{\omega\beta}\right) \qquad (55)$$

where $\mathbf{A}_\omega$, $\mathbf{B}_\omega$, $\mathbf{H}_\omega$, $\mathbf{Z}_\omega$ and $\mathbf{L}_{\omega\beta}$ are functions of $\mathbf{u}_\omega''$. In order to obtain definite expressions for these functions, they have to be expanded in a convenient set of orthonormal functions, the Sonine polynomials (Ferziger and Kaper, 1972)

$$S_k^n\left(x\right) = \sum_{p=0}^{n} \frac{\Gamma\left(k+n+1\right)}{(n-p)!p!\Gamma\left(k+p+1\right)}\left(-x\right)^p \qquad (56)$$

where Γ denotes the gamma function. To obtain practical results these series have to be appropriately truncated. The number of terms retained in this expansions corresponds to the different Enskog approximations. Jenkins and Mancini retain only the first terms of the expansions for $\mathbf{A}_\omega$, $\mathbf{B}_\omega$, $\mathbf{H}_\omega$, $\mathbf{Z}_\omega$ and $\mathbf{L}_{\omega\beta}$. The coefficients of such expansions can be uniquely determined by imposing the conditions that n_ω, $\mathbf{U}_s$ and T_s in the Maxwellian distribution (54) be the local values of the density species ω, of the mass average velocity and of the mixture temperature. Moreover ϕ_ω must satisfy the following conditions:

$$\int f_\omega^{(0)} \phi_\omega d\mathbf{c}_\omega = 0 \qquad (57)$$

$$\sum_\omega \int f_\omega^{(0)} \phi_\omega m_\omega \mathbf{c}_\omega d\mathbf{c}_\omega = 0 \qquad (58)$$

and

$$\sum_\omega \int f_\omega^{(0)} \phi_\omega m_\omega \left(\mathbf{c}_\omega - \mathbf{U}_\omega\right)^2 d\mathbf{c}_\omega = 0 \qquad (59)$$

where $\left(\mathbf{c}_\omega - \mathbf{U}_\omega\right)^2 = \left[\mathbf{c}_\omega - \mathbf{U}_\omega\right] \cdot \left[\mathbf{c}_\omega - \mathbf{U}_\omega\right]$. Forms of such a coefficients are developed in the appendix.

Lathouwers and Bellan:

The single particle distribution function in (46) is evaluated at contact point during collision by Taylor expansion:

$$f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}\right) = \left[1 + \frac{d_\omega}{2}k_i\frac{\partial}{\partial r_i} + \left(\frac{d_\omega}{2}\right)^2 \frac{k_i k_j}{2!}\frac{\partial^2}{\partial r_i \partial r_j}\right] f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r}\right) \qquad (60)$$

the $\omega-$particle distribution is assumed to be equal to the equilibrium Maxwellian distribution

$$f_\omega^{(1)}\left(\mathbf{c}_\omega, \mathbf{r}, t\right) = f_\omega^{(0)}\left(\mathbf{c}_\omega, \mathbf{r}, t\right) = \frac{n_\omega}{\left(\frac{4}{3}\pi q_\omega^2\right)^{3/2}} \exp\left(-\frac{3\left(\mathbf{c}_\omega - \mathbf{U}_\omega\right)^2}{4q_\omega^2}\right) \qquad (61)$$

which satisfies

$$\int f_\omega^{(1)} d\mathbf{c}_\omega = n_\omega \tag{62}$$

$$\int \mathbf{c}_\omega f_\omega^{(1)} d\mathbf{c}_\omega = n_\omega \mathbf{U}_\omega \tag{63}$$

$$\int \frac{1}{2} \left[\mathbf{c}_\omega - \mathbf{U}_\omega\right] \cdot \left[\mathbf{c}_\omega - \mathbf{U}_\omega\right] f_\omega^{(1)} d\mathbf{c}_\omega = n_\omega q_\omega^2 \tag{64}$$

Gourdel and Simonin /Fede and Simonin:
The spatial dependence of the single particle distribution, with respect to the particle size, is neglected in (46),

$$f_\omega^{(1)} \left(\mathbf{c}_\omega, \mathbf{r} + \frac{d_\omega}{2}\mathbf{k}, t\right) = f_\omega^{(1)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) \tag{65}$$

Following Grad (1949), the single particle distribution function $f_\omega^{(1)}$ is provided as a series expansion of Hermite polynomials. Grad proposes to make a third-order approximation, which is a reasonable assumption if the flow is not varying too quickly.

$$f_\omega^{(1)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) = \left[1 - a_{\omega,i} \frac{\partial}{\partial c_{\omega,i}} + \frac{a_{\omega,ij}}{2!} \frac{\partial^2}{\partial c_{\omega,i}\, \partial c_{\omega,j}} - \frac{a_{\omega,ijk}}{3!} \frac{\partial^3}{\partial c_{\omega,i}\, \partial c_{\omega,j}\, \partial c_{\omega,k}}\right] f_\omega^{(0)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) \tag{66}$$

where $f_\omega^{(0)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right)$ is given by (61) . It can be shown (Jenkins and Richman, 1985) that the coefficients a_i, a_{ij}, a_{ijk} which depend on $\mathbf{r}$ and t but not on $\mathbf{c}$, are related to n^{th} order ($n \leq 3$) velocity moments (n_ω, $\mathbf{U}_\omega$, q_ω^2, $\langle \mathbf{u}'_\omega \mathbf{u}'_\omega \rangle$).

