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Probability Density Function Modeling of Evaporating Droplets Dispersed in Isotropic Turbulence

R. V. R. Pandya* and F. Mashayek†
University of Illinois at Chicago, Chicago, Illinois 60607

A statistical closure scheme is used to obtain an approximate equation for probability density function to predict the statistical properties of interest of collisionless evaporating droplets suspended in isothermal isotropic turbulent flows. The resulting Fokker–Planck equation has nonlinear, time-dependent drift and diffusion coefficients that depend on the statistical properties of the droplet slip velocity. Approximate analytical expressions for these properties are derived, and the equation is solved numerically after implementing the path-integral approach. The time evolution of various statistical properties related to the droplet diameter are then calculated and compared with the data available from the stochastic (Mashayek, F., "Stochastic Simulations of Particle-Laden Isotropic Turbulent Flow," *International Journal of Multiphase Flow*, Vol. 25, No. 8, 1999, pp. 1575–1599) and direct numerical (Mashayek, F., Jaberi, F. A., Miller, R. S., and Givi, P., "Dispersion and Polydispersity of Droplets in Stationary Isotropic Turbulence," *International Journal of Multiphase Flow*, Vol. 23, No. 2, 1997, pp. 337–355) simulations.

Nomenclature

A_0 = deterministic linear operator
A_1 = stochastic linear operator
A_1' = fluctuation over ensemble average of A_1
B_M = transfer number
C = constant in Eq. (34)
d_d = droplet diameter
G = short-time propagator
K = drift coefficient in Eq. (11)
k = turbulence kinetic energy
L = Gaussian white noise
P = phase space density
p = probability density function
Q = diffusion coefficient in Eq. (11)
Re = Reynolds number
S = magnitude of the droplet slip velocity
Sc = Schmidt number
T_f = fluid temperature
T_L = fluid integral timescale
$T_{\mathcal{R}}$ = integral timescale in Eq. (15)
t = time variable
$\boldsymbol{u}$ = velocity of the fluid in the vicinity of the droplet
u_i = components of $\boldsymbol{u}$, $i = 1, 2, 3$
u' = rms of fluctuating velocity in any direction
V = droplet volume
$\boldsymbol{v}$ = droplet velocity
v_i = components of $\boldsymbol{v}$, $i = 1, 2, 3$
$\boldsymbol{x}$ = droplet position in physical space
Y_s = vapor mass fraction at the droplet surface
Y_∞ = vapor mass fraction far from the droplet
$\boldsymbol{Z}$ = vector process
α = level of fluctuations
β = $1/\tau_d$
Γ_1 = mass diffusivity coefficient
ϵ = turbulent viscous dissipation
θ = droplet temperature phase space variable
κ = depletion rate
μ = fluid viscosity
ν = μ/ρ_f
ρ = density
τ = time variable
τ_c = autocorrelation time for A_1'
τ_d = droplet time constant
τ_E = Eulerian integral timescale
τ_k = Kolmogorov time scale

Subscripts

d = droplet properties
f = fluid properties
0 = value at time $t = 0$

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*Postdoctoral Fellow, Department of Mechanical Engineering, 842 West Taylor Street.
†Associate Professor, Department of Mechanical Engineering, 842 West Taylor Street. Senior Member AIAA.

Introduction

THE important phenomenon of spray combustion creates a physical situation of evaporating droplet-laden turbulent flows that is similar in nature to the situations encountered in plasma physics, aerosol science, and flame synthesis of nanoparticles. In these situations, particles/droplets move under the influence of forces, for example, molecular, hydrodynamic, electromagnetic, thermal, and interparticle, that are stochastic in nature. The collision, coagulation, and coalescence of the particles, if they occur, would further add to the complexity of the phenomena. A major task in such studies is to predict various statistical properties of flow variables for particles/droplets from the first principle. An attempt to predict such properties of interest requires 1) forming of an equation for the phase space density of the variables by using the Liouville theorem in conjunction with the equations describing the transport of the variables and 2) obtaining the closed form for the ensemble average (over various realizations) of the phase space density equation that represents the probability density function (PDF) equation for the variables. The process of ensemble average introduces several unkown terms in the PDF equation, and their predictions require tackling problems that are similar in nature to the well-known closure problem of fluid turbulence with an enhanced complexity due to the presence of the dispersed phase.

The theoretical approaches to the fluid turbulence closure problem have their roots in quantum and statistical physics and have led to the development of various renormalization techniques[1,2] in physical and Fourier spaces following the pioneering theory, direct interaction approximation (DIA), of Kraichnan.[3] DIA and its Lagrangian counterpart, Lagrangian-history DIA (LHDIA),[4] have been also applied by Orszag and Kraichnan[5] in the phase space of probability density methods to analyze the turbulence in a Vlasov plasma, and their work has provided a foundation to tackle the closure problems of two-phase flows in the framework of PDF approaches.

Subsequently, Reeks[6–8] and Hyland et al.[9] obtained a kinetic equation of nonevaporating droplets suspended in a turbulent flow in the PDF framework by applying LHDIA, which preserves the symmetry of the phenomena under a random Galilean transformation. Consequently, the equation is used to derive a complete set of continuum equations and constitutive relations for a two-fluid model of a particle-laden flow. This approach of arriving at a two-fluid model is also mathematically robust in deriving the boundary conditions for dispersed phase. Recently, Hyland et al.[10] rederived the equations in a functional formalism using the Furutsu–Novikov theorem, which has been first used by Derevich and Zaichik,[11,12] Derevich,[13] Zaichik,[14] and Derevich[15] for two-phase turbulent flows. Pozorski and Minier[16] have also obtained an identical kinetic equation by applying a different closure scheme, proposed by Van Kampen,[17] that is central in the study of nonlinear stochastic differential equations of quantum and statistical physics.

