Supplementary Material: Guide for Employing Inhomogeneity-Dependent Constitutive Closures for the Fluid-Particle Drag Force

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1 Introduction

This Supplementary Material provides a detailed guide for employing the inhomogeneity-dependent drag models that were developed over the course of this study as constitutive relations for larger-scale simulations of fluidized beds. The extent of inhomogeneities is quantified by one of two sub-grid quantities: the scalar variance of the particle volume fraction and a normalized measure for the drift flux. Each of these sub-filter quantities is estimated using a scale-similar approach. The scalar variance of the particle volume fraction, $\overline{(\phi')^2}$, is defined as:

$$\overline{(\phi')^2} = \overline{\phi^2} - \overline{\phi}^2. \tag{1}$$

The drift flux, $\overline{\phi}\widetilde{\boldsymbol{v}}_{drift}$, is defined as:

$$\overline{\phi}\widetilde{\boldsymbol{v}}_{drift} = \overline{\boldsymbol{u}_{slip}\phi} - \widetilde{\boldsymbol{u}}_{slip}\overline{\phi}, \tag{2}$$

A normalized measure for the drift flux is given as:

$$v_d = \frac{\left(\overline{\phi}\widetilde{\boldsymbol{v}}_{drift}\right)\cdot\widetilde{\boldsymbol{u}}_{slip}}{\widetilde{\boldsymbol{u}}_{slip}\cdot\widetilde{\boldsymbol{u}}_{slip}}. \tag{3}$$

Since the constitutive closures for the fluid-particle drag force derived in the current study are applied to larger-scale simulations of fluidized beds at the scale of the base fluid grid, $\overline{\phi}$ is defined as the particle volume fraction at the base grid scale, and $\widetilde{\boldsymbol{u}}_{slip}$ is the slip velocity at the base grid scale. In terms of these quantities, the dimensionless drag force, F, is defined as:

$$F = \frac{\overline{\boldsymbol{F}}_{fp}\cdot\widetilde{\boldsymbol{u}}_{slip}}{3\pi\mu_f d_p\widetilde{\boldsymbol{u}}_{slip}\cdot\widetilde{\boldsymbol{u}}_{slip}}, \tag{4}$$

where μ_f is the fluid viscosity, d_p is the particle diameter, and $\overline{\boldsymbol{F}}_{fp}$ is the fluid-particle interaction force per particle.

Section 2 in this document focuses on the $\overline{(\phi')^2}$-dependent drag model, and section 3 details the v_d-dependent drag model.

2 $\overline{(\phi')^2}$-dependent drag model

The $\overline{(\phi')^2}$-dependent drag model is proposed as an interpolation of the drag at the high and low St limits:

$$F\left(\overline{\phi}, \tilde{St}, \overline{(\phi')^2}\right) = \alpha\left(\tilde{St}\right)F_{high\,St}\left(\overline{\phi}, \overline{(\phi')^2}\right) + \left(1-\alpha\left(\tilde{St}\right)\right)F_{low\,St}\left(\overline{\phi}, \overline{(\phi')^2}\right), \tag{5}$$

where the interpolation function, α, is found to be:

$$\alpha\left(\tilde{St}\right) = \frac{1}{2}\left(1 + \frac{\tilde{St}-7}{\tilde{St}+7}\right). \tag{6}$$

In equations 5 and 6, the modified Stokes number, $\tilde{St}$, is defined as:

$$\tilde{St} = \frac{\rho_p \left|\widetilde{\boldsymbol{u}}_{slip}\right| d_p}{18\mu_f \left(1-\overline{\phi}\right)}. \tag{7}$$

