Summary of MFIX Equations

Refer to this document as:
S. Benyahia, M. Syamlal, T.J. O'Brien, "Summary of MFIX Equations 2012-1", From URL https://mfix.netl.doe.gov/documentation/MFIXEquations2012-1.pdf , January 2012.

Modifications to the previous version
https://mfix.netl.doe.gov/documentation/MFIXEquations2005-4-4.pdf

- Added note stating that all transport equations are solved in non-conservative form.

Table of Contents

The purpose of this document is to summarize the current set of equations in MFIX. This document will be updated when the equations in MFIX are revised or errors in this document needs to be fixed. The equations are listed here without any explanation, to expedite the publication of this document. Some details about the equations may be found in the two previous MFIX documents [1, 2]; be aware that some of the equations in those documents have been revised. Refer to the readme file for the keywords (to be used to set up an MFIX simulation) for selecting the different equation choices presented here.

Please note that all transport equations in MFIX are solved in non-conservative form by subtracting the continuity equation from their conservative form.

A. Governing equations

Einstein summation convention implied only on subscripts *i* and *j*.

Continuity equations for solids phases m = 1, M:

$$\frac{\partial}{\partial t}\left(\varepsilon_m \rho_m\right) + \frac{\partial}{\partial x_i}\left(\varepsilon_m \rho_m U_{mi}\right) = \sum_{n=1}^{N_m} R_{mn} \tag{A1}$$

Continuity equation for gas phase g:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \frac{\partial}{\partial x_i}\left(\varepsilon_g \rho_g U_{gi}\right) = \sum_{n=1}^{N_g} R_{gn} \tag{A2}$$

Momentum equations for solids phases m = 1, M:

$$\left[\frac{\partial}{\partial t}\left(\varepsilon_m \rho_m U_{mi}\right) + \frac{\partial}{\partial x_j}\left(\varepsilon_m \rho_m U_{mj} U_{mi}\right)\right] = -\varepsilon_m \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{mij}}{\partial x_j} + I_{gmi} - \sum_{k=1}^{M} I_{kmi} + \varepsilon_m \rho_m g_i \tag{A3}$$

Momentum equations for gas phase g:

$$\left[\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g U_{gi}\right) + \frac{\partial}{\partial x_j}\left(\varepsilon_g \rho_g U_{gj} U_{gi}\right)\right] = -\varepsilon_g \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{gij}}{\partial x_j} - \sum_{m=1}^{M} I_{gmi} + f_{gi} + \varepsilon_g \rho_g g_i \tag{A4}$$

Granular temperature equations for solids phases m = 1, M

$$\frac{3}{2}\rho_m\left[\frac{\partial \varepsilon_m \Theta_m}{\partial t} + \frac{\partial \varepsilon_m U_{mj} \Theta_m}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\kappa_m \frac{\partial \Theta_m}{\partial x_i}\right) + \tau_{mij}\frac{\partial U_{mi}}{\partial x_j} + \Pi_m - \varepsilon_m \rho_m J_m \tag{A5}$$

Energy balance equations for solids phases m = 1, M

$$\varepsilon_m \rho_m C_{pm} \left[\frac{\partial T_m}{\partial t} + U_{mj} \frac{\partial T_m}{\partial x_j} \right] = -\frac{\partial q_{mi}}{\partial x_i} - \gamma_{gm} \left(T_m - T_g \right) - \Delta H_m + \gamma_{Rm} \left(T_{Rm}^4 - T_m^4 \right) \tag{A6}$$

Energy balance equation for gas phase g:

$$\varepsilon_g \rho_g C_{pg} \left[\frac{\partial T_g}{\partial t} + U_{gj} \frac{\partial T_g}{\partial x_j} \right] = -\frac{\partial q_{gi}}{\partial x_i} + \sum_{m=1}^{M} \gamma_{gm} \left(T_m - T_g \right) - \Delta H_g + \gamma_{Rg} \left(T_{Rg}^4 - T_g^4 \right) \tag{A7}$$

Species balance equations for solids phases m = 1, M

$$\frac{\partial}{\partial t}\left(\varepsilon_m \rho_m X_{mn} \right) + \frac{\partial}{\partial x_i}\left(\varepsilon_m \rho_m U_{mi} X_{mn} \right) = \frac{\partial}{\partial x_i}\left(D_{mn} \frac{\partial X_{mn}}{\partial x_i} \right) + R_{mn} \tag{A8}$$

Species balance equation for gas phase g:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g X_{gn} \right) + \frac{\partial}{\partial x_i}\left(\varepsilon_g \rho_g U_{gi} X_{gn} \right) = \frac{\partial}{\partial x_i}\left(D_{gn} \frac{\partial X_{gn}}{\partial x_i} \right) + R_{gn} \tag{A9}$$

B. Kinetic Theory

Constitutive equations

This is a modified Princeton model [3]. Modifications include the ad-hoc extension of kinetic theory to polydisperse systems (more than one solids phase), which guarantees that two identical solids phases will behave same as one solids phase.