Van Kampen[18,19] originally proposed a cumulant expansion method for the solution of linear stochastic differential equations written for a vector. Later, the closure problem of nonlinear equations was tackled, by the same method, via first translating the equation into a linear form for the phase-space density for the vector using Liouville's equation (see Ref. 17). In the next section, this same closure scheme is applied to solve the closure problem posed by the linear equation for the phase-space density $P(\tau_d, t)$ of the droplet time constant τ_d at time t in stationary isotropic turbulence. In the general case of evaporating droplets in turbulent flows, a complete description would require solving the ensemble average of the equation for the phase-space density P having $(\boldsymbol{x}, \boldsymbol{v}, \theta, \tau_d, t)$ as the phase-space variables for the droplet, with the velocity $\boldsymbol{u}$ and the temperature T_f of the fluid as external variables. The fluid variables can be included in the list of phase-space variables.[16] In this preliminary study, we consider only τ_d and t as the phase-space variables, and the complete description is postponed until a future study.

Fokker–Planck Equation for $p(\tau_d, t)$

In this paper, we consider a stationary isotropic turbulent flow in which a large number of identical spherical droplets of diameter $d_d = d_{d0}$ are introduced simultaneously at different locations with velocity $\boldsymbol{v} = \boldsymbol{v}_0 = a\boldsymbol{u}(t = t_0)$ at time $t = t_0 = 0$. We assume that these droplets remain spherical and do not breakup or collide with each other and that their volume $V = (\pi d_d^3)/6$ decreases due to the evaporation, which is described by the depletion rate κ as a function of the stochastic variable $S = |\boldsymbol{u} - \boldsymbol{v}|$ that represents the magnitude of the droplet slip velocity. For this case, using the Liouville's theorem and the Lagrangian equation for $\mathrm{d}\tau_d/\mathrm{d}t$, an equation for the phase-space density $P(\tau_d, t)$ for the droplet time constant $\tau_d = (\rho_d d_d^2/18\mu)$ can be written as

$$\frac{\partial}{\partial t}[P(\tau_d, t)] + \frac{\partial}{\partial \tau_d}\left[\frac{\mathrm{d}\tau_d}{\mathrm{d}t} P(\tau_d, t)\right] = 0 \tag{1}$$

where

$$\frac{\mathrm{d}\tau_d}{\mathrm{d}t} = -\frac{\rho_d}{18\mu}\kappa = -A - B\tau_d^{0.25} S^{0.5}$$

$$A = \frac{4\rho_d}{9\mu}\Gamma_1 \ln(1 + B_M), \qquad B = 0.3 A Sc_d^{0.333}\left(\frac{18\rho_f}{\nu\rho_d}\right)^{0.25}$$

$$B_M = \frac{Y_s - Y_\infty}{1 - Y_s} \tag{2}$$

are obtained from the Ranz and Marshall formula for evaporating droplets.[20] The ensemble average (denoted by $\langle\ \rangle$) of $P(\tau_d, t)$ over all realizations of the flow gives an exact equation for the PDF $p(\tau_d, t)$:

$$\frac{\partial}{\partial t}[p(\tau_d, t)] - \frac{\partial}{\partial \tau_d}[Ap(\tau_d, t)] = \frac{\partial}{\partial \tau_d}\left[B\tau_d^{0.25}\bar{\mathcal{R}} p(\tau_d, t)\right] + \frac{\partial}{\partial \tau_d}\left[B\tau_d^{0.25}\langle \mathcal{R}' P(\tau_d, t)\rangle\right] \tag{3}$$

with the terms, present on the right-hand side of Eq. (3), that pose the closure problem. These ensemble average terms are 1) $\langle \mathcal{R}' P(\tau_d, t)\rangle$ and 2) $\bar{\mathcal{R}}$, where $\bar{\mathcal{R}}$ is the average value of $S^{0.5}$ and $\mathcal{R}'$ is the fluctuating part of $S^{0.5}$. The first term can be tackled by the well-known turbulence closure schemes and would produce an expression that requires prior knowledge of statistical properties related to S along the trajectory of the droplet, information that is also required for the second term. The prediction of the statistical properties of the flow variables along the droplet trajectory in a general flow situation remains as yet another challenge,[21] and enhances the complexity of turbulence closure problems in two-phase flows.

The cumulant expansion closure method for linear stochastic equations, proposed by Van Kampen,[17–19] is used here to obtain an approximate expression for $\langle \mathcal{R}' P(\tau_d, t)\rangle$. We now briefly discuss the method using the notation of Pozorski and Minier's paper.[16] Van Kampen[17–19] solved the closure problem posed by a linear stochastic differential equation for a vector process $\boldsymbol{Z}$, written as

$$\frac{\mathrm{d}\boldsymbol{Z}(t)}{\mathrm{d}t} = [A_0 + \alpha A_1(t)]\boldsymbol{Z}(t) \tag{4}$$

where the linear operators A_0 and A_1 are deterministic and stochastic in nature, respectively, and α is the level of fluctuations. A_0 is constant in time, and when ensemble average of A_1 is time dependent, the proposed solution[16,17] is written as

$$\frac{\mathrm{d}\langle \boldsymbol{Z}(t)\rangle}{\mathrm{d}t} = \left[A_0 + \alpha\langle A_1(t)\rangle + \alpha^2 \int_0^t \left\langle A_1'(t) e^{\tau A_0} A_1'(t - \tau)\right\rangle e^{-\tau A_0}\,\mathrm{d}\tau\right]\langle \boldsymbol{Z}(t)\rangle \tag{5}$$

for $\alpha\tau_c \ll 1$, where $A_1'(t) = A_1 - \langle A_1\rangle$ and τ_c is the autocorrelation time for A_1'. In case of a single random oscillator problem where $\langle A_1(t)\rangle = 0$ and $A_1'(t)$ has Gaussian distribution, this approximate equation (5) yields the exact solution.[18] Though, in the present case, the conditions $\alpha\tau_c \ll 1$ and distribution for A_1' being Gaussian are not satisfied, in general, we examine Van Kampen's method,[17–19] along with the other involved approximations for their performance.