In equation 5, the high and low St limit drag relations are written as:

$$F_{high\,St}\left(\overline{\phi}, \overline{(\phi')^2}\right) = F_{0,high\,St}\left(\overline{\phi}\right) - a_{high\,St}\left(\overline{\phi}\right)\frac{\overline{(\phi')^2}/b_{high\,St}\left(\overline{\phi}\right)}{1+\overline{(\phi')^2}/b_{high\,St}\left(\overline{\phi}\right)}, \tag{8}$$

$$F_{low\,St}\left(\overline{\phi}, \overline{(\phi')^2}\right) = F_{0,low\,St}\left(\overline{\phi}\right) - a_{low\,St}\left(\overline{\phi}\right)\frac{\overline{(\phi')^2}/b_{low\,St}\left(\overline{\phi}\right)}{1+\overline{(\phi')^2}/b_{low\,St}\left(\overline{\phi}\right)}, \tag{9}$$

In equation 8, $F_{0,high\,St}$, $a_{high\,St}$, and $b_{high\,St}$ are defined as:

$$F_{0,high\,St}\left(\overline{\phi}\right) = 8.54\frac{\overline{\phi}}{1-\overline{\phi}} + \left(1-\overline{\phi}\right)^3\left(1+4.11\sqrt{\overline{\phi}}\right), \tag{10}$$

$$a_{high\,St}\left(\overline{\phi}\right) = 5.70 - 221\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{2.5}\left(1-\frac{\overline{\phi}}{\phi_{max}}\right)^4, \tag{11}$$

$$b_{high\,St}\left(\overline{\phi}\right) = 0.0220 - 240\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{6}\left(1-\frac{\overline{\phi}}{\phi_{max}}\right)^{10}, \tag{12}$$

while in equation 9, $F_{0,low\,St}$, $a_{low\,St}$, and $b_{low\,St}$ are defined as:

$$F_{0,low\,St}\left(\overline{\phi}\right) = 6.69\frac{\overline{\phi}}{1-\overline{\phi}} + \left(1-\overline{\phi}\right)^3\left(1+4.09\sqrt{\overline{\phi}}\right), \tag{13}$$

$$a_{low\,St}\left(\overline{\phi}\right) = 9.39 - 2100\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{3}\left(1-\frac{\overline{\phi}}{\phi_{max}}\right)^7, \tag{14}$$

$$b_{low\,St}\left(\overline{\phi}\right) = 0.0220 - 283\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{5}\left(1-\frac{\overline{\phi}}{\phi_{max}}\right)^{12}. \tag{15}$$

In all of these equations, $\phi_{max} = 0.64$.

Using equations 5-15, the $\overline{(\phi')^2}$-dependent drag model is defined. However, since $\overline{(\phi')^2}$ is a sub-grid quantity, a scale-similar approach is needed to estimate it. This methodology is detailed in section 2.1.

2.1 Scale-similar approach for estimating $\overline{(\phi')^2}$

Since $\overline{(\phi')^2}$ is a sub-grid scale measure for the extent of inhomogeneities, we employ a scale-similar approach to estimate this quantity. In order to utilize this approach, $\overline{(\phi')^2}$ is estimated using the following scale-similar form:

$$\overline{(\phi')^2} = \kappa_1' f_1\left(\frac{\overline{\phi}}{\phi_{max}}\right) g_1'\left(\frac{\Delta_f}{d_p}\right). \tag{16}$$

In equation 16, $f_1\left(\overline{\phi}/\phi_{max}\right)$ is defined as:

$$f_1\left(\frac{\overline{\phi}}{\phi_{max}}\right) = \left(\frac{\overline{\phi}}{\phi_{max}}\right)^{n_1}\left(1-\frac{\overline{\phi}}{\phi_{max}}\right)^{m_1}, \tag{17}$$

where $n_1 = 1.37$, $m_1 = 3.00$, and $\phi_{max} = 0.64$. For the purposes of applications to larger-scale systems, $g_1'\left(\Delta_f/d_p\right)$ is defined as:

$$g_1'\left(\frac{\Delta_f}{d_p}\right) = \left(\frac{\Delta_f}{d_p}\right)^2, \tag{18}$$

where Δ_f is the base fluid grid size of the larger-scale simulation system.

