https://doi.org/10.5194/gmd-2022-247
Preprint. Discussion started: 21 October 2022

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AerSett v1.0: A simple and straightforward model for the settling speed of big spherical atmospheric aerosol.

Sylvain Mailler[1,2], Laurent Menut[1], Arineh Cholakian[1], and Romain Pennel[1]

[1]LMD/IPSL, École Polytechnique, Institut Polytechnique de Paris, ENS, PSL Research University, Sorbonne Université, CNRS, Palaiseau France

[2]École des Ponts-ParisTech, Marne-la-Vallée, France

Correspondence: Sylvain Mailler (sylvain.mailler@lmd.ipsl.fr)

Abstract. This study introduces AerSett v1.0 (AERosol SETTling version 1.0), a model giving the settling speed of big spherical aerosols in the atmosphere without going through an iterative equation resolution. We prove that, for all spherical atmospheric aerosols with diameter D up to $1000\,\mu\mathrm{m}$, this direct and explicit method based on the drag coefficient formulation of Clift and Gauvin (1971) gives results within 2% of the exact solution obtained from numerical resolution of a non-linear fixed-point equation. This error is acceptable considering the uncertainties on the drag coefficient formulations themselves. For $D < 100\,\mu\mathrm{m}$, error is below 0.5%. We hope that with this simple and straightforward model, more Chemistry-Tranport models and General Circulation models will be able to take into account large-particle correction to the settling speed of big spherical aerosol particles in the atmosphere, without performing an iterative and time-consuming calculation.

1 Introduction

The goal of this article is to give a simple, robust and computationnally efficient expression to calculate the terminal fall speed of spherical atmospheric aerosol, including the large-particle correction term of Clift and Gauvin (1971). As discussed thoroughly in Goossens (2019), several parameterizations exist for the drag coefficient, each of them fitting the reference data only in part. These parametrizations give drag coefficients which differ between them and from measurements by a few percents. Among these parameterizations, the Clift and Gauvin (1971) and Cheng (2009) seem to perform better according to the objective scores presented in Table 2 of Goossens (2019).

While large-particle correction is only marginal for small dust particles, the issue of giant dust particle has emerged in the recent years in air quality modelling. Such particles have been observed *in situ* (van der Does et al. (2018)), but climate models still miss the coarsest dust particles (Adebiyi and Kok (2020)). Many reasons such as not accounting for particle's non sphericity (Mallios et al. (2020)), electric charges, convective injection of particles high in the atmosphere, could contribute to this underestimation (Adebiyi and Kok (2020)), but the recent focus on these giant particles highlights the need for a robust and efficient way of calculating the settling speed of particles with diameter $D > 10\,\mu m$. Until now, the gravitational settling speed in most chemistry-transport models is calculated with a plain Stokes formulation and a free-slip correction for the smallest particles through a Cunningham correction factor, following Zhang et al. (2001), and with no large-particle correction (*e.g.*, Sič et al. (2015), Rémy et al. (2019), Shu et al. (2021)). An exception to this is the recent development exposed by Drakaki

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et al. (2022) in the GOCART-AFWA dust scheme of WRFV4.2.1. In that study, the Clift and Gauvin (1971) drag coefficient correction is taken into account by a bisection method, performed once for each of the model size bins. These authors highlight that taking into account a drag-coefficient correction for large dust particles is important. They do so by applying the Clift and Gauvin (1971) drag correction. Drakaki et al. (2022) also remark that much better agreement between model and observations is reached when, apart for applying the Clift and Gauvin (1971) drag correction factor, the settling speed of dust particles is reduced by an empirical factor of 80%, and conclude that there is still much to learn on the processes that explain why large dust particles can stay airborne long enough to match observation. Since it has been highlighted by Drakaki et al. (2022) that taking into account the Clift and Gauvin (1971) drag correction is important for representing the settling of large dust particles, the present study aims at giving an explicit and straightforward formula to obtain the terminal fall speed of a spherical particle as a function of the physical parameters of the dust particles and the surrounding air.

In section 2, we review the basic equations that govern the settling speed of spherical aerosol particle in the atmosphere; in Section 3 we lay the basis for a new methodology for finding the settling speed of the particle as a function of the particle and surrounding gas parameters. In section 4, we apply this method to the case of the drag coefficient parameterization of Clift and Gauvin (1971) and give an approximated expression of the large-particle correction factor, before concluding in Section 5 by summarizing the method we propose for the calculation of the settling speed of large spherical aerosol particles as well as future prospects for improving the representation of the settling speed of large aerosol particles in chemistry-transport models.