Solids stresses:

$$\tau_{mij} = \left(-P_m + \eta \mu_b \frac{\partial U_{mi}}{\partial x_i} \right) \delta_{ij} + 2 \mu_m S_{mij} \tag{B1}$$

where

$$S_{mij} = \frac{1}{2}\left(\frac{\partial U_{mi}}{\partial x_j} + \frac{\partial U_{mj}}{\partial x_i} \right) - \frac{1}{3} \frac{\partial U_{mi}}{\partial x_i} \tag{B2}$$

Solids pressure:

$$P_m = \varepsilon_m \rho_m \Theta_m \left[1 + 4\eta \sum_{n=1}^{M} \left(\varepsilon_n g_{0,mn} \right) \right] \tag{B3}$$

Solids viscosity:

$$\mu_m = \left(\frac{2+\alpha}{3}\right)\left[\frac{\mu_m^*}{g_{0,mm}\eta(2-\eta)}\left(1+\frac{8}{5}\eta\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\right)\left(1+\frac{8}{5}\eta(3\eta-2)\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\right)+\frac{3}{5}\eta\mu_b\right] \tag{B4}$$

$$\mu_m^* = \frac{\rho_m \varepsilon_m g_{0,mm}\Theta_m \; \mu}{\rho_m \sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\Theta_m + \left(\frac{2\beta\mu}{\rho_m \varepsilon_m}\right)} \tag{B5}$$

$$\mu = \frac{5}{96}\rho_m d_p \sqrt{\pi\Theta_m} \tag{B6}$$

$$\mu_b = \frac{256}{5\pi}\mu\varepsilon_m \sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right) \tag{B7}$$

Solids conductivity:

$$\kappa_m = \left(\frac{\kappa_m^*}{g_{0,mm}}\right)\left[\begin{array}{l}\left(1+\frac{12}{5}\eta\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\right)\left(1+\frac{12}{5}\eta^2(4\eta-3)\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\right)\\ +\frac{64}{25\pi}(41-33\eta)\eta^2\left(\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\right)^2\end{array}\right] \tag{B8}$$

$$\kappa_m^* = \frac{\rho_m \varepsilon_m g_{0,mm}\Theta_m \; \kappa}{\rho_m \sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)\Theta_m + \left(\frac{6\beta\kappa}{5\rho_m \varepsilon_m}\right)} \tag{B9}$$

$$\kappa = \frac{75\rho_m d_p \sqrt{\pi\Theta_m}}{48\eta(41-33\eta)} \tag{B10}$$

Collisional dissipation:

$$J_m = \frac{48}{\sqrt{\pi}}\eta(1-\eta)\frac{\sum_{n=1}^{M}\left(\varepsilon_n g_{0,mn}\right)}{d_p}\Theta_m^{3/2} \tag{B11}$$

$$\eta = \frac{1+e}{2} \tag{B12}$$

Exchange terms:

$$\Pi_m = -3\beta\,\Theta_s + \frac{81\varepsilon_m \mu_g^2 \left|\mathbf{u}_g - \mathbf{u}_m\right|^2}{g_{0,mm} d_p^3 \rho_m \sqrt{\pi\Theta_m}} \qquad \text{(B13)}$$

Algebraic granular energy equation
MFIX offers an option to solve algebraic granular energy equation, which is derived by equating the production to dissipation. Note that this is equation was revised in 2005.

