Comment on “A New One-Equation Model of Fluid Drag for Irregularly Shaped Particles Valid Over a Wide Range of Reynolds Number” by F. Dioguardi et al.

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Abstract With this comment we want to clarify a number of aspects of the paper recently published by Dioguardi, Mele, and Dellino “A New One-Equation Model of Fluid Drag for Irregularly Shaped Particles Valid Over a Wide Range of Reynolds Number” (hereafter referred to as DMD2018). In particular, we show that contrary to the conclusions of DMD2018, the model of Bagheri and Bonadonna (2016, https://doi.org/10.1016/j.powtec.2016.06.015), hereafter referred to as BB2016, is the best model in predicting the drag and terminal velocity of particles measured by DMD2018, as demonstrated here by comparison of estimation errors. The discrepancy is mainly due to a production error (misplaced parentheses) introduced in BB2016 during the publication process and partly due to the incorrect methodology used by DMD2018 to calculate particle terminal velocity. Here we present the correct sets of equations and methodology to show that typo-free model of BB2016 outperforms all existing drag models including the new model suggested by DMD2018.

1. Comments on the DMD2018 Methodology

The two main objectives of this comment paper are to present the correct equations of Bagheri and Bonadonna (2016) already published in an errata corrige (Bagheri & Bonadonna, 2019, hereafter referred to as BB2019) and discuss their impact on the results and conclusions of DMD2018. The typos introduced in Bagheri and Bonadonna (2016) during production significantly decrease the accuracy of the proposed model, and therefore, most conclusions of DMD2108 concerning the model of BB2016 are illinformed. We want to highlight here that DMD2018 are not to blame for using the wrong sets of equations since BB2019 was published after their paper. Nonetheless, we also have some additional concerns related to their numerical strategy that we deemed necessary to point out in order to provide the readers with an accurate assessment of existing drag models. These concerns are related to DMD2018’s incorrect definition of particle Reynolds number and their incorrect methodology used to benchmark drag models.

More specifically, DMD2018 defined the particle Reynolds number using particle terminal velocity rather than the relative particle velocity (see equation (3) in DMD2018). Thus, the definition of DMD2018 is a special case that is only applicable when particles are at the terminal velocity. In addition, it should be noted that the terminal velocity is a function of the drag coefficient, which is a function of the Reynolds number that, in turn, depends on the particle velocity. For this reason, an iterative-corrective scheme is usually employed to calculate these quantities. DMD2018 provide a Matlab code (as supporting information) to calculate the particle terminal velocity using an iterative scheme; however, they do not use this same method for benchmarking drag models against their measurements. Instead, in their spreadsheet calculations (Data S1: jgrb52485-sup-0002-2017JB014926-ds01.xlsx, Excel 2007 spreadsheet), DMD2018 first calculate the drag coefficient for a given model using the Reynolds number calculated from a measured velocity, then they use this drag coefficient in an equation that balances the drag force with the gravity and buoyancy forces to recalculate the particle terminal velocity. As a result, this calculated terminal velocity does not agree with the measured velocity used to initially calculate the particle Reynolds number.

As stated above, the appropriate strategy to assess drag models is to determine particle velocity through an iterative-corrective procedure, for example, as it is done in the DMD2018 Matlab code. Another strategy is to directly use the drag model in the particle equation of motion, then track the particle as it falls and stop the simulation when the particle has reached its terminal velocity. Although this procedure is vastly used
Table 1
The (Typo-Free) General Correlation for Estimating the Average Drag Coefficient, $C_D$, of Freely Falling Solid Non-spherical Particles in Liquids or Gases

$$C_D = \frac{24k_s}{Re} \left[ 1 + 0.125 \left( \frac{Re k_s}{k_b} \right)^{2/3} \right] + \frac{0.46k_b}{16k_s^{1/3}} \text{ valid for } Re < 3 \times 10^5$$

where

$$k_s = \left( F_S^{1/3} + F^{-1/3}_S \right) / 2$$

$$F_S = f \epsilon d_{eq}^3 \left( \frac{d_{eq}}{LIS} \right) \text{, or in case of ellipsoids : } F_S = f \epsilon d_{eq}^3$$

$$k_N = 10s_1 \left( -\log(F_S) \right)^2$$

$$s_2 = 0.45 + 10/\left( \exp(2.5 \log^2 + 30 \right)$$

$$\beta_2 = 1 - 37/\left( \exp(3 \log^2 + 100 \right)$$

$$F_N = f^2 \epsilon \left( d_{eq}^3 / LIS \right) \text{, or in case of ellipsoids : } F_N = f^2 \epsilon$$

Note. The original equations (not shown here) are presented by BB2016, which have typos in the misplaced parentheses in denominator of $s_2$ and $\beta_2$ equations and the $\beta_2$ power in $k_N$ equation. Here we only present the typo-free equations; see Bagheri and Bonadonna (2019) for more details.

in the literature for tracking particles in various types of flows (e.g. Bagheri et al., 2012; Daitche, 2013; Maxey & Riley, 1983; Onishi et al., 2015) and for estimating terminal velocity of particles in quiescent flows (Chang & Yen, 1998), we have developed and verified a new code (supporting information). Nonetheless, any iterative approach that can find the velocity at which the drag force is balanced with the particle weight is adequate for solving this problem. Here we prefer to use the free-fall iterative approach since it is a physically guided iterative scheme, which provides a history of dynamics of particle fall and could, for example, be used to check whether or not the falling distance in the experiment was sufficient.

