Gas/Solids Turbulence models implemented in MFIX

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Purpose
The purpose of this document is to describe the governing and constitutive relations of turbulence models recently implemented in MFIX. Simonin [1, 2] and Ahmadi [3] models along with Jenkins [4] small frictional boundary condition are available for download from the development webpage of MFIX (www.mfix.org).

Governing equations

Continuity equation index m=1 (gas) or 2 (solids).

$$\frac{\partial}{\partial t}\left(\alpha_m \rho_m\right) + \frac{\partial}{\partial x_i}\left(\alpha_m \rho_m U_{mi}\right) = 0$$

Momentum equation

$$\alpha_m \rho_m \left[\frac{\partial U_{mi}}{\partial t} + U_{ml}\frac{U_{mi}}{\partial x_j}\right] = -\alpha_m \frac{\partial P_1}{\partial x_i} + \frac{\partial \tau_{mij}}{\partial x_j} + I_{mi} + \alpha_m \rho_m g_i$$

Turbulence modeling in the continuous phase $k_1 = \frac{1}{2}\langle u_1 u_1 \rangle$

$$\alpha_1 \rho_1 \left[\frac{\partial k_1}{\partial t} + U_{1j}\frac{\partial k_1}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_1 \frac{\mu_1^t}{\sigma_k}\frac{\partial k_1}{\partial x_i}\right) + \alpha_1 \tau_{1ij}\frac{\partial U_i}{\partial x_j} + \prod_{k1} - \alpha_1 \rho_1 \varepsilon_1$$

$$\alpha_1 \rho_1 \left[\frac{\partial \varepsilon_1}{\partial t} + U_{1j}\frac{\partial \varepsilon_1}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_1 \frac{\mu_1^t}{\sigma_\varepsilon}\frac{\partial \varepsilon_1}{\partial x_i}\right) + \alpha_1 \frac{\varepsilon_1}{k_1}\left(C_{1\varepsilon}\tau_{1ij}\frac{\partial U_i}{\partial x_j} - \rho_1 C_{2\varepsilon}\varepsilon_1\right) + \prod_{\varepsilon 1}$$

Turbulence modeling of the dispersed phase $\Theta_s = \frac{1}{3}\langle u_2 u_2 \rangle$

$$\alpha_2 \rho_2 \left[\frac{\partial \Theta_s}{\partial t} + U_{2j}\frac{\partial \Theta_s}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_2 \rho_2 \kappa_2 \frac{\partial \Theta_s}{\partial x_i}\right) + \alpha_2 \rho_2 \tau_{2ij}\frac{\partial U_{2i}}{\partial x_j} + \prod_{k2} - \alpha_2 \rho_2 \varepsilon_2$$

Constitutive relations

Stress tensor

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

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

Solids pressure

For Simonin or granular model:

$$P_2 = \alpha_2 \rho_2 \Theta_s \left[1 + 2\alpha_2 g_0 (1+e)\right]$$

For Ahmadi model:

$$P_2 = \alpha_2 \rho_2 \Theta_s \left[(1 + 4\alpha_2 g_0) + 1/2(1 - e^2)\right]$$

Solids shear viscosity

For Simonin:

$$\mu_2 = \alpha_2 \rho_2 \left(\nu_2^{kin} + \nu_2^{col}\right)$$

$$\nu_2^{kin} = \left[\frac{2}{3}k_{12}\eta_t + \Theta_s (1 + \zeta_{c2}\alpha_2 g_0)\right]\tau_2$$

$$\nu_2^{col} = \frac{8}{5}\alpha_2 g_0 \frac{(1+e)}{2}\left(\nu_2^{kin} + d_p \sqrt{\frac{\Theta_s}{\pi}}\right)$$

For Ahmadi:

$$\mu_2 = \left[1 + \left(\tau_1^t / \tau_{12}^x\right)\left(1 - \alpha_2 / \alpha_2^{\max}\right)^3\right]^{-1}\left[0.1045\left(1/g_0 + 3.2\alpha_2 + 12.1824 g_0 \alpha_2^2\right) d_p \rho_2 \sqrt{\Theta_s}\right]$$

Solids bulk viscosity

For Simonin:

$$\lambda_2 = \frac{5}{3}\alpha_2 \rho_2 \nu_2^{col}$$

For Ahmadi:

$$\lambda_2 = \frac{5}{3}\left[1 + \left(\tau_1^t / \tau_{12}^x\right)\left(1 - \alpha_2 / \alpha_2^{\max}\right)^3\right]^{-1}\left[0.1045\left(12.1824 g_0 \alpha_2^2\right) d_p \rho_2 \sqrt{\Theta_s}\right]$$

