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Some accuracy related issues in two-fluid hydrodynamic sub-grid modeling of gas-solid riser flows

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- Filtered two-fluid modeling applied in large scale simulations (LSS) of fluidized gas-solid flows require closure models for filtered parameters.
- Closure models may be derived from results of highly resolved simulations (HRS) with microscopic two-fluid modeling.
- In usual HRS, gas sub-grid turbulence is filtered, and related effects over the predicted meso-scale flow field are lost.



- An analysis is performed where gas phase sub-grid turbulence is artificially induced through a forcing function procedure.
- Highly resolved simulations are performed for fluidized gas-solid flows typical of risers, applying microscopic two-fluid modeling over periodic boundaries, under different domain average solid fractions and gas flow Reynolds numbers, with and without gas sub-grid turbulence.
- Filtering is performed over the predictions, and relevant meso-scale filtered parameters are derived.
- Then, the filtered parameters are evaluated as for their possible correlation to gas sub-grid turbulence.

Microscopic two-fluid formulation

 $\frac{\partial}{\partial t} \left(\rho_{g} \phi_{g} \right) + \nabla \cdot \left(\rho_{g} \phi_{g} \boldsymbol{v}_{g} \right) = 0$ $\frac{\partial}{\partial t} (\rho_{\rm s} \phi_{\rm s}) + \nabla \cdot (\rho_{\rm s} \phi_{\rm s} \boldsymbol{v}_{\rm s}) = 0$ Forcing on gravity $\frac{\partial}{\partial t} \left(\rho_{g} \phi_{g} \boldsymbol{v}_{g} \right) + \nabla \cdot \left(\rho_{g} \phi_{g} \boldsymbol{v}_{g} \boldsymbol{v}_{g} \right) = - \phi_{g} \nabla \cdot \boldsymbol{\sigma}_{g} - \boldsymbol{M}_{I} + (1 + c_{t} f) \rho_{g} \phi_{g} \boldsymbol{g}$ $\frac{\partial}{\partial t} (\rho_{s} \phi_{s} \boldsymbol{v}_{s}) + \nabla \cdot (\rho_{s} \phi_{s} \boldsymbol{v}_{s} \boldsymbol{v}_{s}) = - \nabla \cdot \boldsymbol{\sigma}_{s} - \phi_{s} \nabla \cdot \boldsymbol{\sigma}_{g} + \boldsymbol{M}_{I} + \rho_{s} \phi_{s} \boldsymbol{g}$ $\boldsymbol{\sigma}_{\ell} = \left[\mathbf{P}_{\ell} - \left(\lambda_{\ell} + \frac{2}{3} \mu_{\ell} \right) (\nabla \cdot \boldsymbol{v}_{\ell}) \right] \boldsymbol{I} - 2 \mu_{\ell} \boldsymbol{s}_{\ell} \qquad \boldsymbol{s}_{\ell} = \frac{1}{2} \left[\nabla \boldsymbol{v}_{\ell} + (\nabla \boldsymbol{v}_{\ell})^{\mathrm{T}} \right] - \frac{1}{2} \left(\nabla \cdot \boldsymbol{v}_{\ell} \right) \boldsymbol{I}$ $\ell = g, s$ $\mu_{s} = \frac{(2+\alpha)}{3} \left\{ \frac{\xi^{*}}{g_{0}n(2-n)} \left(1 + \frac{8}{5}\phi_{s}\eta g_{0} \right) \left(1 + \frac{8}{5}\eta(3\eta - 2)\phi_{s}g_{0} \right) + \frac{6}{5}\eta\mu_{b} \right\} \qquad P_{s} = \rho_{s}\phi_{s} \left(1 + 4\eta\phi_{s}g_{0} \right) \Theta$ $M_{\rm I} = \beta (v_g - v_s)$ Drag model - Wen and Yu (1966) $\frac{3}{2} \left[\frac{\partial}{\partial t} (\rho_{s} \phi_{s} \Theta) + \nabla \cdot (\rho_{s} \phi_{s} \boldsymbol{v}_{s} \Theta) \right] = -\boldsymbol{\sigma}_{s} : \nabla \boldsymbol{v}_{s} + \nabla \cdot (\kappa_{s} \nabla \Theta) + \Gamma_{slip} - J_{coll} - J_{vis}$ Kinetic Theory of Granular Flows -Lun et al. (1984)

(A complete formulation can be found in Agrawal et al., 2001)

- Restination of the strong and the

Forcing function derived from an Uhlenbeck-Ornstein stochastic process (Pope, 2000; Eswaram & Pope, 1988):

$$f_{t+\Delta t} = \left(1 - \frac{\Delta t}{\tau^*}\right) f_t + \sqrt{\frac{2\Delta t \sigma^2}{\tau^*}} R_G$$

Δt - time step.

- σ^2 variance of a flow relevant parameter with normal distribution.
- τ^* characteristic time scale associated to the dominant frequency in the temporal series of the concerning parameter.
- R_G ramdomic number with normal distribution determined by Park-Miller's algorithm.

