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Statistical Properties and Numerical Implementation of a Model for Droplet Dispersion in a Turbulent Gas*

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We explore the statistical properties of a model proposed by Dukowicz for calculating the dispersion of spray droplets due to turbulent gas motions. The distributions of turbulent velocity and position changes are derived, making no assumptions concerning the relative magnitudes of the drag time, turbulence correlation time, and the time at which the distributions are evaluated. We also tell how the model is implemented in the computer program KIVA and give some computational examples.

I. INTRODUCTION

In introducing his particle model for calculating liquid sprays, Dukowicz [1] also proposed a method for calculating the dispersion of the spray droplets by turbulent gas motions. The purpose of this paper is to explore some of the statistical properties of this turbulent dispersion model and to tell how we have implemented it in the KIVA [2] computer program. According to the method of Dukowicz, we add to the mean gas velocity $\mathbf{u}$, a fluctuating component $\mathbf{u}'$, where each component of $\mathbf{u}'$ is distributed according to the Gaussian

$$G(u') = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{u'^2}{2\sigma^2}\right). \tag{1}$$

In (1), σ is the standard deviation:

$$\sigma = \sqrt{2/3Q}, \tag{2}$$

where Q is the gas turbulent kinetic energy. Dukowicz proposed taking $\mathbf{u}'$ to be a piecewise constant function of time, changing discontinuously after each passage of the turbulence correlation time t_d. The time t_d corresponds physically to an eddy breakup time or to a time for a droplet to traverse an eddy.

The sum $\mathbf{u}+\mathbf{u}'$ is then the gas velocity that the droplet "sees" and that is used

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in computing the momentum transfer between the droplet and the gas. More precisely, the acceleration of a droplet is given by

$$\frac{d\mathbf{v}}{dt} = A(\mathbf{u} + \mathbf{u}' - \mathbf{v}) + \mathbf{g}, \tag{3}$$

where $\mathbf{v}$ is the droplet velocity, $\mathbf{g}$ the acceleration due to gravity, and A is the drag function. For liquid droplets in a gas one can use, with sufficient accuracy [3],

$$A = \frac{3}{8}\frac{\rho_g}{\rho_l}\frac{|\mathbf{u} + \mathbf{u}' - \mathbf{v}|}{r} c_D, \tag{4}$$

where ρ_g and ρ_l are the gas and liquid densities, r is the droplet radius, and c_D is the drag coefficient.

In conjunction with particle methods for calculating sprays, this model for the turbulent dispersion of droplets is now almost universally used [4–7]. The main differences in the proposed formulations are in the methods for choosing the turbulence correlation time t_d. Although interesting and important, we will not deal with this question here.

The question that motivates this paper is the following. How do we solve (3) in numerical calculations when the computational time-step Δt is larger, possibly by several orders of magnitude, than t_d? This question is not addressed in Ref. [1 or 4–7]. When $\Delta t < t_d$, we can solve (3) directly by finite difference approximation and thereby account for such effects as nonlinearity due to dependence of A on the relative velocity. When $\Delta t > t_d$, direct solution of (3) using time-step Δt is no longer possible because more than one value of $\mathbf{u}'$ is "seen" by a droplet in time Δt. One approach to this problem is to simply restrict Δt to be smaller than t_d and solve (3) directly. This approach would be computationally inefficient, however, in circumstances where we could, in the absence of this time-step restriction, compute with Δt much larger than t_d. This is because the equations would have to be solved $\Delta t/t_d$ times more often to compute to a given problem time. To remedy this inefficiency one might consider a time-step splitting method in which the droplet equation of motion (3) is solved with a time-step δt that is less than t_d, and the gas-phase equations are solved with longer time-step Δt. While more attractive than the first approach, a time-step splitting method will still be inefficient when Δt is much larger than t_d, because then one must choose a fluctuating velocity $\mathbf{u}'$ and solve Eq. (3) at least $\Delta t/t_d$ times for each gas-phase time-step Δt.

When $\Delta t > t_d$, the solution method we propose involves choosing random velocity and position changes for each droplet from probability distributions that we will derive for the droplet turbulent velocity and position changes. Thus, independent of how small t_d is relative to Δt, our method requires the choice of only two random numbers for each droplet and each time-step Δt, one to determine its turbulent velocity change and one to determine its turbulent position change.

To simplify the analysis, the turbulent distributions will be derived assuming the

parameters A, Q, and t_d are constant for a given droplet during the time interval Δt. The assumption that Q and t_d are constant for time Δt will be approximately satisfied in our numerical calculations. This is because droplets usually travel no more than one cell size Δx in the time Δt. Thus, assuming the turbulence field is well resolved by the numerical calculation, Q and t_d will be nearly constant and equal to their values in the computational cell in which the droplet is located during the time-step.