Gas turbulent viscosity

For Simonin or k-epsilon:

$$\mu_1^t = \rho_1 C_\mu \frac{k_1^2}{\varepsilon_1}$$

For Ahmadi:

$$\mu_1^t = \rho_1 C_\mu \left[1 + \left(\tau_{12}^x / \tau_1^t\right)\left(\alpha_2 / \alpha_2^{\max}\right)^3\right]^{-1} \frac{k_1^2}{\varepsilon_1}$$

Solids granular conductivity

For Simonin:

$$\kappa_2 = \alpha_2 \rho_2 \left(\kappa_2^{kin} + \kappa_2^{col}\right)$$

$$\kappa_2^{kin} = \left(9/10\, k_{12}\eta_t + \frac{3}{2}\Theta_s \left(1 + \varpi_c \alpha_2 g_0\right)\right)\left(\frac{9/5}{\tau_{12}^x} + \frac{\xi_c}{\tau_2^c}\right)^{-1}$$

$$\kappa_2^{col} = 18/5\, \alpha_2 g_0 \frac{(1+e)}{2}\left(\kappa_2^{kin} + 5/9 d_p \sqrt{\frac{\Theta_s}{\pi}}\right)$$

For Ahmadi:

$$\kappa_2 = 0.1306 \rho_2 d_p \left(1+e^2\right)\left(1/g_0 + 4.8\alpha_2 + 12.1184 g_0 \alpha_2^2\right)\sqrt{\Theta_s}$$

Radial distribution function (g_0) and drag term(β)

User-defined through g_0.f and drag_gs.f (not part of this study).

Granular energy dissipation

For granular, Simonin or Ahmadi:

$$\varepsilon_2 = 12\left(1-e^2\right)\alpha_2^2 \rho_2 g_0 \frac{\Theta_s^{3/2}}{d_p}$$

Turbulence interaction terms

For Simonin:

$$\Pi_{k1} = \beta\left(k_{12} - 2k_1\right)$$

$$\Pi_{\varepsilon 1} = C_{3\varepsilon}\left(\varepsilon_1 / k_1\right)\Pi_{k1}$$

$$\Pi_{k2} = \beta\left(k_{12} - 3\Theta_s\right)$$

$$k_{12} = \frac{\eta_t}{1 + \left(1 + X_{21}\right)\eta_t}\left(2k_1 + 3X_{21}\Theta_s\right)$$

For Ahmadi:

$$\Pi_{k1} = \beta\left(3\Theta_s - 2k_1\right)$$

$$\Pi_{\varepsilon 1} = 0$$

$$\Pi_{k2} = \beta\left(\frac{2k_1}{1 + \tau_{12}^x / \tau_1} - 3\Theta_s\right)$$

Time scales and constants definition

Particle relaxation time:

$$\tau_{12}^{x} = \frac{\alpha_2 \rho_2}{\beta}$$

Time-scale of turbulent eddies:

$$\tau_1^t = \frac{3}{2} C_\mu \frac{k_1}{\varepsilon_1}$$

Fluid Lagrangian integral time-scale:

$$\tau_{12}^{t} = \frac{\tau_1^t}{\sqrt{1 + C_\beta \xi_r^2}}$$

$$\xi_r^2 = \frac{3\left|\mathbf{U}_r\right|^2}{2k_1}$$

$$C_\beta = 1.8 - 1.35\cos^2(\theta)$$

Ratio between the Lagrangian integral time scale and the particle relaxation time:

$$\eta_t = \frac{\tau_{12}^t}{\tau_{12}^x}$$

Collisional time-scale:

$$\tau_2^c = \frac{d_p}{6\alpha_2 g_0 \sqrt{16\Theta_s / \pi}}$$

New time-scale in Simonin model

$$\frac{1}{\tau_2} = \frac{2}{\tau_{12}^x} + \frac{\sigma_c}{\tau_2^c}$$

Constants in $k - \varepsilon$ model:

σ_k, σ_ε, $C_{1\mu}$, $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$ = 1.0, 1.3, 0.09, 1.44, 1.92, and 1.22, respectively.

