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Neural-Network-Based Filtered Drag Model for Gas-Particle Flows

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Abstract

Filtered two-fluid model (fTFM) for gas-particle flows require closures for the sub-filter scale corrections to interphase drag force and the stresses, the former being more significant. In this study, we have formulated a neural-network-based model to predict the sub-grid drift velocity, which is then used to estimate the drag correction. As a part of the neural network model development effort, we derived a transport equation for drift velocity and then performed a budget analysis to conclude that an algebraic model for drift velocity in terms of the filtered variables that are resolved in a fTFM simulation is adequate, and the model should include the filtered gas-phase pressure gradient as a marker in addition to the filtered particle volume fraction and the filtered gas-solid slip velocity. Both \textit{a priori} and \textit{a posteriori} analyses reveal that the present model for drift velocity when used in a fTFM simulation is able to capture the fine-grid simulation results quite well.

\textit{Keywords:} drift velocity two-fluid model sub-grid modeling filtering approach drag force fluidized bed

1. Introduction

Gas-particle flows in industrial devices such as circulating and turbulent fluidized beds are inherently unstable. They exhibit temporal and spatial inhomogeneities that take the form of bubble-like voids as well as clusters and streamers (e.g. Shaffer et al. (2013); Kolehmainen et al. (2013)). While Euler-Euler and Euler-Lagrange simulations using fine grids do reveal the formation of such dynamic meso-scale structures, it is not practical to resolve them at all scales in
large-scale process units (Agrawal et al., 2001; Ozel et al., 2013, 2017b). In most industrial-scale applications, the macro-scale flow structures are of the greatest concern as a result of their influence on gas-particle contacting and reaction rates; and, it has raised the following question: Can one probe the effects of design choices on macro-scale flow structures via “coarse” simulations in a reliable manner?

Coarse simulations, by definition, would not resolve the meso-scale (sub-grid) structures. It is now known that the coarse simulations yield grossly incorrect predictions unless the consequences of the sub-grid structures on the resolved flow are taken into account Agrawal et al., 2001; Wang et al., 2009; Parmentier et al., 2012; Ozel et al., 2013; Cloete et al., 2017). This has led to the development of models such as the filtered two-fluid model (fTFM) in which the effects of sub-filter scale fluctuations on resolved flow appear as corrections to the gas-particle drag force and effective stresses in both phases, which require additional constitutive models (Igci et al., 2008; Igci and Sundaresan, 2011; Parmentier et al., 2012; Ozel et al., 2013; Schneiderbauer and Pirker, 2014; Schneiderbauer, 2017; Milioli et al., 2013; Sarkar et al., 2016; Cloete et al. 2018c). Among these, the drag correction has been shown through budget analysis to be most important Parmentier et al., 2012; Ozel et al., 2013), and the stress corrections are only of secondary importance in most applications. Using an uncorrected microscopic drag model in coarse simulations of dense fluidized beds leads to a significant over-prediction of the drag force, which in turn leads to an over-prediction of bed height Parmentier et al., 2012; Schneiderbauer and Pirker, 2014; Cloete et al., 2018c).

Several different modeling approaches have been pursued in the literature to estimate the drag correction in coarse simulations, which are summarized in a recent review article (Sundaresan et al., 2018). Explicit models include the Energy Minimization Multi-Scale model (Li and Kwauk, 1994; Wang et al., 2008) and corrections expressed as functions of the filter size and the resolved variables (Igci et al., 2008; Igci and Sundaresan, 2011; Schneiderbauer and Pirker, 2014; Milioli et al., 2013; Sarkar et al., 2016; Schneiderbauer, 2017). Other modeling approaches express the drag correction in terms of filter size, filtered variables and additional sub-filter scale metrics such as the drift velocity Parmentier et al., 2012; Ozel et al., 2013, 2017a; Schneiderbauer and Saeedipour, 2018), the scalar variance of particle volume fraction Ozel et al., 2013, 2017a; Schneiderbauer, 2017), and large-scale fluctuations kinetic energy per unit mass associated with sub-filter scale velocity fluctuations Schneiderbauer, 2017). While including one or more of these
sub-filter scale metrics has been found to lead more accurate estimates of drag correction Ozel et al., 2017a), additional models are needed to estimate these metrics, which introduce errors Rubinstein et al., 2017). This brings up the following question: How can one estimate the relevant sub-grid metrics more accurately? The present manuscript is concerned with modeling the drift velocity.

The primary dependent variables in fTFM are the filtered particle volume fraction $\bar{\phi}_s$, and the phase-weighted (Favre-averaged) velocities of the gas ($\bar{\boldsymbol{u}}_g$) and particle phases ($\bar{\boldsymbol{u}}_s$). As drag force on a particle depends on the gas velocity experienced by it, the filtered drag force can be expected to depend on the average gas velocity experienced by the particles, which is different from the $\bar{\boldsymbol{u}}_g$ in fTFM Parmentier et al., 2012; Ozel et al., 2013) and analogously in the framework of Reynolds-averaged kinetic theory by Fox (2014) and Capecelatro et al. (2015, 2016). The difference between these two velocities, referred to as the drift velocity ($\bar{\boldsymbol{v}}_s$), has been found to be an excellent marker to estimate the drag correction Parmentier et al., 2012; Ozel et al., 2013, 2017a; Rubinstein et al., 2017; Schneiderbauer and Saeedipour, 2018). These studies found that scale-similarity and approximate deconvolution models yield a good estimate of the local drift velocity in a priori analysis for small filter sizes. Furthermore, coarse-grid fTFM simulations, incorporating the scale-similarity model for the drift velocity and a drift velocity based correction to the drag coefficient, have been shown to produce predictions of bed height in 2-D fluidized beds that are close to those observed in fine-grid simulations Parmentier et al., 2012). However, challenges still remain in the implementation of scale-similarity approach to coarse-grid simulations because a second level filtering is required, and a posteriori studies of approximate deconvolution models are lacking. Additionally, recent studies have found that the accuracy of the scale-similarity model degrades as filter size increases Ozel et al., 2017a; Rubinstein et al., 2017), pointing to the need for improved models to estimate the drift velocity.