Assuming A is constant will certainly introduce some errors in practical spray calculations, but including the effects of a nonlinear drag law will be very difficult. The drag function A is constant if the drop Reynolds number

$$\mathrm{Re} = \frac{2\rho_g |\mathbf{u} + \mathbf{u}' - \mathbf{v}| r}{\mu_g} \tag{5}$$

is small compared to unity, where μ_g is the gas viscosity. In this so-called Stokes regime [3],

$$c_D = 24/\mathrm{Re}, \tag{6}$$

which, combined with (4), gives A constant. Although many droplets will be small enough that $\mathrm{Re} < 1$, in practical sprays Re can be as large as 1000 [3]. For large Reynolds numbers c_D is nearly constant, and a quadratic drag law would be more appropriate. There appears, however, to be no alternative to the assumption of a linear drag law because use of a nonlinear law renders intractable the problem of deriving probability distributions for droplet turbulent displacements. We point out that the errors incurred in making this assumption are confined to the calculated turbulent displacements of droplets whose correlation times t_d are less than Δt and for which $\mathrm{Re} \gtrsim 1$.

Using these assumptions, we first derive for the Dukowicz model the distributions of droplet turbulent velocity and position changes. No assumptions are made concerning the relative magnitudes of the drag time $1/A$, the turbulence correlation time t_d, and the time $t = \Delta t$ at which the distributions are evaluated. Under the additional restrictive assumptions that $t \gg 1/A$ and $t \gg t_d$, it is shown that the distribution of drop turbulent displacements x' in each coordinate direction is Gaussian with variance $\sigma_{x'}^2 = \sigma^2 t t_d$ and depends on the drag function A only through the dependence of t_d on A. Since a distribution that follows a diffusion law has $\sigma_{x'}^2 = 2Dt$, where D is the diffusion coefficient, droplets spreading obeys a diffusion law with diffusion coefficient $D = \frac{1}{2}\sigma^2 t_d$ under the very restrictive assumptions that Q, t_d, and A are constant for times $t \gg 1/A$ and $t \gg t_d$.

We next derive the conditional distribution of droplet turbulent position changes, given that the turbulent velocity change is known. This result is used to derive a general criterion for neglecting droplet turbulent velocity changes in numerical calculations. We show in particular that in numerical calculations with time-step size Δt, if $\Delta t \gg 1/\mathrm{A}$ and $\Delta t \gg t_d$ then to calculate accurately the turbulent diffusion

of a droplet in physical space, one can neglect random changes in the droplet's velocity. When $1/A \gg \Delta t \gg t_d$, this is not true, and on each time-step one must compute random changes to both the droplet's physical location and velocity. We give the numerical algorithm that is used under general circumstances in the KIVA program to compute the turbulent displacement of a droplet and compare theoretical distributions of droplet turbulent position change with calculated distributions using $\Delta t/t_d = 0.1$ and $\Delta t/t_d = 10.0$.

II. The Distributions of Droplet Turbulent Velocity and Position Change

A. *The Distribution of Turbulent Velocity Changes*

We want to solve the Langevin [8] equation (3), where each component of $\mathbf{u}'$ is distributed according to (1). Since A is constant, formal solution of (3) gives

$$v - u(1 - e^{-At}) - \frac{1 - e^{-At}}{A} g = e^{-At}\left(v_0 + \int_0^t e^{At'} A u' \, dt'\right) \tag{7}$$

for each component v of the drop velocity. In (7) v_0 is the initial droplet velocity, whose value may also be governed by a distribution function. Equation (7) says that the probability distribution of the quantity on the left-hand side equals that of the right. With w' equal to the change in droplet velocity because of turbulence interactions,

$$w' = e^{-At} \int_0^t e^{At'} A u' \, dt', \tag{8}$$

we seek to find the probability $P(w')\,dw'$ that w' lies in $(w', w' + dw')$.

Since u' is held constant for turbulence correlation time t_d, we have for $Nt_d \leqslant t < (N+1)t_d$,

$$\begin{aligned} w' &= e^{-At} \sum_{k=1}^{N} \left(u'_k \int_{(k-1)t_d}^{kt_d} e^{At'} A \, dt'\right) + \int_{Nt_d}^{t} u'_{N+1} e^{A(t'-t)} A \, dt' \\ &= \sum_{k=1}^{N} w_k(t) + u'_{N+1}(1 - e^{A(Nt_d - t)}), \end{aligned} \tag{9}$$

where

$$w_k(t) = e^{-At}(1 - e^{-At_d})\, e^{Akt_d} u'_k$$

and u'_k is the gas velocity fluctuation when $(k-1)t_d < t < kt_d$. Since the occurence of u'_k is Gaussian with deviation σ, the occurrence of w_k is Gaussian with deviation

$$e^{-At}(1 - e^{-At_d})\, e^{Akt_d} \sigma.$$

We now use the result that if $P(w_1)$ and $P(w_2)$ are Gaussian with deviations σ_1 and σ_2 and if w_1 and w_2 are uncorrelated, then $P(w_1+w_2)$ is Gaussian with deviation $\sqrt{\sigma_1^2+\sigma_2^2}$ [9]. Applying this result to Eq. (9) shows w' is Gaussian with deviation $\sigma_{w'}$, where

$$\sigma_{w'}^2=\left\{e^{-2At}(e^{At_d}-1)\frac{e^{2At_dN}-1}{e^{At_d}+1}+(1-e^{A(Nt_d-t)})^2\right\}\sigma^2. \tag{10}$$

This is the formula we seek concerning the distribution of drop velocity changes.