$$a_{\omega,ij} = \left\langle u'_{\omega,i} u'_{\omega,j} \right\rangle_\omega - \frac{2}{3} q_\omega^2 \delta_{ij} \tag{67}$$

and

$$a_{\omega,ijm} = \left\langle u'_{\omega,i} u'_{\omega,j} u'_{\omega,m} \right\rangle_\omega \tag{68}$$

after carried out derivatives, the general form of approximation (66) is

$$f_\omega^{(1)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) = \left[1 + \frac{a_{\omega,i}}{\left(\frac{2}{3} q_\omega^2\right)} C_i + \frac{a_{\omega,ij}}{2\left(\frac{2}{3} q_\omega^2\right)^2} C_i C_j + \frac{a_{\omega,ijk}}{9\left(\frac{2}{3} q_\omega^2\right)^3} C_i C_j C_k\right] f_\omega^{(0)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) \tag{69}$$

where

$$C_{\omega,i}(\mathbf{r}, t) = c_{\omega,i} - U_{\omega,i}(\mathbf{r}, t) \tag{70}$$

Straightforward integration shows that eq. (9) places no constraint on the series (66) , whereas for the velocity moment of order 1 we find that

$$a_{\omega,i} = 0 \tag{71}$$

Furthermore, in view of the definition of the temperature, the following restriction must be imposed

$$a_{\omega,ii} = 0 \tag{72}$$

Grad introduces a simpler model to reduce the number of unknowns from 20 to 13. The closure of 13-moment system on the third-order moment tensor is written

$$a_{\omega,ijk} = \frac{1}{5} \left(a_{\omega,imm} \delta_{jk} + a_{\omega,jmm} \delta_{ik} + a_{\omega,kmm} \delta_{ij}\right) \tag{73}$$

When formulation (69), restrictions (71) , (72) and the contracted form (73) of a_{ijk} are used, the approximate single particle velocity distribution function may be written as

$$f_\omega^{(1)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) = \left[1 + \frac{a_{\omega,ij}}{2\left(2/3\ q_\omega^2\right)^2} C_{\omega,i} C_{\omega,j} + \frac{a_{\omega,imm}}{10\left(2/3\ q_\omega^2\right)^2} \times \left(\frac{1}{2/3\ q_\omega^2} C_{\omega,j} C_{\omega,j} - 5\right) C_{\omega,i}\right] f_\omega^{(0)} \left(\mathbf{c}_\omega, \mathbf{r}, t\right) \tag{74}$$

Collisional source terms

Momentum:

Lathouwers and Bellan:
The collisional source term is obtained by analytic integration of (22) using (46), (60) and (61), assuming a small mean relative velocity between species with respect to the turbulent velocity fluctuations ("low drift regime").

$$\left|\mathbf{U}_\omega - \mathbf{U}_\beta\right|^2 \ll \left(q_\omega^2 + q_\beta^2\right) \tag{75}$$

the collision source term in the momentum equation is written,

$$\boldsymbol{\chi}_{\omega\beta} \left(m_\omega \mathbf{U}_\omega\right) = -\frac{m_\omega\ m_\beta}{m_\omega + m_\beta} \frac{\left(1 + e_{\omega\beta}\right)}{6} \frac{n_\omega}{\tau_{\omega\beta}^c} \times \left[\left[\mathbf{U}_\omega - \mathbf{U}_\beta\right] - \frac{d_{\omega\beta}}{8} \sqrt{\frac{\pi}{3}\left(q_\omega^2 + q_\beta^2\right)}\ \nabla \ln \frac{n_\omega}{n_\beta}\right] \tag{76}$$

with the inter-particle collision time $\tau_{\omega\beta}^c$ given by

$$\tau_{\omega\beta}^c = \left[4 d_{\omega\beta}^2 g_{\omega\beta} n_\beta \sqrt{\frac{\pi}{3}\left(q_\omega^2 + q_\beta^2\right)}\right]^{-1} \tag{77}$$

Gourdel and Simonin / Fede and Simonin:
The collisional source term is obtained by analytic integration of (22) using (46), (65) and (66) for the computation of the $\boldsymbol{\chi}_{\omega\beta}$ and accounting for the small mean relative velocity between species.

