Answer to Reviewer comment RC1 on the manuscript “New straightforward formulae for the settling speed of prolate spheroids in the atmosphere: theoretical background and implementation in AerSett v2.0.2.”

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We are grateful to Reviewer Carlos Alvarez Zambrano for his careful reading of our manuscript and his insightful questions and suggestions. This document is a contribution to the discussion and not a formal answer in view of the final publication, therefore we will address only the reviewer comments that refer to the scientific content of the manuscript. Reformulations will be addressed for the final submission if we are invited to submit this study to GMD.

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1 Transcript of the Reviewer Comment RC1

1.1 Summary

In this paper, the authors deduced two equations for calculating the settling velocity of atmospheric particles with elongated spheroidal shapes, considering both horizontal and vertical orientations. The first formulation relies solely on theoretical reasoning. The second method is based on drag expressions derived from numerical simulations using computational fluid dynamics (CFD). Their findings indicate that these two formulations yield comparable results, with a deviation, based on the mean particle diameter, within 2% and 10% for particles falling horizontally. The authors also implemented their formulations into a Fortran-based model to calculate dust transport.

1.2 Overall Evaluation

The manuscript is well-written, and the authors have done a great job deducing the equations and providing explanations for the reasoning behind them. However, certain sections of the paper, including those related to the formulation deduction, could benefit from additional explanations and discussion. With the incorporation of extra clarifications and/or inclusion of details, in my opinion, this manuscript will ultimately make a good
contribution to the atmospheric dust transport community. Below, I include some questions and comments that could enhance the quality of this paper.

1. I recommend that the authors provide a brief description of AerSett v2.0.2 in the Introduction section, as not everyone may be familiar with this module previously published by (almost) the same authors.

2. Line 67: I suggest changing the expression "might be tricky" to a more formal expression, such as "pose challenges.”

3. Line 69: It would be advisable to include the definition of the aspect ratio, even though it is defined later in the document.

4. Abstract and Line 85: It is not clear if the authors implemented both formulations as mentioned in Line 85, or if they used the equation obtained from the first approach, as stated in the Abstract.

5. Equation 10: Define x in the D(x).

6. Equation 11: Is $v_\infty$ the settling velocity for prolate spheroid-shaped particles? If so, what is the main difference with $U^{(\lambda,\phi)}$?

7. Section 2.3: Why is the slip correction factor needed? Is the correction being applied to the whole range of particle sizes? To determine the applicability of the slip-correction factor, the Knudsen number (Kn), the ratio of the mean free path to the particle diameter, needs to be observed. Depending on the calculated value of Kn, the correction may be relevant or not. However, the mean free path depends on the pressure, density, and dynamic viscosity of the air. This raises a question for the authors: do the calculations include variations in these air parameters, or was only a constant pressure considered? I recommend that the authors explore in detail the impact and applicability of the slip correction and include in the paper a discussion of for what particle sizes and/or air pressures the correction is important.

8. Equation 29: Define u in $F_{cg}(u)$.

9. Line 195: The authors state that Eq. 31 provides an accuracy better than 2.5%. However, it is not clear what was the reference used to calculate/compare the results of this equation.

10. Conclusions: I suggest that the authors expand the discussion of the limitations of this formulation. They can explore, for example: i) how other orientation values would change their findings. Although the authors stated that particles tend to fall horizontally, it is also known that during the particle lifespan, they change their orientation. ii) Are there any ideas on how to incorporate porosity into each particle for this new formulation?

2 Answers

2.1 Comment 1. Adding a description of AerSett v2.0.2

We agree that a description of the module is missing in the introduction, since this module is not (hopefully, not yet) well-known to the community. If we are invited to submit an updated version for final publication we will add this missing piece in the introduction.

2.2 Comment 4. Did we implement both methods?

Line 85 in the manuscript says that “In Section 4 we will present the implementation of both these methods in AerSett v2.0”, but Abstract says that “we provide an implementation of the first of these methods in AerSett v2.0.2, a module written in Fortran.”. The Reviewer is right in spotting an inconsistency here. The statement in the Abstract is correct, only the first of these method is implemented. In the end of section 3 of the manuscript, we explain why we consider that using the first formulation is more simple and accurate enough for atmospheric sciences.
2.3 Comment 5. Equation 10: Define \( x \) in the \( D(x) \).