We can check that (10) is correct in two limiting cases. When $At\gg 1$ and $At_d\gg 1$, it is seen from (10) that $\sigma_{w'}\approx\sigma$ except for short periods of time when

$$Nt_d<t<Nt_d+1/A.$$

In this limit the droplets are tightly coupled to the gas and, accordingly, the distributions of droplet and gas velocities coincide.

In the second limit when both t and t_d are small compared to the droplet drag time $1/A$, we obtain from (10)

$$\sigma_{w'}^2=A^2t_d^2\sigma^2\left\{N+\left(N-\frac{t}{t_d}\right)^2\right\}. \tag{11}$$

With $t/t_d=N$, this reduces to

$$\sigma_{w'}=At_d\sigma\sqrt{t/t_d}, \tag{12}$$

which is the result one naively obtains by assuming the fluctuating velocity follows a random walk with deviation $At_d\sigma$ each step for $N=t/t_d$ steps. The result (12) can be misleading. It is only valid when $t\ll 1/A$. When $t\to\infty$, $\sigma_{w'}$ given by (12) grows without bound, but Eq. (10) shows $\sigma_{w'}$ is bounded by σ. In fact, one can show that $\sigma_{w'}^2$ is less than the expression obtained from (10) by substituting $t=Nt_d$:

$$\sigma_{w'}^2\leqslant\left[\frac{1-e^{-At_d}}{1+e^{-At_d}}(1-e^{-2At})\right]\sigma^2.$$

Thus, as one would expect, the width of the distribution of droplet random velocities cannot exceed the width of the distribution of gas random velocities.

Equation (9) can be put in a more compact form that will be useful later. By defining

$$\Psi(t)=\begin{cases}0 & t\leqslant 0\\ t & t>0,\end{cases}$$

Equation (9) can be rewritten

$$w'(t)=\sum_{k=1}^{\infty}\{e^{-A\Psi[t-kt_d]}-e^{-A\Psi[t-(k-1)t_d]}\}\,u_k'. \tag{13}$$

B. *The Distribution of Turbulent Position Changes*

We now derive the distribution of drop position changes. The random displacement of a droplet is given by

$$x'(t) = \int_0^t w'(t')\, dt'. \tag{14}$$

Substituting (13) into (14) and using

$$\int_0^t e^{-A\Psi(t'-kt_d)}\, dt' = t - \Psi(t-kt_d) + \frac{1}{A}\left(1 - e^{-A\Psi(t-kt_d)}\right) \tag{15}$$

gives

$$x'(t) = \sum_{k=1}^{\infty} \left[\Psi[t-(k-1)t_d] - \Psi[t-kt_d] + \frac{1}{A}\left\{e^{-A\Psi[t-(k-1)t_d]} - e^{-A\Psi[t-kt_d]}\right\} \right] u'_k. \tag{17}$$

Thus if $Nt_d \leqslant t < (N+1)t_d$, by definition of Ψ we have

$$x'(t) = \sum_{k=1}^{N} \left[t_d + \frac{1}{A} e^{-A(t-kt_d)}(e^{-At_d} - 1) \right] u'_k + \left[t - Nt_d + \frac{e^{A(Nt_d - t)} - 1}{A} \right] u'_{N+1}. \tag{18}$$

Applying the law for the sum of uncorrelated Gaussian variables [9], we obtain for the variance of x'

$$\sigma_{x'}^2 = \left\{ A^2 t_d^2 N - 2At_d e^{-At}(e^{ANt_d} - 1) + \frac{1 - e^{-At_d}}{1 + e^{-At_d}} e^{-2At}(e^{2ANt_d} - 1) + [A(t - Nt_d) - 1 + e^{A(Nt_d - t)}]^2 \right\} \frac{\sigma^2}{A^2}. \tag{19}$$

We can derive from (19) an interesting result concerning the asymptotic value of $\sigma_{x'}^2$ for large times. When $t \gg t_d$, one can show that $\sigma_{x'}^2$ is asymptotic to the expression obtained by replacing N in Eq. (19) with t/t_d; that is,

$$\sigma_{x'}^2 \sim \left[A^2 t_d\, t - 2At_d(1 - e^{-At}) + \frac{1 - e^{-At_d}}{1 + e^{-At_d}}(1 - e^{-2At}) \right] \frac{\sigma^2}{A^2}. \tag{20}$$