Our code is used here to calculate the drag coefficient of particles based on various drag models (the code is available for download as a Jupyter notebook written in Python 3 as supporting information). Models considered in the code are those of (i) Clift and Gauvin (1971), that is, equation (20) in DMD2018; (ii) Haider and Levenspiel (1989), that is, equation (6) in BB2016; (iii) Ganser (1993), that is, equation (17) in DMD2018; (iv) BB2016, that is, equation (34) and Table 8 in BB2016 (also see BB2019); and (v) the new model presented in equation (14) of DMD2018. As mentioned above, there are some typos in equations (30) and (31) and Table 8 of BB2016 available at the Powder Technology website. For clarification, the correct set of equations is shown here in Table 1 (G. Bagheri & Bonadonna, 2019).

The code calculates particle velocity by solving the particle equation of motion for a falling particle (e.g., equation (4) in Bagheri et al., 2013), considering only buoyancy, drag, and gravitational forces. The Basset history force term and added-mass forces are neglected in the calculations, which is an acceptable assumption only for sufficiently high particle-to-fluid density ratios or for particles falling with negligible acceleration relative to the surrounding fluid (e.g., after the particle reaches its terminal velocity). It is assumed that the terminal velocity is reached when the magnitude of particle acceleration falls below 0.001 m/s².

1.1. Recalculation of DMD2018 Results
We first verified the implementation of our methods by reproducing the drag coefficients of 26 freely falling spherical particles, calculated from measurements by Pettyjohn and Christiansen (1948) and Christiansen and Barker (1965), at Reynolds numbers between 0.01 and 20,000 (section 1.1 of the Python code). By using our code together with the spherical model of Clift and Gauvin (1971), we calculated drag coefficients of spherical particles with mean (equation (1)) and maximum errors of 4.6% and 9.8%, respectively. Furthermore, the mean error in replicating measured
terminal Reynolds number is 2.4%. This exercise verifies correct implementation of the code considering the
fact that the spherical drag coefficient obtained from the model of Clift and Gauvin (1971) is associated with
an inherent uncertainty of −4% to +6% (see Table 5.1 in Clift et al., 2005).

The verified code is further used to benchmark various drag models against drag measurements carried out
by DMD2018 (section 1.2 of the Python code). Figure 1 and Table 2 summarize results of this benchmark.
Mean relative error for a given quantity is defined as follows:

\[
\text{value mean rel. err. } \% = \left( \frac{1}{N} \right) \sum_{i=1}^{N} \left| \text{value}_{\text{code}} - \text{value}_{\text{ref}} \right| \times 100/\text{value}_{\text{ref}} \tag{1}
\]

where \( N \) is the number of data points and \( \text{ref} \) and \( \text{code} \) indicate the reference values from measurements and
simulation values obtained by the code, respectively. Similarly, root-mean-square error (RMSE) is defined as
follows:

\[
\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (\text{value}_{\text{code}} - \text{value}_{\text{ref}})^2}{N}} \tag{2}
\]

As shown in Figure 1 and Table 1, BB2016 is associated with the lowest error in estimating the drag coefficient
and terminal velocity of irregular particles in all the considered criteria, which are mean relative drag and
terminal velocity errors, and RMSE of terminal velocity. The next best model considering relative errors
is the model of Ganser (1993), which is closely followed by the model of DMD2018. If we consider RMSE
errors (equation (2)), however, DMD2018 is the second most accurate model and that of Ganser (1993) is
the third most accurate. Drag coefficients predicted by the corrected BB2016 model are compared to those
calculated from measurements by DMD2018 in Figure 2, which again confirms that the BB2016 estimations
are associated with low errors unlike what is shown in Figure 4 of DMD2018.

![Figure 2. Particle Reynolds number versus drag coefficient measured by DMD2018 against those estimated by the model of BB2016 (i.e., the typo-free version presented in Table 1).](image-url)
2. Conclusions

We have demonstrated that the typo-free equations of BB2016 presented in BB2019 are associated with the lowest mean relative errors for estimating the drag and terminal velocity of particles measured by DMD2018 averaged across all Reynolds numbers, followed by the model of Ganser (1993), DMD2018, and Haider and Levenspiel (1989). The code and database used here to reproduce and investigate the results presented by DMD2018 can be found as supporting information.

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