Numerical study on fluidization of binary mixture of particles using SOM- KTGF-MP

(second-order moment of kinetic theory of granular flow for multi-type particles)

Dan Sun

National Institute of Clean-and-Low-Carbon Energy, China

2023 NETL Workshop on Multiphase Flow Science, 1st - 2nd Aug. 2023

Kinetic theory of granular flow (KTGF)

Numerical method for fluidization

- Lagrangian (CFD-DEM ...)
- Eulerian (TFM with KTGF)



Large-scale simulation for fluidized bed using Eulerian method with KTGF **KTGF**





Challenge of Eulerian method for fluidization

Multi-scale structure of gas-particle flow in fluidized risers

Core-annulus pattern

- dilute particles flow upward in the core of the reactor.
- dense particles flow downward close to the wall.

EMMS model for drag correction [Li 1987]

- multi-scale structure: dilute & dense
- drag force modelling for dilute & dense phases separately.

Multi-scale structure in risers [EMMS 1987]

- Dense phase: particle clusters
- Dilute phase: dispersed particles



KTGF simulation for dense & dilute phase

Particles in dense phase concentration well predicted by KTGF



Exp.

KTGF (Jung 2006)

Particles in dilute phase concentration failed in predicting velocity gradient using classic KTGF

KTGF

volume fraction

 $\begin{array}{c} 0 & 0.0002 & 0.0004 & 0.0006 & 0.0008 \\ (1) Classic KTGF, ewt = -0.999 \end{array}$

(2) Classic KTGF, ewt = -0.99

(3) Classic KTGF, ewt = -0.95



Second-order moment KTGF (SOM-KTGF)

Particles in dilute phase concentration Velocity gradient were well predicted using SOM-KTGF



SOM-KTGF model

Solve M_{ij} by PDE

$$\frac{\partial}{\partial t} \left(\varepsilon_{s} \rho_{s} M_{ij} \right) + \frac{\partial}{\partial x_{k}} \left(\varepsilon_{s} \rho_{s} u_{sk} M_{ij} \right) = \\ -\frac{\partial}{\partial x_{k}} \left(\varepsilon_{s} \rho_{s} A_{s} M_{kij} \right) - \frac{\partial}{\partial x_{i}} \left(\varepsilon_{s} \rho_{s} B_{s} M_{jkk} \right) - \frac{\partial}{\partial x_{j}} \left(\varepsilon_{s} \rho_{s} B_{s} M_{ikk} \right) \\ -\frac{\partial}{\partial x_{k}} \left(\kappa^{c} \frac{\partial \Theta}{\partial x_{k}} \delta_{ij} \right) - \frac{\partial}{\partial x_{i}} \left(\kappa^{c} \frac{\partial \Theta}{\partial x_{j}} \right) - \frac{\partial}{\partial x_{j}} \left(\kappa^{c} \frac{\partial \Theta}{\partial x_{i}} \right) \\ -2\beta \left(M_{ii} - \overline{C_{qi} C_{si}} \right) + \gamma_{ii}$$

SOM-KTGF

SOM-KTGF extends the capability of KTGF to predict particles from the dense to median concentration.

[Powder Tech. 390: 354-368]

Conservation equation for particles, KTGF

Conservation of momentum in KTGF

$$\frac{\partial}{\partial t}(\varepsilon_{s}\rho_{s}u_{si}) + \frac{\partial}{\partial x_{j}}(\varepsilon_{s}\rho_{s}u_{si}u_{sj}) = -\frac{\partial}{\partial x_{j}}(\rho_{s}\varepsilon_{s}A_{s}M_{ij})$$
$$-\varepsilon_{s}\frac{\partial p_{g}}{\partial x_{i}} - \frac{\partial p_{s}^{c}}{\partial x_{i}} + \frac{\partial \tau_{sij}^{c}}{\partial x_{j}} + \beta u_{gs,i} + \varepsilon_{s}\rho_{s}g_{i}$$

Second-order moment of fluctuating velocity of particles,

$$\boldsymbol{M_{ij}} = \begin{bmatrix} C_i C_i & C_i C_j & C_i C_k \\ C_i C_j & C_j C_j & C_j C_k \\ C_i C_k & C_j C_k & C_z C_z \end{bmatrix}$$

Fluctuating velocity of particles

$$C_i = u_i - \overline{u_i}$$
$$A_s = 1 + \frac{4}{5}(1+e)\varepsilon_s g_0$$

Classic-KTGF, solve M_{ij} by

<u>Normal stress</u>, i = j

by Granular temperature, θ , PDE.

