HZDR baseline closures for Euler-Euler modelling of isothermal poly-dispersed multiphase flows with inhomogeneous MUSIG

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The department of Computational Fluid Dynamics at the Helmholtz-Zentrum Dresden – Rossendorf (HZDR) has promoting a baseline concept for the definition of closures for Euler-Euler modelling of poly-dispersed multiphase flows (Lucas et al., 2016, Rzehak et al., 2017).

1. Bubble forces

a. Drag force

$$\mathbf{F}_D = -\frac{3}{4d_B} C_D \rho_L \alpha_G \left|\mathbf{u}_G - \mathbf{u}_L\right| \ (\mathbf{u}_G - \mathbf{u}_L)$$

The drag coefficient for single bubble is calculated according to the work of Ishii and Zuber (1979)

$$\begin{aligned}
C_D &= \max\left(C_{D,sphere}, \min\left(C_{D,ellipse}, C_{D,cap}\right)\right), \text{ where} \\
C_{D,sphere} &= \frac{24}{\mathrm{Re}_p}\left(1 + 0.1\ \mathrm{Re}_p^{0.75}\right) \\
C_{D,ellipse} &= \frac{2}{3}\sqrt{\mathrm{Eo}} \\
C_{D,cap} &= \frac{8}{3}
\end{aligned}$$

where Re_p and Eo are particle Reynolds number and Eötvös number, respectively.

b. Virtual mass force

$$\mathbf{F}_{VM} = -\alpha_G \rho_L C_{VM} \left(\frac{D\mathbf{u}_G}{Dt} - \frac{D\mathbf{u}_L}{Dt}\right)$$

The virtual mass coefficient is set to constant, i.e. $C_{VM} = 0.5$.

c. Lift force

$$\mathbf{F}_L = -C_L \rho_L \alpha_G (\mathbf{u}_G - \mathbf{u}_L) \times rot(\mathbf{u}_L)$$

The lift force coefficient is calculated according to the Tomiyama correlation (Tomiyama, 2002).

$$C_L = \begin{cases} \min[0.288\tanh(0.121\mathrm{Re}_p), f(Eo_d)] & Eo_d < 4 \\ f(Eo_d) \qquad\qquad\qquad\qquad\qquad\qquad\quad for & 4 < Eo_d < 10 \\ -0.27 & Eo_d > 10 \end{cases}$$

$$with \quad f(Eo_d) = 0.00105Eo_d^3 - 0.0159Eo_d^2 - 0.0204Eo_d + 0.474$$

$$Eo_d = \frac{g(\rho_L - \rho_G)d_H^2}{\sigma}, \; d_H = d_B\sqrt[3]{1+0.163Eo^{0.757}}$$

d. Turbulent dispersion force

The turbulent dispersion force is calculated by the Favre averaging drag force (FAD) model (Burns et al., 2004).

$$\mathbf{F}_{TD} = -\frac{3}{4}C_D\frac{\alpha_G}{d_B}\left|\mathbf{u}_G - \mathbf{u}_L\right|\frac{\mu_L^{turb}}{\sigma_{TD}}\left(\frac{\mathrm{grad}\,\alpha_G}{\alpha_G} - \frac{\mathrm{grad}\,\alpha_L}{\alpha_L}\right)$$

with σ_{TD} = 0.9.

e. Wall lubrication force

$$\mathbf{F}^{wall} = \frac{2}{d_B}C_W\rho_L\alpha_G\left|\mathbf{u}_G - \mathbf{u}_L\right|^2\hat{\mathbf{y}}$$

The wall force coefficient C_W is calculated according to the work of Hosokawa et al. (2002)

$$C_W = f(Eo)\left(\frac{d_B}{2y}\right)^2, \quad \text{with } f(Eo) = 0.0217\ Eo$$

and $\hat{\mathbf{y}}$ is the wall normal vector and y is the distance to the wall.