In the present case, the closure problem of nonlinear stochastic equation (2) can be transformed into a linear stochastic equation for scalar process $P(\tau_d, t)$, that is, Eq. (1). We write the equation for $P(\tau_d, t)$ as

$$\frac{\partial}{\partial t} P(\tau_d, t) = -\frac{\partial}{\partial \tau_d}\left[F^{(0)}(\tau_d) P(\tau_d, t)\right] - \frac{\partial}{\partial \tau_d}[F(\tau_d, t) P(\tau_d, t)] - \frac{\partial}{\partial \tau_d}\left[F^{(1)}(\tau_d, t) P(\tau_d, t)\right] \tag{6}$$

with $F^{(0)}(\tau_d) = -A$, $F(\tau_d, t) = -B\tau_d^{0.25}\bar{\mathcal{R}}$ and $F^{(1)}(\tau_d, t) = -B\tau_d^{0.25}\mathcal{R}'$. Comparing Eq. (6) with Eq. (4), we obtain

$$A_0 = -\frac{\partial}{\partial \tau_d} F^{(0)}(\tau_d), \qquad \alpha\langle A_1\rangle = -\frac{\partial}{\partial \tau_d} F(\tau_d, t)$$

$$\alpha A_1' = -\frac{\partial}{\partial \tau_d} F^{(1)}(\tau_d, t) \tag{7}$$

and, using Eq. (5), the closed equation for $p(\tau_d, t) = \langle P(\tau_d, t)\rangle$ can be written as

$$\frac{\partial}{\partial t} p(\tau_d, t) = -\frac{\partial}{\partial \tau_d}\left[F^{(0)}(\tau_d) p(\tau_d, t)\right] - \frac{\partial}{\partial \tau_d}[F(\tau_d, t) p(\tau_d, t)] + \frac{\partial}{\partial \tau_d}\int_0^t \mathrm{d}\tau \left\langle F^{(1)}(\tau_d, \tau) e^{\tau A_0} \frac{\partial}{\partial \tau_d} F^{(1)}(\tau_d, t - \tau)\right\rangle \times e^{-\tau A_0} p(\tau_d, t) \tag{8}$$

The action of $e^{\tau A_0}$ on any function $f(\tau_d)$ is given by the following[16,17]:

$$e^{\tau A_0} f(\tau_d) = f\left(\tau_d^{-\tau}\right)\frac{\mathrm{d}\left(\tau_d^{-\tau}\right)}{\mathrm{d}(\tau_d)} \tag{9}$$

where τ_d is the value of the particle time constant at time t and τ_d^{τ} is the value at time $t+\tau$ along the trajectory that is determined from

$$\frac{\mathrm{d}\tau_d}{\mathrm{d}t} = F^{(0)}(\tau_d) = -A \tag{10}$$

Simplifying Eq. (8), by making use of Eq. (9), we obtain a Fokker–Planck equation:

$$\frac{\partial}{\partial t}[p(\tau_d,t)] = -\frac{\partial}{\partial \tau_d}[K(\tau_d,t)p(\tau_d,t)] + \frac{1}{2}\frac{\partial^2}{\partial \tau_d^2}[Q(\tau_d,t)p(\tau_d,t)] \tag{11}$$

with

$$K(\tau_d,t) = F^{(0)}(\tau_d) + F(\tau_d,t) + \int_0^t \mathrm{d}\tau \left\langle \frac{\partial F^{(1)}(\tau_d,t)}{\partial \tau_d} F^{(1)}\left(\tau_d^{-\tau}, t-\tau\right)\right\rangle \frac{\mathrm{d}(\tau_d)}{\mathrm{d}\left(\tau_d^{-\tau}\right)} \tag{12}$$

$$\frac{1}{2}Q(\tau_d,t) = \int_0^t \mathrm{d}\tau \left\langle F^{(1)}(\tau_d,t)F^{(1)}\left(\tau_d^{-\tau}, t-\tau\right)\right\rangle \frac{\mathrm{d}(\tau_d)}{\mathrm{d}\left(\tau_d^{-\tau}\right)} \tag{13}$$

Equation (10) gives

$$\tau_d^{-\tau} = \tau_d + A\tau, \qquad \frac{\mathrm{d}(\tau_d)}{\mathrm{d}\left(\tau_d^{-\tau}\right)} = 1 \tag{14}$$

and to proceed, we now introduce the ad hoc approximation

$$\frac{\left\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'\left(\tau_d^{-\tau}, t-\tau\right)\right\rangle}{\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle} \cong \exp\left(-\frac{\tau}{T_{\mathcal{R}}}\right) \tag{15}$$

Here $T_{\mathcal{R}}$ is a constant and represents the integral timescale for the correlation of $\mathcal{R}'$ and, possibly, depends on the size of the droplets and slip velocity. The resulting expressions for K and Q in the present case, after substituting for $F^{(0)}$, F, and $F^{(1)}$, incorporating the approximation (15) into Eqs. (12) and (13), and using Eq. (14), are

$$K(\tau_d,t) = -A - B\tau_d^{0.25}\bar{\mathcal{R}} + \int_0^t \mathrm{d}\tau\ 0.25B^2\tau_d^{-0.75} \times \left[\left(\tau_d^{-\tau}\right)^{0.25}\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle \exp\left(-\frac{\tau}{T_{\mathcal{R}}}\right)\right] + \int_0^t \mathrm{d}\tau\, B^2\tau_d^{0.25}\left(\tau_d^{-\tau}\right)^{0.25}\left\langle \frac{\partial \mathcal{R}'(\tau_d,t)}{\partial \tau_d}\mathcal{R}'\left(\tau_d^{-\tau}, t-\tau\right)\right\rangle \tag{16}$$

$$\frac{1}{2}Q(\tau_d,t) = \int_0^t \mathrm{d}\tau\, B^2\tau_d^{0.25}\left(\tau_d^{-\tau}\right)^{0.25} \times \left[\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle \exp\left(-\frac{\tau}{T_{\mathcal{R}}}\right)\right] \tag{17}$$

The last two terms in Eq. (16), contributing to the drift coefficient K, arise due to the nonzero gradients of $F^{(1)}$ in τ_d. Note that these types of terms in PDF modeling of two-phase turbulent flows, which contain nonzero gradients of the stochastic variable in the phase space, account for the additional forces on particles due to inhomogeneities in fluid turbulence.[7] Because the expression for $\langle[\partial \mathcal{R}'(\tau_d,t)/\partial\tau_d]\mathcal{R}'(\tau_d^{-\tau}, t-\tau)\rangle$ and also the direct numerical simulation (DNS) data are not available, we do not include the last term on the right-hand side of Eq. (16) in the numerical computation to follow.