The collisional source term in the momentum equation is

$$\boldsymbol{\chi}_{\omega\beta} \left(m_\omega \mathbf{U}_\omega\right) = -\frac{m_\omega m_\beta}{m_\omega + m_\beta} \frac{\left(1 + e_{\omega\beta}\right)}{2} \times \frac{n_\omega}{\tau_{\omega\beta}^c} \left[\mathbf{U}_\omega - \mathbf{U}_\beta\right] H_1(z) \tag{78}$$

with the inter-particle collision time $\tau_{\omega\beta}^c$ given by

$$\tau_{\omega\beta}^c = \left[4 d_{\omega\beta}^2 g_{\omega\beta} n_\beta \sqrt{\frac{\pi}{3}\left(q_\omega^2 + q_\beta^2\right)} H_0(z)\right]^{-1} \tag{79}$$

here H_0 and H_1 are given as function of z which characterize the competition between the mean slip and the fluctuating relative velocity in the collision mechanism,

$$z = \frac{3\left(\mathbf{U}_\omega - \mathbf{U}_\beta\right)^2}{4\left(q_\omega^2 + q_\beta^2\right)} \tag{80}$$

H_0 is written as

$$H_0(z) = \left[\frac{\exp(-z)}{2} + \frac{\sqrt{\pi z}}{2} \operatorname{erf}\left(\sqrt{z}\right)\left(1 + \frac{1}{2z}\right)\right]^{-1} \tag{81}$$

which can be approximated by

$$H_0^*(z) = \left[\sqrt{1 + \pi z / 4}\right]^{-1} \tag{82}$$

the behavior of this two last expressions are in good agreement (Fig.2).

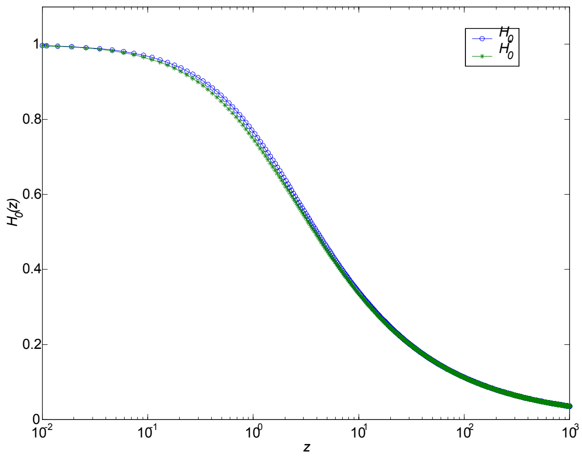

Fig. 2 Curves for $H_0(z)$ from equations (81) and (82).

complementary definition is

$$H_1(z) = \frac{\frac{\exp(-z)}{\sqrt{\pi z}}\left(1+\frac{1}{2z}\right)+\operatorname{erf}\left(\sqrt{z}\right)\left(1+\frac{1}{z}-\frac{1}{4z^2}\right)}{\frac{\exp(-z)}{\sqrt{\pi z}}+\operatorname{erf}\left(\sqrt{z}\right)\left(1+\frac{1}{2z}\right)} \tag{83}$$

The corresponding H_1 curve is on Fig. 3

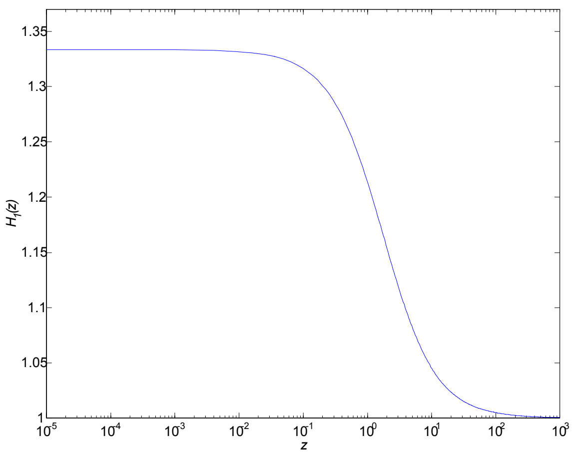

Fig. 3 Curve for $H_1(z)$.

Kinetic Energy:

Jenkins and Mancini:

The source term in the energy equation for total rate of energy dissipation per unit volume is

$$\chi\left(\frac{m_\omega u_\omega^{"\,2}}{2}\right) = g_{\omega\beta}^2 d_{\omega\beta}^2 n_\omega n_\beta \frac{m_\omega}{m_\omega+m_\beta} \tag{84}$$
$$\times\left(1-e_{\omega\beta}\right)\left(\frac{2\pi\left(m_\omega+m_\beta\right)T_s^3}{m_\omega m_\beta}\right)^{1/2}$$

T_s is the mixture temperature given by equation (33).

Lathouwers and Bellan:

The collisional source term in the kinetic energy equation is resulting from the effects of energy redistribution among particle species and of the dissipation due to inelastic collisions,

$$\chi_{\omega\beta}\left(m_\omega q_\omega^2\right) = -\frac{m_\omega\ m_\beta}{\left(m_\omega+m_\beta\right)^2}\frac{n_\omega}{\tau_{\omega\beta}^c}\frac{\left(1+e_{\omega\beta}\right)}{3}$$
$$\times\left[\frac{\left(1-e_{\omega\beta}\right)}{2}m_\beta\left(q_\omega^2+q_\beta^2\right)+\left(m_\omega q_\omega^2-m_\beta q_\beta^2\right)\right] \tag{85}$$

for particles of same species, the collision source term leads,

$$\boldsymbol{\chi}_{\omega\omega}\left(m_\omega q_\omega^2\right) = -\frac{1}{12}m_\omega\frac{n_\omega}{\tau_{\omega\omega}^c}\left(1-e_{\omega\omega}^2\right)q_\omega^2 \tag{86}$$

and

$$\tau_{\omega\omega}^c = \left[4d_\omega^2 g_{\omega\omega} n_\omega\sqrt{\frac{2\pi}{3}q_\omega^2}\right]^{-1} \tag{87}$$