2. Turbulence

a. Liquid phase

The k-ω-SST model with additional source terms for bubble-induced turbulence (BIT) is recommended:

$$\frac{\partial}{\partial t}\left(\alpha_L\rho_L k_L\right) + \nabla\cdot\left(\alpha_L\rho_L\mathbf{u}_L k_L\right)$$
$$= \nabla\cdot\left(\alpha_L\left(\mu_L^{mol} + \frac{\mu_L^{turb}}{\sigma_k}\right)\nabla k_L\right) + \alpha_L\left(\mathbf{T}_L^{Re} : \nabla\mathbf{u}_L - \rho_L\varepsilon_L\right) + S_L^k$$

$$\frac{\partial}{\partial t}\left(\alpha_L\rho_L\varepsilon_L\right) + \nabla\cdot\left(\alpha_L\rho_L\mathbf{u}_L\varepsilon_L\right)$$
$$= \nabla\cdot\left(\alpha_L\left(\mu_L^{mol} + \frac{\mu_L^{turb}}{\sigma_\varepsilon}\right)\nabla\varepsilon_L\right) + \alpha_L\frac{\varepsilon_L}{k_L}\left(C_{\varepsilon P}\mathbf{T}_L^{Re} : \nabla\mathbf{u}_L - C_{\varepsilon D}\rho_L\varepsilon_L\right) + S_L^\varepsilon$$

The BIT source terms, S_L^k and S_L^ε are calculated according to a model derived from DNS (Direct Numerical Simulation) of bubble column (Ma et al., 2017).

$$S_L^k = \min\left(0.18\,\mathrm{Re}_p^{0.23},1\right)\mathbf{F}_D \cdot \left|\mathbf{u}_G - \mathbf{u}_L\right|$$

$$S_L^\varepsilon = 0.3C_D\frac{S_L^k}{\tau}\text{, with } \tau = \frac{d_B}{\left|\mathbf{u}_G - \mathbf{u}_L\right|}$$

The source term in the ω–equation is derived from the relation between k, ε and ω

$$S_L^\omega = \frac{1}{C_\mu k_L}S_L^\varepsilon - \frac{\omega_L}{k_L}S_L^k$$

b. Near-wall treatment

The automatic near-wall treatment presented in Menter et al. (2003) is used.
The flux (wall shear stress) for the momentum equation is computed from

$$F_u = -\rho_L u_\tau u^*$$

$$u^* = \sqrt[4]{\left(\sqrt{\frac{\mu_L}{\rho_L}\left|\frac{\Delta u_L}{\Delta y}\right|}\right)^4 + \left(\sqrt{C_\mu^{1/2}k_L}\right)^4}$$

$$u_\tau = \sqrt[4]{\left(\sqrt{\frac{\mu_L}{\rho_L}\left|\frac{\Delta u_L}{\Delta y}\right|}\right)^4 + \left(\frac{\kappa\mathbf{u}_L}{\ln\left(y^+\right)+C}\right)^4}$$

where $\frac{\Delta u_L}{\Delta y}$ is the velocity gradient over the first cell adjacent to the wall, and for a smooth wall the constant C has a value around 2.28.

The flux for the k-equation is assumed to be zero.

$$F_k = 0$$

For the ω-equation, an algebraic expression is specified instead of the flux, which is a blend between the analytical expression for ω in the logarithmic region and the corresponding expression in the sublayer:

$$\omega_w = \sqrt{\omega_s^2 + \omega_l^2}\ ,$$

$$\text{with } \omega_s = \frac{6\mu_L}{0.075\Delta y^2} \text{ and } \omega_l = \frac{1}{C_\mu^{1/2}\kappa y}$$

c. Gas phase

$$\mu_L^{turb} = \frac{\rho_G}{\rho_L} \cdot \frac{\mu_L^{turb}}{\sigma}$$

The turbulent Prandtl number σ is set to 1.0.

3. The inhomogeneous MUSIG model

The poly-dispersity of bubbles is considered by the inhomogeneous MUSIG model (Krepper et al., 2008), which is a kind of class method. A transport equation for the volume fraction of each size group is solved.

$$\frac{\partial}{\partial t}\left(\alpha_{G,j}\rho_G f_i\right) + \nabla \cdot \left(\alpha_{G,j}\rho_G f_i \,\mathrm{u}_{G,j}\right) = B_{C,i} - D_{C,i} + B_{B,i} - D_{B,i}$$

The terms on the right hand side are birth rate, death rate of the size group i due to coalescence and break of bubbles. These integro-differential terms have to be solved by an appropriate discretization algorithm preserving the bubble number and mass (Liao et al., 2017). In addition, kernels describing the coalescence and breakup rate are required to close the equation.

