On the Evaluation of the Collection Kernel for the Coalescence of Water Droplets

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ABSTRACT

Two anomalies are described which arise in the kernel for stochastic droplet collection when it is specified by the formula of Scott and Chen for the linear collision efficiency $y(R,r)$ and by the formula of Wobus *et al.* for the droplet terminal velocity $V(R)$. It is pointed out that if accurate values for $y(R,r)$ are to be obtained for a given droplet pair by interpolation using data for specific droplet pairs, then for large droplet radii ($R \lesssim 30$ μm) it is desirable that these data be tabulated for 2-μm intervals of R. It is shown that if the difference in terminal velocities of two droplets is computed from a formula approximating $V(R)$ and composed of various functions $V^*(R)$ applicable over adjoining domains of R, then it is necessary that these functions be constructed so that the formula and its derivatives, at least up to *second* order, are everywhere continuous. An improved formula for $V(R)$ satisfying this criterion is described.

1. Introduction

The development of a continuous size distribution of water droplets is described, for any droplet radius r, by a nonlinear integrodifferential "collection" equation relating the time-derivative of the spectral number density of droplets $n(r,t)$ to the rate at which droplets collide and coalesce to create or destroy r-droplets (Twomey, 1964). The fundamental physical quantity appearing in this equation is a collection kernel $K(R,r)$ giving that portion of the volume of air swept out per unit time by a droplet of radius R in which a droplet of smaller radius r must lie in order to collide and coalesce with the R-droplet. Assuming each droplet is spherical and any collision is followed by coalescence, the kernel may be written as

$$K(R,r)=\pi R^2 y^2(R,r)[V(R)-V(r)], \qquad (1)$$

where $y(R,r)$ is the linear collision efficiency of the relative motion of the droplets and $V(R)$ the terminal velocity of a droplet of radius R. These two functions must be specified in order to solve the collection equation for the droplet spectrum. The best numerical formulas for these functions would seem to be found in the work of Scott and Chen (1970) who derive approximate formulas for the efficiency y, and in the work of Wobus *et al.* (1971), who provide rational functions $V^*(R)$ approximating the actual terminal velocity $V(R)$. In this paper we point out two anomalies which arise in the behavior of K when specified by these formulas. We also present a new formula for the terminal velocity free of the drawbacks found in the formula of Wobus *et al.* [Incidentally, these drawbacks appear in the terminal velocity formulas of Berry and Pranger (1974).]

2. The collision efficiency

Scott and Chen (1970) present two different methods for calculating y. Their second method, using Eqs. (3), (5), (6) and (9) of their paper, requires less calculation and has a larger domain of validity than does their first method, which is limited to $R \lesssim 200$ μm. Because the accuracy of either method is essentially equal, the second would seem to be more efficacious. Its results are discussed here.

First, however, we note that in Eq. (8) of Scott and Chen the first right-hand bracket should be placed just after the cosine term and the correct form for B in their Eq. (9) should be

$$B=1.587/R+32.73/R^2+344(20/R)^{1.56} \times\exp[-(R-10)/15]\sin[\pi(R-10)/63]/R^2. \qquad (2)$$

The formulas for y given by Scott and Chen approximately match the theoretical results of Davis and Sartor (1967) at the droplet radii $R=10$, 20, 25 and 30 μm, and those of Shafrir and Neiburger (1963) at $R=40$, 60, 80 and 136 μm. Thus, the formulas provide an inter-

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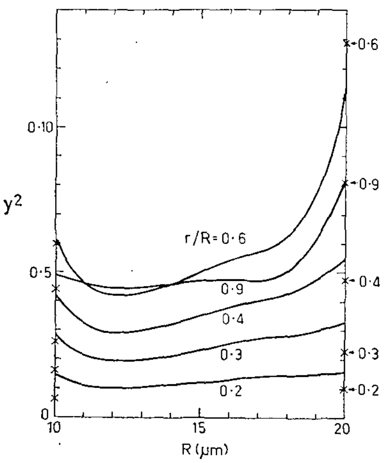

FIG. 1. Dependence of the square of the linear collision efficiency $y^2(R,r)$ upon droplet radius R, from Scott and Chen (1970). The actual results of Davis and Sartor (1967) are given on the two vertical axes by the small crosses, labelled on the right-hand axis according to (r/R) value. The order of the crosses on the left-hand axis is identical except for the uppermost two, which are reversed.

polation for R in the range 10 to 136 μm and an extrapolation for smaller and larger R.