2 Basic equations

We will follow the notations of Mallios et al. (2020). The terminal fall speed v_∞ of a spherical particle with diameter D is given by:

$$\frac{1}{2}C_d A_p \rho_{air} v_\infty^2 = (\rho_p - \rho_{air}) V_p g, \tag{1}$$

Where C_d is the drag coefficient, A_p the projected area of the particle normal to the flow, ρ_{air} the density of air, ρ_p the density of the settling particle, v_∞ the final fall velocity for the particle, V_p the particle volume and g the acceleration of gravity.

In the case of spherical particles, for extremely small Reynolds numbers, Stokes (1851) has shown that:

$$C_d = \frac{12}{Re}, \tag{2}$$

with

$$Re = \frac{\rho_{air} D v_\infty}{2\mu}, \tag{3}$$

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where μ is the dynamic viscosity of air. Eq. 2 holds only for extremely small Reynolds number ($Re < 0.1$), and Clift and Gauvin (1971) has given an empirical expression of C_d as a function of Re, which holds for $Re < 10^5$:

$$C_d = \frac{12}{Re}\left(1 + 0.2415\, Re^{0.687}\right) + \frac{0.42}{1 + \frac{19019}{Re^{1.16}}}, \tag{4}$$

where exponents 0.687 and 1.16 and coefficients 0.2415, 0.42 and 19019 are empirical numbers that permit Eq. 4 to fit experimental data. Hereinafter, we will refer to Eq. 4 as the Clift-Gauvin formula.

Equations 1 and 4 are two equations for two unknowns, v_∞ and C_d. For small Reynolds numbers ($Re < 0.1$), Eq. 4 reduces to Eq. 2 and we obtain:

$$v_\infty^{Stokes} = \frac{D^2\,(\rho_p - \rho_{air})\,g}{18\mu}. \tag{5}$$

If the Reynolds number exceeds 0.1, Eq 2 does not hold, and v_∞ does not have an analytical expression. The solution to Eq. 2 can be obtained by the iterative method described in Van Boxel. The results of this numerical calculation is shown in Fig. 1. Fig. 1a shows that the Stokes equation (Eq. 5) gives excellent results for $D < 10\,\mu\text{m}$, but that the deviations from it due to departure of the drag coefficient from Eq. 2 are strong when D exceeds $10\,\mu\text{m}$. In terms of Reynolds number, the deviation begins to be considerable when the Reynolds number reaches or exceeds 0.1, reaching -30% when $D \simeq 100\,\mu\text{m}$, and -90% when $D \simeq 1000\,\mu\text{m}$. While particles with diameter $D \simeq 1000\,\mu\text{m}$ are not a concern for chemistry-transport modelling, these with $D \simeq 100\,\mu\text{m}$ are an emerging concern, due to recent observations of particles with such diameters far away from their source (van der Does et al. (2018)).

Solving Eq. 1 with the iterative method of van Boxel (1998) demands several iterations when the diameter of the particle gets close to $100\,\mu\text{m}$. This is why we will expose a way to estimate v_∞ from the characteristics of the problem in a straightforward way.

3 Expressing v_∞ from the parameters of the problem

To slightly generalize matters, let us rewrite Eq. 4 as:

$$C_d = \frac{12}{Re}\left(1 + f\,(Re)\right), \tag{6}$$

where f is a function characterizing the deviation of C_d from its Stokes (1851) expression.

Injecting Eq. 6 into Eq. 1, with $A_p = \frac{\pi D^2}{4}$ and $V_p = \frac{\pi D^3}{6}$, we obtain:

$$v_\infty = \frac{D^2\,(\rho_p - \rho_{air})\,g}{18\mu} \times \frac{1}{(1 + f\,(Re))} \tag{7}$$