Eq. 10 in the manuscript is as follows:

\[
C_D(Re) = \frac{A \lambda, \phi}{Re} \mathcal{D}(Re), \text{ with } \lim_{x \to 0^+} \mathcal{D}(x) = 1. \tag{10}
\]

In this equation, \( x \) is the infinitesimal quantity going to zero in \( \lim_{x \to 0^+} \mathcal{D}(x) = 1 \), it is just a dummy variable name. However, introducing a dummy variable here is not indispensable, and may just induce confusion, therefore in case of resubmission we will clarify the meaning by rewriting Eq. 10 as:

\[
C_D(Re) = \frac{A \lambda, \phi}{Re} \mathcal{D}(Re), \text{ with } \lim_{Re \to 0^+} \mathcal{D}(Re) = 1, \tag{10}
\]

2.4 Comment 6.

Eq. 11 and the surrounding text are as follows:

\[
v_\infty = \frac{4}{3} \frac{(\rho_p - \rho) g d^2_{eq}}{A \lambda, \phi \mu \mathcal{D}(Re)} = \frac{U \lambda, \phi}{\mathcal{D}(Re)}, \tag{11}
\]

where \( U \lambda, \phi = \frac{4}{3} \frac{(\rho_p - \rho) g d^2_{eq}}{A \lambda, \phi \mu} \) is the settling velocity of a prolate spheroid with aspect ratio \( \lambda \) and orientation angle \( \phi \), under the Stokes law for prolate spheroids.

In these equations, \( v_\infty \) is the settling velocity for a prolate spheroid-shaped particle, and \( \frac{U \lambda, \phi}{\mathcal{D}(Re)} \) is the settling speed of the same particle under the Stokes law. More explicitly, \( v_\infty \) includes the large-particle drag correction, while \( U \lambda, \phi \) does not. Therefore, \( U \lambda, \phi \) has an exact analytic expression \( U \lambda, \phi = \frac{4}{3} \frac{(\rho_p - \rho) g d^2_{eq}}{A \lambda, \phi \mu} \), already known from past theoretical works as detailed in the introduction, while \( v_\infty \) includes \( \mathcal{D}(Re) \), a drag-correction term that accounts for deviations from the creeping-flow regime that occur for larger Reynolds number.

This distinction will be made more explicit in the manuscript if we are invited to submit a final version of this manuscript.

2.5 Comment 7. on the slip-correction factor

We agree that this discussion is important, however it has been done for the case of spherical particles in Mailler et al. (2023) (their Section 5). The conclusions of this figure are not changed in any substantial way for prolate spheroidal particles. In short, the main point-by-point answer to your questions on this point are:

- The slip-correction is needed to take into account the fact that for the smallest particles, their size is comparable to the free mean path of air molecules so that air does not behave like a continuous fluid. We can develop this point in the introduction.

- yes, the correction is applied for the whole range of particle sizes. However, for particles with diameter \( D > 10 \, \mu m \), this correction is almost negligible (see Fig. 4 of Mailler et al. (2023)).

- Regarding the atmospheric conditions used for this manuscript, only Figures 2 and 5 in the manuscript depend on particular atmospheric conditions. These figures have been produced with \( P = 101325 \, Pa \) and \( T = 298.15 \, K \). This choice is not specified in the manuscript, we will specify it in a revised version.

- Regarding the influence of atmospheric pressure, temperature and viscosity, Fig. 4 of Mailler et al. (2023) shows that the impact of both the slip-correction and the large-particle drag correction on the settling speed for spherical particles, as a function of particle size and of atmospheric pressure (temperature and viscosity being calculated from pressure using the US Standard Atmosphere).
• We feel that Fig. 4 of [Mailler et al. (2023)], which is a pressure-diameter diagram, gives an indication as of for which diameters and pressures are slip-correction and/or large-particle drag corrections relevant. We agree that this part of the conclusions of [Mailler et al. (2023)] needs to be reminded to the Reader in a future version of this manuscript, probably in the introduction. The present manuscript complements this already existing discussion by discussing for which particles eccentricity correction may become substantial (for which we answer in the conclusion that differences begin to be substantial for aspect ration greater than 2).