Now we obtain approximate expressions for $\bar{\mathcal{R}}$ and $\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle$ before solving the Fokker–Planck equation (11). We write the square of the magnitude of the droplet slip velocity S^2 in terms of its ensemble average $S_1 = \langle S^2\rangle$ and its fluctuation part $S_1' = S^2 - S_1$ so that

$$\langle (S^2)^n\rangle = S_1^n\left\langle (1 + S_1'/S_1)^n\right\rangle \tag{18}$$

and using the binomial expansion we obtain $\langle (S^2)^n\rangle$, up to second order in the binomial expansion, written as

$$\langle (S^2)^n\rangle = S_1^n\left\{1 - [n(n-1)/2](1 - \langle S^2S^2\rangle/S_1S_1)\right\} \tag{19}$$

$\forall n \le 2$. Here n is a real number, and the terms up to the second order in the binomial expansion give the exact expression when $n = 1$ or 2. For the case of isotropic turbulence, we assume Gaussian distributions for u_i and v_i and obtain

$$\langle S^2S^2\rangle \big/ S_1S_1 = \tfrac{15}{9} \tag{20}$$

by incorporating

$$u_iu_j = u_iv_j = v_iv_j = 0 \quad \text{when } i \ne j \tag{21}$$

$$\langle u_iu_jv_kv_l\rangle = \langle u_iu_j\rangle\langle v_kv_l\rangle + \langle u_iv_k\rangle\langle u_jv_l\rangle + \langle u_iv_l\rangle\langle u_jv_k\rangle \tag{22}$$

$$\langle u_iu_ju_kv_l\rangle = \langle u_iu_j\rangle\langle u_kv_l\rangle + \langle u_iu_k\rangle\langle u_jv_l\rangle + \langle u_iv_l\rangle\langle u_ju_k\rangle \tag{23}$$

$$\langle u_iu_ju_ku_l\rangle = \langle u_iu_j\rangle\langle u_ku_l\rangle + \langle u_iu_k\rangle\langle u_ju_l\rangle + \langle u_iu_l\rangle\langle u_ju_k\rangle \tag{24}$$

Substituting Eq. (20) into Eq. (19) and for $n = 0.25$, we obtain

$$\langle (S^2)^{0.25}\rangle = \bar{\mathcal{R}} = \tfrac{15}{16}\langle (u_iu_i + v_iv_i - 2u_iv_i)\rangle^{0.25} \tag{25}$$

and for $n = 0.5$, we obtain the ensemble average value of S:

$$\langle S\rangle = \tfrac{11}{12}\langle (u_iu_i + v_iv_i - 2u_iv_i)\rangle^{0.5} \tag{26}$$

with usual summation convention over repeated subscript i. Now

$$\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle = \langle (S^{0.5} - \bar{\mathcal{R}})(S^{0.5} - \bar{\mathcal{R}})\rangle = \langle S^{0.5}S^{0.5}\rangle - \langle S^{0.5}\rangle\langle S^{0.5}\rangle \tag{27}$$

Using Eqs. (19) and (20) with appropriate values for n, we obtain from Eq. (27)

$$\langle \mathcal{R}'(\tau_d,t)\mathcal{R}'(\tau_d,t)\rangle \cong 0.03776\langle S^2\rangle^{0.5} \cong 0.03776\langle (u_iu_i + v_iv_i - 2u_iv_i)\rangle^{0.5} \tag{28}$$

To obtain the expressions for $\langle v_iv_i\rangle$ and $\langle u_iv_i\rangle$, we use the equation of motion for a droplet:

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \frac{u_i - v_i}{\tau_d} \tag{29}$$

Integration of this equation gives

$$v_i(t) = v_i(t=0)e^{-t/\tau_d} + \frac{1}{\tau_d}\int_0^t \exp\left(\frac{s-t}{\tau_d}\right)u_i(s)\,\mathrm{d}s \tag{30}$$

where we assume the initial velocity of the droplet as proportional to the fluid velocity in the vicinity of the droplet with proportionality constant a, written as

$$v_i(t=0) = au_i(t=0) \tag{31}$$

Multiplying Eq. (30) by $u_i(t)$, taking the ensemble average, and incorporating the following relation

$$\langle u_i(t)u_i(s)\rangle = \langle u_i(t)u_i(t)\rangle \exp[(s-t)/\tilde{T}_L] \qquad \forall\, s \le t \tag{32}$$

we obtain after simplification

$$\langle v_i(t)u_i(t)\rangle = \langle u_i(t)u_i(t)\rangle\left\{ae^{(-t/\tau_d - t/\tilde{T}_L)} + \left[\beta\tilde{T}_L/(\beta\tilde{T}_L + 1)\right]\left[1 - \exp(-\beta t - t/\tilde{T}_L)\right]\right\} \tag{33}$$

where $\beta = 1/\tau_d$ and $\tilde{T}_L$ represents the fluid integral timescale and is approximated by[9]

$$\tilde{T}_L = C(k/\epsilon) \tag{34}$$

where C is a constant, k is the turbulence kinetic energy of the fluid, and ϵ is the viscous dissipation. Similarly, we obtain an expression for $\langle v_i(t)v_i(t)\rangle$, written as