$$\Theta_m = \left\{ \frac{-K_{1m}\varepsilon_m D_{mii} + \sqrt{K_{1m}^2 (D_{mii})^2 \varepsilon_m^2 + 4K_{4m}\varepsilon_m [K_{2m}(D_{mii})^2 + 2K_{3m}(D_{mij} D_{mij}))]}}{2\varepsilon_m K_{4m}} \right\}^2 \qquad \text{(B14)}$$

$$K_{1m} = 2(1+e_{mm})\rho_m g_{0_{mm}} \qquad \text{(B15)}$$

$$K_{2m} = 4 d_{pm}\rho_m (1+e_{mm})\varepsilon_m g_{0_{mm}} / (3\sqrt{\pi}) - \frac{2}{3}K_{3m} \qquad \text{(B16)}$$

$$K_{3m} = \frac{d_{pm}\rho_m}{2}\left\{ \frac{\sqrt{\pi}}{3(3-e_{mm})}[0.5(3e_{mm}+1) + 0.4(1+e_{mm})(3e_{mm}-1)\varepsilon_m g_{0_{mm}}] + \frac{8\varepsilon_m g_{0_{mm}}(1+e_{mm})}{5\sqrt{\pi}} \right\} \qquad \text{(B17)}$$

$$K_{4m} = \frac{12(1-e_{mm}^2)\rho_m \, g_{0mm}}{d_{pm}\sqrt{\pi}} \qquad \text{(B18)}$$

C. Frictional Stress Models

Schaeffer model
This model [4] is used at the critical state when the solids volume fraction exceeds the maximum packing limit.

$$P_c = \begin{cases} 10^{24}\left(\varepsilon^* - \varepsilon_g\right)^{10} & \varepsilon_g < \varepsilon^* \\ 0 & \varepsilon_g \geq \varepsilon^* \end{cases} \qquad \text{(C1)}$$

(Note that the constant in the code is 10^{25} dyne/cm^2).

$$\mu_f = \begin{cases} \min\left(\dfrac{P_c \sin(\phi)}{\sqrt{4 I_{2D}}} \dfrac{\varepsilon_s}{\sum_{m=1}^{M} \varepsilon_m}, \mu_s^{\max} \right) & \varepsilon_g < \varepsilon^* \\ 0 & \varepsilon_g \ge \varepsilon^* \end{cases} \tag{C2}$$

$$\mu_s^{\max} = 100 \tag{C3}$$

(Note that this constant in the code is 1000 poise).

$$\mu_f^{bulk} = 0 \tag{C4}$$

$$I_{2D} = \frac{1}{6}\left[\left(D_{s,11} - D_{s,22}\right)^2 + \left(D_{s,22} - D_{s,33}\right)^2 + \left(D_{s,33} - D_{s,11}\right)^2 \right] + D_{s,12}^2 + D_{s,23}^2 + D_{s,31}^2 \tag{C5}$$

$$D_{s,ij} = \frac{1}{2}\left(\frac{\partial u_{s,i}}{\partial x_j} + \frac{\partial u_{s,j}}{\partial x_i} \right) \tag{C6}$$

Princeton model

This model [5] is a modification of Savage model that accounts for strain-rate fluctuations. Also the frictional model influences the flow behavior at solids volume fractions below maximum packing ($\varepsilon_{sf}^{\min} = 0.5$).

$$P_c = \begin{cases} 10^{24}\left(\varepsilon^* - \varepsilon_g\right)^{10} & \varepsilon_g < \varepsilon^* \\ Fr \dfrac{\left(\left(1-\varepsilon_g\right) - \varepsilon_s^{\min}\right)^r}{\left(\varepsilon_g - \varepsilon^*\right)^s} & \varepsilon^* \le \varepsilon_g < \left(1 - \varepsilon_{sf}^{\min}\right) \\ 0 & \varepsilon_g \ge \left(1 - \varepsilon_{sf}^{\min}\right) \end{cases} \tag{C7}$$

Where Fr =0.05, r= 2, s=5. (Note that the constants in the code are 0.5 and 10^{25} dyne/cm^2).

$$\frac{P_f}{P_c} = \left(1 - \frac{\nabla \cdot \mathbf{v}}{n\sqrt{2}\sin(\phi)\sqrt{\mathbf{S}:\mathbf{S} + \Theta / d_p^2}} \right)^{n-1} \frac{\varepsilon_s}{\sum_{m=1}^{M} \varepsilon_m} \tag{C8}$$

$$\mu_f = \frac{\sqrt{2} P_f \sin(\phi)}{\sqrt{\mathbf{S}:\mathbf{S} + \Theta / d_p^2}} \left\{ n - (n-1)\left(\frac{P_f}{P_c}\right)^{\frac{1}{n-1}} \right\} \frac{\varepsilon_s}{\sum_{m=1}^{M} \varepsilon_m} \tag{C9}$$