KTGF

 $\langle M_{ii} \rangle = M_{ii} + M_{jj} + M_{kk} = 3\theta$

Shear stress , $i \neq j$

by pseudo kinetic(eddy) viscosity

$$\boldsymbol{M_{ij}} = \left[\frac{10\rho_s d_p \sqrt{\theta \pi}}{96(1+e)g_0}\right] \times \left\{\frac{1}{2} \left[\nabla u_s + (\nabla u_s)^T\right]\right\}$$

Boussinesq hypothesis

Equilibrium status can be achieved byfrequent interparticle collisions indense particle flow.



Fluidized riser

Normal stress

<*M*ii>

Granular temperature (m/s)²

0.1

Prediction using classic KTGF & SOM-KTGF

Normal stress



Anisotropic ratio of normal stress > 1, high when volume fraction $\alpha_s < 0.01$.

Shear stress by Classic KTGF higher than stress by SOM-KTGF, esp. when $\alpha_s < 0.01$.

1E-3

Volume fraction of particles

Second order moment by

viscosity in Classic KTGF PDE in SOM-KTGF

0.01

Shear Stress

Mii

SOM-KTGF is essential for dilute-phase particles, when $\alpha_s < 0.01$.

Shear stress

0.8

0.4

0.0

-0.4

-0.8

1E-3

0.01

Second order moment $(m/s)^2$

SOM-KTGF

Simulation with SOM-KTGF(FW-SOM)

Spouted fluidized bed



- High fidelity prediction.
- Able to describe the interface between the spouted and annulus zone.
- Volume fraction of particles across dense to dilute regions.

Fluidized riser



- Four-way coupled SOM (FW-SOM)
- Increasing with the particle volume fraction, anisotropic ratios of turbulent intensity,
 - increase in dilute phase
 - reduce in dense phase.

SOM-KTGF well predicts both dense & dilute phases, from dense to median concentrations.

Dense concentration inter-particle collision

7



Dilute concentration Non-equilibrium

SOM-KTGF for Multi-type Particles

Conservation PDE

Continuity equation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m u_{m,i}) = 0$$

Momentum equation

$$\frac{\partial}{\partial t}(\alpha_{m}\rho_{m}u_{mi}) + \frac{\partial}{\partial x_{j}}(\alpha_{m}\rho_{m}u_{m,i}u_{m,j}) = \sum_{l=1,m} \left[\chi(m_{m}C_{m,i})_{l}\right] - \frac{\partial}{\partial x_{j}}\left(\alpha_{m}\rho_{m}M_{m,ij} + \sum_{l=1,m} \left[\psi(m_{m}C_{m,i})_{l}\right]\right) + F_{m,i} - \alpha_{m}\frac{\partial p_{g}}{\partial x_{i}}$$

Second-order moment conservation

$$\begin{aligned} &\frac{\partial}{\partial t} \left(\alpha_m \rho_m M_{m,ij} \right) + \frac{\partial}{\partial x_k} \left(\alpha_m \rho_m u_{m,k} M_{m,ij} \right) = + \Pi_{d,m,ij} \\ &+ \sum_{l=1}^{l=1} \left[\chi \left(m_m C_{m,i} C_{m,j} \right)_l \right] - \frac{\partial}{\partial x_k} \left(\alpha_m \rho_m M_{m,kij} + \sum_{l=1}^{l=1} \left[\psi_k \left(m_m C_{m,i} C_{m,j} \right)_l \right] \right) \\ &- \left\{ \left[\alpha_m \rho_m M_{m,ik} + \sum_{l=1}^{l=1} \left[\psi_k \left(m_m C_{m,i} \right)_l \right] \right] \frac{\partial u_{m,ij}}{\partial x_k} + \left[\alpha_m \rho_m M_{m,jk} + \sum_{l=1}^{l=1} \left[\psi_k \left(m_m C_{m,j} \right)_l \right] \right] \frac{\partial u_{m,ij}}{\partial x_k} \right\} \end{aligned}$$

SOM-KTGF-MP

- Derived based on kinetic theory with interparticle collisions.
- Momentum exchange between particles and multi-type particles, $\chi(m_m C_{m,i})_l$.
- Energy/Stress exchange between particles and multi-type particles, $\chi(m_m C_{m,i} C_{m,j})_l$.