$$\langle v_i(t)v_i(t)\rangle = \langle u_i(t)u_i(t)\rangle \exp(-2\beta t)\left(a^2 + \frac{2a\beta\tilde{T}_L}{\beta\tilde{T}_L - 1} \times \left[\exp\left(\beta t - \frac{t}{\tilde{T}_L}\right) - 1\right] + \frac{2\beta^2\tilde{T}_L}{\beta\tilde{T}_L + 1}\left\{\frac{\exp(2\beta t) - 1}{2\beta} - \frac{\tilde{T}_L}{\beta\tilde{T}_L - 1}\left[\exp\left(\beta t - \frac{t}{\tilde{T}_L}\right) - 1\right]\right\}\right) \tag{35}$$

when $\beta\tilde{T}_L \neq 1$ and

$$\langle v_i(t)v_i(t)\rangle = \langle u_i(t)u_i(t)\rangle \exp(-2\beta t) \times \left(a^2 + 2a\beta t + \frac{2\beta^2\tilde{T}_L}{\beta\tilde{T}_L + 1}\left[\frac{\exp(2\beta t) - 1}{2\beta} - t\right]\right) \tag{36}$$

when $\beta\tilde{T}_L = 1$. Note that, in the limit $t \to \infty$, Eqs. (33), (35), and (36) become identical to the equations obtained by Tchen (see Ref. 22). These expressions for $\langle v_i(t)u_i(t)\rangle$ and $\langle v_i(t)v_i(t)\rangle$ are obtained by keeping τ_d fixed during the time integration, to obtain the analytical form and, thus, are approximate and valid for the case of slowly evaporating droplets. We also require an expression for $T_{\mathcal{R}}$, and as a first approximation we take it to be equal to $\tilde{T}_L$. In the next section we discuss a numerical method to solve the Fokker–Plank equation (11).

Numerical Procedure

A discrete form of the Langevin equation equivalent to the Fokker–Planck equation (11) can be written as[17]

$$\tau_d(t+\Delta t) - \tau_d(t) = \tau K[\tau_d(t), t] + \{Q[\tau_d(t'), t']\}^{\frac{1}{2}} \int_t^{t+\Delta t} L(s)\,\mathrm{d}s \tag{37}$$

where $L(s)$ is a Gaussian white noise with $\langle L\rangle = 0$ and $\langle L(t)L(s)\rangle = \delta(t-s)$, δ is the Dirac delta function, and $t' = t + \eta\Delta t$ with $0 \leq \eta \leq 1$. For $\eta = 0$, Eq. (37) (known as the Ito equation) is equivalent to Eq. (11).

Instead of numerically solving the Ito equation (37) or using one of the existing finite difference methods to compute Eq. (11), we choose a well-established path-integral method for the solution of the Fokker–Plank equation because the number of independent variables is small. The use of yet another method, namely, the stochastic particle approach, is preferable in systems with many independent variables.

Wehner and Wolfer[23–25] proposed a numerical method, based on the path-integral formalism, to solve nonlinear Fokker–Planck equations. In this method, the equation

$$p(\tau_d, t+\tau) = \int \mathrm{d}\tau_d'\, G(\tau_d, \tau_d', \tau)\, p(\tau_d', t) \tag{38}$$

which relates the PDF $p(\tau_d, t+\tau)$ at time $t+\tau$ to the known PDF $p(\tau_d, t)$ at time t is used iteratively. Here τ is a small time step that is constrained as

$$0 < \tau < \text{minimum value of} \frac{Q(\tau_d, t)}{[K(\tau_d, t)]^2} \text{at } t \tag{39}$$

and $G(\tau_d, \tau_d', \tau)$ is the short-time propagator given by the relation[25,26]

$$G(\tau_d, \tau_d', \tau) = \left[\frac{1}{2\pi\tau Q(\tau_d', t')}\right]^{\frac{1}{2}} \times \exp\left\{-\frac{[\tau_d - \tau_d' - \tau K(\tau_d', t')]^2}{2\tau Q(\tau_d', t')}\right\} \tag{40}$$

where $t' = t + \eta\tau$ with $0 \leq \eta \leq 1$. For the present computation, we select $\eta = 0$ because this value obtains exact drift coefficient $K(\tau_d, t)$ even for finite value of τ (Ref. 25).

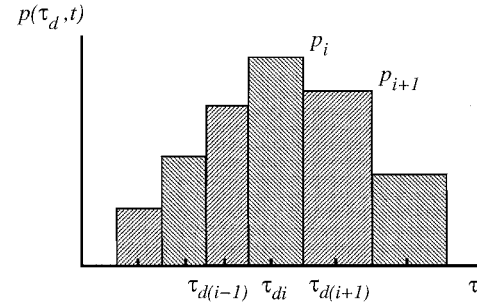

Fig. 1 Histogram representation of PDF.

To compute Eq. (38), $p(\tau_d, t)$ is assumed to be represented by a histogram (Fig. 1) over N discrete points (τ_{di}; $i = 1, 2, \ldots, N$) in the τ_d domain as

$$p(\tau_d, t) = \sum_{i=1}^{N} \psi(\tau_d - \tau_{di})\, p_i(t) \tag{41}$$

Here

$$\psi(\tau_d - \tau_{di}) = \begin{cases} 1 & \text{for } \left[\tau_{di} + \tau_{d(i-1)}\right]/2 \leq \tau_d \\ & \leq \left[\tau_{di} + \tau_{d(i+1)}\right]/2 \\ 0 & \text{otherwise} \end{cases} \tag{42}$$

$p_i(t)$ is the value of $p(\tau_d, t)$ at discrete points τ_{di}, and the spacing between two discrete points is given by the relation

$$\tau_{d(i+1)} - \tau_{di} = \{\tau Q[\tau_{d(i+1)}, t]\}^{\frac{1}{2}} \tag{43}$$