Fig. 1 shows y^2 for R in the range 10–20 μm and for various values of r/R as computed by the second method of Scott and Chen. It is seen that the method does not yield a monotonic value of y^2; there is a local minimum near $R=12$ μm, a minimum about 30% less than the value at $R=10$ μm, and the curvature of y^2 is negative for R in the neighborhood of 16 μm. Furthermore, the curves generally predict values for y^2 differing considerably from those given by a simple linear interpolation between the actual values of Davis and Sartor, denoted by the crosses on the vertical axes. The error is about +50% for $r/R=0.2$ and 0.3, and about −40% for $r/R=0.6$ and 0.9.

Although the Scott-Chen formula is designed to match y not just for $R=10$ and 20 μm but over a wider range of R, the very poor fit exhibited here in this range of small droplet sizes is disturbing. This anomalous behavior for y^2 probably would lead to incorrect and misleading predictions for the importance of collection in the initial development of a droplet spectrum. This development is surely a critical factor in determining the time required for precipitable drops to appear in a cloud.

The original source of this poor approximation for the collision efficiency of small collector droplets would seem to be the paucity of published data to which an approximate formula can be matched. A satisfactory formula for y in this interval probably would require as its basis theoretical calculations of y at (say) 2-μm intervals of R, rather than the 10-μm, or at best 5-μm, intervals published to date (Davis, 1972; Klett and Davis, 1973). This is especially important for R in the range 10–30 μm, where the collision efficiency increases most rapidly and not, incidentally, where most cloud droplets initially are found. Until such detailed knowledge of the collision efficiency is obtained, a linear or at most quadratic interpolation between its presently known values would seem to be all that is justified.

In obtaining a better formula for the collision efficiency in the future it would seem preferable to find approximate expressions for y^2 rather than for y, since it is y^2 that is required in (1) for the collection kernel. For the same relative error in these two quantities y will contribute to the kernel at least twice the error of y^2.

3. The terminal velocity

Wobus *et al.* (1971) give two methods for calculating the terminal velocity of water droplets in air. The function $V^*(R)$ is found in each case by matching the experimental results of Gunn and Kinzer (1949) with rational functions applicable over various adjoining domains of R. Since their second method [Eq. (4) in their paper] is at least as accurate as the first and, in addition, has a more correct asymptotic behavior as R approaches infinity, it would appear to be the better choice for evaluating the contribution to the collection kernel due to the difference in droplet terminal veloci-

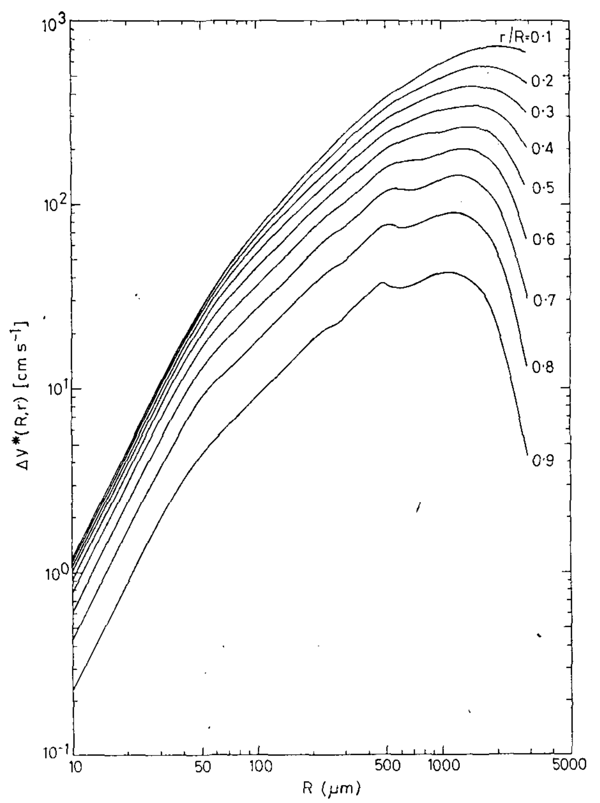

FIG. 2. The relative terminal velocity, $\Delta V^*(R,r)$, computed with Eq. (4) of Wobus *et al.* (1971).

ties. Nevertheless, the values it yields for K have an anomalous behavior. This is apparent from Fig. 2, showing the relative terminal velocity, $\Delta V^*(R,r) \equiv V^*(R)-V^*(r)$, for various R and for r/R fixed and computed using Eq. (4) of Wobus *et al.* In the neighborhood of $R=230$ and 450 μm the velocity $\Delta V^*(R,r)$ behaves anomalously, and because here the collision efficiency y^2 is essentially constant at its geometric value $(1+r/R)^2$, this behavior will extend to the kernel K. The behavior in Fig. 2 is simply understood by noting that the above two radii, along with $R=50$ μm, happen to be junction points for the Wobus functions approximating V.