If in addition $At \gg 1$, one can use (20) to show that

$$\sigma_{x'}^2 \sim \sigma^2 t t_d. \tag{21}$$

The interesting and perhaps puzzling feature of this result is that the drag time $1/A$

does not appear in it. One might naively expect $\sigma_{x'}$ to increase with increasing A. This is in contrast to the asymptotic behavior of $\sigma_{w'}^2$, for which one can show from (10) that

$$\sigma_{w'}^2 \sim \frac{1-e^{-At_d}}{1+e^{-At_d}}\sigma^2, \tag{22}$$

when $t = Nt_d$. As one would intuitively expect, the width of the velocity distribution increases with increasing A—that is, as the drops become more tightly coupled to the gas.

One can easily understand Eq. (21) in the limit when $At_d \gg 1$. In this case the drop follows the gas and the root-mean-square amplitude of its fluctuating velocity will be σ. Each turbulence correlation time t_d the drop will undergo a random displacement σt_d, and after $N = t/t_d$ random displacements we have

$$\sigma_{x'} = \sigma t_d \sqrt{\frac{t}{t_d}} = \sigma t_d^{1/2} t^{1/2}.$$

Although the root-mean-square velocity fluctuation decreases with decreasing A, $\sigma_{x'}$ does not decrease because the fluctuating drop velocity persists for a longer time as A decreases. For example, when $At_d \ll 1$, Eq. (22) shows that

$$\sigma_{w'} \approx \left(\frac{At_d}{2}\right)^{1/2} \sigma.$$

This velocity will persist for a time approximately equal to $1/A$ and the drop will undergo approximately tA displacements. Thus the random displacement will be

$$\sigma_{x'} \approx (At_d)^{1/2}\sigma \qquad 1/A \qquad \sqrt{tA} \qquad \approx \sigma t_d^{1/2} t^{1/2}.$$

velocity — time per displacement — square root of number of displacements

C. *Conditional Distribution of Turbulent Position (Velocity) Changes Given that the Droplet's Turbulent Velocity (Position) Change is Known*

Another question that arises in the next section of this report is given that a droplet's random displacement at time t is x_0', what is the probability distribution of its random velocity w'? The question can also be reversed: given that a droplet's random velocity component is w_0', what is the distribution of its random displacement x'? We answer the second question. The first question can be answered using the same approach.

First we introduce some notation. From Eqs. (13) and (15) we have for the random velocity w' and position x' of a droplet,

$$w' = \sum_{k=1}^{\infty} a_k u_k' \tag{23}$$

and

$$x' = \sum_{k=1}^{\infty} b_k u'_k, \tag{24}$$

where

$$a_k(t) = e^{-A\Psi[t-kt_d]} - e^{-A\Psi[t-(k-1)t_d]} \tag{25}$$

and

$$b_k(t) = \Psi[t-(k-1)t_d] - \Psi[t-kt_d] - \frac{1}{A}a_k(t) = \int_0^t a_k(t')\,dt'. \tag{26}$$

We decompose x' into two terms:

$$x' = \lambda_x \sum_k a_k u'_k + \sum_k (b_k - \lambda_x a_k) u'_k = x'_a + x'_b, \tag{27}$$

where

$$\lambda_x = \left(\sum_k a_k b_k\right) \Big/ \left(\sum_k a_k^2\right). \tag{28}$$

This value of λ_x is chosen so that x'_a and x'_b are statistically independent random variables. To see that this is so, we first show they are uncorrelated:

$$\begin{aligned}
\overline{x'_a x'_b} &= \overline{\left[\sum_k \lambda_x a_k u'_k\right]\left[\sum_j (b_j - \lambda_x a_j) u'_j\right]} \\
&= \lambda_x \sum_{k,j} (a_k b_j - \lambda_x a_k a_j)\, \overline{u'_k u'_j} \\
&= \lambda_x \sum_k (a_k b_k - \lambda_x a_k^2) \overline{(u'_k)^2} \\
&= \lambda_x \left[\sum_k a_k b_k - \frac{\sum_j a_j b_j}{\sum_j a_j^2} \sum_k a_k^2\right] \sigma^2 \\
&= 0.
\end{aligned}$$

We also know x'_a and x'_b are jointly normal, since they are linear combinations of independent Gaussian variables [9]. The statistical independence of x'_a and x'_b then follows from the facts that they are jointly normal and uncorrelated [9].