Substituting Eq. (41) in Eq. (38) and then integrating it over the interval from $[\tau_{di} + \tau_{d(i-1)}]/2$ to $[\tau_{di} + \tau_{d(i+1)}]/2$ gives

$$p_i(t+\tau) = \sum_{j=1}^{N} T_{ij}(\tau)\, p_j(t) \tag{44}$$

where the propagator matrix $T_{ij}(\tau)$ is defined as

$$T_{ij}(\tau) = \frac{2}{\tau_{d(i+1)} - \tau_{d(i-1)}} \int_{[\tau_{di} + \tau_{d(i-1)}]/2}^{[\tau_{di} + \tau_{d(i+1)}]/2} \mathrm{d}\tau_d \times \left[\int_{[\tau_{dj} + \tau_{d(j-1)}]/2}^{[\tau_{dj} + \tau_{d(j+1)}]/2} \mathrm{d}\tau_d'\, G(\tau_d, \tau_d', \tau)\right] \tag{45}$$

Because of the approximations involved in the representation of p and the truncation errors introduced during the computation of Eq. (44), the discrete representation $p_i(t)$ is renormalized to

$$\left\{2 \Big/ \sum_j \left[\tau_{d(j+1)} - \tau_{d(j-1)}\right] p_j(t)\right\} p_i(t) \tag{46}$$

before using it again in the right-hand side of Eq. (44) for the next iteration in time.

In our case, at time $t = 0$, $Q(\tau_d, 0) = 0$ and, consequently, inequality (39) cannot be satisfied by a nonzero value of τ. At $t = 0$, we consider $p(\tau_d, 0) = \delta(\tau_d - \tau_{d0})$ and obtain an approximate expression for the PDF at $t = 0.012\tau_E$ using Eqs. (38) and (40) with $\eta = 1$,

$$p(\tau_d, 0.012\tau_E) = \left[\frac{1}{2\pi \times 0.012\tau_E Q(\tau_{d0}, 0.012\tau_E)}\right]^{\frac{1}{2}} \times \exp\left\{-\frac{[\tau_d - \tau_{d0} - 0.012\tau_E K(\tau_{d0}, 0.012\tau_E)]^2}{2 \times 0.012\tau_E Q(\tau_{d0}, 0.012\tau_E)}\right\} \tag{47}$$

where τ_E is the Eulerian integral timescale and is given by[27]

$$\tau_E = 0.2904\,[(u')^2/\epsilon] \tag{48}$$

where u' is the root mean square of the fluctuating velocity in any arbitrary direction.

All of the integrals appearing in Eqs. (16), (17), and (45) are calculated using Simpson's method. Furthermore, to reduce the time of computation, integrals appearing in Eqs. (16) and (17) are calculated in the beginning of the computation at discrete points (τ_{dj}, t_j) with spacing $\tau_{dj} - \tau_{d(j-1)} = 0.004\tau_E$ and $t_j - t_{(j-1)} = 0.004\tau_E$ over the entire domain of (τ_d, t) and stored in a matrix. Linear interpolation is then used first along the t axis and then along the τ_d axis to obtain values of integral terms at points lying between these discrete points during the computation. Once the PDF is known, the statistical properties related to τ_d can be calculated.

Results and Discussion

In this section we compare the present numerical solutions obtained for the derived Fokker–Planck equation (11) with the data available from the stochastic[27] (STH) and DNS[28] studies. In DNS, the fluid phase velocity u_i is simulated using the Navier–Stokes (N–S) equations. The trajectories and sizes of the droplets are obtained by solving the Lagrangian equations for their position X_i, velocity v_i, and time constant τ_d, using the computed values for u_i at the droplet location. Then the average over many trajectories is taken to obtain the statistical properties of interest for the case of isotropic turbulence. In STH, instead of solving the N–S equations, u_i at the particle location is obtained, from known statistical properties for u_i in isotropic turbulence, by using a method proposed by Lu (see Ref. 27). Using these synthetic values of u_i along the particle trajectory, the Lagrangian equations for X_i, v_i, and τ_d are integrated in time to obtain various statistical properties.

For numerical solution of the Fokker–Planck equation, we use $\nu = 2.6 \times 10^{-4}$ m^2/s, $\epsilon = 3.987 \times 10^{-6}$ m^2/s^3, $u' = 0.0185$ m/s, $\tau_k = 8.229$ s, and $\rho_d/\rho_f = 10^3$, which are identical to the values used in the DNS and STH studies. We assume that at $t = 0$ the velocity of the droplets is perfectly correlated with the fluid velocity in their vicinity, that is, $a = 1$. We also assume a delta function for $p(\tau_d, t)$ at $t = 0$ that gives an approximate expression for PDF at $t = 0.012\tau_E$ through Eq. (47). Using this $p(\tau_d, 0.012\tau_E)$ now as an initial condition at $t = 0.012\tau_E$, we obtain numerical solutions for cases having different values for τ_{d0}, τ_{ec} $(= A\tau_E/0.29)$, and Sc_d.

All of the cases are calculated for two different values for constant C that appears in Eq. (34) and assuming $T_{\mathcal{R}} = \tilde{T}_L$, which is the only unknown parameter. In the following discussions, the present results are referred to as ANL1 when $C = 0.482$, a value suggested by Hyland et al.,[9] and ANL2 when $C = 0.2826$, a value used in the stochastic study.[27]

The performance of the model strongly depends on its accuracy in predicting the statistical properties related to S. One such property, the mean droplet Reynolds number,

$$\langle Re_d \rangle = \left(\frac{18\tau_p}{\nu \rho_d/\rho_f} \right)^{\frac{1}{2}} \langle S \rangle \tag{49}$$

is calculated using Eq. (26) for various values of τ_d for nonevaporating droplets, and the results are compared with the DNS and STH data in Fig. 2. For each curve, the DNS results show a transient region in which the mean droplet Reynolds number $\langle Re_d \rangle$ increases from zero at $t = 0$ and becomes almost constant at sufficiently large times. The value of the mean droplet Reynolds number $\langle Re_d \rangle$ exceeds this constant value in the later stages of the transient region, which here onward is referred to as second region for the sake of discussion.