In matching $V(R)$ with a sequence of adjoining curves two types of error may occur. One is associated with the degree of fit within the particular domain covered by a given curve. The second is associated with any mismatch between curves at their junction points and near these points this error will affect the "smoothness" of the approximation. Wobus *et al.* (1971) reduced the first type of error below the experimental errors in Gunn and Kinzer's (1949) original data. They attempted to reduce the second type of error by requiring that $V^*(R)$ be continuous and have a continuous first derivative at the junction points. These two continuity requirements are sufficient if the approximating function $V^*(R)$ is to be smooth.

In the present case, however, we are seeking a smooth approximation to the *difference* in terminal velocities. This requires that $\Delta V^*(R,r)$ be continuous and have a continuous first derivative. For r/R near unity, where the anomalous behavior in Fig. 2 is most prominent, $\Delta V^*(R,r)$ behaves similarly to the derivative of V^*. Thus, for $\Delta V^*(R,r)$ to be smooth it is necessary that both the first and second derivatives of $V^*(R)$ be continuous.

Fig. 3 displays dV^*/dR computed with the Wobus formula and shows that the second derivative is far from being continuous. Comparison with Fig. 2 shows the effect of this on $\Delta V^*(R,r)$. The next section describes an improved formula for the terminal velocity specifically constructed to have a continuous second derivative.

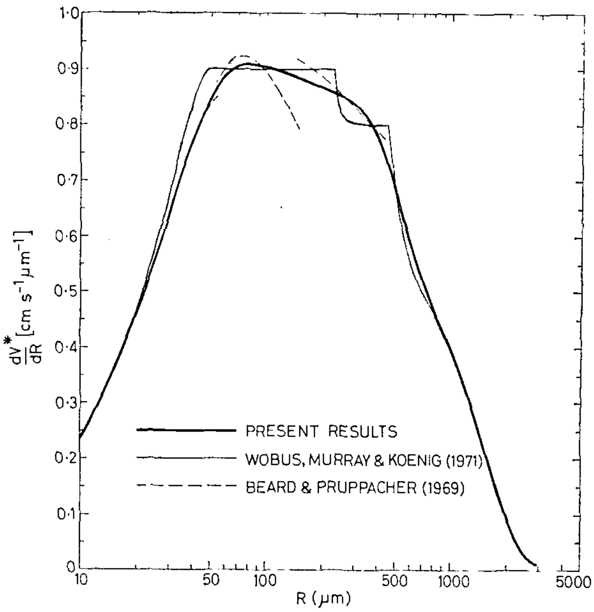

FIG. 3. The first derivative of $V^*(R)$ computed with the improved formula in Section 4 (heavy solid line), computed with the formula of Wobus *et al.* (light solid line), and computed from the drag relationships of Beard and Pruppacher in Eqs. (5) (broken line).

4. An improved terminal velocity formula

An approximate, continuous formula for the terminal velocity $V(R)$, having continuous first *and* second derivatives everywhere, has been obtained and is now described. This formula has five parts (sections) with junction points at $R=15$, 35, 300 and 800 μm. The first section predicts Stokesian terminal velocities. The second section interpolates between these velocities and those predicted by the third section from the experimental work of Pruppacher and Steinberger (1968) and Beard and Pruppacher (1969). The fourth section interpolates between these velocities and those of the fifth section, given by the Wobus formula. This last section of the formula includes none of the Wobus junction points. The velocity formula is based on the assumption that the atmospheric pressure is 1013 mb, the temperature 20C, and the relative humidity 100%. All algebraic quantities in it have their cgs values.

For droplets <15 μm radius, the terminal velocity is given by the Stokes formula:

$$V^*(R)=(2/9)[g(\rho_l-\rho_a)/\eta]R^2,\quad 0\leqslant R\leqslant 0.0015 \text{ cm},\quad (3)$$

where g is the acceleration of gravity, ρ_l the density of the liquid droplet, ρ_a the air density, and η the dynamic viscosity of the air. Stokesian velocities are restricted to droplets <15 μm radius having Reynolds numbers $Re<0.05$. This cutoff value is much less than the usual value of $Re\approx 1$ and is used because Maxworthy (1965) and Pruppacher and Steinberger (1968) suggest that Stokes flow around spheres may actually occur only for such small Reynolds numbers.