Here, the coefficient n is set differently depending on whether the granular assembly experiences a dilatation or compaction:

$$n = \begin{cases} \dfrac{\sqrt{3}}{2\sin(\phi)} & \nabla \cdot \mathbf{v} \geq 0 \\ 1.03 & \nabla \cdot \mathbf{v} < 0 \end{cases} \tag{C10}$$

$$\mu_f^{bulk} = -\frac{2}{3}\mu_f \tag{C11}$$

D. Interface Momentum Transfer

Gas/solids momentum interface exchange:

$$I_{gmi} = \beta_{gm}\left(u_{gi} - u_{mi}\right) \tag{D1}$$

Solids/solids momentum exchange:

$$I_{kmi} = \beta_{km}\left(u_{ki} - u_{mi}\right) \tag{D2}$$

Wen-Yu drag correlation

$$\beta_{gm} = \frac{3}{4} C_D \frac{\rho_g \varepsilon_g \varepsilon_m \left|\mathbf{u}_g - \mathbf{u}_m\right|}{d_{pm}} \varepsilon_g^{-2.65} \tag{D3}$$

$$C_D = \begin{cases} 24/\mathrm{Re}\left(1 + 0.15\,\mathrm{Re}^{0.687}\right) & \mathrm{Re} < 1000 \\ 0.44 & \mathrm{Re} \geq 1000 \end{cases} \tag{D4}$$

$$\mathrm{Re} = \frac{\rho_g \varepsilon_g \left|\mathbf{u}_g - \mathbf{u}_m\right| d_{pm}}{\mu_g} \tag{D5}$$

Gidaspow drag correlation

$$\beta_{gm} = \begin{cases} \frac{3}{4} C_D \frac{\rho_g \varepsilon_g \varepsilon_m \left| \mathbf{u}_g - \mathbf{u}_m \right|}{d_{pm}} \varepsilon_g^{-2.65} & \varepsilon_g \geq 0.8 \\ \frac{150 \varepsilon_s \left(1-\varepsilon_g\right) \mu_g}{\varepsilon_g d_{pm}^2} + \frac{1.75 \rho_g \varepsilon_m \left| \mathbf{u}_g - \mathbf{u}_m \right|}{d_{pm}} & \varepsilon_g < 0.8 \end{cases} \quad \text{(D6)}$$

$$C_D = \begin{cases} 24/\mathrm{Re}\left(1+0.15\,\mathrm{Re}^{0.687}\right) & \mathrm{Re} < 1000 \\ 0.44 & \mathrm{Re} \geq 1000 \end{cases} \quad \text{(D7)}$$

$$\mathrm{Re} = \frac{\rho_g \varepsilon_g \left| \mathbf{u}_g - \mathbf{u}_m \right| d_{pm}}{\mu_g} \quad \text{(D8)}$$

Hill-Koch-Ladd drag correlation
(valid for one solids phase only)

The drag correlation of Hill, Koch and Ladd [6, 7] was modified [12] and implemented in MFIX.

$$\beta_{gm} = 18 \mu_g \left(1-\varepsilon_m\right)^2 \varepsilon_m \frac{F}{d_{pm}^2} \quad \text{(D9)}$$

The drag force (F) is given as:

$$F = 1 + 3/8\,\mathrm{Re} \qquad \varepsilon_s \leq 0.01 \; and \; \mathrm{Re} \leq \frac{\left(F_2 - 1\right)}{\left(3/8 - F_3\right)} \quad \text{(D10)}$$

$$F = F_0 + F_1 R_e^2 \qquad \varepsilon_s > 0.01 \; and \; \mathrm{Re} \leq \frac{F_3 + \sqrt{F_3^2 - 4F_1\left(F_0 - F_2\right)}}{2F_1} \quad \text{(D11)}$$

$$F = F_2 + F_3\,\mathrm{Re} \qquad \begin{cases} \varepsilon_s \leq 0.01 \; and \; \mathrm{Re} > \frac{\left(F_2 - 1\right)}{\left(3/8 - F_3\right)} \\ \varepsilon_s > 0.01 \; and \; \mathrm{Re} > \frac{F_3 + \sqrt{F_3^2 - 4F_1\left(F_0 - F_2\right)}}{2F_1} \end{cases} \quad \text{(D12)}$$