Figure 2 suggests that the value of $C = 0.482$, represented by ANL1, gives closer comparisons with DNS data in the region where the mean droplet Reynolds number $\langle Re_d \rangle$ becomes almost constant. In contrast, $C = 0.2826$, represented by ANL2, gives better predictions in the initial transient region. Also note that the values of the mean droplet Reynolds number $\langle Re_d \rangle$ as predicted by ANL2 are consistently greater than the predictions of ANL1. The overshoot in the second region is not captured properly by any of the three STH, ANL1, or ANL2 predictions. In Fig. 2b, we show the curves for $a = 0$, that is, when the droplets are at rest at $t = 0$. In this case the mean droplet Reynolds number $\langle Re_d \rangle$ has a finite value equal

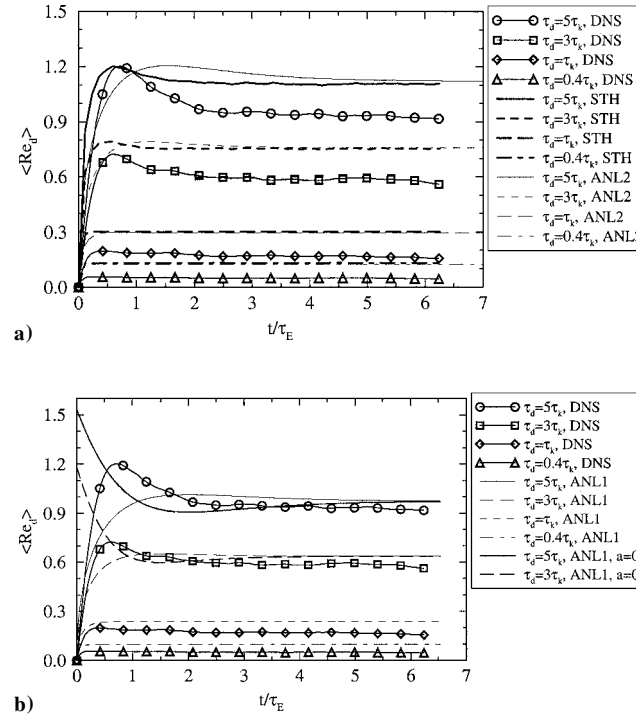

Fig. 2 Temporal variations of the mean droplet Reynolds number as calculated by STH,[27] DNS[28] and present analytical (ANL1, ANL2) expressions.

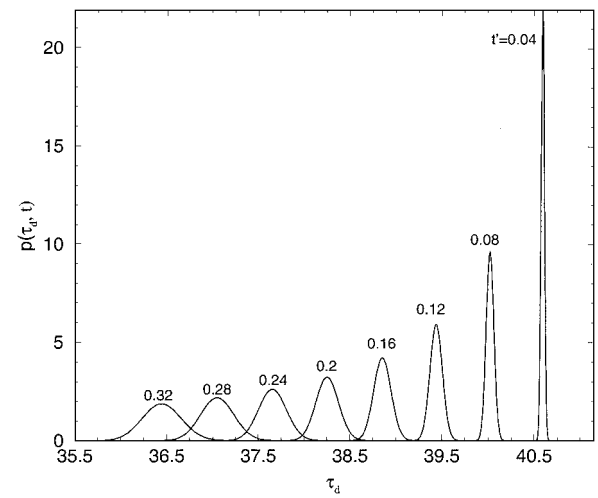

Fig. 3 PDF $p(\tau_d, t)$ at different times $t' = t/\tau_E$ for $\tau_{d0} = 5\tau_k$, $\tau_{ec} = 5\tau_k$, and $Sc_d = 1$.

to $\frac{11}{12}\{18\tau_p/[\nu(\rho_d/\rho_f)]\}^{1/2}\langle u_i u_i \rangle^{0.5}$ at $t = 0$. These curves finally merge with the curves for $a = 1$ after a sufficiently long period of time in the region where the mean droplet Reynolds number $\langle Re_d \rangle$ is almost constant.

Figure 3 shows a typical temporal behavior of the PDF $p(\tau_d, t)$ as predicted by the Fokker–Planck equation. For the delta function as an initial condition for PDF, all droplets have identical time constant τ_{d0} at $t = 0$. In time, the peak of the PDF shifts toward the lower values of τ_d, and the curves spread, due to the nonzero diffusion coefficient $Q\ \forall t > 0$, indicating an increase in polydispersity. Because the area under a PDF curve should be unity, this spreading causes a decrease in the peak value and is attributed to the stochastic term containing B, which is present in Eq. (2) as a convective correction term for temporal variation of τ_d.

In Fig. 4, temporal variations of $\langle (\tau_d/\tau_{d0})^{1/2} \rangle$ are shown for $\tau_{d0} = 5\tau_k$, $\tau_{ec} = 5\tau_k$, and $Sc_d = 5$ along with the DNS and STH data. The STH curve is closer to the DNS as compared to ANL1 and

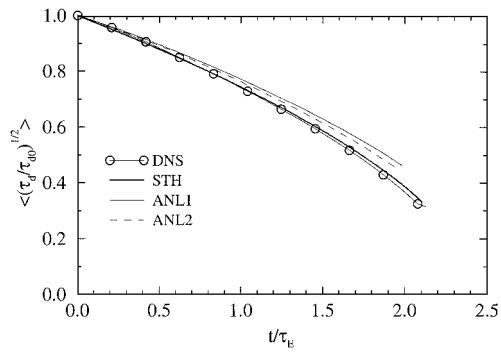

Fig. 4 Temporal variations of $\langle(\tau_d/\tau_{d0})^{1/2}\rangle$ for $\tau_{d0} = 5\tau_k$, $\tau_{ec} = 5\tau_k$, and $Sc_d = 5$.