2.6 Comment 8. define \( u \) in \( F_{cg}(u) \)

\( u \) is just a dummy variable here, it has no meaning outside of Eq. 29. We will try to rewrite / add a precision at this point if we find a good way to make this clearer.

2.7 Comment 9. Where does the 2.5% accuracy come from?

In line 195 and around, the following statement is made, for which the Reviewers asks for precisions.

“Eq. 18 with \( C_D \) as expressed in Eq. 27 yields:

\[
S = (F_{cg}(R \cdot S))^{-1}. \tag{30}
\]

An equivalent fixed-point equation has been solved in [Mailler et al. (2023)] (their Eqs. 13 and 16), yielding the following approximated expression for \( S(R) \):

\[
S(R) = 1 - \left[ 1 + \left( \frac{R}{4.880} \right)^{-0.4335} \right]^{-1.905}, \tag{31}
\]

which holds with an accuracy better than 2.5% for the \( Re < 1000 \).”

The justification of this statement is at the core of [Mailler et al. (2023)], so that we will make it clearer in a future version that the reader is refered to that study for the details of this assertion. The assertion of 2.5% is relative to the loss of accuracy when solving Eq. 30 using explicit expression 31 to obtain the solution right away instead of performing an iterative resolution of Eq. 30.

We agree that we have to clarify what we mean by “[Eq. 31] holds with an accuracy better than 2.5% for the \( Re < 1000 \).” We do not claim that the accuracy is better than 2.5% relative to real-world data or to an exact theoretical solution (which is not known). We mean that the loss of accuracy in using the explicit formula instead of resolving the fixed-point equation is less than 2.5%, which as we discuss in [Mailler et al. (2023)] is not a considerable accuracy loss since the Clift-Gauvin formula itself has an uncertainty around 7% compared to real-world measurement and to other comparable formulations (Goossens, 2019).

We could clarify this by changing sentence in line 195 by: “As discussed in [Mailler et al. (2023)], using this explicit formula instead of numerically solving Eq. 30 induces a loss of less than 2.5% in accuracy for \( Re < 1000 \), which is not critical since, the uncertainty of the Clift-Gauvin formula itself (and of other comparable drag-coefficient formulations) is around 7% when compared to field measurement (Goossens, 2019).

2.8 Comment 10. Expand the conclusions and discuss the limitations

We agree that the discussion could be enhanced and in particular the limitations of the present approach could be discussed further. Two points in particular are suggested by the Reviewer.

1. intermediate orientations We agree that intermediate orientations have to be dealt with. From methods based on mechanics and statistical physics, [Mallios et al. (2021)] have determined probability distribution functions (PDFs) for particle’s attack angle as a function of their aspect ratio and of the other characteristics of the particle and of the fluid (assuming particles shaped as prolate spheroids). Based on these PDFs the authors have calculated the average attack angle of particles with different sizes. They showed that particles with sizes less than \( \approx 2 \mu m \) are in principle randomly oriented, while particles with sizes larger than \( \approx 20 \mu m \) tend to fall on average horizontally oriented. A future
line of work is to find theoretical and/or heuristic ways to extend our findings to the intermediate orientations and to obtain an expression of the instant settling speed for each possible attack angle. Then, this expression could be integrated on all attack angles (weighted by the PDF of the attack angle) to obtain the resulting average settling speed for a given particle depending on particle’s shape and fluid’s characteristics. Further work needs to be done towards this direction, but we can add this as a discussion element, and also discuss how addressing only horizontal and vertical orientations for the moments limits the possible use of our results.

2. porosity As long as the particle shape is not affected, porosity can be included easily into our equation system. Let us say that the minerals composing the particle have an overall density $\rho_m$, but has porosity $\phi$. Then, its apparent density $\rho_p$ is $\rho_p = \rho_m (1 - \phi)$, so that we can use the exact same approach we develop in the manuscript, modulating the value of $\rho_p$ to take porosity into account.

Other limitations include the fact that we have provided expressions for prolate spheroids, but other shapes can occur, in particular oblate spheroids, triaxial spheroids or more irregular shapes. These limitations will be discussed more in-depth as well if we are invited to submit a revised version.

On behalf of the all the authors,

Sylvain Mailler

References