$$= v_\infty^{Stokes} \times \frac{1}{(1 + f\,(Re))} \tag{8}$$

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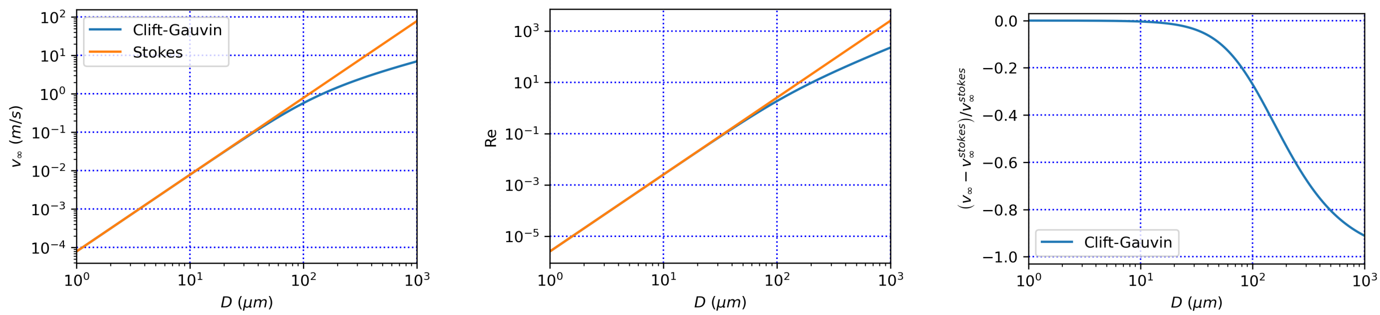

(a) (b) (c)

Figure 1. (a) Terminal fall speed of a spherical particle with $\rho = 2650\,\mathrm{kg\,m^{-3}}$ in air with $P = 101325\,\mathrm{Pa}$ and $T = 293.15\,\mathrm{K}$ as a function of diameter with C_d from equations 4 (blue) and 5 (orange). (b) Reynolds number from equations 4 (blue) and 5 (orange), and (c) relative difference of v_∞ from v_∞^{Stokes}

Of course, Eq. 8 does not give an explicit formulation of v_∞ since Re depends on v_∞ (Eq. 3). However, we are looking for a way to take advantage of Eq. 8 to obtain an explicit estimate of v_∞, so that we introduce the deviation of v_∞ from v_∞^{Stokes}, δ, as:

$$v_\infty = v_\infty^{Stokes}(1+\delta) \tag{9}$$

The terminal Reynolds number of the particle is equal to:

$$Re = \frac{\rho_{air} D v_\infty^{Stokes}(1+\delta)}{2\mu} = (1+\delta)\frac{\rho_{air} D^3 (\rho_p - \rho_{air}) g}{36\mu^2} \tag{10}$$

Let us introduce:

$$R = \frac{\rho_{air} D^3 (\rho_p - \rho_{air}) g}{36\mu^2} \tag{11}$$

R is the Reynolds number of the particle if it would have if it would be falling at speed v_∞^{Stokes}: we will call it the *virtual Reynolds number*. The Reynolds number of the particle falling at its corrected settling speed v_∞ is $R(1+\delta)$. With these modifications, Eq. 8 can be rewritten as:

$$1+\delta = \frac{1}{1+f((1+\delta)R)} \tag{12}$$

In this equation, R is a non-dimensional number that depends on the characteristics of the problem (Eq. 11), and f is the relative deviation of the drag coefficient C_d from $\frac{12}{Re}$ (Eq. 6). Independantly of the formulation of $f(Re)$, the relative deviation δ of v_∞ from v_∞^{Stokes} is the solution of the fixed-point equation 12. Therefore, δ is a function of R, and only of R, which we will note $\delta(R)$. In other words the terminal fall speed of particles can be expressed as:

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$$v_\infty = \frac{D^2\left(\rho_p - \rho_{air}\right)g}{18\mu} \times \left(1+\delta\left(R\right)\right), \text{ with} \quad (13)$$

$$R = \frac{\rho_{air} D^3\left(\rho_p - \rho_{air}\right)g}{36\mu^2}. \quad (14)$$

This shows that the dependance of v_∞ on parameters D, ρ_p, ρ_{air}, g, μ and on function $f\left(Re\right)$ has a very specific form, and that, if one wants to tabulate the solutions, the values of $\delta\left(R\right)$ could be obtained once and for all solving Eq. 12 for the entire relevant range of the possible values of R (where the virtual Reynolds number R is defined by Eq. 11), instead of tabulating v_∞ for all the possible combinations of D, ρ_p, ρ_{air}, g and μ.