With this in mind, we develop in the present study a neural-network-based model for predicting the drift velocity. To deduce markers for the predictive model, we first derived a transport equation for the drift velocity, and then performed budget analysis using simulation data. We found that, in addition to filtered solid volume fraction and phase velocities as identified in previous studies Parmentier et al., 2012; Ozel et al., 2013, 2017a; Schneiderbauer and Saeedipour, 2018), the filtered gas-phase pressure gradient is an essential marker for the accurate estimation of
drift velocity. Then, we employed neural network approach to build a predictive model for the drift velocity based on filtered fine-grid simulation results. This model is shown to be excellent in predicting the drift velocity in a priori analysis with a Pearson correlation coefficient of up to 0.99 with various filter sizes. This neural-network-based model was then used in coarse-grid fTFM simulations to demonstrate good agreement with fine-grid simulation results.

The paper is organized as follows. In section 2, we present the two-fluid model (TFM), and briefly outline the filtering procedure and the final fTFM; we then sketch the derivation of the transport equation for drift velocity. In section 3, we describe fine-grid TFM simulations of a fluidization test problem whose results are then used to perform a priori budget analysis of various terms in the transport equation for drift velocity; this analysis reveals the potential markers for modeling drift velocity. Section 4 outlines how a simple neural network closure model is formulated for drift velocity. Section 5 is devoted to a posteriori analysis, assessing the performance of fTFM supplemented with a neural-network-based model for drift velocity. The key findings are then summarized in section 6.

2. Model Development

The two-fluid model for non-reacting flow of a mixture of gas and uniformly sized particles is given by Eq.(1)-(4) below:

\[
\frac{\partial}{\partial t} (\rho_s \phi_s) + \nabla \cdot (\rho_s \phi_s \mathbf{u}_s) = 0 \\
\frac{\partial}{\partial t} (\rho_g \phi_g) + \nabla \cdot (\rho_g \phi_g \mathbf{u}_g) = 0 \\
\frac{\partial}{\partial t} \rho_s \phi_s \mathbf{u}_s + \nabla \cdot (\rho_s \phi_s \mathbf{u}_s \mathbf{u}_s) = -\nabla \cdot \mathbf{\sigma}_g - \phi_s \nabla \cdot \mathbf{\sigma}_g + \mathbf{F}_d + \rho_g \phi_g \mathbf{g} \\
\frac{\partial}{\partial t} \rho_g \phi_g \mathbf{u}_g + \nabla \cdot (\rho_g \phi_g \mathbf{u}_g \mathbf{u}_g) = -\phi_g \nabla \cdot \mathbf{\sigma}_g - \mathbf{F}_d + \rho_s \phi_s \mathbf{g}
\]

Here, \( \rho_g \) and \( \rho_s \) are gas and particle densities; \( \phi_s \) and \( \phi_g \) are solid and gas volume fractions; \( \mathbf{u}_s \) and \( \mathbf{u}_g \) are solid and gas phase velocities; \( \mathbf{\sigma}_g \) and \( \mathbf{\sigma}_s \) are phase stress tensor associated with gas and solid phases; \( \mathbf{F}_d \) is the interphase interaction force per unit volume of the mixture exerted by the gas on the solid phase. The principal part of this interaction force in the case
of gas-particle flow is the drag force, for which we use the well-known Wen & Yu’s drag law (Wen and Yu, 1966). In most gas-particle flows of interest in turbulent and circulating fluidized beds, the deviatoric part of $\sigma_g$ is unimportant (Agrawal et al., 2001), leaving gas pressure as the only important component of $\sigma_g$. The kinetic theory of granular materials (e.g. Lun et al. (1984a); Gidaspow (1994)) is widely used to close $\sigma_g$, which requires an additional transport equation for the granular temperature (e.g., see Lun et al. (1984a); Gidaspow (1994); Garzo and Dufty (1999); Koch (1990); Agrawal et al. (2001) and van Wachem et al. (2001)).

It is well established that the above system of equations, when applied to turbulent or circulating fluidized beds, manifest persistent fluctuations down to the scale of a few particle diameters (Ozel et al., 2013; Sarkar et al., 2016). As noted in the Introduction, when these structures are not resolved using fine grids, the bed height in a fluidized bed is over-predicted (Parmentier et al., 2012; Schneiderbauer et al., 2013). fTFM seeks to average over the fine structures that one does not want to resolve (Agrawal et al., 2001; Parmentier et al., 2012; Ozel et al., 2013). Towards this end, the filtered variables over a filter size $\Delta_f$ are defined as follows.

The filtered phase volume fraction is

$$\bar{\phi}_i(x, t) = \int_R^r \phi_i(r, t) G_{\Delta_f}(r - x) d\mathbf{r}, \quad i = s, g. \quad (5)$$

Similarly, the filtered phase velocity is defined as

$$\bar{\mathbf{u}}_i(x, t) = \frac{1}{\phi_i} \int_R^r G_{\Delta_f}(r - x) \phi_i(r, t) \mathbf{u}_i(r, t) d\mathbf{r}, \quad i = s, g. \quad (6)$$

Here, $G_{\Delta_f}(r - x)$ is a filter kernel function which satisfies $\int_R^r G_{\Delta_f}(r) d\mathbf{r} = 1$. The box filter kernel employed in all the results presented here is given by

$$G_{\Delta_f}(r - x) = \begin{cases} \frac{1}{\Delta^3}, & \text{if } |j| - x_j| \leq \frac{\Delta_f}{2}, \quad j = x, y, z \\ 0, & \text{otherwise}. \end{cases} \quad (7)$$