And the coefficients are defined as follows:

$$F_0 = \begin{cases} (1-w)\left[\dfrac{1+3\sqrt{\varepsilon_s/2}+(135/64)\varepsilon_s\ln(\varepsilon_s)+17.14\varepsilon_s}{1+0.681\varepsilon_s-8.48\varepsilon_s{}^2+8.16\varepsilon_s{}^3}\right]+w\left[10\dfrac{\varepsilon_s}{(1-\varepsilon_s)^3}\right] & 0.01<\varepsilon_s<0.4 \\ 10\dfrac{\varepsilon_s}{(1-\varepsilon_s)^3} & \varepsilon_s \geq 0.4 \end{cases}$$

(D13)

$$F_1 = \begin{cases} \sqrt{\dfrac{2}{\varepsilon_s}}/40 & 0.01<\varepsilon_s\leq 0.1 \\ 0.11+0.00051\exp(11.6\varepsilon_s) & \varepsilon_s>0.1 \end{cases}$$ (D14)

$$F_2 = \begin{cases} (1-w)\left[\dfrac{1+3\sqrt{\varepsilon_s/2}+(135/64)\varepsilon_s\ln(\varepsilon_s)+17.89\varepsilon_s}{1+0.681\varepsilon_s-11.03\varepsilon_s{}^2+15.41\varepsilon_s{}^3}\right]+w\left[10\dfrac{\varepsilon_s}{(1-\varepsilon_s)^3}\right] & \varepsilon_s<0.4 \\ 10\dfrac{\varepsilon_s}{(1-\varepsilon_s)^3} & \varepsilon_s \geq 0.4 \end{cases}$$

(D15)

$$F_3 = \begin{cases} 0.9351\varepsilon_s+0.03667 & \varepsilon_s<0.0953 \\ 0.0673+0.212\varepsilon_s+0.0232/(1-\varepsilon_s)^5 & \varepsilon_s\geq 0.0953 \end{cases}$$ (D16)

$$\mathrm{Re} = \frac{\rho_g(1-\varepsilon_m)\left|\mathbf{u}_g-\mathbf{u}_m\right|d_{pm}}{2\mu_g}$$ (D17)

$$w = e^{(-10(0.4-\varepsilon_s)/\varepsilon_s)}$$ (D18)

Syamlal and O'Brien

$$\beta_{gm} = \frac{3\,\varepsilon_m\,\varepsilon_g\,\rho_g}{4V_{rm}^2\,d_{pm}}\left(0.63+4.8\sqrt{V_{rm}/Re_m}\right)^2\left|\mathbf{u}_g-\mathbf{u}_m\right|$$ (D19)

$$V_{rm} = 0.5\left(A-0.06\,Re_m+\sqrt{(0.06\,Re_m)^2+0.12\,Re_m(2B-A)+A^2}\right)$$ (D20)

$$A = \varepsilon_g^{4.14} \tag{D21}$$

$$B = \begin{cases} 0.8\,\varepsilon_g^{1.28} & \text{if } \varepsilon_g \le 0.85 \\ \varepsilon_g^{2.65} & \text{if } \varepsilon_g > 0.85 \end{cases} \tag{D22}$$

$$Re_m = \frac{d_{pm}\left|\mathbf{u}_g - \mathbf{u}_m\right|\rho_g}{\mu_g} \tag{D23}$$

Solids/solids momentum exchange coefficient

$$\beta_{km} = 3(1+e)\left(\frac{\pi}{2} + c_{fkm}\frac{\pi^2}{8}\right)\frac{\left(d_{p,m} + d_{p,k}\right)^2}{2\pi\left(\rho_m d_{p,m}^3 + \rho_k d_{p,k}^3\right)}\rho_m \rho_k g_{0,mk}\left|\mathbf{u}_m - \mathbf{u}_k\right| + s_{coef} P_c \tag{D19}$$

c_{fkm} : Constant defined in input file (no default value assigned)

s_{coef} : Constant defined in input file with default value of zero. (See reference [10] and [11] for details)

E. Correlations for maximum packing

This section provides description of two empirical correlations for computing the solids maximum packing in polydisperse systems by Yu and Standish [8] and Fedors and Landel [9]. To use these correlations, the numbering of the solids phases was rearranged in MFIX to start with the coarsest to the finest powder.