4 The $\delta\left(R\right)$ function in the Clift-Gauvin case

Now, we proceed supposing that the expression of C_d as a function of Re is that of Clift et al. (2005) (Eq. 4), yielding the following expression for $f\left(Re\right)$:

$$f(Re) = 0.2415 Re^{0.687} + \frac{Re}{12} \times \frac{0.42}{1+\frac{19019}{Re^{1.16}}} \quad (15)$$

Equation 12 can be solved iteratively (as described in, *e.g.*, Van Boxel 1998). The resulting function $\delta\left(R\right)$ is shown on Fig. 2a. Due to the sigmoid shape of $f=\delta\left(R\right)$, fitting it with a logistic function of $\ln R$ is tempting, and gives relatively good results. However, a generalized logistic function gives an even better agreement with the exact solution (Fig. 2a). The equation obtained with this fit is:

$$\delta(R) \simeq -\left(1+\mathrm{e}^{0.4335(\ln R - 0.8921)}\right)^{-1.905} \quad (16)$$

$$\simeq -\left(1+\left(\frac{R}{2.440}\right)^{0.4335}\right)^{-1.905} \quad (17)$$

This expression of $f(R)$ yields an error relative to the exact solution $< 1\%$ up to $Re = 10$ and $< 2.5\%$ up to $Re = 10^3$ (Fig. 2b). Considering that Goossens (2019) indicate that the Clift-Gauvin empirical formulation of the drag coefficient (Eq. 4) is true within 7% of the reference drag coefficient values of Lapple and Sheperd (1940), approximating δR by the generalized logistic function given in Eq. 17 is accurate enough not to degrade the evaluation of the terminal fall speed, at least until $Re = 10^3$, which is well beyond the typical range of Reynolds number for atmospheric aerosol in free fall (Fig. 1). Figure 2c indeed shows that the error commited by applying the fit formula (Eq. 17) instead of actually solving Eq. 12 is in fact smaller than the discrepancy between the Clift and Gauvin (1971) formulation and the Cheng (2009) parameterization. The Clift et al. (2005) and Cheng (2009) drag formulations being the two best performing formulations according to the objective scores presented in Goossens (2019) (their Table 2), this confirms that the error introduced by using Eq. 17 instead of the exact solution of Eq. 12 is smaller than the uncertainty of state-of-the-art drag coefficient formulations.

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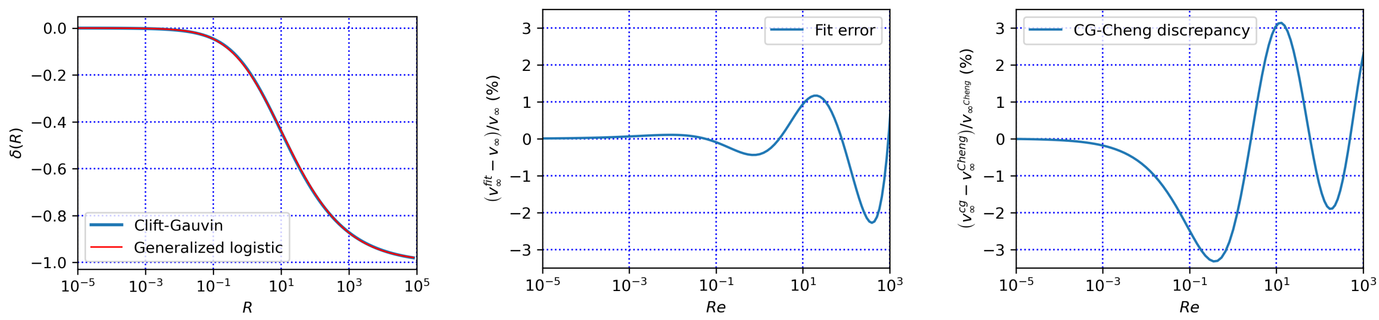
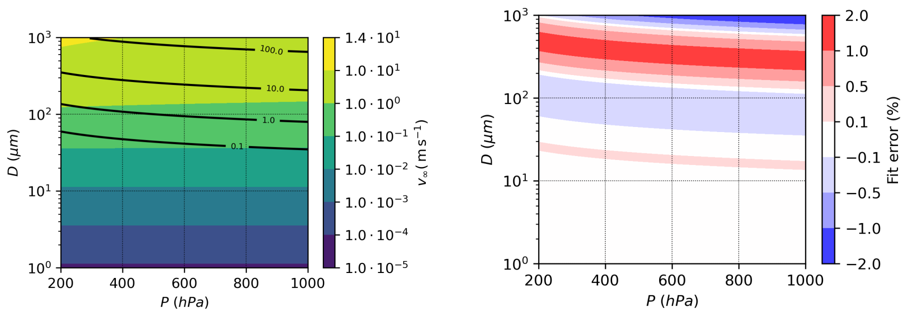


(a) (b) (c)

Figure 2. (a) δR (solution of Eq. 12) as a function of R when f is defined from the Clift-Gauvin expression (Eq. 15). The red line is a fit of the solution by a generalized logistic function (Eq. 17). (b) percent error of the fitted expression of v_∞ relative to the exact solution. (c) Percent difference of the settling speed v_∞ calculated with the Clift and Gauvin (1971) parameterization relative to the one calculated with the Cheng (2009) parameterization.