Filtering Eq.(1)-(4), one obtains

$$\frac{\partial (\rho_s \bar{f}_s \bar{u}_s)}{\partial t} + \nabla \cdot (\rho_s \bar{f}_s \bar{u}_s \bar{u}_s) = -\nabla \cdot \mathbf{U}_s - \nabla \cdot \bar{\sigma}_s - \sum_{g, s, g} \bar{\phi}_g \nabla \cdot \bar{\sigma}_g - \sum_{g, s, g} \bar{F}_d + \bar{F}_d + \rho_s \bar{f}_s \bar{g}$$

$$\frac{\partial (\rho_g \bar{f}_g \bar{u}_g)}{\partial t} + \nabla \cdot (\rho_g \bar{f}_g \bar{u}_g \bar{u}_g) = -\nabla \cdot U_{s, g, s} - \bar{\phi}_g \nabla \cdot \bar{\sigma}_g - \sum_{g, s, g} \bar{F}_d - F_{d, s, g} + \rho_g \bar{f}_g \bar{g}$$

$$\frac{\partial (\rho_s \bar{f}_s \bar{u}_s)}{\partial t} + \nabla \cdot (\rho_s \bar{f}_s \bar{u}_s \bar{u}_s) = -\nabla \cdot \mathbf{U}_s - \nabla \cdot \bar{\sigma}_s - \sum_{g, s, g} \bar{F}_d + \bar{F}_d + \rho_s \bar{f}_s \bar{g}$$

$$\frac{\partial (\rho_g \bar{f}_g \bar{u}_g)}{\partial t} + \nabla \cdot (\rho_g \bar{f}_g \bar{u}_g \bar{u}_g) = -\nabla \cdot U_{s, g, s} - \bar{\phi}_g \nabla \cdot \bar{\sigma}_g - \sum_{g, s, g} \bar{F}_d - F_{d, s, g} + \rho_g \bar{f}_g \bar{g}$$

(8)

(9)
Here, $\sigma_s$ and $\sigma_g$ denote solid and gas stresses, respectively; see Ozel et al. (2013) for explicit definitions of filtered and sub-grid terms in Eqs. (8) and (9). The symbol $\vec{F}_d$ is the drag force computed at the filtered solid volume fraction and the filtered phase velocities. The terms in Eq. (8) and (9) requiring constitutive modeling are:

$$F_{d, sgs} = \beta(\bar{u}_g - \bar{u}_s) - \beta'(\bar{\bar{u}}_g - \bar{\bar{u}}_s)$$

$$U_{i, sgs} = \rho_i \phi_i \bar{u}_i - \rho_i \bar{\bar{\phi}}_i \bar{\bar{u}}_i, \quad i = s, g$$

$$\Sigma_{g, sgs} = \phi_g \nabla \cdot \sigma_g - \bar{\phi}_g \nabla \cdot \bar{\sigma}_g$$

$$\Sigma_{s, sgs} = \nabla \cdot \bar{\sigma}_s - \nabla \cdot \bar{\sigma}_s$$

Here, $\beta'$ denotes the drag coefficient computed using the microscopic drag force model at the filtered solid volume fraction and the filtered phase velocities. The symbol $\sigma_s$ is the solid phase stress evaluated using the filtered solid volume fraction and the filtered solid phase velocity field. The symbol $\Sigma_{i, sgs}$ comes about because of the fact that the filtered stress is, in general, not the same as the stress evaluated at the filtered quantities.

Before presenting the results, averaging definitions are listed that would be helpful for readers. The symbol $\langle , \rangle$ refers to a domain-averaged variable, $\langle \rangle_t$ refers to a time-domain averaged variable and $\langle \rangle_{i,j}$ refers to a time-surface $(i, j)$ averaged variable.

Fig. 1: Budget analysis of the filtered solid phase momentum equation in the gravity direction. Each term is scaled by total weight of solid in the domain. See Eqs. (8)- (13) for explicit definitions of terms.

Budget analysis by Parmentier et al. (2012) has revealed that in dense fluidized beds, $F_{d, sgs}$ is important, while $U_{i, sgs}$ and $\Sigma_{g, sgs}$ are less important. In the present study, we found similar results, as demonstrated in Fig. 1. The magnitude of sub-grid scale contribution to drag force increases substantially as the filter size increases, whereas Reynolds stress-like term, $U_{s, sgs}$ and sub-grid scale gas-phase pressure gradient term which constitutes the majority of $\Sigma_{g, sgs}$ have negligible magnitude at various filter sizes. We also observe that the sub-grid scale kinetic theory
term, $\sum_{i,sgs}$ increases with the filter size. Although the sub-grid scale kinetic theory term should be considered for fTFM according to budget analysis, its effect is anticipated to be significantly less than the sub-grid scale drag force. With this in mind, we only focus on modeling $F_{d,sgs}$ in this study, and the stress correction terms are left to be investigated in future studies. The reader is referred to the literature (e.g. see Ozel et al. (2013); Milioli et al. (2013); Sarkar et al. (2016); Cloete et al. (2018a)) for modeling of $U_{i,sgs}$ and $\sum_{g,sgs}$. It was shown by Parmentier et al. (2012) and Ozel et al. (2013) and ascertained in several other studies (Ozel et al., 2017a; Rubinstein et al., 2017; Schneiderbauer and Saeedipour, 2018; Cloete et al., 2018b) that to a very good approximation

$$F_{d,sgs} \approx \beta \cdot \vec{v}_d$$

where $\vec{v}_d$ is the drift velocity given by

$$\vec{v}_d = \frac{\phi_s}{\phi_g} u_g - \vec{u}_{sgs}$$

In the present study, we aim to develop a closure model for the drift velocity, using which we can compute the sub-grid contribution of the filtered drag force. To identify essential markers for the model, we started by formulating a transport equation by reorganizing Eqs. (1)-(15), followed by filtering. This leads to

$$\frac{\partial \vec{v}_d}{\partial t} + \nabla \cdot (\vec{v}_d \vec{u}_g) = \mathcal{X}^{sgs} + \mathcal{Y}^{sgs} - \nabla \cdot \mathcal{A}^{sgs} + \mathcal{B}^{sgs} - \mathcal{C}^{sgs} - \mathcal{D}^{sgs}$$

$$+ \mathcal{F}^{sgs} - \frac{\phi_s}{\phi_g} \mathcal{K}^{sgs} + \frac{1}{\phi_g} \nabla \cdot \mathcal{L}^{sgs} - \nabla \cdot \mathcal{I}^{sgs} + \nabla \cdot \mathcal{H}^{sgs}$$

Here, $\mathcal{X}^{sgs}$ and $\mathcal{Y}^{sgs}$ are given by

$$\mathcal{X}^{sgs} = \frac{1}{\phi_g} \left( \frac{\phi_s}{\rho_g} \nabla p_g - \frac{\phi_s}{\rho_g} \nabla p_{sgs} \right)$$

$$\mathcal{Y}^{sgs} = \frac{1}{\phi_g} \frac{\vec{F}_d}{\rho_g} - \frac{1}{\phi_g} \frac{\vec{F}_d}{\rho_g}$$

where $p_g$ is the gas pressure, and $\vec{F}_d$ is given by $\beta(\vec{u}_g - \vec{u}_s)$ as appeared in the first term on the right-hand-side of Eq. (10). Expressions for all the other terms, which we will show by the budget analysis (see below) to be much less important than $\mathcal{X}^{sgs}$ and $\mathcal{Y}^{sgs}$, are presented in Table 1.
budget analysis also shows that $\mathcal{X}^{sgs}$ and $\mathcal{Y}^{sgs}$ almost balance each other with similar magnitude and opposite signs, indicating that an algebraic equation is sufficient for modeling drift velocity.