Let us now return to our original question. Assume the random velocities are such that $\sum_k a_k u'_k = w'_0$. What is the probability distribution of x'? By Eq. (27) and the statistical independence of x'_a and x'_b,

$$x' = \lambda_x w'_0 + x'_b, \tag{29}$$

where

$$\begin{aligned}\sigma_{x_b'}^2 &= \sum_k (b_k - \lambda_x a_k)^2 \sigma^2 \\ &= \sum_k (b_k^2 - 2\lambda_x a_k b_k + \lambda_x^2 a_k^2)\sigma^2 \\ &= \left[\sum_k b_k^2 - 2\frac{(\sum_k a_k b_k)^2}{\sum_k a_k^2} + \frac{(\sum_k a_k b_k)^2}{\sum_k a_k^2}\right]\sigma^2 \\ &= \left[\sum_k b_k^2 - \frac{(\sum_k a_k b_k)^2}{\sum_k a_k^2}\right]\sigma^2 \\ &= \sigma_{x'}^2 - \lambda_x^2 \sigma_{w'}^2. \end{aligned} \tag{30}$$

Thus the occurence of x' is Gaussian with mean value $\lambda_x w_0'$ and variance $\sigma_{x'}^2 - \lambda_x^2 \sigma_{w'}^2$. Similarly it can be shown that if the u_k' are such that $x_0' = \sum_k b_k u_k'$, then the probability distribution of w' is Gaussian with mean value $\lambda_w x_0'$ and variance

$$\sigma_{w'_a}^2 = \sigma_{w'}^2 - \lambda_w^2 \sigma_{x'}^2,$$

where

$$\lambda_w = \left(\sum_k a_k b_k\right) \Big/ \left(\sum_k b_k^2\right). \tag{31}$$

Detailed formulas for

$$\sum_{k=1}^{\infty} a_k^2 = \frac{\sigma_{w'}^2}{\sigma^2}$$

and

$$\sum_{k=1}^{\infty} b_k^2 = \frac{\sigma_{x'}^2}{\sigma^2}$$

are given in (10) and (19). One can show using (25) and (26) that

$$\sum_{k=1}^{\infty}{}' a_k b_k = t_d[e^{-A(t-Nt_d)} - e^{-At}] + (t - Nt_d)[1 - e^{-A(t-Nt_d)}] - \frac{1}{A}\sum_{k=1}^{\infty} a_k^2 \tag{32}$$

for times t such that $Nt_d \leqslant t < (N+1)t_d$.

D. *Neglect of Turbulent Velocity Changes in Numerical Calculations*

In numerical calculations we are primarily interested in predicting accurately the turbulent displacement of a droplet in physical space after each passage of time

$t = \Delta t$, where Δt is the computational time-step. A natural question to ask is when can one ignore turbulent changes in velocity space when calculating a droplet's turbulent displacement in physical space.

It turns out that although one can ignore turbulent velocity changes in the limit of very large time-steps, in general one must include them for accuracy. From Eq. (30) it is necessary and sufficient to have $\lambda_x^2 \sigma_{w'}^2 \ll \sigma_{x'}^2$ in order to ignore turbulent velocity changes. One easily shows this condition is equivalent to the condition

$$\sum_{k=1}^{\infty} a_k^2 \sum_{k=1}^{\infty} b_k^2 \gg \left(\sum_{k=1}^{\infty} a_k b_k \right)^2. \tag{33}$$

Equation (33) is a very complicated constraint on the times t, t_d, and $1/A$, but we can show that when $t \gg t_d$ and $t \gg 1/A$, then (33) is satisfied. First one shows that when $At \gg 1$,

$$\sum_{k=1}^{\infty} a_k^2$$

is bounded below by

$$\frac{1 - e^{-At_d}}{2}$$

and

$$\sum_{k=1}^{\infty} a_k b_k$$

is bounded above by t_d. Since (21) shows that

$$\sum_{k=1}^{\infty} b_k^2 \sim t t_d$$

for $t \gg t_d$ and $At \gg 1$, we have

$$\sum_{k=1}^{\infty} a_k^2 \sum_{k=1}^{\infty} b_k^2 \geqslant t t_d \frac{1 - e^{-At_d}}{2} \gg t_d^2 > \left(\sum_{k=1}^{\infty} a_k b_k \right)^2. \tag{34}$$

The requirement that $t \gg 1/A$ is necessary above. That is, if $At \ll 1$ and $t \gg t_d$, then one can show that constraint (33) fails. This is the case when we have a very large droplet whose drag time is long compared to the computational time-step, which is in turn long compared to the turbulence time scale.