Constants in Simonin model:

$$\zeta_{c2} = 2/5\,(1+e)(3e-1)$$

$$\varpi_c = (1+e)^2 (2e-1)/100$$

$$\zeta_c = (1+e)(49-33e)/100$$

$$\sigma_c = (1+e)(3-e)/5$$

$$X_{21} = \frac{\alpha_2 \rho_2}{\alpha_1 \rho_1}$$

Jenkins small frictional limit boundary condition

$$\mu_2 \frac{\partial u_2}{\partial x}\bigg|_w = P_2 \tan(\phi_w) \frac{u_2}{|u_2|}$$

$$\kappa_2 \frac{\partial \Theta_s}{\partial x}\bigg|_w = P_2 \sqrt{3\Theta_s}\, \frac{3}{8}\left[\frac{7}{2}(1+e_w)\tan^2(\phi_w) - (1-e_w)\right]$$

ϕ_w : angle of internal friction at the wall defined in mfix.dat (default value is zero).
Appendix A shows a generalization of Jenkins BC to a 2-D plane.

Wall functions for gas phase turbulence boundary condition

$$\frac{\partial u_1}{\partial x}\bigg|_w = \frac{\rho_1 \kappa u_1 C_{1\mu}^{1/4} k_1^{1/2}}{(\mu_1 + \mu_1^t)\ln(E\, x^*)}$$

$$x^* = \frac{\rho_1 C_{1\mu}^{1/4} k_1^{1/2} \Delta x / 2}{\mu_1}$$

Modifications of source terms for k_1 and ε_1 at wall-adjacent fluid cells:

$$production\ of\ k_1 = \alpha_1\ \tau_{1ij} \frac{\partial u_{1i}}{\partial x_j} = \alpha_1 \rho_1 \sqrt{C_{1\mu}}\, k_1 \frac{u_1}{\Delta x / 2 \ln(E\, x^*)}$$

$$dissipation\ of\ k_1 = \alpha_1 \rho_1 \varepsilon_1$$

$$\varepsilon_1 = \frac{C_{1\mu}^{3/4} k_1^{3/2}}{\kappa \Delta y / 2}$$

Apply zero flux for k_1 and ε_1 at walls:

$$\frac{\partial k_1}{\partial x}\bigg|_w = 0$$

$$\frac{\partial \varepsilon_1}{\partial x}\bigg|_w = 0$$

Some remarks in implementing these models in MFIX

- With $k-\varepsilon$ turbulence model, wall functions are applied to all walls (NSW, FSW and PSW) except undefined wall types.
- k_2 as defined by Simonin [1, 2] was replaced by the definition of granular temperature Θ_s already existing in MFIX. Simonin and Ahmadi models were changed accordingly to fit this definition.
- When SIMONIN or AHMADI keywords are set to true, $k-\varepsilon$ model and the full granular energy are automatically solved (even when set to false in mfix.dat).

- Assumed a certain form for Ahmadi [3] bulk viscosity and granular conductivity. Communicated to Ahmadi my assumptions, and may change the code depending on his response.
- When JENKINS and GRANULAR keyword are set to true, BC_JJ_PS is set to one for all walls to make use of the Johnson and Jackson boundary condition in MFIX.
- The definition of μ in Jenkins paper [4] was changed to $\tan(\phi_w)$ to make use of this already defined keyword in MFIX.
- Single particle drag used in calc_mu_s.f to define τ_{12}^{x} in case of very dilute conditions.
- For very dilute flows where Ep_s may get below 1E-04, I suggest that a user modifies toleranc_mod.f to reduce Dil_ep_s and zero_ep_s. As an example, I simulated a turbulent particle-laden jet and had to set dil_ep_s to 1E-10. This relatively low value of dil_ep_s was suggested by Simonin who solves the solids momentum in the entire computational domain (even when solids is non-existent) to reduce granular temperature production at interfaces between very dilute regions (where solids momentum is not solved) and regions where solids momentum is solved.

Nomenclature

$C_{1\mu}$, $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$: constants in the gas turbulence model.
d_p: particle mean diameter.
e: particle-particle restitution coefficient.
e_w: particle-wall restitution coefficient.
E: constant in wall function formulation equal to 9.81.
g_0 : radial distribution function at contact.
I_{im}: momentum exchange
k_1: turbulent kinetic energy of gas phase.
k_{12}: cross-correlation of gas and solids fluctuating velocities.
κ_2: conductivity of solids turbulent energy.
P_m: pressure of phase m.
S_{mij} : mean strain-rate tensor.
U_m, V_m: averaged velocity of phase m.

Greek letters:
α_m: volume fraction of phase m.
β : drag coefficient.
Δx: width of computational cell next to the wall.
ε_1: turbulent energy dissipation in the gas phase.
ε_2: dissipation of solids fluctuating energy due to inter-particle collisions.
ζ_c and ϖ_c: constants depending on particle restitution coefficient.
η_t: ratio between Lagrangian and particle relaxation time scales.

