Holloway, Yin, and Sundaresan drag relation implementation in MFIX:

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Drag formulation and implementation:

<u>*Drag formulation:*</u>

The Holloway, Yin and Sundaresan (HYS)[1] drag relation is an extension to an earlier drag relation proposed by Yin and Sundaresan (YS)[2, 3] for low-Reynolds number polydisperse suspensions with particle-particle relative motion (in the local average sense). The HYS extension accounts for the effect of finite Reynolds number on the fluid-particle drag experienced by particles in polydisperse suspensions using the inertial correction originally proposed by Beetstra *et al*. [4] for monodisperse fixed beds. Below we briefly present the form of the drag relation, and discuss its implementation in MFIX.

The fluid-particle drag in a polydisperse suspension in the high Stokes number limit is given as follows according to YS [2, 3]:

$$f_{Di} = -\beta_{ii}\Delta U_i - \sum_{i \neq j} \beta_{ij}\Delta U_j \tag{1}$$

where f_{Di} is the fluid-particle drag *per unit volume suspension* on the *i*th particle type in a bidisperse suspension, β_{ij} is the dimensional friction coefficient of the *i*th particle *per unit volume suspension* due to the relative motion of a particle of type *j* (in the local average sense), and ΔU_i and ΔU_j is the relative velocity of particles of type *i* and *j* relative to the fluid.

When $\Delta U_i = \Delta U_j$, the fluid-particle drag relation given in eq. (1) must reduce to a fixed bed drag relation. To ensure that such a condition is satisfied a fixed bed drag coefficient β_i is introduced into the fluid-particle drag relation given in eq. (1) as follows

$$f_{Di} = -\left(\beta_i - \sum_{i \neq j} \beta_{ij}\right)\Delta U_i - \sum_{i \neq j} \beta_{ij}\Delta U_j \tag{2}$$

where β_i is the fixed bed friction coefficient given by

$$\beta_i = \frac{18(1-\phi)\phi_i \mu_f}{d_i^2} F^*_{Di-fixed}. \tag{3}$$

In eq. (3), ϕ represents the total particle volume fraction, ϕ_i is the volume fraction of the ith particle species, μ_f is the fluid viscosity, d_i is the diameter of the *i*th particle species, and $F^*_{Di-fixed}$ is the dimensionless fluid-particle drag on a particle of type *i* in a polydisperse fixed bed ($F^{*}_{Di-fixed}$ is made dimensionless by dividing by the Stokes drag, namely $3\pi d_i \mu_f (1-\phi)\Delta U$).

The fluid-particle drag experienced by a particle of type *i* in a polydisperse fixed bed has been shown by YS[3] to be related to the fluid-particle drag experienced by a particle in a monodisperse fixed bed as follows

$$F^{*}_{Di-fixed} = \frac{1}{1-\phi} + \left(F^{*}_{D-fixed} - \frac{1}{1-\phi} \right)\left(a y_i + (1-a) y_i^2 \right) \tag{4}$$

where $F^{*}_{D-fixed}$ is the dimensionless fluid-particle drag experienced by a particle in a monodisperse fixed bed as given by van der Hoef *et al*. [5] in the following expression

$$F_{D-fixed} = \frac{10\phi}{(1-\phi)^2} + (1-\phi)^2\left(1+1.5\sqrt{\phi}\right). \tag{5}$$

In eq. (4), *a* represents a cubic polynomial of volume fraction given as

$$a = 1 - 2.66\phi + 9.096\phi^2 - 11.338\phi^3, \tag{6}$$

and y_i is the ratio of the *i*th particle diameter to the Sauter mean diameter. The Sauter mean diameter can be defined for an *n*-component mixture as

$$\langle d \rangle = \frac{\sum_i n_i d_i^3}{\sum_i n_i d_i^2} \tag{7}$$

where n_i is the number density of a particle of type *i*.