Gourdel and Simonin / Fede and Simonin:

the collisional source term in the kinetic energy equation for unlike particle species is

$$\chi_{\omega\beta}\left(m_\omega q_\omega^2\right) = \frac{m_\omega m_\beta}{\left(m_\omega+m_\beta\right)^2}\frac{1+e_{\omega\beta}}{2}\frac{n_\omega}{\tau_{\omega\beta}^c}\left[m_\beta\left(1+e_{\omega\beta}\right)\right. \tag{88}$$
$$\times\left[\mathbf{U}_\omega-\mathbf{U}_\beta\right]^2 H_1(z) - \frac{16}{3}\left(\frac{m_\beta}{2}\left(1-e_{\omega\beta}\right)\left[q_\omega^2+q_\beta^2\right]\right.$$
$$\left.\left.+\left[m_\omega q_\omega^2-m_\beta q_\beta^2\right]\right)\right]$$

The collisional source term in the kinetic energy equation for the same particle species is written

$$\chi_{\omega\omega}\left(m_\omega q_\omega^2\right) = -\frac{2}{3}m_\omega\frac{n_\omega}{\tau_{\omega\omega}^c}\left(1-e_{\omega\omega}^2\right)q_\omega^2 \tag{89}$$

and

$$\tau_{\omega\omega}^c = \left[4d_\omega^2 g_{\omega\omega} n_\omega\sqrt{\frac{2\pi}{3}q_\omega^2}\right]^{-1} \tag{90}$$

Collisional flux terms

Momentum:

Jenkins and Mancini:

The collisional flux term of linear momentum $\boldsymbol{\theta}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right)$ in (40) is given by

$$\boldsymbol{\theta}_{\omega\beta}\left(m_\omega\mathbf{U}_\omega\right) = \frac{1}{12}\pi g_{\omega\beta}d_{\omega\beta}^3 n_\omega n_\beta T_s\mathbf{I} - \frac{1}{15}\pi g_{\omega\beta}d_{\omega\beta}^3 n_\omega n_\beta T_s \tag{91}$$
$$\times\left[b_{\omega o}\left(\frac{m_\beta}{m_\omega+m_\beta}\right)+\left(2\pi T_s\frac{m_\omega m_\beta}{m_\omega+m_\beta}\right)^{1/2}\frac{d_{\omega\beta}}{2}\right]$$
$$\times\left[\frac{1}{2}\nabla\mathbf{U}_s+\frac{1}{2}\left(\nabla\mathbf{U}_s\right)^T-\frac{1}{3}\nabla\cdot\mathbf{U}_s\mathbf{I}\right]+O(\epsilon)$$

where the coefficient $b_{\omega o}$ is, for $\omega \neq \beta$, given by

$$b_{\omega o} = 5\left(b_\omega\left[n_\omega + \frac{2}{5}K_{\omega\omega} + \frac{4}{5}K_{\omega\beta}\left(\frac{m_\beta}{m_\omega + m_\beta}\right)\right] + \frac{32}{3}\left[\frac{\pi}{2}\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^3}\right]^{1/2} \times \frac{d_{\omega\beta}^2}{4}\left[n_\beta + \frac{2}{5}K_{\beta\beta} + \frac{4}{5}K_{\omega\beta}\left(\frac{m_\beta}{m_\omega + m_\beta}\right)\right]\right) \left(g_{\omega\beta}n_\omega n_\beta T_s^{1/2}\left[b_\omega b_\beta - \frac{32}{9}d_{\omega\beta}^4\pi \times \left(\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^3}\right)\right]\right)^{-1} \quad (92)$$

where coefficient b_ω is

$$b_\omega = 10d_{\omega\beta}^2\left(\frac{\pi}{2}\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^3}\right)^{1/2}\left(\frac{2}{3} + \frac{2}{5}\frac{m_\omega}{m_\beta}\right) + 2\frac{n_\beta g_{\beta\beta}}{n_\omega g_{\omega\beta}}d_{\beta\beta}^2\left(\frac{\pi}{m_\beta}\right)^{1/2} \quad (93)$$

and $K_{\omega\beta}$ is

$$K_{\omega\beta} = \frac{1}{12}\pi n_\omega n_\beta d_{\omega\beta}^3 g_{\omega\beta} \quad (94)$$

Lathouwers and Bellan:

The collisional flux term of linear momentum is obtained by analytic integration of (23) using (46), (60) and (61)

$$\boldsymbol{\theta}_{\omega\beta}(m_\omega \mathbf{U}_\omega) = P_{\omega\beta}\mathbf{I} - \mu_{\omega\beta}^\omega\left[\nabla\mathbf{U}_\omega + \nabla\mathbf{U}_\omega^T - (\nabla\cdot\mathbf{U}_\omega)\mathbf{I}\right] - \mu_{\omega\beta}^\beta\left[\nabla\mathbf{U}_\beta + \nabla\mathbf{U}_\beta^T - (\nabla\cdot\mathbf{U}_\beta)\mathbf{I}\right] \quad (95)$$

here the pressure is given by

$$P_{\omega\beta} = \frac{1}{36}\pi g_{\omega\beta}d_{\omega\beta}^3 n_\omega n_\beta\frac{m_\omega m_\beta}{m_\omega + m_\beta} \times (1 + e_{\omega\beta})\left(q_\omega^2 + q_\beta^2\right) \quad (96)$$

complementary definitions are

$$\mu_{\omega\beta}^\omega = \frac{d_{\omega\beta}^2\pi n_\omega}{240}\frac{m_\omega m_\beta^2}{(m_\omega + m_\beta)^2} \times \frac{(1 + e_{\omega\beta})}{\tau_{\omega\beta}^c}\frac{\left(q_\omega^2 + q_\beta^2\right)}{q_\omega^2} \quad (97)$$

and

$$\mu_{\omega\beta}^\beta = \frac{d_{\omega\beta}^2\pi n_\omega}{240}\frac{m_\beta m_\omega^2}{(m_\omega + m_\beta)^2} \times \frac{(1 + e_{\omega\beta})}{\tau_{\omega\beta}^c}\frac{\left(q_\omega^2 + q_\beta^2\right)}{q_\beta^2} \quad (98)$$

Kinetic Energy:

Jenkins-Mancini:

The collisional heat flux is

$$\boldsymbol{\theta}_{\omega\beta}\left(m_\omega q_\omega^2\right) = \left(\frac{T_s}{m_\omega}\right)^{1/2} d_{\omega\beta}^3 g_{\omega\beta}\pi n_\omega n_\beta\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^2} \left[a_{\omega 1} - \frac{d_{\omega\beta}}{3}\left(\pi\left(\frac{m_\beta}{m_\omega + m_\beta}\right)\right)^{-1/2}\right]\nabla T_s - \left(\frac{T_s^3}{8}\right)^{1/2}\frac{1}{3}d_{\omega\beta}^3 g_{\omega\beta}\pi n_\omega n_\beta\left[m_\omega^{-1/2} \times (nt_{\omega o}\mathbf{d}_\omega + a_{\omega o}\nabla\ln T_s)\left(\frac{m_\omega - m_\beta}{m_\omega + m_\beta}\right) + m_\beta^{-1/2}(nt_{\beta o}\mathbf{d}_\beta + a_{\beta o}\nabla\ln T_s)\right] + O\left(\epsilon^{3/2}\right) \quad (99)$$

where the coefficient $a_{\omega 1}$ is, for $\omega \neq \beta$, given by

$$a_{\omega 1} = 15\left(a_\omega m_\beta^{1/2}\left[n_\omega + \frac{3}{5}K_{\omega\omega} + \frac{12}{5}K_{\omega\beta}\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^2}\right] + 54\left[\pi m_\omega/2(m_\omega + m_\beta)\right]^{1/2}\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^2}\frac{d_{\omega\beta}^2}{4} \times \left[n_\beta + \frac{3}{5}K_{\beta\beta} + \frac{12}{5}K_{\omega\beta}\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^2}\right]\right)\left(2\sqrt{2}g_{\omega\beta} \times n_\omega n_\beta(m_\omega m_\beta)^{1/2}\left[\frac{729}{8}d_{\omega\beta}^4\pi\frac{m_\omega^2 m_\beta^2}{(m_\omega + m_\beta)^5} - a_\omega a_\beta\right]\right)^{-1} \quad (100)$$

the definition for a_ω is

$$a_\omega = 10d_{\omega\beta}^2\left(\frac{\pi m_\omega}{m_\beta(m_\omega + m_\beta)}\right)^{1/2}\left[\frac{3}{2}\left(\frac{m_\beta}{m_\omega + m_\beta}\right)^2 + \frac{13}{20}\left(\frac{m_\omega}{m_\omega + m_\beta}\right)^2 + \frac{4}{5}\left(\frac{m_\omega m_\beta}{(m_\omega + m_\beta)^2}\right)\right] + \frac{n_\beta g_{\beta\beta}}{n_\omega g_{\omega\beta}}2d_{\beta\beta}^2\left(\frac{\pi}{m_\beta}\right)^{1/2} \quad (101)$$

and complementary expressions which are included in (99) are

$$t_{\omega o} = \left(\frac{3}{32}d_{\omega\beta}^2\rho n_\omega\right)\left(\frac{(m_\omega + m_\beta)m_\beta}{\pi}\right)^{1/2} \quad (102)$$

$$a_{\omega o} = \left(\frac{1}{2}\rho\right)\left((m_\omega + m_\beta)m_\beta\right)^{1/2} n_\beta\left(\left(\frac{m_\beta}{m_\omega + m_\beta}\right)^{3/2} a_{\omega 1} - \left(\frac{m_\omega}{m_\omega + m_\beta}\right)^{3/2} a_{\beta 1}\right) \quad (103)$$