4. Bubble coalescence & breakup

The models presented in Liao et al. (2015) are used to calculate the coalescence and breakup rate.

a. Coalescence

$$\Gamma(i,j) = \frac{\alpha_{\max}}{\alpha_{\max} - \alpha_r} \left\{ \begin{array}{ll} \left\{ \begin{array}{ll} \frac{\pi}{4}\left(d_i + d_j\right)^2 u_{rel,turb}\ \lambda_{inertial}, & \left(d_i + d_j > \eta\right) \\ 0.5\frac{\pi}{4}\left(d_i + d_j\right)^2 u_{rel,eddy}\ \lambda_{viscous}, & \left(d_i + d_j \le \eta\right) \end{array} \right. & \\ +0.5\frac{\pi}{4}\left(d_i + d_j\right)^2 u_{rel,shear}\ \lambda_{eff} & \\ +0.5\frac{\pi}{4}\left(d_i + d_j\right)^2 u_{rel,buoy}\ \lambda_{eff} & \\ +0.5\frac{\pi}{4}\left(u_{rel,wake,i}\Theta_i + u_{rel,wake,j}\Theta_j\right) & \end{array} \right\},$$

with

$$\lambda_{inertial} = \exp\left\{-C_{eff}\left(\frac{\rho_l d_{eq}}{\sigma}\right)^{0.5} \max\left(u_{rel,turb}, u_{rel,shear}, u_{rel,buoy}\right)\right\}$$

$$\lambda_{viscous} = \exp\left\{-\frac{3\mu_l d_{eq}\dot{\gamma}_{eddy}}{4\sigma} \ln\left[\frac{\pi\sigma d_{eq}^2}{32A_H}\right]^{1/3}\right\} ,$$

$$\lambda_{eff} = \begin{cases} \lambda_{inertial} & \left(d_i + d_j > \eta\right) \\ \lambda_{viscous} & \left(d_i + d_j \le \eta\right) \end{cases}$$

and

$$u_{rel,turb} = C_{turb}\sqrt{2}\varepsilon^{1/3}\left(d_i^{2/3} + d_j^{2/3}\right)^{1/2} \qquad \text{(turbulent fluctuation)}$$

$$u_{rel,eddy} = C_{eddy}\frac{0.5}{\pi}\left(d_i + d_j\right)\dot{\gamma}_{eddy} \qquad \text{(eddy-capture)}$$

$$u_{rel,shear} = C_{shear}\frac{0.5}{\pi}\left(d_i + d_j\right)\dot{\gamma}_b \qquad \text{(velocity shear)} \quad ,$$

$$u_{rel,buoy} = C_{buoy}\left|u_{T,i} - u_{T,j}\right| \qquad \text{(buoyancy)}$$

$$u_{rel,wake,i} = C_{wake,i}u_{T,i}C_{D,i}^{1/3} \qquad \text{(wake-entrainment)}$$

and

$$\Theta_i = \begin{cases} \dfrac{\left(d_i - 0.5d_{crit}\right)^6}{\left[\left(d_i - 0.5d_{crit}\right)^6 + \left(0.5d_{crit}\right)^6\right]} & \left(d_i \ge 0.5d_{crit}\right) \\ 0 & \text{else} \end{cases} ,$$

$$d_{crit} = 4\sqrt{\left(\frac{\sigma}{g\Delta\rho}\right)},\ \eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4},\ d_{eq} = \frac{2d_i d_j}{d_i + d_j},$$

and

$$\dot{\gamma}_{eddy} = \sqrt{\frac{\rho_l\varepsilon_l}{\mu_l}}$$

$$\dot{\gamma}_b = \left[2\left(\frac{\partial u_l}{\partial x}\right)^2 + 2\left(\frac{\partial u_l}{\partial y}\right)^2 + 2\left(\frac{\partial w_l}{\partial z}\right)^2 + \left(\frac{\partial u_l}{\partial y} + \frac{\partial v_l}{\partial x}\right)^2 + \left(\frac{\partial u_l}{\partial z} + \frac{\partial w_l}{\partial x}\right)^2 + \left(\frac{\partial w_l}{\partial y} + \frac{\partial v_l}{\partial z}\right)^2\right]^{1/2}$$

Finally, A_H is the (material dependent) Hamaker constant. For twi air-water interafces, its value is about $3.7\text{x}10^{-20}$J.