III. Numerical Considerations and Computational Examples

The computer program KIVA [2] aims to solve such problems as the motion of an ensemble of spray droplets in a turbulent gas. For these applications, we must solve an equation of the form

$$\frac{\partial f}{\partial t} + \nabla_x \cdot (f\mathbf{v}) + \nabla_v \cdot \left(f \frac{d\mathbf{v}}{dt} \right) = 0, \tag{35}$$

where f is the probability distribution of the droplets and $d\mathbf{v}/dt$ is given by (3). The function f is defined so that $f(\mathbf{x}, \mathbf{v}, \mathbf{r}, t)\, d\mathbf{x}\, d\mathbf{v}\, d\mathbf{r}$ is the probable number of drops in the spatial interval $(\mathbf{x}, \mathbf{x} + d\mathbf{x})$ with velocities in the range $(\mathbf{v}, \mathbf{v} + d\mathbf{v})$ and radii in the interval $(r, r + dr)$ at time t. In the spray literature [3], Eq. (35) is known as the spray equation and can be considerably more complicated when vaporization, collisions, or droplet breakup must be taken into consideration. A rigorous derivation [10] of (32) reveals that because $d\mathbf{v}/dt$ has a distribution of values, diffusion-like terms will arise also on the right-hand side of Eq. (35). To derive the exact forms of these terms, would be interesting but beyond the scope of this work. If the gas velocity $\mathbf{u}$, drag function A, turbulent kinetic energy Q, and turbulent time scale t_d were all constant, then Eq. (35) could be solved analytically using the methods of the previous section. In practice these quantities vary in time, and thus (35) must be solved numerically. In this section we tell how (35) is solved numerically in KIVA.

Among the many methods [10] for solving (35), the stochastic particle method of Dukowicz [1] has become widely used for spray applications. In this method the spray is represented by an ensemble of computational particles, each particle representing a number of drops N_p with identical location $\mathbf{x}_p$, velocity $\mathbf{v}_p$, and radius r_p. The drops move relative to a computational mesh on which gas phase properties $\mathbf{u}$, Q, and t_d are calculated. The time-dependent solution is advanced through a sequence of time-steps Δt, using finite difference approximations to (3) to solve for the particle position $\mathbf{x}_p^{n+1}$ and velocities $\mathbf{v}_p^{n+1}$ at time $t^{n+1} = t^n + \Delta t$. The approximate distribution function f is obtained from the formula

$$f(\mathbf{x}, \mathbf{v}, r, t^{n+1})\, \Delta\mathbf{x}\, \Delta\mathbf{v}\, \Delta r = \sum_p N_p, \tag{36}$$

where the summation is over all computational particles with positions $\mathbf{x}_p^{n+1}$ in the interval $(\mathbf{x}, \mathbf{x} + \Delta\mathbf{x})$ velocities $\mathbf{v}_p^{n+1}$ in the interval $(\mathbf{v}, \mathbf{v} + \Delta\mathbf{v})$, and radii in the interval $(r, r + \Delta r)$ at time t^{n+1} and where the space, velocity, and radius increments are small compared to the scales for change in f but large enough to contain many computational particles.

For each particle we choose one of two numerical procedures for updating that particle position and velocity. The choice depends on the relative magnitudes of Δt and t_d. When $\Delta t < t_d$, which is often the case, the most convenient method for

finding $\mathbf{x}_p^{n+1}$ and $\mathbf{v}_p^{n+1}$ is to solve (3) directly by finite difference approximations. In KIVA we use the approximations

$$\frac{\mathbf{v}_p^{n+1}-\mathbf{v}_p^n}{\Delta t}=A_p^n(\mathbf{u}_p^{n+1}+\mathbf{u}_p'-\mathbf{v}_p^{n+1})+\mathbf{g} \tag{37}$$

and

$$\frac{\mathbf{x}_p^{n+1}-\mathbf{x}_p^n}{\Delta t}=\mathbf{v}_p^n, \tag{38}$$

where $\mathbf{u}_p^{n+1}$ is the advanced-time gas velocity at the location of the particle. The gas turbulent velocity $\mathbf{u}_p'$ is held fixed for a number of computational cycles N such that

$$(N-1)\,\Delta t<t_d\leqslant N\,\Delta t,$$

where t_d is the local turbulence time.

When $\Delta t\geqslant t_d$, we make the assumptions of and use the results of the previous section. Since we cannot assume that Δt is much larger than the droplet drag time $1/A$, we must add random changes to both the droplet's position and velocity. The particle velocity and position are updated using

$$\frac{\mathbf{v}_p^{n+1}-\mathbf{v}_p^n}{\Delta t}=A_p^n(\mathbf{u}_p^{n+1}-\mathbf{v}_p^{n+1})+\mathbf{g}+\frac{\mathbf{w}'}{\Delta t} \tag{39}$$

and

$$\frac{\mathbf{x}_p^{n+1}-\mathbf{x}_p^n}{\Delta t}=\mathbf{v}_p^n+\frac{\mathbf{x}'}{\Delta t}, \tag{40}$$

where $\mathbf{w}'$ and $\mathbf{x}'$ are turbulent velocity and position changes that are calculated as

$$\alpha=\sum a_k^2=\frac{}{1+e^{-A t_d}}(1-e^{-2A\,\Delta t}),$$

$$\beta=\sum b_k^2=\Delta t t_d-2t_d\frac{1-e^{-A\,\Delta t}}{A}+\frac{\alpha}{A^2},$$

and

$$\gamma=\sum a_k b_k=t_d(1-e^{-A\,\Delta t})-\frac{\alpha}{A}.$$

These formulas are obtained from Eqs. (10), (19), and (32) by substituting $\Delta t=Nt_d$. Each component w' of $\mathbf{w}'$ is then chosen randomly from a Gaussian distribution with variance $\sigma_{w'}^2=\alpha\sigma^2$. The scalar λ_x is obtained from $\lambda_x=\gamma/\alpha$, and then the random displacement x' in each coordinate direction is calculated from