Lathouwers and Bellan:

the collisional heat flux of particle kinetic energy is

$$\boldsymbol{\theta}_{\omega\beta}\left(m_\omega q_\omega^2\right) = \frac{2}{3}\left(K_{\omega\beta}^\omega\nabla q_\omega^2 + K_{\omega\beta}^\beta\nabla q_\omega^2\right) \quad (104)$$

where

$$K_{\omega\beta}^\omega = \frac{1}{96}d_{\omega\beta}^2 n_\omega\frac{m_\omega m_\beta^2}{(m_\omega + m_\beta)^2}\frac{(1 + e_{\omega\beta})}{\tau_{\omega\beta}^c}\left(\frac{q_\beta^2}{q_\omega^2}\right) \quad (105)$$

$$K_{\omega\beta}^\beta = \frac{1}{96}d_{\omega\beta}^2 n_\omega\frac{m_\omega^2 m_\beta}{(m_\omega + m_\beta)^2}m_\omega\frac{(1 + e_{\omega\beta})}{\tau_{\omega\beta}^c}\left(\frac{q_\omega^2}{q_\beta^2}\right) \quad (106)$$

Gourdel and Simonin/Fede and Simonin:

The spatial dependence of the single particle distribution, with respect to the particle size, neglected in (65) leads to ignore the collisional flux term in momentum and fluctuating kinetic energy balance.

Kinetic flux terms

Jenkins and Mancini:

The kinetic flux contribution to the effective stress tensor is

$$n_\omega m_\omega \left\langle \mathbf{u}^{"}_\omega \mathbf{u}^{"}_\omega \right\rangle_\omega = n_\omega T_s \mathbf{I} - n_\omega T_s b_{\omega o} \quad (107)$$

$$\left(\frac{1}{2}\nabla \mathbf{U}_s + \frac{1}{2}\left(\nabla \mathbf{U}_s\right)^T - \frac{1}{3}\nabla \cdot \mathbf{U}_s \mathbf{I}\right) + O\left(\epsilon\right)$$

with $b_{\omega o}$ given by eq. (92).

The kinetic flux in the kinetic energy equation is

$$n_\omega m_\omega \left\langle \left[\mathbf{u}^{"}_\omega \cdot \mathbf{u}^{"}_\omega\right] \mathbf{u}^{"}_\omega \right\rangle_\omega = \frac{5}{4} n_\omega a_{\omega 1} \left(2T_s/m_\omega\right)^{1/2} \nabla T_s \quad (108)$$

$$+\frac{5}{2} n_\omega \left(T_s^3/2m_\omega\right)^{1/2} \left(nt_{\omega o}\mathbf{d}_\omega + a_{\omega o}\nabla \ln T_s\right) + O\left(\epsilon^{3/2}\right)$$

where $a_{\omega o}$and $a_{\omega 1}$ are given by (103) and (100), respectively.

Lathouwers and Bellan:

The chosen form of particle distribution function at equilibrium leads to following kinetic transport of momentum:

$$n_\omega \left\langle u'_{\omega,i} u'_{\omega,j} \right\rangle_\omega = \frac{2}{3} n_\omega q_\omega^2 \mathbf{I} \quad (109)$$

and the corresponding kinetic flux in energy equation is

$$n_\omega \left\langle \left[\mathbf{u}'_\omega \cdot \mathbf{u}'_\omega\right] u'_{\omega,i} \right\rangle_\omega = 0 \quad (110)$$

such assumption is generally valuable only in dense flows ($\alpha_\omega \geq 0.1$) corresponding to the so-called collisional regime.

Gourdel and Simonin:

The kinetic flux terms of momentum and energy in the model are not taken in to account.

Closure

models for fluid-particle interaction terms

Jenkins and Mancini:

They consider no contribution of the fluid force on the particle, consequently

$$\frac{\mathbf{F}_\omega}{m_\omega} = \mathbf{g} \quad (111)$$

Lathouwers and Bellan:

The force acting on a single particle is written

$$\frac{\mathbf{F}_\omega}{m_\omega} = \mathbf{g} - \frac{1}{\rho_\omega}\nabla \overline{p}_g - \frac{\mathbf{u}_\omega - \mathbf{u}_g}{\tau^F_{g\omega}} \quad (112)$$

whith the particle relaxation time $\tau^F_{g\omega}$,

$$\frac{1}{\tau^F_{g\omega}} = \frac{3}{4}\frac{\rho_g}{\rho_\omega d_\omega} C_{d_\omega}\left(\mathrm{Re}_\omega\right)\left|\mathbf{u}_\omega - \mathbf{u}_g\right| \quad (113)$$

The drag coefficient C_{d_ω} is based on two separate empirical correlations valid for dilute (Wen et Yu, 1965) and dense (Ergun's relation) particulate flows, respectively,

$$C_{d_\omega}\left(\mathrm{Re}_\omega\right) = W C_d^{wy}\left(\mathrm{Re}_\omega\right) + \left(1-W\right) C_d^{Eg}\left(\mathrm{Re}_\omega\right) \quad (114)$$

where W is a switch function described on (118). According to Wen and Yu (1965), C_d^{wy} is

$$C_d^{wy}\left(\mathrm{Re}_\omega\right) = \begin{cases} \frac{24}{\mathrm{Re}_\omega}\alpha_g^{-1.7}\left(1+0.15\,\mathrm{Re}_\omega^{0.687}\right) & \mathrm{Re} < 1000 \\ 0.44\alpha_g^{-1.7} & \text{for} \quad \mathrm{Re} \geq 1000 \end{cases} \quad (115)$$

the particle Reynolds number is

$$\mathrm{Re}_\omega = \frac{\alpha_\omega \left|\mathbf{u}_\omega - \mathbf{u}_g\right| d_\omega}{\nu_g} \quad (116)$$