Table 1: Definition of sub-grid terms on the right-hand-side of the transport equation for drift velocity, Eq. (16).

<table>
<thead>
<tr>
<th>Sub-Grid Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{A}^{sgs}$</td>
<td>$\bar{u}_k \nabla \cdot \bar{u}_k - \bar{u}_k \nabla \cdot \bar{u}_k$</td>
</tr>
<tr>
<td>$\mathcal{B}^{sgs}$</td>
<td>$\nabla \cdot (\phi \bar{u}_k) - \bar{u}_k \nabla \cdot (\bar{\phi} \bar{u}_k)$</td>
</tr>
<tr>
<td>$\mathcal{C}^{sgs}$</td>
<td>$\nabla \cdot (\phi \bar{u}_k) - \bar{u}_k \nabla \cdot (\bar{\phi} \bar{u}_k)$</td>
</tr>
<tr>
<td>$\mathcal{D}^{sgs}$</td>
<td>$\bar{\rho}_s \nabla \cdot \bar{\tau}_s - \bar{\rho}_s \nabla \cdot \bar{\tau}_s$</td>
</tr>
<tr>
<td>$\mathcal{E}^{sgs}$</td>
<td>$\phi \bar{u}_k \bar{u}_k - \bar{\phi} \bar{u}_k \bar{u}_k$</td>
</tr>
<tr>
<td>$\mathcal{F}^{sgs}$</td>
<td>$\bar{u}_k \bar{u}_k - \bar{u}_k \bar{u}_k$</td>
</tr>
<tr>
<td>$\mathcal{G}^{sgs}$</td>
<td>$\phi \bar{u}_k \bar{u}_k - \bar{\phi} \bar{u}_k \bar{u}_k$</td>
</tr>
</tbody>
</table>

In general, one need to model drift velocity as a vector for an anisotropic drag closure model. The importance of this anisotropic effect has been presented in a recent study undertaken by Cloete et al. (2018b). Cloete et al. (2018b) found that the effect of anisotropy on the filtered drag force model increased with increasing filter size; in the present study, however, we did not observe the effect of filter size on the degree of anisotropy. Additionally, predicting anisotropic drag using a neural network model (the modeling approach in this study given in Section 4) will face a challenge in meeting Galilean invariance, rotational invariance in particular. This issue arises from non-linear structure of the neural network. If one rotates the input vectors by a given angle, the output would need to be rotated by the same angle in order to satisfy rotational invariance. However, general architecture of neural networks does not satisfy this constraint (Ling et al., 2016). To resolve this issue, machine learning practitioners have used Galilean invariant
input features, which effectively resolves the problem. For the present drag problem, this would imply a local coordinate system that would satisfy Galilean invariance inherently. In our study we use gravity to span this local coordinate system, but this will leave two other axes arbitrary. Natural choices for locking the remaining directions would be either local slip velocity, slip velocity gradient or pressure gradient. Currently, it is not known which of these vectors correlate the most with the anisotropic drag, and hence what would be the best way to span the local coordinate system. In the present study, we will use an isotropic drag law in conjunction with the gravity direction to resolve this issue and leave general Galilean invariant anisotropic drag modeling for a future work. Furthermore, as the lateral components of the velocities were in significantly smaller magnitude than that in the flow direction, any model we constructed using them proved to be mostly unreliable in \textit{a posteriori} tests. As the principal motion in fluidized beds is in the vertical direction, estimating the drag correction in the vertical direction is of the greatest importance. Indeed, Igci and Sundaresan (2011), Milioli et al. (2013) and Sarkar et al. (2016) proposed models to estimate the drag correction in the vertical direction and used the same correction in the other directions as well. The same approach is followed in the present study: applying the flow-direction drag correction to lateral force components in all the directions yields (in \textit{a priori} analysis) Pearson correlation coefficients of 0.99 and 0.8 in the vertical and lateral directions respectively. Parmentier et al. (2012) and Ozel et al. (2013) have dynamically adjusted the model parameter in vertical and horizontal directions separately, but it is not known if this extra sophistication affected the predicted bed expansion in a noticeable fashion. In this first study exploring the use of neural-network-based closure for evaluating the drift velocity, we limit our attention to finding the drag correction in the vertical direction and have applied the same correction in the other directions as well.

3. Flow Configuration and Budget Analysis

Simulations of 75 $\mu$m particles (density, $\rho_s = 1500$kg/m$^3$) fluidized by ambient air (density, $\rho_g = 1.3$kg/m$^3$ and kinematic viscosity, $\nu_g = 1.5 \times 10^{-5}$m$^2$/s) in a bed of square cross section (2.025cm×2.025cm×12.25cm) were performed using twoPhaseEulerFoam solver of OpenFOAM 3.x, which solves the TFM equations (Eqs. (1)-(4)). The computational domain with boundary conditions is shown in Fig. 2. The Wen & Yu’s drag law (Wen and Yu, 1966) was used in all the
simulations. A frictional-collisional model (Johnson and Jackson, 1987a) is used to model the solid phase stress. In dilute and moderately dense suspensions where frictional stress transmission through sustained contact network is not present, the stress is closed by kinetic theory where solid phase pressure is modeled according to (Lun et al., 1984a); the shear and bulk viscosities in this regime are modeled using expressions given by (Gidaspow et al., 1991). The granular temperature is found by solving the granular energy transport equation (Gidaspow et al., 1991). The frictional pressure turned on when the solid volume fraction reaches 0.6. The solid phase stress model used in the simulations is summarized in Appendix A. No-slip boundary condition is applied for both the gas and solid phases at walls. The gas velocity is specified at the bottom boundary, which is impermeable to the solids. At the top boundary, the free outlet is imposed for both phases.