(a) (b)

Figure 3. (a) v_∞ from the Clift-Gauvin expression (Eq. 15) as a function of atmospheric pressure P and particle diameter D for an atmospheric particle with density $\rho = 2650\,\mathrm{kg\,m^{-3}}$. Black contours are iso-Re contours. (b) percent error committed by using Eq. 17 instead of solving Eq. 12.

Figure 3a shows that, for all realistic particle size and all realistic atmospheric pressures in the troposphere, the Reynolds number is below 100, and Fig. 3b shows that the error induced by using Eq. 17 to evaluate the solution of Eq. 12 is less than 0.5% for all particles with $D < 100\,\mu\mathrm{m}$, and less than 2% for all particles with diameter less than $D < 1000\,\mu\mathrm{m}$: this shows that the domain of applicability of Eq. 17 largely covers the size range of giant dust particles (for which typical diameter is below or around $100\,\mu\mathrm{m}$).

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5 Conclusions

As a conclusion, we have found that the following method is suitable to evaluate the terminal fall speed of aerosol in the atmosphere:

$$v_\infty^{Stokes} = \frac{D^2\,(\rho_p - \rho_{air})\,g}{18\mu}\;; \tag{18}$$

$$R = \frac{\rho_{air} D v_\infty^{Stokes}}{2\mu}\;; \tag{19}$$

$$v_\infty = v_\infty^{Stokes} \times \left[1 - \left(1 + \left(\frac{R}{2.440}\right)^{0.4335}\right)^{-1.905}\right]. \tag{20}$$

Equations 18, 19 and 20 constitute the AerSett model v1.0 (AerSett for AERosol SETTling). The error induced by applying this model compared to an iterative calculation of v_∞ is less than 0.5% for particles with diameter $D < 100\,\mu\mathrm{m}$ and less than 2% for particles with $D < 1000\,\mu\mathrm{m}$ (Fig. 3b). Particles with larger diameters fall so rapidly that they are not relevant as atmospheric aerosol: other parameterizations exist for the falling hydrometeors (Khvorostyanov and Curry (2005)), taking into account the shape of snow flakes, the deformation of raindrops due to their speed etc. We have shown that the error due to using Eq. 20 is smaller than the uncertainty that exists between different state-of-the-art formulations of the drag coefficient, showing that this error is not a problem for modelling.

While the correction introduced by Eq. 20 relative to v_∞^{Stokes} is small for particles with diameter $D < 10\,\mu m$ (Fig. 1c), it is about 25% for a particle with diameter $D \simeq 100\,\mu m$, a typical diameter for giant dust particles. So if chemistry-transport models are to represent the observed giant dust particles (which is still a challenge), large-particle correction for the gravitational settling speeds need to be taken into account, and we think that Eq. 20, valid well beyond the typical diameter range of giant dust particles (Fig. 3b), is the simplest available method to do it.

Of course, this method takes into account only the velocity dependance due to the dependance of the drag coefficient on the Reynolds number, typically important for large particles, and not the free-slip correction factor C_c which is necessary for large Knudsen numbers, for which the most frequent formulation is that of Davies (1945) used in the Zhang et al. (2001) parameterization of dry deposition.

To go further in understanding the settling speed of giant dust particles and be able to represent them in chemistry-transport models, it is needed to extend simple models such as AerSett to the case of non-spherical particles, and give simple and straightforward estimates of the correction factor δ not only as a function of particle density and diameter, as in the present study, but also including other factors such as particle excentricity which have been shown to have a strong impact on the settling speed of dust particles (Mallios et al. (2020) and references therein).

Code availability. All the simulations and figures have been performed with python scripts available according to the GNU General Public License v3.0 at the following doi: 10.5281/zenodo.7139284

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Author contributions. All authors have contributed to the article by stirring the ideas, writing and correcting the paper and providing bibliographical reference. SM has developed the Python scripts used to produce the plots..

Competing interests. None.

Acknowledgements. The Authors acknowledge the developers of the python modules `thermo` (Caleb Bell and Contributors[1] and `scipy` (Virtanen et al. (2020)), used for our numerical treatment of the problem.

[1] https://github.com/CalebBell/thermo

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