The Ergun's relation is written

$$C_d^{Eg}\left(\mathrm{Re}_\omega\right) = \left(1-\alpha_g\right)\frac{200}{\mathrm{Re}_\omega} + \frac{7}{3} \quad (117)$$

The switch function W is choosen arbitrarely to insure a rapid continuous transition from (115) to (117)when the gas volumetric fraction value α_g is below 0.8,

$$W = \arctan\left(150\left(\alpha_g - 0.8\right)\right)/\pi + 1/2 \quad (118)$$

The behavior for drag coefficient on Ergun, Wen-Yu and Lathouwers-Bellan expressions are showed in Fig. 4 for differents Reynolds numbers.

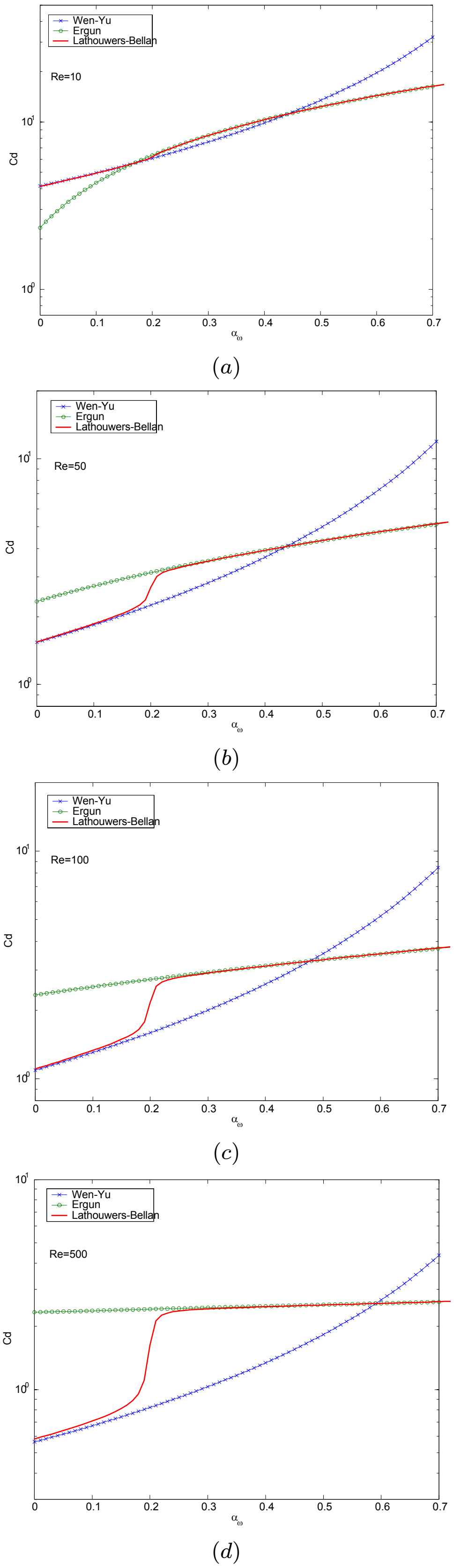

Fig.4 Cd from Ergun, Wen-Yu and Lathouwers-Bellan
(a) Re=10, (b) Re=50, (c) Re=100, (d) Re=500

The averaged fluid-particle interaction terms in the particulate momentum and kinetic energy equations, (25) and (27) respectively, are derived by averaging from the force exerted on a single particle.

The mean momentum interphase transfer rate is written,

$$\left\langle \frac{\mathbf{F}_\omega}{m_\omega} \right\rangle = \mathbf{g} - \frac{1}{\rho_\omega}\nabla \overline{p}_g - \frac{1}{\langle \tau^F_{g\omega} \rangle} (\mathbf{U}_\omega - \mathbf{U}_g) \tag{119}$$

where

$$\frac{1}{\langle \tau^F_{g\omega} \rangle} = \frac{3}{4}\frac{\rho_g}{\rho_\omega d_\omega} C_{d\omega} (\langle \mathrm{Re}_\omega \rangle) |\mathbf{U}_\omega - \mathbf{U}_g| \tag{120}$$

$$\langle \mathrm{Re}_\omega \rangle = \frac{\alpha_\omega |\mathbf{U}_\omega - \mathbf{U}_g| d_\omega}{\nu_g} \tag{121}$$

The kinetic energy equation fluid-particle interaction term is assumed to be negligeable for heavy particles, then

$$\left\langle \frac{\mathbf{F}_\omega}{m_\omega} \cdot \mathbf{u}'_\omega \right\rangle_\omega \approx 0 \tag{122}$$

Gourdel and Simonin:

The external force acting on a single particle is written,

$$\frac{\mathbf{F}_\omega}{m_\omega} = \mathbf{g} - \frac{1}{\rho_\omega}\nabla \overline{p}_g - \frac{\mathbf{u}_\omega - \mathbf{u}_g}{\tau^F_{g\omega}} \tag{123}$$

with the particle relaxation time $\tau^F_{g\omega}$,

$$\frac{1}{\tau^F_{g\omega}} = \frac{3}{4}\frac{\rho_g}{\rho_\omega d_\omega} C_{d_\omega} (\mathrm{Re}_\omega) |\mathbf{u}_\omega - \mathbf{u}_g| \tag{124}$$

The drag coefficient C_{d_ω} is also based on the two separate empirical correlations valid for dilute (Wen et Yu, 1965) and dense (Ergun's relation) particulate flows, respectively, but with a different continuous transition between both correlations occuring at α_g value smaller ($\alpha_g < 0.7$) than the Lathouwers and Bellan's proposition ($\alpha_g \approx 0.8$),

$$C_{d\omega}(\mathrm{Re}_\omega) = \begin{cases} C^{wy}_{d\omega}(\mathrm{Re}_\omega) & \alpha_g \geq 0.7 \\ \min\left(C^{wy}_{d\omega}(\mathrm{Re}_\omega),\ C^{Eg}_{d\omega}(\mathrm{Re}_\omega)\right) & \alpha_g < 0.7 \end{cases} \tag{125}$$

The mean momentum interphase transfer rate is derived by averaging from (123) as

$$\left\langle \frac{\mathbf{F}_\omega}{m_\omega} \right\rangle = \mathbf{g} - \frac{1}{\rho_\omega}\nabla \overline{p}_g - \frac{1}{\langle \tau^F_{g\omega} \rangle}\mathbf{V}_{r\omega} \tag{126}$$

where $\mathbf{V}_{r\omega} = \langle \mathbf{u}_\omega - \mathbf{u}_g \rangle$, the mean relative velocity, is written,

$$\mathbf{V}_{r\omega} = \mathbf{U}_\omega - \mathbf{U}_g - \mathbf{V}_{d\omega} \tag{127}$$

with the fluid-particle turbulent drift velocity $\mathbf{V}_{d\omega}$ accounting for the correlation between the gas turbulent velocity and the instantaneous particle distribution,

$$\mathbf{V}_{d\omega} = \langle \mathbf{u}'_g \rangle_\omega \tag{128}$$

the drift velocity accounts for the turbulent dispersion induced by the particle transport by gas eddies and is generally negligible in dense fluidized beds. Following Simonin et al. (1991), the non linear dependence of the particle relaxation time on the instantaneous relative velocity is modelled as

$$\frac{1}{\langle \tau^F_{g\omega} \rangle} = \frac{3}{4}\frac{\rho_g}{\rho_\omega d_\omega} C_{d\omega} (\langle \mathrm{Re}_\omega \rangle) \langle |\mathbf{u}_\omega - \mathbf{u}_g| \rangle \tag{129}$$

the averaged Reynolds number is

$$\langle \mathrm{Re}_\omega \rangle = \frac{\alpha_\omega \langle |\mathbf{u}_\omega - \mathbf{u}_g| \rangle d_\omega}{\nu_g} \quad (130)$$

and

$$\langle |\mathbf{u}_\omega - \mathbf{u}_g| \rangle = \sqrt{V_{r\omega,i} V_{r\omega,i} + \left\langle v'_{r\omega,i} v'_{r\omega,i} \right\rangle_\omega} \quad (131)$$

The kinetic energy equation fluid-particle interaction term is written,

$$\left\langle \frac{\mathbf{F}_\omega \cdot \mathbf{u}'_\omega}{m_\omega} \right\rangle = -\frac{2q_\omega^2 - q_{g\omega}}{\langle \tau_{g\omega}^F \rangle} \quad (132)$$

where the covariance fluid-particle is

$$q_{g\omega} = \langle \mathbf{u}'_g \cdot \mathbf{u}'_\omega \rangle_\omega \quad (133)$$

generally negligible in dense fluidized beds.

The fluid-particle interaction term in the kinetic energy equation reduces to a dissipation effect. Its influence has to be compared with the dissipation induced by inelastic collisions and becomes negligeable when $n_\omega / \langle \tau_{g\omega}^F \rangle << \sum (1 - e_{\omega\beta}^2) n_\beta / \tau_{\omega\beta}^c$.

Concluding Remarks

Expressions have been given for the modeling of turbulent non-reacting gas-solid flows by classical transport equations, continuity and momentum equations which are closed for the interfacial momentum transfer, the stress tensor in the particle phase, the drift velocity, the fluid-particle velocity correlation tensor and the second-order velocity moment in both phases. The models were only possible with simplifying asuptions. The collision model is based on binary encounters between particles in translational motion. In contrast, the bed material is a polydispersed suspension of rigid, nonspherical, rotating particles, where the anisotropy level can be high. Some specific problems are the value of the constants included in the equations, the treatment of the wall region and the form of the coupling term. For the fluid-particle moments a general formulation is possible but two-way coupling is omited. Algebraic models can be derived for homogeneous isotropic turbulence, asymptotic cases. The models formulated need to be solved by numerical methods and further validated against experiments to see to what extent they capture the essential physical mechanisms of turbulent nonreacting gas-particle flows applied to fluidization.

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