The quantity, $\kappa_1^{'}$, which scales with the extent of inhomogeneities present in a fluidized system, is computed as:

$$\kappa_1^{'} = \frac{\widehat{\overline{\phi}^2} - \widehat{\overline{\phi}}^2}{f_1\left(\widehat{\overline{\phi}}/\phi_{max}\right) g_1^{'}\left(\Delta_{f,test}/d_p\right) - f_1\,\widehat{\left(\overline{\phi}/\phi_{max}\right) g_1^{'}}\left(\Delta_f/d_p\right)}, \tag{19}$$

where $\Delta_{f,test}$ is the test filter size. For the purposes of applying the constitutive drag relation to larger-scale systems, $\Delta_{f,test}$ is chosen to be $3\Delta_f$, as this is the minimum test filter size for a simulation with a base fluid grid size of Δ_f. With $\Delta_{f,test} = 3\Delta_f$, the test-filtered quantities are computed as:

$$\hat{q}_{i,j,k} = \frac{1}{27}\sum_{i'=i-1}^{i+1}\left(\sum_{j'=j-1}^{j+1}\left(\sum_{k'=k-1}^{k+1} q_{i',j',k'}\right)\right), \tag{20}$$

where q is a generic system quantity. The use of a test filter in this approach takes advantage of the assumption that due to scale-similarity, the value of $\kappa_1^{'}$ does not change over a range of length scales. Using equations 16-19, the sub-grid quantity $\overline{(\phi')^2}$ can be estimated at the base fluid grid size over the entire fluidized system. Plugging this estimate of $\overline{(\phi')^2}$ into equations 8 and 9, the $\overline{(\phi')^2}$-dependent drag model can be fully implemented as a constitutive closure for larger-scale simulations of fluidized beds.

3 v_d-dependent drag model

The drift flux-dependent drag model is defined as follows:

$$F\left(\overline{\phi}, \tilde{St}, v_d\right) = F_0\left(\overline{\phi}, \alpha\left(\tilde{St}\right)\right) - a\left(\overline{\phi}\right)\frac{v_d/b\left(\overline{\phi}\right)}{1 + v_d/b\left(\overline{\phi}\right)}, \tag{21}$$

where $F_0\left(\overline{\phi}, \alpha\left(\tilde{St}\right)\right)$ is defined as:

$$F_0\left(\overline{\phi}, \alpha\left(\tilde{St}\right)\right) = \frac{F_{0,high\,St}\left(\overline{\phi}\right) + F_{0,low\,St}\left(\overline{\phi}\right)}{2} + \left(\frac{F_{0,high\,St}\left(\overline{\phi}\right) - F_{0,low\,St}\left(\overline{\phi}\right)}{2}\right)\frac{e^{10\left(\alpha\left(\tilde{St}\right)-0.6\right)} - 1}{e^{10\left(\alpha\left(\tilde{St}\right)-0.6\right)} + 1}. \tag{22}$$

In equation 22, $\alpha\left(\tilde{St}\right)$ is defined in equation 6, and $F_{0,high\,St}\left(\overline{\phi}\right)$ and $F_{0,low\,St}\left(\overline{\phi}\right)$ are defined as:

$$F_{0,high\,St}\left(\overline{\phi}\right) = 8.41\frac{\overline{\phi}}{1-\overline{\phi}} + \left(1-\overline{\phi}\right)^3\left(1 + 3.45\sqrt{\overline{\phi}}\right), \tag{23}$$

$$F_{0,low\,St}\left(\overline{\phi}\right) = 6.57\frac{\overline{\phi}}{1-\overline{\phi}} + \left(1-\overline{\phi}\right)^3\left(1 + 3.39\sqrt{\overline{\phi}}\right), \tag{24}$$