Fig. 2: Flow configuration used in the present study.

Results from the fine-grid simulations (mesh size = 3d_p, henceforth referred to as ∆) were used to perform a budget analysis of the terms appearing on the right hand side of Eq. (16). The right hand side of Eq. (16) contains a large number of terms requiring closure models. Budget analysis provides us with a way of identifying the most important terms which must be retained. As we intend to develop an isotropic drag model, we focus on the gravity direction for budget analysis, which is denoted by the non-bold font of the sub-grid terms. With this in mind, we collected a number of snapshots in a statistical steady state and used them to evaluate each of the terms on the right-hand-side of Eq. (16) at various locations in the bed. They were then averaged over the entire bed to obtain typical values for each term. As illustrated in Fig. 3, the first two terms on the right-hand-side of Eq. (16) are much larger in magnitude in the gravity direction than the remaining terms. (We also determined the bed-average of the absolute value of each of the terms and arrived at the same conclusion.) It is clear from Fig. 3 that as the filter size is increased, the first two terms increase in magnitude; they have opposite signs and nearly balance each other. Therefore Eq. (16) can be well approximated by $\nabla \cdot \mathcal{A}^{gs} + \nabla \cdot \mathcal{Y}^{gs} - \nabla \cdot \mathcal{A}^{gs} + \mathcal{B}^{gs} + ... + \nabla \cdot \mathcal{H}^{gs} \sim 0$. With $\nabla \cdot \mathcal{A}^{gs}, \ldots \mathcal{H}^{gs}$ contributing weakly, we can further simplify the equation as $\nabla \cdot \mathcal{A}^{gs} + \mathcal{Y}^{gs} \sim 0$. In view of these findings, we conclude that an algebraic equation for drift velocity is sufficient for gas-particle flows as a first modeling attempt for dense fluidized bed case. The
terms on the left hand side are not important, as the typical magnitude of the left-hand-side is the sum of all the terms on the right, therefore one can readily expect that the left hand side terms would be of the order of \( \mathcal{X}^{sgs} + \mathcal{Y}^{sgs} \), which is much smaller than the magnitude of \( \mathcal{X}^{sgr} \) and \( \mathcal{Y}^{sgr} \) individually. In other words, stipulating that \( \mathcal{X}^{sgr} + \mathcal{Y}^{sgr} \sim 0 \) is a reasonable first approximation for the present study. It is reasonable to anticipate that the terms on the left hand side could be important in liquid-solid and bubbly gas-liquid flows, where other terms on the right may also have to be retained. According to the expression of \( \mathcal{X}^{sgr} \) and \( \mathcal{Y}^{sgr} \) as shown in Eq. (17) and (18), we can also deduce that drift velocity is a function of \( \nabla p_g \), \( \phi_s \), and slip velocity, \( \vec{u}_{slip} \) (calculated by \( \vec{u}_g - \vec{u}_i \)). In this study, we settled for a neural network model to close drift velocity for two reasons: (a) the vast amount of computational data available from the fine-grid simulations can be deployed to construct neural network models using open-source codes quite readily and such a model is adequate for estimating drift velocity; and, (b) good guidance for explicit constitutive model forms is not yet available and developing them would require significant work, whose benefits remain to be demonstrated.

Fig. 3: Budget analysis of the sub-grid terms on the right-hand-side of transport equation for drift velocity (Eq. (16)). The non-bold font of the sub-grid terms indicates that this analysis is done for the gravity direction.

4. Neural Network Closure Models: a priori Analysis

Originally inspired by the learning process of the brain, the neural network approach is widely applied in diverse fields such as natural language processing and image recognition. Its ability to handle large data sets in the training step and yield good predictions makes it a very useful data mining technique for our purpose. Additionally, implementation of the neural network closures into our solver is quite straightforward. With these advantages in mind, we set out to formulate closure models for drift velocity using the fine-grid simulation results obtained for an inlet gas velocity of 0.4 \( u_t \) where \( u_t \) is the terminal settling velocity of a single particle and equal to 0.219 m/s.

The multi-layer perceptrons neural network models for drift velocity involve three hidden
layers. Each hidden layer contains 128, 64, and 16 nodes respectively, and we use ReLU (Rectified Linear Unit with a function form of $f(x) = \max(0, x)$) activation function for all hidden layers. Neural network models were trained using a machine learning library called Keras (Chollet et al., 2015). The model uses the filtered solid volume fraction, gas-phase pressure gradient, and slip velocity as inputs. Such neural network models were determined for different filter sizes: $\Delta_f = 15d_p$, $21d_p$, and $27d_p$.

As an illustration, we present some results for a filter size of $27d_p$, which corresponds to a filter whose length is 9 times that of the mesh used in the fine-grid simulation. To quantify the statistical accuracy of the model, we define the relative error as

$$e_i(x; y) = \frac{x_i - y_i}{y_i}. \quad (19)$$

Fig. 4(a) shows the probability density function of relative error. It can be observed that majority of the error is at zero. Fig. 4(b) shows parity plot of the predicted and exact values of $\bar{\phi}_s \tilde{v}_{d,z}$. Each point represents $\bar{\phi}_s \tilde{v}_{d,z}$ at some location in the bed in one of the snapshots used to train the model. In each of these plots, the abscissa and ordinate are scaled and made dimensionless with $\phi_{\text{max}} u_t$. The points are distributed around the parity line roughly evenly. Models, in general, can be expected to capture the real observations only in a statistical sense, and so some scatter around the parity line is to be expected. As another metric of the quality of predictions, we also computed the Pearson correlation coefficient, which is defined as

$$r(y^*, y) = \frac{\text{cov}(y^*, y)}{\text{std}(y^*) \text{std}(y)}, \quad (20)$$

where $y^*$ and $y$ denote predicted and real value respectively; $\text{cov}$ denotes covariance, and $\text{std}$ denotes standard deviation. The Pearson correlation coefficients corresponding to Fig. 4 were found to be 0.99, which is indicative of a strong correlation between the predicted and resolved quantities. The Pearson correlation coefficients ranges from 0.98 to 0.99 for filter sizes in the range of $15–27d_p$. Furthermore, this predicted flow direction drift velocity is tested using the drag model modified from our recent study (Ozel et al., 2017a):