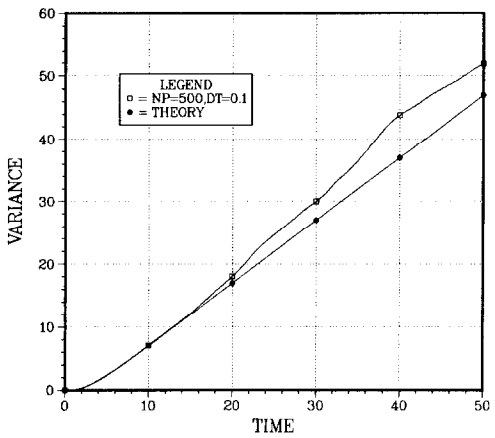

FIG. 1. Theoretical and calculated ($N_p = 500$, $\Delta t = 0.1$) variances in the distributions of drop position.

$x' = \lambda_x w' + x'_b$ where x'_b is chosen randomly from a Gaussian with variance $\sigma^2_{x'_b} = (\beta - \lambda_x^2 \alpha)\sigma^2$.

To confirm both the theory and the numerical implementation of it, we performed calculations with KIVA in which a large number of droplets were initially placed in the center of a large cubical computational cell. The physical parameters were gas velocity $\mathbf{u} = 0$, gravity $\mathbf{g} = 0$, standard deviation of gas velocity fluctuations $\sigma = 1.0$, turbulence correlation time $t_d = 1.0$, and drag function $A = 0.5$. Thus the sole mechanism for droplet motion was the action of turbulent fluctuations on them. We varied the computational time-step Δt and number of droplets and monitored the width of the computed droplet distribution of positions.

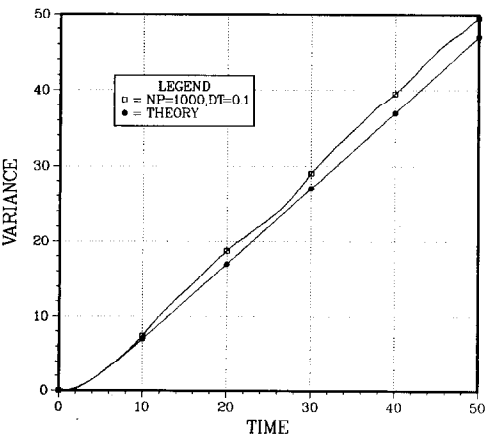

FIG. 2. Theoretical and calculated ($N_p = 1000$, $\Delta t = 0.1$) variances in the distributions of drop position.

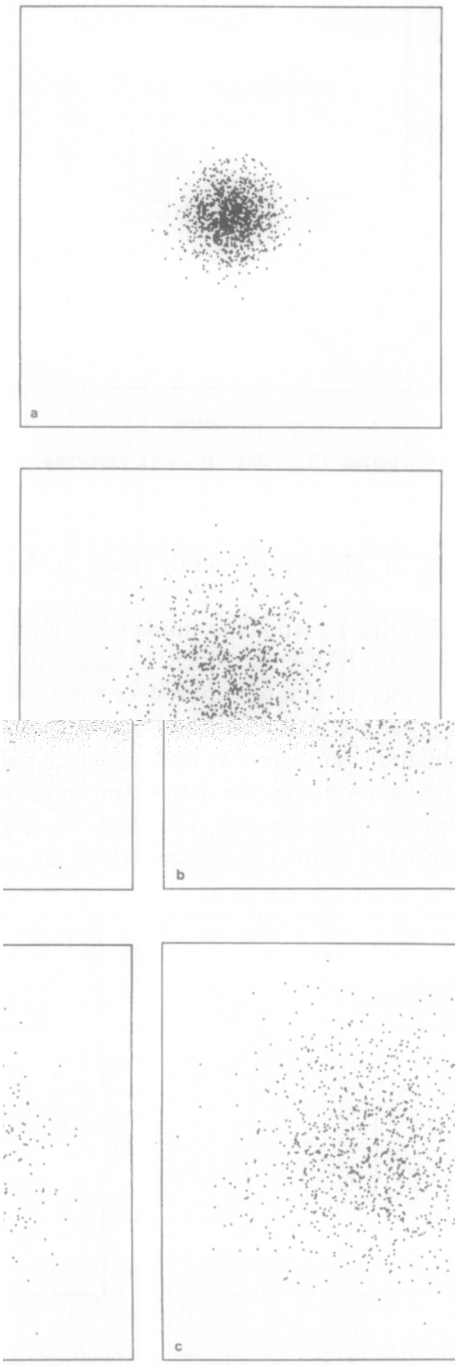

FIG. 3. Calculated ($N_p = 1000$, $\Delta t = 0.1$) drop positions at times $t = 10.0$ (a), 30.0 (b), and 50.0 (c).

