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:

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

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

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

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).

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.