$$\bar{F}_d \approx \tilde{F}_d (1 + \frac{\tilde{v}_{d,z} \tilde{u}_{\text{slip},z}}{\| \tilde{u}_{\text{slip}} \|}) \quad (21)$$
To illustrate the improved performance by including the filtered gas-phase pressure gradient as a third marker, we performed *a priori* analysis for a two-marker neural network model. The two essential variables identified in our previous work include the filtered solid volume fraction, \( \bar{\phi}_s \), and the filtered slip velocity, \( \bar{u}_{slip} \). The results are summarized in Fig. 4 (c) and (d). According to the probability density function, the error is not centered at zero, and the error is more spread out than the three-marker model. The parity plot in Fig. 4 (b) shows that a significant number of points are distributed relatively far away from the parity line. The two-marker model yields a Pearson correlation coefficient of 0.88, which is inferior to the three-marker case. We also compared the three-marker neural network model to the most recent two-marker model developed by Gao et al. (2018), which is based on the model originally proposed by Sarkar et al. (2016). Using Eq. (21), we computed the flow direction filtered drag force with the three-marker neural network model, and a parity plot of the exact versus predicted filtered drag is shown in Fig. 4 (e) along with that from Gao et al. (2018) model in Fig. 4 (f). The points in the parity plot from the three-marker model are apparently closer to the parity line and less scattered. Pearson correlation coefficients of 0.994 and 0.87 were obtained respectively from the neural network and Gao et al. (2018) model. This comparison further indicates that the three-marker neural network model predicts the filtered drag force more accurately with the additional marker of the gas-phase pressure gradient.

Fig. 4: Assessment of model predictions: (a) probability density function of relative error (Eq. (19)) and (b) parity plot between predicted and exact values with the three-marker neural network model \((\bar{\phi}_s, \frac{\partial \bar{p}_g}{\partial z}, \bar{u}_{slip,z})\). (c) probability density function of relative error (Eq. (19)) and (d) parity plot between predicted and exact values with the two-marker neural network model \((\bar{\phi}_s, \bar{u}_{slip,z})\); parity plot of predicted filtered drag versus exact filtered drag for e) the three-marker neural network model f) Gao et al. (2018) model

To implement the neural network model, we saved the output files from the training process using Keras: 1) a JSON file that contains the neural network structure; 2) a HDF5 file that contains weight information required for the evaluation of the neural network model (See the Supplementary Material for JSON and hdf5 files). There files are read by an open-source interface
C++ code (https://github.com/pplonski/keras2cpp) and passed to OpenFOAM twoPhaseEulerFoam solver at the beginning of a simulation. This implementation allows us to read the flow quantities during simulation runtime and evaluate the prediction with the neural network model. With the neural network model and implementation approach, we set out to assess its predictability in the next section.

5. Results and Discussion

Simulations of fluidization were performed in the geometry shown in Fig. 2, using gas and particle properties presented earlier in section 3 with various mesh sizes: $\Delta = 15d_p$, $21d_p$, and $27d_p$. The drift velocity is computed during simulation using the neural network model developed, and the resolved drag force is corrected using a model modified from our recent study (Ozel et al., 2017a) as in Eq. (21).

Panel (a) in Fig. 5 shows a snapshot of the particle volume fraction field at the center plane of a 3-D fine-grid TFM simulation ($\Delta = 3d_p$), whose results were used to perform the budget analysis and neural network model development. Panel (b) shows the same snapshot after filtering with a box filter ($\Delta_f = 27d_p$). Panel (c) is a snapshot from fTFM simulation using the same mesh size of $27d_p$, but with the neural network model for drift velocity. Panel (d) shows a snapshot with a coarse-grid TFM simulation of ($\Delta = 27d_p$) without using any sub-grid correction; as already noted by Parmentier et al. 2012, the bed height is much larger indicating poor prediction. It is readily apparent that fTFM supplemented with corrections from drift velocity affords results that are closer to the fine-grid simulation results shown in Panel (b).

Fig. 5: Snapshots of solid volume fraction: (a) fine-grid simulation with a mesh size of $3d_p$ and Wen & Yu’s drag law (Wen and Yu, 1966) (b) fine-grid simulation results mapped onto a coarse-mesh size of $27d_p$ (c) simulation with a mesh size of $27d_p$ and the neural network model (the drift velocity is predicted with three-marker model and the drag correction is computed by Eq. (21)) (d) simulation with mesh size of $27d_p$ and Wen & Yu’s drag law (Wen and Yu, 1966).

The axial profiles of the solid volume fraction (averaged laterally and temporally) obtained
with fine-grid and coarse-grid simulations are presented in Fig. 6(a) and (b). The solid volume fraction profiles with various mesh sizes ($3d_p$, $15d_p$, $21d_p$, and $27d_p$) and Wen & Yu’s drag law are shown in Fig. 6(a); a clear overestimation of the bed expansion can be observed for the coarse-grid simulations, which is principally due to the over-prediction of the drag force. Fig. 6(b) shows the results of the fine-grid simulation and those of coarse-grid simulations with various mesh sizes where the drag force is corrected by drift velocity computed with the neural network model; in these coarse-grid simulations, the mesh size is the same as the filter size. The filtered model simulation results are close to the fine-grid result for all the three mesh sizes. Fig. 6(c) shows a comparison of fine- and coarse-grid simulation results with various filter sizes using the Gao et al. model. This two-marker constitutive model can decently correct the filtered drag force to be consistent with fine-grid simulation results, but a slight degradation in the performance can be observed when $\Delta = 15d_p$. According to these a posteriori analysis results, the two-marker Gao et al. model and three-marker neural network model are comparable in predicting the filtered drag force in coarse-grid simulations.

Fig. 6: Solid volume fraction profile in the vertical direction with various mesh sizes ($3d_p$, $15d_p$, $21d_p$, and $27d_p$) and (a) Wen & Yu’s drag law (Wen and Yu, 1966), (b) neural network model (the drift velocity is predicted with three-marker model and the drag correction is computed by Eq. (21)). (c) Gao et al. (2018) model. The symbol $< . >_{x,y}$ refers to averaging over $x$ and $y$ directions.