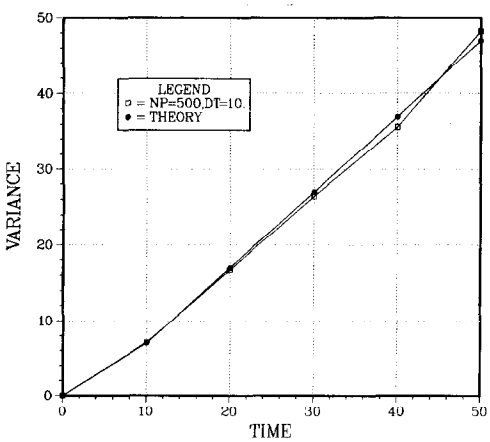

FIG. 4. Theoretical and calculated ($N_p = 500$, $\Delta t = 10.0$) variances in the distributions of drop position.

Figure 1 shows the theoretical (Eq. (19)) and calculated variance in the droplet position distribution when 500 droplets were used and the time-step Δt was 0.1. The two curves follow each other closely until a time of 10.0, after which they slowly drift apart. At $t = 50.0$, the relative difference between the calculated and theoretical variance is 13%. It was suspected that this error was a statistical error and could be reduced by increasing the number of droplets. Figure 2 shows the result of using 1000 computational droplets. The two curves now closely follow each other until $t = 10.0$, and the relative error at $t = 50.0$ is only 6.5%.

Figure 3 shows plots of the computed droplet positions at times $t = 10.0$, 30.0, and 50.0 for the calculation with 1000 droplets. It is seen that the dispersion of the droplets is isotropic.

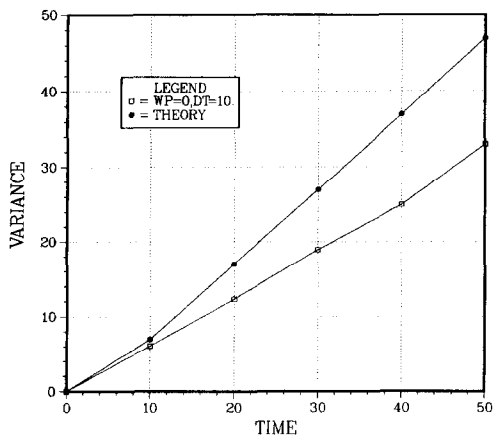

FIG. 5. Theoretical and calculated (ignoring dispersion of drop velocities) variances in the distributions of drop position.

To test the algorithm for dispersing droplets when $\Delta t > t_d$, we performed a calculation with $\Delta t = 10.0$. Figure 4 displays the resulting excellent agreement between calculation and theory.

To show the errors one can make by ignoring droplet dispersion in velocity space we performed a calculation with $\Delta t = 10.0$ and in which no random changes were added to the droplet velocities. Random position changes were chosen on each time-step from Eq. (20) with $t = \Delta t$. As expected, the distribution of droplet positions has a computed variance that is approximately linear in time and agrees with theory only at $t = \Delta t = 10.0$. At $t = 50.0$, the calculated variance is 26% below the theoretical value. This error is not reduced when the number of droplets is increased. Thus, by ignoring dispersion of droplet velocities, one can have large

as 5.0.

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REFERENCES

1. J. K. DUKOWICZ, *J. Comput. Phys.* **35**, 229 (1980).
2. A. A. AMSDEN, *et al.*, Los Alamos National Laboratory Report LA-10245-MS, 1985 (unpublished).
3. G. M. FAETH, *Prog. Energy Combust. Sci.* **3**, 191 (1977).
4. A. D. GOSMAN AND E. IOANNIDES, AIAA paper 81-0323 (1981).
5. F. BOYSAN, W. H. AYERS, AND J. SWITHENBANK, *Trans I Chem E* **60**, 222 (1982).
6. J. S. SHUEN, L.-D. CHEN, AND G. M. FAETH, *AICHE J.* **29**, No. 1, 167 (1983).
7. A. ORMANCEY AND J. MARINON, *Phys. Chem. Hydrodyn.* **5**, Nos. 3/4, 229 (1984).
8. S. CHANDRASEKHAR, *Rev. Mod. Phys.* **15**, No. 1, 1 (1943).
9. A. PAPOULIS, *Probability, Random Variables, and Stochastic Processes*, (McGraw-Hill, New York, 1965) pp. 203, 211, 221.
10. P. J. O'ROURKE, Princeton University Thesis 1532-T, 1981 (unpublished).