For droplet radii between 15 and 35 μm, $V(R)$ is given by

$$V^*(R)=1.443646-3.417072\times10^3R+4.243126\times10^6R^2 -1.263519\times10^9R^3+2.432383\times10^{11}R^4 -1.917038\times10^{13}R^5,\quad 0.0015\leqslant R\leqslant 0.0035 \text{ cm}.\quad (4)$$

This polynomial contains six terms because it is based on the six conditions that $V^*(R)$ and its first and second derivatives be continuous at the two end points, $R=15$ and 35 μm. Although (4) is based only on data at these points, it still predicts for intermediate radii velocities well within those allowed by the errors in the work of

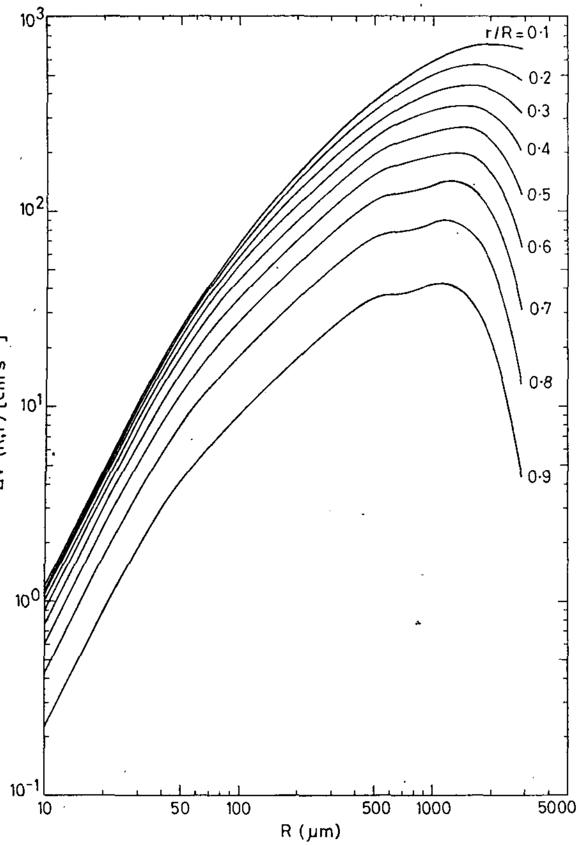

FIG. 4. The relative terminal velocity $\Delta V^*(R,r)$ computed with the improved formula described in Section 4.

Beard and Pruppacher (1969) and of Gunn and Kinzer (1949).

For droplets with radii between 35 and 300 μm, terminal velocities are obtained from the drag data of Beard and Pruppacher (1969). They summarize their data with the following three (least-squares) formulas relating the drag coefficient C_D of a droplet falling at its terminal velocity to its Reynolds number Re:

$$C_D\,\mathrm{Re}^2=24\,\mathrm{Re}[1+0.102\,\mathrm{Re}^{0.955}],\quad 0.2\leqslant \mathrm{Re}\leqslant 2,\qquad (5a)$$

$$C_D\,\mathrm{Re}^2=24\,\mathrm{Re}[1+0.115\,\mathrm{Re}^{0.802}],\quad 2\leqslant \mathrm{Re}\leqslant 21,\qquad (5b)$$

$$C_D\,\mathrm{Re}^2=24\,\mathrm{Re}[1+0.189\,\mathrm{Re}^{0.632}],\quad 21\leqslant \mathrm{Re}\leqslant 200.\qquad (5c)$$

Using

$$C_D\,\mathrm{Re}^2=(32/3)(\rho_l-\rho_a)(\rho_a g/\eta^2)R^3 \qquad (6)$$

to evaluate the left-hand side of Eqs. (5), we can solve them in an iterative manner to obtain Re. The standard procedure is as follows: (i) assume a value for Re (such as 10 for $R\leqslant 100$ μm and 100 for $R>100$ μm); (ii) insert this into the right-hand side of the appropriate equation in (5) [this step requires prior knowledge of the droplet radii corresponding to Re=2 and 21]; and (iii) examine whether the result is equal to $C_D\,\mathrm{Re}^2$ as given by (6) to within some tolerance and if it does not obtain a more correct value for Re by dividing $C_D\,\mathrm{Re}^2$ by the factor in brackets in (5). The final value for Re so obtained yields the terminal velocity.