To further compare the flow behavior inside the bed predicted by fine-grid TFM and coarse-grid fTFM simulations, we present the time-averaged vertical solid flux in the $x$-direction at two different elevations, $z = 0.4L_b$ and $z = 0.8L_b$ ($L_b$ = bed height of fine-grid simulation) in Fig. 4(a) and (b). The solid line refers to the fine-grid ($\Delta = 3d_p$) predictions. The downward flux of solid near the wall region and the up-flow in the core are readily seen. The fTFM simulation results with $\Delta = 27d_p$ and the neural network model at both elevations, shown as filled circles, are comparable to the fine-grid TFM simulation results. On the other hand, the coarse-grid simulation results without drag force
correction, shown as unfilled circles, differ significantly from the fine-grid simulation results.

Fig. 7: Time-averaged vertical solid flux in the axial direction (x-direction) with fine-grid simulation ($\Delta = 3d_p$ + Wen & Yu’s drag law (Wen and Yu, 1966)), coarse-grid simulation ($\Delta = 27d_p$ + Wen & Yu’s drag law (Wen and Yu, 1966)) and coarse-grid simulation with the neural network model ($\Delta = 27d_p$) and the drift velocity is predicted with three-marker model and the drag correction is computed by Eq. (21) at (a) $z = 0.4L_b$ and (b) $z = 0.8L_b$ ($L_b$ is the bed height of fine-grid simulation).

In order to assess the accuracy of drift velocities estimated by the neural-network-based model, we computed the axial variation of temporally and laterally averaged drift flux ($\bar{\phi}_s \bar{v}_d$) from the fTFM simulations and compared it against analogous results obtained by filtering the fine-grid TFM simulation results.

Fig. 8 shows this comparison for a fTFM with a filter sizes of $15d_p$, $21d_p$, and $27d_p$. The drift flux values estimated in the fTFM simulations generally agree with those estimated from the fine-grid results in the interior of the bed away from the top and bottom boundaries; however, sharp differences can be seen at the bottom and near the top surface of the bed, where the magnitude of drift velocity is over-predicted by the neural network model. We attribute this deficiency to the sharp gradients that exist at these two boundaries, whose effects have not been included in our neural network model in which the drift flux at any location is simply related to the filtered solid volume fraction, the filtered slip velocity and the filtered gas-phase pressure gradient. Further refinement of the neural network model, allowing for the influence of the gradients in these markers, could improve the predictions at these boundaries; this will be pursued in a future study.

Fig. 8: Drift flux ($\bar{\phi}_s \bar{v}_d$) profile comparison of filtered fine-grid ($3d_p$) simulation results and coarse-grid simulation results with filter size of: (a) $15d_p$ (b) $21d_p$ (c) $27d_p$ corrected with corresponding neural network model for drift velocity.
We assessed the predictability of the neural network model by applying it to one fluidized bed operated at a different inlet velocity. Fig. 9 shows the solid volume fraction profile in the axial direction obtained from a coarse-grid simulation \((27d_p)\) of a fluidized bed with a higher inlet velocity of 0.15 m/s. (The model was trained using only results from a simulation with an inlet gas velocity of 0.1 m/s.) Compared to the uncorrected case, the neural network model effectively brings the bed expansion closer to the fine-grid simulation results, showing that the neural network model for drift velocity can be applied to conditions beyond the conditions in the training set.

Fig. 9: Solid volume fraction profile in the vertical direction with fine-grid, coarse-grid and coarse-grid with the neural network model simulations. The inlet velocity is 1.5 m/s. The symbol \(<\cdot>_{x,y}\) refers to averaging over \(x\) and \(y\) directions.

According to a priori analysis, the performance of the current neural network model using the filtered gas-phase pressure gradient as a third marker shows significant improvement compared to two-marker neural network model. We performed a posteriori test and come to the same conclusion. A preliminary analysis of the predictions afforded by the neural network model suggests that the drift flux in the vertical direction could be approximated as

\[
\bar{\phi}_s \bar{v}_{g,z} \approx f_1(\bar{\phi}_s) \nabla p_{g,z} / \rho_g + f_2(\bar{\phi}_s, \bar{u}_{dip,z})
\]

(22)

where \(f_1\) and \(f_2\) are suitable constants or functions to fit the data. It then follows that in fTFM, the contribution of the gas-phase pressure gradient shows up in the right hand side as:

\[
-(\bar{\phi}_s + \beta f_1(\bar{\phi}_s)) \nabla p_{g,z}
\]

(23)

As discussed in Zhang and VanderHeyden (2002) and De Wilde (2005), this additional contribution from the pressure gradient can also be modelled as an effective added mass contribution. A more in-depth analysis of this effective added mass contribution will be pursued in a future study.

Fig. 10 shows the solid volume fraction profile in the axial direction of fine-grid TFM simulation and neural-network-based coarse-grid \((27d_p)\) fTFM simulation with and without the filtered gas-phase pressure gradient as a marker to estimate the drift velocity. Leaving out the
filtered gas-phase pressure gradient as an additional marker yields higher bed expansion and significantly different profile in the bulk part of the bed. This comparison indicates that the filtered gas-phase phase pressure gradient plays a significant role in capturing the sub-grid scale drag force contribution in the fTFM.

Fig. 10: Solid volume fraction profile in the vertical direction for neural network models with and without the filtered gas-phase pressure gradient as a third marker. The symbol $< . >_{x,y}$ refers to averaging over $x$ and $y$ directions.

6. Conclusion

In the present study, we have formulated a neural-network-based model to predict the sub-grid drift velocity with the objective of finding a proper way to modify the drag model for microscopic simulation to make it applicable for coarse grid simulation. With the aid of filtering analysis, we derived a transport equation for drift velocity and simplified it through budget analysis. This transport equation enabled us to identify important markers for closing drift velocity. In addition to the two markers explored before, namely the filtered solid volume fraction and slip velocity, we identified the filtered gas-phase pressure gradient as another essential marker for modeling the drift velocity. A neural network model to estimate the drift velocity in terms of the three resolved variables mentioned above and an algebraic relation to estimate drag correction in terms of the drift velocity were incorporated in an OpenFOAM fluid solver for Euler-Euler simulations on coarser mesh grids, and the results are compared against fine-grid Euler-Euler simulation results.