Filtered parameters



$$\begin{split} P_{\text{fil},g} &= \widetilde{P}_{g} - \frac{2}{3} \mu_{g} \left(\nabla \cdot \widetilde{\mathbf{v}}_{g} \right) \\ P_{\text{fil},s} &= \overline{P}_{s} - \overline{\left(\lambda_{s} + \frac{2}{3} \mu_{s} \right)} \overline{\left(\nabla \cdot \mathbf{v}_{s} \right)} \\ \mu_{\text{fil},s} &= \overline{\mu}_{s} \\ H &= 1 - \frac{\beta_{\text{eff}}}{\overline{\beta}} \\ \beta_{\text{eff}} &= \frac{\overline{\beta}(\overline{\mathbf{v}}_{g} - \overline{\mathbf{v}}_{s})}{(\widetilde{\mathbf{v}}_{g} - \widetilde{\mathbf{v}}_{s})} - \frac{\left[\overline{\phi}_{s} \nabla P_{g} - \overline{\phi}_{s} \nabla \overline{P}_{g}\right]}{(\widetilde{\mathbf{v}}_{g} - \widetilde{\mathbf{v}}_{s})} \\ \end{split}$$

$$\begin{aligned} P_{\text{res},\ell} &= \frac{1}{3} \text{tr}(\overline{\mathbf{r}}_{\ell}^{\prime}) \\ \mu_{\text{res},\ell} &= \frac{1}{2} \left[\nabla \widetilde{\mathbf{v}}_{\ell} + \left(\nabla \widetilde{\mathbf{v}}_{\ell} \right)^{T} \right] - \frac{1}{3} \left(\nabla \cdot \widetilde{\mathbf{v}}_{\ell} \right) \mathbf{I} \qquad \ell = g,s \\ \mathbf{v}_{\ell} &= \rho_{\ell} \overline{\phi}_{\ell} \widetilde{\mathbf{v}}_{\ell} \mathbf{v}_{\ell} - \rho_{\ell} \overline{\phi}_{\ell} \widetilde{\mathbf{v}}_{\ell} \\ |\mathbf{E}| &= \sqrt{\frac{1}{2} \mathbf{E} : \mathbf{E}^{T}} = \sqrt{\frac{1}{2} \sum \left(\mathbf{E}_{\text{ij}} \mathbf{E}_{\text{ij}} \right)} \\ |\mathbf{E}_{\text{shear}}| &= \sqrt{\frac{1}{2} \sum \left(\mathbf{E}_{\text{ij}} \mathbf{E}_{\text{ij}} \right)} \end{aligned}$$

Method



- A square filter box is defined embracing a number of grid cells, which is made to sweep all over the domain while calculating inside averages (i.e. filtered data).
- Filtered data are classified while statistically averaged for ranges of suitable markers (binning).
- Filtered solid volume fraction, filtered slip velocity and filtered kinetic energy of solid velocity fluctuations are assumed as suitable markers:

$$\overline{\phi}_{s} \qquad \widetilde{v}_{slip,y} = \widetilde{v}_{g,y} - \widetilde{v}_{s,y} \qquad k_{s} = \frac{1}{2} \underbrace{v_{s,i}' v_{s,i}''}_{i} \cong \frac{1}{2} \frac{tr(\tau_{s,ij}')}{\rho_{s} \overline{\phi}_{s}}$$



Simulations

Simulations were performed with the microscopic two-fluid model of MFIX, for:

- all periodic boundaries
- under prescribed domain average solid fraction and axial gas flux
- 16 cm x 16 cm domain
- 128 x 128 grids

Particulate and gas properties:

$$d_p = 7.5 \times 10^{-5} \text{ m}$$
 $\rho_s = 1500 \text{ kg/m}^3$ $e = 0.9$
 $\rho_g = 1.3 \text{ kg/m}^3$ $\mu_g = 1.8 \times 10^{-5} \text{ kg/(ms)}$ $c_t = 0.06$



Forcing set up

- Fede and Simonin (2006) generated a steady turbulent flow applying Eswaran and Pope's stochastic spectral forcing in Fourier space under gas conditions very close to those applied in the current work.
- Their procedure provided eddies of 12.8 mm (with an average turbulent kinetic energy of 0.00437 m²/s² for a 2D condition), which suits our analysis since we apply numerical grids one order of magnitude smaller than that length. Accounting for that, we currently enforce a gas sub-grid turbulence just as provided by Fede and Simonin.
- As an approximation, the characteristic time scale is replaced with the Lagrangian integral time scale that is provided, and forcing is applied in the physical space over the gravitational term in our gas momentum equation.
- Owing to those assumptions, the resulting turbulence field turns out distorted, so that some calibration procedure is required, which is performed through a forcing multiplying coefficient set in order to recover the correct average turbulent kinetic energy of the turbulent field (i.e. 0.00437 m²/s² for a 2D condition).



From the proposed procedure:





PDFs – to evaluate the importance ranges of the variables





Results - drag coefficiente correction



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Results – filtered solid pressure







Results – filtered solid dynamic viscosity



Results – filtered solid granular temperature





Results – residual pressure for both the phases





Results – filtered kinetic energy of the gas velocity fluctuations







- No significant effects of gas sub-grid turbulence was found for a particular high Stokes number particulate.
- The observed insensitivity of the meso-scale flow to the sub-grid turbulence of the gas phase may be a consequence of the imposition of inappropriate markers (as the statistical averaging that is performed inside bins may be hiding hydrodynamic effects).
- Further work is required for different gas sub-grid turbulence levels and particulates.
- A rigorous reassessment of markers relevance is a major need.



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Thank you very much!