respectively. In equation 21, $a\left(\overline{\phi}\right)$ and $b\left(\overline{\phi}\right)$ are defined as:

$$a\left(\overline{\phi}\right) = 10.95 - 24.82\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{0.5}\left(1 - \frac{\overline{\phi}}{\phi_{max}}\right)^2, \tag{25}$$

$$b\left(\overline{\phi}\right) = -0.093 - 6460\left(\frac{\overline{\phi}}{\phi_{max}}\right)^{8}\left(1 - \frac{\overline{\phi}}{\phi_{max}}\right)^7, \tag{26}$$

where $\phi_{max} = 0.64$.

Using equations 21-26, the v_d-dependent drag model is defined. However, since v_d is a sub-grid quantity, a scale-similar approach is needed to estimate it. This methodology is detailed in section 3.1.

3.1 Scale-similar approach for estimating v_d

Since v_d is a sub-grid scale measure for the extent of inhomogeneities, we employ a scale-similar approach to estimate this quantity. In order to utilize this approach, v_d is estimated using the following scale-similar form:

$$v_d = \kappa_2' f_2\left(\frac{\overline{\phi}}{\phi_{max}}\right) g_2'\left(\frac{\Delta_f}{d_p}\right). \tag{27}$$

In equation 27, $f_2\left(\overline{\phi}/\phi_{max}\right)$ is defined as:

$$f_2\left(\frac{\overline{\phi}}{\phi_{max}}\right) = \left(\frac{\overline{\phi}}{\phi_{max}}\right)^{n_2}\left(1 - \frac{\overline{\phi}}{\phi_{max}}\right)^{m_2}, \tag{28}$$

where $n_2 = 1.44$, $m_2 = 1.84$, and $\phi_{max} = 0.64$. For the purposes of applications to larger-scale systems, $g_2'\left(\Delta_f/d_p\right)$ is defined as:

$$g_2'\left(\frac{\Delta_f}{d_p}\right) = \left(\frac{\Delta_f}{d_p}\right)^2, \tag{29}$$

where Δ_f is the base fluid grid size of the larger-scale simulation system.

The quantity, κ_2', which scales with the extent of inhomogeneities present in a fluidized system, is computed as:

$$\kappa_2' = \frac{\overline{\phi}\,\widehat{\left|\widetilde{\boldsymbol{u}}_{slip}\right|} - \widehat{\overline{\phi}}\left|\widehat{\widetilde{\boldsymbol{u}}_{slip}}\right|}{f_2\left(\widehat{\overline{\phi}}/\phi_{max}\right) g_2'\left(\Delta_{f,test}/d_p\right)\left|\widehat{\widetilde{\boldsymbol{u}}_{slip}}\right| - f_2\left(\overline{\phi}/\phi_{max}\right)\widehat{g_2'\left(\Delta_f/d_p\right)\left|\widetilde{\boldsymbol{u}}_{slip}\right|}}, \tag{30}$$

where $\Delta_{f,test}$ is the test filter size. For the purposes of applying the constitutive drag relation to larger-scale systems, $\Delta_{f,test}$ is chosen to be $3\Delta_f$. With $\Delta_{f,test} = 3\Delta_f$, the test-filtered quantities are computed using equation 20. Using equations 27-30, the sub-grid quantity v_d can be estimated at the base fluid grid size over the entire fluidized system. Plugging this estimate of v_d into equation 21, the v_d-dependent drag model can be fully implemented as a constitutive closure for larger-scale simulations of fluidized beds.

4 Summary

In this Supplementary Material, we have detailed how to utilize the fluid-particle drag models that were derived in this study as constitutive closures in larger-scale simulations of fluidized beds. In section 2.1, we showed how to employ the $\overline{(\phi')^2}$-dependent drag model, and in section 3, we showed how to employ the v_d-dependent drag model. Each of these two drag models accounts for the effects of inhomogeneities within a system, which is not possible with prior drag relations.