The off-diagonal friction coefficient β_{ij} was found by YS [3] to be a function of the harmonic mean of β_i / ϕ_i and β_j / ϕ_j as follows

$$\beta_{ij} = -2\alpha_{ij} \frac{\phi_i \phi_j}{\dfrac{\phi_i}{\beta_i} + \dfrac{\phi_j}{\beta_j}} \tag{8}$$

where

$$\alpha_{ij} = 1.313 \log_{10}\left(\frac{\min(d_i, d_j)}{\lambda} \right) - 1.249. \tag{9}$$

In eq. (11) λ represents the lubrication cutoff. The variable λ can be thought of as the point where lubrication forces level off and remain constant. This term has been left as an adjustable parameter in MFIX. If a value for λ is not specified in the mfix.dat file, a default value of $1\,\mu m$ is specified (roughly the mean free path of a gas) within the drag_gs subroutine located in the drag_gs.f file.

It was recently shown by HYS that the fluid-particle drag relation given by eqs. (1) – (9) can be extended to account for moderate fluid inertia by using an inertial correction proposed by Beetstra *et. al.* [4] for monodisperse fixed beds as follows

$$F^{*}_{D-fixed} = \left(\frac{10\phi}{(1-\phi)^2} + (1-\phi)^2 \left(1+1.5\sqrt{\phi}\right) \right)(1+\chi_{BVK}) \tag{10}$$

where

$$\chi_{BVK} = \frac{0.413\,\mathrm{Re}_{mix}}{240\phi + 24(1-\phi)^4(1+1.5\sqrt{\phi})} \frac{(1-\phi)^{-1} + 3\phi(1-\phi) + 8.4\,\mathrm{Re}_{mix}^{\ -0.343}}{1+10^{3\phi}\,\mathrm{Re}_{mix}^{\ \frac{-(1+4\phi)}{2}}}, \tag{11}$$

and

$$\mathrm{Re}_{mix} = \frac{\Delta U_{mix}(1-\phi)\langle d \rangle}{\nu} \qquad \Delta U_{mix} = \frac{\sum_i \phi_i \Delta U_i}{\sum_i \phi_i}. \tag{12}$$

It should be noted that although the form of the inertial correction is identical to that proposed by Beetstra *et al*.[4] the definition of Re_{mix} differs from the original formulation.

Eqs. (1) – (4) and (6) – (12) represents the fluid-particle drag relation given by HYS, which was recently coded into MFIX.

Drag implementation in MFIX:

The first term in eq. (2) of the HYS drag relation was implemented in the drag_gs subroutine in MFIX, located in drag_gs.f. The second term in eq. (2) was added as a source term to the momentum equations in the source_u_s, source_v_s, source_w_s, source_u_g, source_v_g, and source_w_g subroutines located in the source_u_s.f, source_v_s.f, source_w_s.f, source_u_g.f, source_v_g.f, and source_w_g.f files, respectively. This fluid-particle drag relation has been tested for highly polydisperse systems, as well as monodisperse systems, and yielded good results. This fluid-particle drag relation can also be used in any kinetic theory framework that is currently available in MFIX. However, it should be noted that this fluid-particle drag relation has not been appropriately modified for the coupled discrete element/continuum solver that is available in MFIX.

References:

1. Holloway, W., Yin, X., & Sundaresan, S., Fluid-particle drag in inertial polydisperse gas-solid suspensions. **2009,** (manuscript under preparation).
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3. Yin, X., Sundaresan, S., Fluid-particle drag in low-Reynolds-number polydisperse gas-solid suspensions. *AIChE* **2009,** (in press).
4. Beetstra, R., Van Der Hoef, M.A., & Kuipers, J.A.M. , Drag Force of Intermediate Reynolds Number Flow Past Mono- and Bidisperse Arrays of Spheres. *AIChE* **2007,** 53, 489-501.
5. van der Hoef, M. A., Beetstra, R., Kuipers, J. A. M., Lattice-Boltzmann simulations of low-Reynolds-number flow past mono- and bidisperse arrays of spheres: results for permeability and drag force. *J. Fluid. Mech.* **2005,** 528, 233-254.