Yu-Standish correlation
This correlation can be used for powder mixtures with 2 or more components.

$$\varepsilon^* = 1 - \varepsilon_{s,mixture}^{\max} \tag{E1}$$

$$\varepsilon_{s,mixture}^{\max} = \min\left\{\frac{\varepsilon_{s,i}^{\max}}{1 - \sum_{j=1}^{i-1}\left(1 - \frac{\varepsilon_{s,i}^{\max}}{p_{ij}}\right)\frac{cx_i}{X_{ij}} - \sum_{j=i+1}^{M}\left(1 - \frac{\varepsilon_{s,i}^{\max}}{p_{ij}}\right)\frac{cx_i}{X_{ij}}}\right\} \qquad i = 1, 2, ..., M \tag{E2}$$

$$cx_i = \frac{\varepsilon_{s,i}}{\sum_{j=1}^{M} \varepsilon_{s,j}} \tag{E3}$$

$$X_{ij} = \begin{cases} \dfrac{1-r_{ij}^2}{2-\varepsilon_{s,i}^{\max}} & j < i \\ 1-\dfrac{1-r_{ij}^2}{2-\varepsilon_{s,i}^{\max}} & j \ge i \end{cases} \tag{E4}$$

$$p_{ij} = \begin{cases} \varepsilon_{s,i}^{\max} + \varepsilon_{s,i}^{\max}\left(1-\varepsilon_{s,i}^{\max}\right)\left(1-2.35 r_{ij} + 1.35 r_{ij}^2\right) & r_{ij} \le 0.741 \\ \varepsilon_{s,i}^{\max} & r_{ij} > 0.741 \end{cases} \tag{E5}$$

$$r_{ij} = \begin{cases} \dfrac{d_{p,i}}{d_{p,j}} & i \ge j \\ \dfrac{d_{p,j}}{d_{p,i}} & i < j \end{cases} \tag{E6}$$

$\varepsilon_{s,i}^{\max}, d_{p,i} \quad i = 1, 2, ..., M$ represent the maximum packing and particle diameter of individual powders.

Fedors-Landel correlation

This correlation can only be used for a binary mixture of powders.

$$\varepsilon_{s,mixture}^{\max} = \begin{cases} \left[\left(\varepsilon_{s,1}^{\max} - \varepsilon_{s,2}^{\max}\right) + \left(1-\sqrt{r_{2,1}}\right)\left(1-\varepsilon_{s,1}^{\max}\right)\varepsilon_{s,2}^{\max}\right] \times \\ \quad \left[\varepsilon_{s,1}^{\max} + \left(1-\varepsilon_{s,1}^{\max}\right)\varepsilon_{s,2}^{\max}\right]\dfrac{cx_1}{\varepsilon_{s,1}^{\max}} + \varepsilon_{s,2}^{\max} & cx_1 \le \dfrac{\varepsilon_{s,1}^{\max}}{\varepsilon_{s,1}^{\max} + \left(1-\varepsilon_{s,1}^{\max}\right)\varepsilon_{s,2}^{\max}} \\ \left(1-\sqrt{r_{2,1}}\right)\left[\varepsilon_{s,1}^{\max} + \left(1-\varepsilon_{s,1}^{\max}\right)\varepsilon_{s,2}^{\max}\right] cx_2 + \varepsilon_{s,1}^{\max} & cx_1 > \dfrac{\varepsilon_{s,1}^{\max}}{\varepsilon_{s,1}^{\max} + \left(1-\varepsilon_{s,1}^{\max}\right)\varepsilon_{s,2}^{\max}} \end{cases} \tag{E7}$$

F. Gas momentum equation constitutive models

Stresses

$$\tau_{gij} = 2\mu_{gt} S_{gij} \quad \text{(F1)}$$

where

$$S_{gij} = \frac{1}{2}\left(\frac{\partial U_{gi}}{\partial x_j} + \frac{\partial U_{gj}}{\partial x_i}\right) - \frac{1}{3}\frac{\partial U_{gi}}{\partial x_i}\delta_{ij} \quad \text{(F2)}$$

$$\mu_{gt} = Min(\mu_{\max}, \mu_g + \mu_e) \quad \text{(F3)}$$

$$\mu_e = 2 l_s^2 \varepsilon_g \rho_g \sqrt{I_{2Dg}} \quad \text{(F4)}$$

$$\begin{aligned} I_{2Dg} = {} & \frac{1}{6}\left[\left(D_{g,11} - D_{g,22}\right)^2 + \left(D_{g,22} - D_{s,33}\right)^2 + \left(D_{g,33} - D_{g,11}\right)^2\right] \\ & + D_{g,12}^2 + D_{g,23}^2 + D_{g,31}^2 \end{aligned} \quad \text{(F5)}$$