Values suggested for the adjusted constants are α_{max}= 0.8, C_{turb}= 1.0, C_{eddy}= 1.0, C_{shear}= 1.0, C_{buoy}= 1.0, C_{wake}= 1.0, C_{eff} = 5.0.

b. Breakup

$$\Omega(i,j)=\begin{cases}\dfrac{1}{d_i\sqrt{\rho_l}}\sum_k\sqrt{\tau_k\left(d_i\right)-\tau_{crit}\left(d_i,d_j\right)} & \left(\tau_k>\tau_{crit}\right)\\ 0 & \left(\tau_k\le\tau_{crit}\right)\end{cases},$$

with

$$\tau_k\left(d_i\right)=\begin{cases}\tau_{turb}=B_{turb}\cdot 0.5\rho_l u_{turb,i}^2\approx B_{turb}\rho_l\left(\varepsilon d_i\right)^{2/3} & \left(d_i>\eta\right)\\ \tau_{shear}=B_{shear}\cdot\mu_l\dot{\gamma}_b & \\ \tau_{eddy}=B_{eddy}\cdot\mu_l\dot{\gamma}_{eddy} & \left(d_i\le\eta\right)\\ \tau_{fric}=B_{fric}\cdot 0.5\rho_l u_{T,i}^2 C_{D,i} & \end{cases},$$

and

$$\tau_{crit}\left(d_i,d_j\right)=\max\left(\tau_{crit,1},\tau_{crit,2}\right)$$

$$\tau_{crit,1}=\frac{6\sigma}{d_i}\left[\left(\frac{d_j}{d_i}\right)^2+\left(\frac{d_k}{d_i}\right)^2-1\right]$$

$$\tau_{crit,2}=\frac{\sigma}{\min\left(d_k,d_j\right)}$$

$$d_k=\left(d_i^3-d_j^3\right)^{1/3}$$

Values suggested for the adjusted constants are B_{turb}= 1.0, B_{eddy}= 1.0, B_{shear}= 1.0, B_{fric}= 0.25 are adjusted parameters.

5. References

Lucas, D. et al., 2016. A strategy for the qualification of multi-fluid approaches for nuclear reactor safety. *Nuclear Engineering and Design*, **299**, 2-11

Rzehak, R. et al., 2017. Unified modelling of bubbly flows in pipes, bubble columns, and airlift columns. *Chemical Engineering Science*, **157**, 147-158

Ishii, M. and Zuber, N. 1979. Drag coefficient and relative velocity in bubbly, droplet or particulate flows. *AIChE Journal*, **25**, 843-853

Tomiyama, A. et al. 2002. Transverse migration of single bubbles in simple shear flows. *Chemical Engineering Science*, **57**, 1849-1858

Burns, A. et al., 2004. The Favre averaged drag model for turbulent dispersion in Eulerian multi-phase flows. *5th International Conference on Multiphase Flow, ICMF'04*, Yokohama, Japan, May 30-June 4, 2004

Hosokawa, S. et al., 2002. Lateral migration of single bubbles due to the presence of wall. *Proceedings of ASME FEDSM'02, ASME 2002 Fluids Engineering Division Summer Meeting*, Montreal, Quebec, Canada, July 14-18, 2002

Ma, T. et al., 2017. Direct numerical simulation-based Reynolds-averaged closure for bubble-induced turbulence. *Physical Review Fluids*, **2**, 034301
Menter, F. et al., 2003. The SST turbulence model with improved wall treatment for heat transfer predictions in gas turbines. Proceedings of the International Gas Turbine Congress 2003, Tokyo, November 2-7, 2003
Krepper, E. et al., 2008. The inhomogeneous MUSIG model for the simulation of polydispersed flows. *Nuclear Engineering and Design*, **238**, 1690-1702
Liao, Y. et al., 2017. Approximate solution of population balance equation for binary breakup processes. *Chemical Engineering Science*, submitted
Liao, Y. et al., 2015. Baseline closure model for dispersed bubbly flow: Bubble coalescence and breakup. *Chemical Engineering Science*, **122**, 336-349