SOM-KTGF-MP and classic KTGF-MP

Flux due to collisions in momentum equations (pressure tensor)

SOM-KTGF-MP

$$\psi_{j} (mC_{m,i})_{l} = \frac{\pi d_{ml}^{3}}{6} \frac{m_{l}m_{m}}{m_{0}} (1 + e_{ml})g_{ml}n_{l}n_{m} \left(\frac{m_{l}m_{m}}{4\Theta_{l}\Theta_{m}}\right)^{\frac{3}{2}} \\ + \frac{1}{5} \frac{m_{l}^{2}m_{m}^{2}}{m_{0}^{2}} \left(\frac{a_{l,ij}^{(2)}}{\Theta_{m}^{2}} + \frac{a_{m,ij}^{(2)}}{\Theta_{l}^{2}}\right)R_{3} \\ \times \left\{ -\frac{m_{l}m_{m}}{m_{0}} \frac{d_{ml}}{5} \frac{1}{\sqrt{\pi}}R_{1} \left[\frac{1}{\Theta_{l}} \left(\frac{\partial u_{l,k}}{\partial x_{k}} + \frac{\partial u_{l,i}}{\partial x_{j}} + \frac{\partial u_{l,j}}{\partial x_{i}}\right) + \frac{1}{\Theta_{m}} \left(\frac{\partial u_{m,k}}{\partial x_{k}} + \frac{\partial u_{m,i}}{\partial x_{j}} + \frac{\partial u_{m,j}}{\partial x_{i}}\right) \right] \right\}$$

Classic KTGF-MP (Iddir & Arastoopour [2005])

$$\psi(mC_{m,i})_{l} = \frac{d_{ml}^{3}}{48} \frac{m_{l}m_{m}}{m_{0}} (1 + e_{ml})g_{ml}n_{l}n_{m} \left(\frac{m_{l}m_{m}}{\Theta_{l}\Theta_{m}}\right)^{\frac{3}{2}} \\ \times \left\{ \pi R_{0}\bar{I} - \frac{\sqrt{\pi}}{3} d_{ml} \frac{m_{l}m_{m}}{m_{0}} R_{1} \left[\frac{6}{5} \left(\frac{\nabla^{s} \vec{v_{m}}}{\Theta_{m}} + \frac{\nabla^{s} \vec{v_{l}}}{\Theta_{l}}\right) \\ + \left(\frac{\nabla \cdot \vec{v_{m}}}{\Theta_{m}} + \frac{\nabla \cdot \vec{v_{l}}}{\Theta_{l}}\right) \bar{I} \right] \right\}$$

 $\frac{\text{SOM-KTGF}(l=m)}{\psi_j(m_m c_{m,i})_m} = 2\rho_m \alpha_m^2 (1+e_m) g_0 \Theta_m \delta_{ij}$ $-\frac{4}{5} \rho_m \alpha_m^2 \sigma_m (1+e_m) g_0 \sqrt{\frac{\Theta_m}{\pi}} \begin{bmatrix} \left(\frac{\partial u_{mi}}{\partial x_j} + \frac{\partial u_{mj}}{\partial x_i}\right) \\ + \frac{\partial u_{mk}}{\partial x_k} \delta_{ij} \end{bmatrix}$ $+\frac{4}{5} \rho_m \alpha_m^2 (1+e_m) g_0 a_{m,ij}^{(2)}$

SOM-KTGF-MP for fluidization

Fluidized riser with two sizes of particles.



- Binary particles moving together.
- *d_p* = 120 μm, 185 μm.



- Simulation comparison with experimental data.
- Velocities of binary particles were close.

SOM-KTGF-MP for fluidization

Fluidized riser with two types (density) of particles.



- More high-density particles at bottom.
- $\rho_p = 655 \text{ kg/m}^3$, 2400 kg/m³.



- Granular temp. higher for low-density particles.
- Anisotropic turbulence high when $\alpha_s < 0.01$.

Conclusion

- SOM-KTGF, as an Eulerian method, extends the capability of KTGF to predict particles from the dense to median concentrations.
- SOM-KTGF (FW-SOM) can well predict both the dense and dilute phases in fluidization with multi-scale structures.
- SOM-KTGF is essential in the dilute phase of particles in fluidization,
 - when the volume fraction of particles is less than 0.01,
 - where exist particle-particle collisions, but less frequent to be equilibrium and unable to satisfy the Boussinesq hypothesis.
- SOM-KTGF-MP was proposed to predict particle flows with various types of particles with different diameters and densities, in the Eulerian framework.
- The simulations of two-size and two-type particles in fluidized risers demonstrated the capability of SOM-KTGF-MP.

Acknowledge

Funded by Education Ministry of China through the Grant Excellent Doctoral Student (学术新人奖) 2010, and finally hosted by National Institute of Clean-and-Low-Carbon Energy.