Porous media model

$$f_{gi} = -\frac{\mu_g}{c_1} U_{gi} - \frac{c_2}{2}\rho_g \left(\sqrt{U_{gj} U_{gj}}\right) U_{gi} \quad \text{(F6)}$$

G. Gas/Solids Turbulence models

The gas/solids turbulence models are given in Benyahia 2005. The equations are not reproduced here because of a small inconsistency in the notation.

H. Energy equation constitutive models

Interphase heat transfer

$$\gamma_{gm} = C_{pg} R_{gm} \Big/ \left[\exp\left(\frac{C_{pg} R_{gm}}{\gamma_{gm}^0}\right) - 1\right] \quad \text{(H1)}$$

$$\gamma_{gm}^0 = 6\kappa_g \varepsilon_m Nu_m \Big/ d_m^2 \quad \text{(H2)}$$

$$Nu_m = \left(7 - 10\varepsilon_g + 5\varepsilon_g^2\right)\left(1 + 0.7\,\mathrm{Re}_m^{0.2}\,\mathrm{Pr}^{1/3}\right) + \left(1.33 - 2.4\varepsilon_g + 1.2\varepsilon_g^2\right)\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3} \quad \text{(H3)}$$

Gas and solids conduction

$$q_{mi} = -\kappa_m \frac{\partial T_m}{\partial x_i} \tag{H4}$$

$$q_{gi} = -\kappa_g \frac{\partial T_g}{\partial x_i} \tag{H5}$$

Heats of reaction

$$\begin{aligned} -\Delta H_m &= \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)dT \right] \varepsilon_g \rho_g \left(\frac{\partial X_{gn}}{\partial t} + U_{gi} \frac{\partial X_{gn}}{\partial x_i} \right) \\ &\approx \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)dT \right] \left(R_{mn} - X_{mn} \sum_{n'=1}^{N_m} R_{mn'} \right) \end{aligned} \tag{H6}$$

$$-\Delta H_g \approx \sum_n \left[\left(H_{g,ref} \right)_n + \int_{T_{ref}}^{T_g} C_{pgn}(T)dT \right] \left(R_{gn} - X_{gn} \sum_{n'=1}^{N_g} R_{gn'} \right) \tag{H7}$$

Nomenclature

c_1	Permeability of porous media; m^2
c_2	Inertial resistance factor of porous media; m^{-1}
C_{pg}	Specific heat of the fluid phase; J/kg·K
C_{fkm}	Coefficient of friction for solids phases k and m
C_{pm}	Specific heat of the m^{th} solids phase; J/kg·K
d_{pm}	Diameter of the particles constituting the m^{th} solids phase; m
D_{gij}	Rate of strain tensor, fluid phase; s^{-1}
D_{mij}	Rate of strain tensor, solids phase-m; s^{-1}
D_{gn}	Diffusion coefficient of nth gas-phase species, kg/m·s
D_{mn}	Diffusion coefficient of nth solids-phase-m species-n, kg/m·s
e_{km}	Coefficient of restitution for the collisions of m^{th} and k^{th} solids phases
f_{gi}	Fluid flow resistance due to porous media; N/m^3
g_i	Acceleration due to gravity; m/s^2
g_{0m}	Radial distribution function at contact
$(H_{m,ref})_n$	Enthalpy of m^{th} solids phase, species n at T_{ref}; J/m^3
$(H_{g,ref})_n$	Enthalpy of fluid phase, species n at T_{ref}; J/m^3
ΔH_g	Heat of reaction in the fluid phase; $J/m^3 \cdot s$
ΔH_m	Heat of reaction in the m^{th} solids phase; $J/m^3 \cdot s$
i, j	Indices to identify vector and tensor components; summation convention is used only for these indices.
I_{2Dg}	Second invariant of the deviator of the strain rate tensor for gas phase; s^{-2}
I_{2Ds}	Second invariant of the deviator of the strain rate tensor for solids phase 1; s^{-2}
k_g	Fluid-phase conductivity; J/m·K·s
k_{pm}	Conductivity of material that constitutes solids phase m; J/m·K·s
k_{sm}	Solids phase m conductivity; J/m·K·s
l_s	A turbulence length-scale parameter; m
m	Index of the m^{th} solids phase. "m=0" indicates fluid phase
M	Total number of solids phases
Mw	Average molecular weight of gas
n	Index of the nth chemical species
N_g	Total number of fluid-phase chemical species
N_m	Total number of solids phase m chemical species
Nu_m	Nusselt number
P_g	Pressure in the fluid phase; Pa
P_m^p	Pressure in Solids phase m, plastic regime; Pa
P_m^v	Pressure in Solids phase m, viscous regime; Pa
Pr	Prandtl number
q_{gi}	Fluid-phase conductive heat flux; $J/m^2 \cdot s$
q_{mi}	Solids-phase m conductive heat flux; $J/m^2 \cdot s$
R	Universal gas constant; $Pa \cdot m^3/kmol \cdot K$
Re_m	m^{th} solids phase particle Reynolds number
R_{km}	Ratio of solids to fluid conductivity
R_{mk}	Rate of transfer of mass from m^{th} phase to k^{th} phase. k or m = 0 indicates fluid phase; $kg/m^3 \cdot s$