Comparisons of instantaneous snapshots, axial variations of cross-sectional average solid volume fraction and axial component of the drift velocity, and lateral variation of axial solid flux profile at different elevations show clearly that the new neural-network-based drift velocity model for drag correction provides an effective way of reproducing the coarse features of the fine-grid simulation results in coarse-grid simulations.

Some shortcomings in the neural network model to estimate the drift velocity remain near the top and bottom boundaries, which could be remedied by including the effect of gradients in the marker variables. Further, albeit small, improvement of the filtered model predictions could come by including a model for the sub-grid stresses. These remain to be explored in future studies.
The dependency of the drag correction on local gas-phase pressure gradient is a new finding in this study. It immediately suggests a closer investigation of this dependence and what it means to how one partitions the overall fluid-part interaction force in a component associated with the slowly varying gas phase stress (principally pressure gradient) and one associate with the rapid variation on the particle scale as the fluid moves around the particle; these should be explored in future studies.

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Appendix-A: Solid Stress Closures

The solid stress tensor $\sigma_s$ in Eq. (3) is defined by

$$\sigma_s = (p_s - \lambda_s \nabla \cdot u_s)I - \mu_s \left( \nabla u_s + \nabla u_s^T - \frac{2}{3} (\nabla \cdot u_s)I \right) \quad (A1)$$

where $p_s$ is the granular pressure, $\lambda_s$ is the bulk viscosity and $\mu_s$ is the shear viscosity. These terms are defined as follows (Gidaspow (1994)):

$$p_s = \phi_s \rho_s \left[ 1 + 2 \phi_s g_0 (1 + e_c) \right] \Theta, \quad (A2)$$

$$\lambda_s = \frac{4}{3} \phi_s^2 \rho_s d_p g_0 (1 + e_c) \sqrt{\frac{\Theta}{\pi}}, \quad (A3)$$

$$\mu_s = d_p \sqrt{\Theta} \left[ \frac{4}{5} \phi_s g_0 \frac{1 + e_c}{\sqrt{\pi}} + \frac{1}{15} \sqrt{\pi} g_0 (1 + e) \phi_s^2 + \frac{1}{6} \sqrt{\pi} \phi_s + \frac{10}{96} \frac{\sqrt{\pi}}{(1 + e_c) g_0} \right] \quad (A4)$$

where $\Theta$ is granular temperature, $e_c$ is the restitution coefficient (equal to 0.9 in this study), $g_0$ is the radial distribution function at contact and $d_p$ is the particle diameter. The transport equation for granular temperature is

$$\frac{\partial}{\partial t} \left( \rho_s \phi_s \Theta \right) + \nabla \cdot \left( \rho_s \phi_s u_s \Theta \right) = \nabla \cdot (\kappa_p \nabla \Theta) - \sigma_s : \nabla u_s - 12 (1 - e_c^2) \frac{\phi_s^2 \rho_s g_0 \Theta \gamma^2}{d_p \sqrt{\pi}} - 3 \beta \Theta \quad (A5)$$

with the granular temperature conductivity $\kappa_p$ given by
\[ \kappa_p = 2 \rho \phi_s^2 d_p (1 + e') g_0 \sqrt{\frac{\Theta}{\pi}}. \]  

(6)

The radial distribution function at contact, \( g_0 \), is given by

\[ g_0 = \left( 1 - \left( \frac{\phi_s}{\phi_{s,\text{max}}} \right)^{1/3} \right)^{-1}. \]  

(7)

where the packing solid volume fraction \( \phi_{s,\text{max}} \) is equal to 0.64.

The frictional solid pressure, \( p_{s,f} \), is added to the granular pressure when \( \phi_s > \phi_{s,f,\text{min}} \). By following Johnson and Jackson (1987a), it is defined as

\[ p_{s,f} = a \left( \frac{\phi_s - \phi_{s,f,\text{min}}}{\phi_{s,\text{max}} - \phi_s} \right)^b. \]  

(8)

Here, the minimum solid volume fraction for the frictional solid pressure, \( \phi_{s,f,\text{min}} \), is set to 0.6. In Eq. (A8), \( a, b \) and \( c \) are empirical constants and equal to 2, 2, and 5 respectively. The constant \( a \) is with a unit of \( \text{Pa} \).

The frictional shear viscosity, \( \mu_{s,f} \), is also accounted for when \( \phi_s > \phi_{s,f,\text{min}} \). It is given by

\[ \mu_{s,f} = A p_{s,f} \sin \theta \]  

(9)

with the internal angle of friction, \( \theta \), which is set to 28.5° and the model constant, \( A \), which is equal to 1/2 with a unit of time.

References


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Figure 1

\[ \langle \phi_s \rangle / \langle \rho_s \rangle \]

\[ \frac{\langle \phi_s \rangle}{\langle \rho_s \rangle} | g | \]

\[ \Delta / \Delta_f \]

Symbols:
- \( \bar{\phi}_s \)
- \( \nabla \cdot \bar{\sigma}_g \)
- \( \Sigma_{g, sgs} \)
- \( \nabla \cdot \tilde{\sigma}_s \)
- \( \Sigma_{s, sgs} \)
- \( \tilde{F}_d \)
- \( F_{d, sgs} \)
- \( U_{i, sgs} \)
Figure 2

Free Outlet

Walls
Gas: No-slip
Solid: No-slip

Inlet

3.0375 cm
$\phi_s = 0.55$

2.025 cm

Gas Flow
$u = 0.1$ m/s
Figure 3
Figure 4

(a) PDF

(c) PDF

(e) PDF

(b) 

(d) 

(f)
Figure 6
Figure 7
Figure 8

(a) $\Delta = 15 \, d_p$ + NN model
Filtered, $\Delta = 3 \, d_p$

(b) $\Delta = 21 \, d_p$ + NN model
Filtered, $\Delta = 3 \, d_p$

(c) $\Delta = 27 \, d_p$ + NN model
Filtered, $\Delta = 3 \, d_p$
Figure 10

- $\Delta = 27 \delta_p + $ NN model (Two markers)
- $\Delta = 27 \delta_p + $ NN model (Three markers)
- $\Delta = 3 \delta_p + $ Wen & Yu's drag law