θ : angle between mean particle velocity and mean relative velocity.
Θ_s : granular temperature
κ : Von Karmen constant of value: 0.42.
λ_2 : bulk viscosity in the solids phase.
μ : coefficient of friction.
μ_m^t : turbulent eddy viscosity for phase m.
ν_m^t : turbulent kinematic viscosity for phase m.
Π : turbulence exchange terms.
ρ_m : density of phase m.
σ_{mij} : viscous stress tensor of phase m.
σ_k , σ_ε : constants in the gas turbulence model of values: 1.0, 1.3, respectively.
$\sum_{mij}$: effective stress tensor.
τ_{12}^x : particle relaxation time scale.
τ_{12}^t : eddy-particle interaction time scale.
τ_1^t : energetic turbulent eddies time scale.
τ_2^c : collisional time scale.
τ_{mij} : Reynolds stresses for phase m.
ϕ_w : angle of internal friction at walls.
ω_c : constant depending on particle restitution coefficient.

Indices:
col: collisional
i, j, k: indices used to represent spatial direction and in Einstein summation convention
m: phase m, takes values 1 and 2 for gas and solids phases.
max: maximum packing
kin: kinetic
s, p: solids or particulate phase.
w: wall

References

[1] Balzer, G., Simonin, O., Boelle, A. and Lavieville, J., 1996. A unifying modelling approach for the numerical prediction of dilute and dense gas-solid two phase flow, CFB5, *5th Int. Conf. on Circulating Fluidized Beds*, Beijing, China.

[2] Simonin, O., "Continuum modeling of dispersed two-phase flows, in **Combustion and Turbulence in Two-Phase Flows**, Von Karman Institute of Fluid Dynamics Lecture Series 1996-2, 1996.

[3] Cao, J. and Ahmadi, G., 1995. Gas-particle two-phase turbulent flow in a vertical duct. *Int. J. Multiphase Flow*, Vol. 21 No. 6, pp. 1203-1228.

[4] Jenkins, J.T. and Louge, M.Y., 1997. On the Flux of Fluctuating Energy in a Collisional Grain Flow at a Flat Frictional Wall, *Phys. Fluids* **9** (10), pp. 2835-2840.

Appendix A. Derivation of Jenkins BC for a 2-D surface

Previously, the Jenkins BC was expressed as:

$$-\mu_2 \frac{\partial u_2}{\partial x}\bigg|_w = P_2 \tan(\phi_w)\frac{u_2}{|u_2|} \quad (1)$$

where u_2 is a velocity component of the solids velocity.

Let's look at equation (1) in Tardos paper for non-cohesive particles or equation (2) of Jenkins and Louge paper:

$$\tau = \sigma \tan(\phi_w) \quad (2)$$

Where τ is the shear stress at the wall and σ is normal stress (Coulomb law of friction).

To illustrate how to derive a similar equation in an Eulerian frame of reference, let's choose a wall surface in the X-Y coordinate system and the normal to this surface will be in the Z-direction. Then, we can express the total stress at the wall as:

$$T \bullet \vec{n} = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{bmatrix} \bullet \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} T_{13} \\ T_{23} \\ T_{33} \end{bmatrix} \quad (3)$$

The normal stress to the wall is defined as:

$\sigma = T_{33}$, which in terms of absolute value can be expressed as:

$$\sigma = \left| -P_s + 2\mu_s \frac{\partial w}{\partial z} \right| \cong P_s \quad (4)$$

Here we assume that the total force to the wall is approximated by the solids pressure.

Now for the shear stresses, let's express the tangential force on the wall knowing that:

$$\begin{cases} T_{13} = 2\mu_s D_{13} = \mu_s \dfrac{\partial u}{\partial z} \\ T_{23} = 2\mu_s D_{23} = \mu_s \dfrac{\partial v}{\partial z} \end{cases} \quad (5)$$

Graphically in an X-Y plane, the tangential force on a wall can be represented in the following diagram:

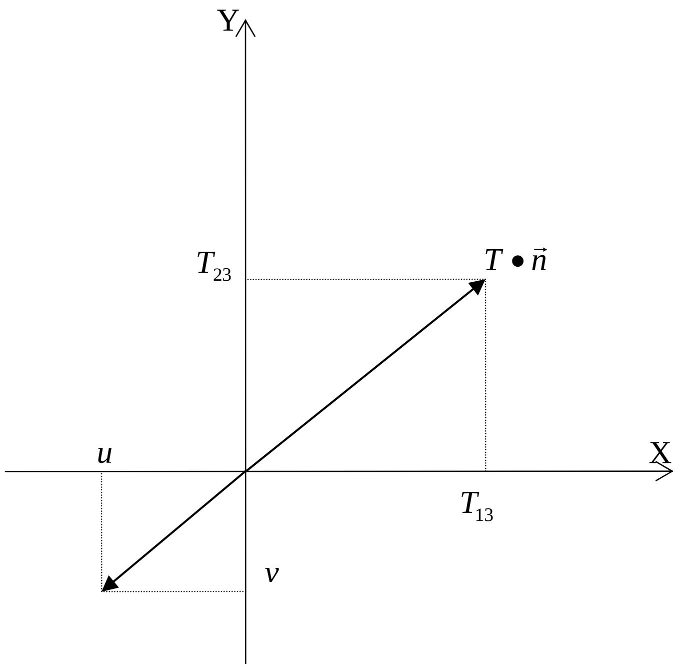

Figure 1 Construction of a tangential force that is acting opposite but exactly on the same line as the velocity vector

We can see from Figure 1 that the magnitude of the frictional force τ is expressed as:

$$\tau = \sqrt{T_{13}^2 + T_{23}^2} = \mu_s \sqrt{2D_{13}^2 + 2D_{23}^2} = \mu_s \sqrt{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2} \tag{6}$$

Combining equations (2, 4 and 6) we obtain:

$$\mu_s \sqrt{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2} = P_s \tan(\phi_w) \tag{7}$$

Let's go back to Figure 1 and notice that the frictional force is aligned with the velocity vector at the wall but has an opposite sign. Thus we can relate unit components of these vectors in the following:

$$\begin{cases} \dfrac{u}{\sqrt{u^2 + v^2}} = -\dfrac{T_{13}}{\sqrt{T_{13}^2 + T_{23}^2}} \\ \dfrac{v}{\sqrt{u^2 + v^2}} = -\dfrac{T_{23}}{\sqrt{T_{13}^2 + T_{23}^2}} \end{cases} \tag{8}$$

Rearranging equation (8) and using equations (5 and 7) we can write:

$$\begin{cases} -u = \left[\mu_s \dfrac{\sqrt{u^2 + v^2}}{P_s \tan(\phi_w)} \right] \dfrac{\partial u}{\partial z} \\ -v = \left[\mu_s \dfrac{\sqrt{u^2 + v^2}}{P_s \tan(\phi_w)} \right] \dfrac{\partial v}{\partial z} \end{cases} \tag{9}$$

In terms of code implementation in MFIX, we can notice after rearranging equation (9) that it is very similar to Johnson and Jackson BC and the same code can, thus, be used for this boundary condition:

$$\begin{cases} -\dfrac{\partial u}{\partial z} - \left[\dfrac{P_s \tan(\phi_w)}{\mu_s \sqrt{u^2 + v^2}} \right] u = 0 \\ -\dfrac{\partial v}{\partial z} - \left[\dfrac{P_s \tan(\phi_w)}{\mu_s \sqrt{u^2 + v^2}} \right] v = 0 \end{cases} \tag{10}$$

One issue with this BC that is not encountered in the JJ BC is that the term $\sqrt{u^2 + v^2}$ has to be expressed explicitly.

In a one dimensional flow situation where, say, the main flow velocity is along the v direction, one can reduce equation (10) assuming $u = 0$ and obtain the following:

$$-\frac{\partial u}{\partial z} - \left[\frac{P_s \tan(\phi_w)}{\mu_s} \right] \frac{u}{|u|} = 0 \tag{11}$$

One can notice that equations (1) and (11) are identical, which is a validation of the limit of equation (10) in a 1-D flow.

For a general surface where *r* is a distance normal to a wall, we can express (noting the normal velocity to wall should be set to zero) Jenkins BC as:

$$\begin{cases} -\dfrac{\partial u}{\partial r} - \left[\dfrac{P_s \tan(\phi_w)}{\mu_s \sqrt{u^2 + v^2 + w^2}} \right] u = 0 \\ -\dfrac{\partial v}{\partial r} - \left[\dfrac{P_s \tan(\phi_w)}{\mu_s \sqrt{u^2 + v^2 + w^2}} \right] v = 0 \\ -\dfrac{\partial w}{\partial r} - \left[\dfrac{P_s \tan(\phi_w)}{\mu_s \sqrt{u^2 + v^2 + w^2}} \right] w = 0 \end{cases} \tag{12}$$