R_{gn}	Rate of production of the nth chemical species in the fluid phase; $kg/m^3 \cdot s$
R_{mn}	Rate of production of the nth chemical species in the m^{th} solids phase; $kg/m^3 \cdot s$
t	Time; s
T_g	Thermodynamic temperature of the fluid phase; K
T_m	Thermodynamic temperature of the solids phase m; K
T_{Ref}	Reference temperature; K
T_{Rg}	Fluid phase radiation temperature; K
T_{Rm}	Solids phase-m radiation temperature; K
U_{gi}	Fluid-phase velocity vector; m/s
U_{mi}	m^{th} solids-phase velocity vector; m/s
x_i	i^{th} Coordinate Direction; m
X_{gn}	Mass fraction of the n^{th} chemical species in the fluid phase
X_{mn}	Mass fraction of the n^{th} chemical species in the m^{th} solids phase

GREEK LETTERS

β_{gm}	Coefficient for the interphase force between the fluid phase and the m^{th} solids phase; $kg/m^3 \cdot s$
β_{km}	Coefficient for the interphase force between the k^{th} solids phase and the m^{th} solids phase; $kg/m^3 \cdot s$
γ_{gm}	Fluid-solids heat transfer coefficient corrected for interphase mass transfer; $J/m^3 \cdot K \cdot s$
γ_{gm}^0	Fluid-solids heat transfer coefficient not corrected for interphase mass transfer; $J/m^3 \cdot K \cdot s$
γ_{Rg}	Fluid-phase radiative heat transfer coefficient; $J/m^3 \cdot K^4 \cdot s$
γ_{Rm}	Solids-phase-m radiative heat transfer coefficient; $J/m^3 \cdot K^4 \cdot s$
	Granular energy dissipation due to inelastic collisions; $J/m^3 \cdot s$
ε_g	Volume fraction of the fluid phase (void fraction)
	Packed-bed (maximum) solids volume fraction
ε_m	Volume fraction of the m^{th} solids phase
η	Function of restitution coefficient
Θ_m	Granular temperature of phase m; m^2/s^2
λ_{rm}	Solids conductivity function
λ^v_m	Second coefficient of solids viscosity, viscous regime; $kg/m \cdot s$
μ_e	Eddy viscosity of the fluid phase; $kg/m \cdot s$
μ_g	Molecular viscosity of the fluid phase; $kg/m \cdot s$
μ_{gmax}	Maximum value of the turbulent viscosity of the fluid phase; $kg/m \cdot s$
μ_{gt}	Turbulent viscosity of the fluid phase; $kg/m \cdot s$
μ^p_m	Solids viscosity, plastic regime; $kg/m \cdot s$
μ^v_m	Solids viscosity, viscous regime; $kg/m \cdot s$
ξ_{mk}	$\xi_{mk} = 1$ if $R_{mk} < 0$; else $\xi_{mk} = 0$.
ρ_g	Microscopic (material) density of the fluid phase; kg/m^3
ρ_m	Microscopic (material) density of the m^{th} solids phase; kg/m^3
τ_{gij}	Fluid-phase stress tensor; Pa
τ_{mij}	Solids phase m stress tensor; Pa
φ	Angle of internal friction, also used as general scalar
φ_k	Contact area fraction in solids conductivity model

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