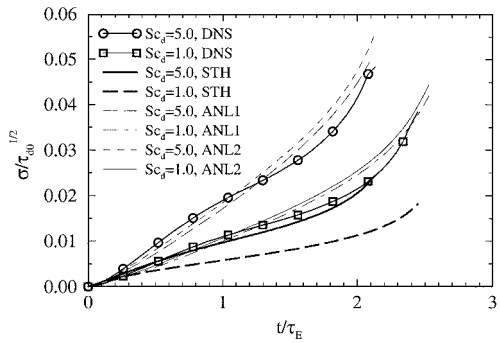

Fig. 5 Temporal variations of the standard deviation of $\tau_d^{1/2}$ at different droplet Schmidt numbers for $\tau_{d0} = 5\tau_k$ and $\tau_{ec} = 5\tau_k$.

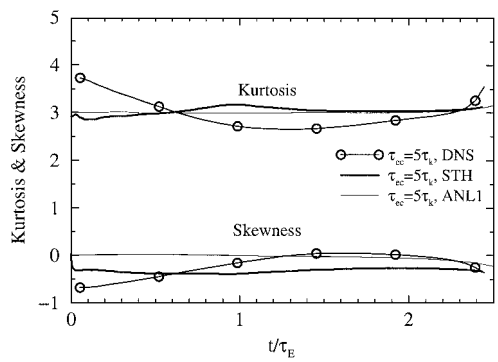

Fig. 6 Temporal variations of the skewness and kurtosis of $\tau_d^{1/2}$ for $\tau_{d0} = 5\tau_k$, $\tau_{ec} = 5\tau_k$, and $Sc_d = 1$.

ANL2. Figure 4 shows that ANL2 predicts a larger value for effective average evaporation rate (as compared to that predicted by ANL1), which makes the ANL2 curve closer to the DNS. This behavior of ANL2 is mainly because the predicted value of the mean droplet Reynolds number $\langle Re_d\rangle$ is greater in this case as compared to the case of ANL1.

In Fig. 5, the temporal variations of the normalized standard deviation, $\sigma/\tau_{d0}^{1/2}$, of $\tau_d^{1/2}$ are shown for $\tau_{d0} = 5\tau_k$ and $\tau_{ec} = 5\tau_k$ for $Sc_d = 1$ and 5. The DNS results indicate that $d\sigma/dt$ is not a monotonic function of t. The present predictions are better compared to the STH, which predicts much narrower (thinner) droplet size distribution, for the reasons discussed in Ref. 27, and gives smaller values for σ as compared to DNS results. Figure 5 shows that values from ANL2 predictions are greater than the ANL1 results. This is due mainly to the greater values of the mean droplet Reynolds number $\langle Re_d\rangle$ and, consequently, a greater value of Q in the Fokker–Planck equation in the case of ANL2. Although the present predictions for σ are in good agreement with the DNS, the PDF model is not capable of capturing the minute temporal behavior of $d\sigma/dt$, apparently due to the difficulty in properly capturing the second region in the temporal variation of the mean droplet Reynolds number $\langle Re_d\rangle$, as shown in Fig. 2.

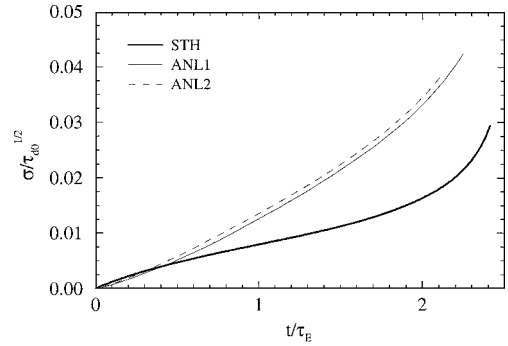

Fig. 7 Temporal variations of the standard deviation of $\tau_d^{1/2}$ for $\tau_{d0} = 10\tau_k$, $\tau_{ec} = 10\tau_k$, and $Sc_d = 1$.

The temporal behavior of higher-order moments as computed from the calculated PDF is shown in Fig. 6 for $\tau_{d0} = 5\tau_k$, $\tau_{ec} = 5\tau_k$, and $Sc_d = 1$. The present solution does not predict the true temporal behavior of the skewness and kurtosis of $\tau_d^{1/2}$. The underlying reason for this behavior is not clear to us, but it could be due to the approximate initial condition, Eq. (47), used for $p(\tau_d, t)$ at $t = 0.012\tau_E$, which is Gaussian in nature.

In Fig. 7, the standard deviation of $\tau_d^{1/2}$ for $\tau_{d0} = 10\tau_k$, $\tau_{ec} = 10\tau_k$, and $Sc_d = 1$ as predicted is shown along with the STH data. Figure 6, in conjunction with Figs. 4 and 5, suggests that the predictions are not very sensitive to the value of C in the range of 0.2826–0.482 and that the present predictions for the standard deviation are better as compared to the STH results when assessed against the DNS data.

Conclusions

The objective of this study has been to obtain a kinetic or PDF equation that governs the temporal behavior of distribution of the droplet size, in terms of its time constant, in an isotropic turbulence where the stochastic nature in droplet evaporation occurs solely due to the convective correction term, that is, the term containing B on the right-hand side of Eq. (2). To obtain the closed governing equation, the cumulant expansion closure method of Van Kampen has been used, which has already found its success in the derivation of kinetic equation for nonevaporating particles dispersed in turbulent flows.[16] The resulting equation has been computed using a path-integral-based numerical scheme, and the results have been compared with the DNS data for the purpose of assessment. Present predictions for the mean and the root mean square of $\tau_d^{1/2}$ have been found in good agreement with DNS data, whereas the predictions of higher-order moments, that is, skewness and kurtosis, exhibit some deviations. The results presented here, indicate that the Fokker–Planck equation could be used for a detail parametric study of the phenomena of evaporating droplets in isotropic turbulence with different initial conditions for $p(\tau_d, t)$.

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J. R. Bellan
Associate Editor