The disadvantage in so using these three separate formulas is that at the junction points Re=2 and 21 they predict discontinuous values for $V^*(R)$ and its derivatives (see Fig. 3). It has been possible to eliminate this drawback with a single least-squares approximation to Eqs. (5), namely

$$C_D\,\mathrm{Re}^2=24\,\mathrm{Re}[1+0.10229\,\mathrm{Re}^{0.94015+y}],\quad 0.2\leqslant \mathrm{Re}\leqslant 200,\quad 0.0035\leqslant R\leqslant 0.0300\text{ cm} \qquad (7)$$

where

$$y=-2.44461\times10^{-2}\ln \mathrm{Re}-6.98404\times10^{-3}(\ln \mathrm{Re})^2+8.88634\times10^{-4}(\ln \mathrm{Re})^3.$$

Solving (7) in the iterative manner described above yields values for $V^*(R)$ well within the errors ascribed to Eq. (5) by Beard and Pruppacher (1969).

Eq. (7) was obtained by approximating

$$\ln[(C_D\,\mathrm{Re}/24)-1],$$

as predicted by (5), by an nth-order Forsythe (1957) polynomial in ln Re. A value of $n=4$ gave the best fit, being close to the data and still free of unwanted oscillations. Sixty-four data points were used in the fitting process. These were composed of three sets of 20 points each, spaced equally in terms of ln Re over each of the intervals in Eqs. (5), and four additional points at Re=0.2, 2, 21 and 200. At the junction points Re=2 and 21, $\ln[(C_D\,\mathrm{Re}/24)-1]$ was assumed to equal the mean of the two values predicted by the two adjoining formulas. Although (7) is valid over the same range of Reynolds numbers as (5), corresponding to radii in the range 23.5 to 433.2 μm, it is used here for radii in the somewhat reduced range of 35 to 300 μm. This results in no real loss of accuracy for $V^*(R)$ or for $\Delta V^*(R,r)$ and permits a smoother transition between velocities obtained with (7) and those obtained for small droplets with the Stokes formula (3) and for very large drops ($R>800$ μm) with formula (9) (described below).

Although the Wobus formula has no junction points for $R>450$ μm, and for these radii could be used to obtain $V^*(R)$, it was found that a smooth transition between the velocities predicted by it and by Eq. (7) required an interpolating polynomial covering the droplet radii from 300 to 800 μm. This polynomial has the form

$$V^*(R)=3.510302\times10^1+2.865716\times10^3R+2.559450\times10^5R^2-5.064069\times10^6R^3+3.971905\times10^7R^4-1.135044\times10^8R^5,\quad 0.0300\leqslant R\leqslant 0.0800\text{ cm}. \qquad (8)$$

The fifth and last section of the velocity formula is simply that portion of the Wobus formula which is valid for droplets with radii between 800 and 2900 μm (the upper limit of the Gunn and Kinzer data). For the sake of completeness it is listed here:

$$V^*(R) = -[554.5/D] + 921.5 - [4\times 10^{-3}/(R-0.0210)],\quad 0.0800 \leqslant R \leqslant 0.2900 \text{ cm}, \qquad (9)$$

where

$$D = 2.036791\times 10^5 x^5 - 3.815343\times 10^4 x^4 + 4.516634\times 10^3 x^3 - 8.020389\times 10^1 x^2 + 1.44274121\times 10^1 x + 1,$$

and

$$x = R - 0.0450.$$

Fig. 4 displays the relative terminal velocity $\Delta V^*(R,r)$ calculated with the above improved formula. The anomalous behavior found in Fig. 2 no longer appears. This can be attributed to the care taken here to ensure that the second derivative of the velocity is continuous at the junction points (see Fig. 3). (Tests showed that the slight dip in the curves in Fig. 4, for large r/R and for R between 500 and 1000 μm, apparently occurs because the Wobus formula predicts slightly too large values for dV^*/dR for R in the range 800–1200 μm. Their formula is still used, however, because of its asymptotic properties at larger R.)

5. Summary

Two anomalies have been described which arise in the kernel for stochastic droplet collection when it is specified by the formula of Scott and Chen (1970) for the linear collision efficiency $y(R,r)$ and by the formula of Wobus *et al.* (1971) for the droplet terminal velocity $V(R)$. It has been pointed out that if accurate values for $y(R,r)$ are to be obtained for a given droplet pair by interpolation using data for specific droplet pairs, then for large droplet radii $R \lesssim 30$ μm it is desirable that these data be tabulated for 2-μm intervals of R. It has been shown that if the difference in terminal velocities of two droplets is computed from a formula approximating $V(R)$ and composed of various functions $V^*(R)$ applicable over adjoining domains of R, then it is necessary that these functions be constructed so that the formula and its derivatives, at least up to *second* order, are everywhere continuous. An improved formula for $V(R)$ satisfying this criterion has been described.

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