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Statistical modeling of sprays using the droplet distribution function

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Theoretical foundations of a statistical spray modeling approach based on the droplet distribution function (ddf), which was originally proposed by Williams [Phys. Fluids 1, 541 (1958)], are established. The equation governing the ddf evolution is derived using an alternative approach. The unclosed terms in the ddf evolution equation are precisely defined, and the regime of applicability of current models is discussed. The theory of point processes is used to rigorously establish the existence of a disintegration of the ddf in terms of a spray intensity, which is the density of expected number of spray droplets in physical space, and the joint probability density function (jpdf) of velocity and radius conditional on physical location. Evolution equations for the spray intensity and the conditional jpdf of velocity and radius are derived. The intensity evolution equation contains a sink term corresponding to droplet vaporization, hitherto missing in previous derivations of this equation. This sink term is essential in order to correctly represent the vaporization phenomenon. Problems with numerical convergence of computed solutions to the ddf evolution are discussed, and criteria for establishing convergence are proposed. The study also shows how quantities predicted by ddf-based spray models can be compared to experimental measurements. © 2001 American Institute of Physics. [DOI: 10.1063/1.1344893]

I. INTRODUCTION

Spray modeling is a research topic of great practical importance. Faeth1 has reviewed different spray modeling approaches. The focus of this paper is on a particular statistical approach to spray modeling, which was originally proposed by Williams.2 In this modeling approach the statistical properties of a spray are characterized by a droplet distribution function (ddf). Based on physical principles, Williams derived an evolution equation for the ddf, which is called the spray equation. The spray equation is of fundamental importance in spray modeling. The ddf approach has been further extended by O’Rourke3 to dense sprays, and it forms the basis of the spray model in several simulation codes4–7 which are widely used in industry, academia, and research laboratories around the world.

The ddf approach is a mathematical model for the physical spray. One motivation for understanding the basis of the modeling approach is to clearly state the underlying assumptions. This is done with a view to verifying the extent to which physical sprays actually satisfy these assumptions. Furthermore, in the ddf approach the relationship between observable properties of the physical system and properties of the mathematical model is not readily apparent. Understanding the mathematical basis of the modeling approach is a crucial step in establishing these relationships. It is also essential to making the connection between experimentally measured quantities and those predicted by the mathematical model.

While spray models based on the ddf approach are used extensively, there are certain outstanding fundamental questions concerning the ddf modeling approach that remain unresolved. These questions may be grouped under the following categories:

1. Modeling: The spray equation contains unclosed terms corresponding to the acceleration and vaporization of spray droplets. These unclosed terms must be modeled. The following important questions need to be answered in this context:
   (a) What is the precise form of the unclosed terms in the ddf evolution equation and how can they be quantified in simple canonical flows?
   (b) What is the regime of validity of current sub-models for these unclosed terms?
   (c) How do the quantities predicted by ddf-based spray models relate to experimentally measured spray statistics, and what constitutes a meaningful comparison of model prediction and experiment?

2. Computations: Studies by Abraham and co-workers8,9 indicate possible numerical convergence problems with spray computations based on the ddf approach. Recently Subramaniam and O’Rourke10 have conclusively shown that a particular numerical implementation (KIVA–3) of a ddf-based spray model does not show empirical evidence of numerical convergence. Therefore, understanding the numerical resolution requirements arising from the spray model also motivates a re-examination of the fundamentals of the ddf approach. In particular, convergence criteria for computations of solutions to the ddf evolution equation need to be established.
The foundations of the statistical representation of a spray as a point process are established in Ref. 11, where it is shown that the ddf can be expressed as the superposition of weighted single-particle probability density functions corresponding to a surrogate droplet ensemble. The ddf is then established to be the density of expected number of droplets in a position-velocity-radius space, and this defines which events associated with the ensemble of spray droplets it is capable of characterizing. In that work it was also shown that there are fundamental differences between spray theory and the standard kinetic theory of ideal gases. These fundamental differences between spray and kinetic theory warrant a careful re-examination of the spray modeling approach using the droplet distribution function.

The present work uses the ideas developed in Ref. 11 to address the aforementioned outstanding fundamental questions concerning the ddf modeling approach. The results of this work are applicable to a wide variety of sprays, but for some exceptions. For simplicity, droplet collisions, coalescence, and breakup are neglected. This is not due to any fundamental limitation of the formulation itself, but rather due to the fact that these are not central to the main conclusions of this study, and yet their inclusion unnecessarily complicates the equations. Additional terms will appear in the equations derived in this work, if these effects are to be included. Also any electromagnetic interactions among the droplets are neglected in this study.

The paper begins with a derivation of the spray equation from first principles that is different from previous derivations. Then the exact nature of the unclosed terms in the spray equation, and the regime of applicability of current modeling approaches are discussed. Also the use of direct numerical simulations (DNS) to quantify the unclosed terms in canonical flows is noted.

The ddf approach to spray modeling and plasma kinetic theory share a common mathematical foundation in the theory of stochastic point processes. The details of this mathematical basis are given in an appendix for the interested reader, where the implications of the underlying assumptions are also discussed. It is noteworthy that Edwards and Marx have also used an approach based on the theory of stochastic point processes to characterize statistics of sprays.

The theory of point processes rigorously establishes the disintegration of the ddf as a product of two quantities, namely: (i) the spray intensity, which is the density of expected number of droplets in physical space, and (ii) the joint probability density function (jpdf) of velocity and radius conditioned on physical location. [Disintegration is the formal term from point process theory for expressing the density of the expectation measure as a product of two quantities, one of which is a conditional probability density (p. 604 DV13). In this work this term is preferred to the term ‘decomposition’ which has a special meaning in the context of random measures.] The relation between the ddf and the conditional jpdf of velocity and radius is useful in comparing ddf predictions to experimental measurements. These properties of the ddf are explained in the section following the spray equation derivation.

The evolution equation for the spray intensity, and for the conditional jpdf of velocity and radius, as implied by the ddf evolution equation are derived. Archambault et al. have derived similar equations for nonvaporizing sprays, but there are important differences when vaporization effects are considered. It is shown in this study that the intensity evolution equation contains a sink term corresponding to droplet vaporization, which has not been reported in previous derivations of this equation. The sink term is essential to represent inhomogeneities that arise in the intensity as a result of a spatially inhomogeneous mean gas-temperature field.

The evolution of global spray properties, such as the expected total spray mass, as implied by the ddf evolution equation are derived. Two criteria for characterizing the numerical convergence of computed solutions to the ddf evolution equation are proposed in this work. A summary of results, and the important conclusions of this study, conclude the paper.

II. THE SPRAY EQUATION

Consider a spray in a finite flow domain \( \mathcal{R} \) in physical space as an ensemble of spherical droplets, or droplets that can be characterized by a single length scale parameter. At time \( t \) the total number of spray droplets \( N_s(t) \) is a non-negative integer-valued random variable, which is finite with probability 1. The \( i \)th spray droplet is characterized by its position vector \( \mathbf{X}_{(i)}(t) \) (which is defined as the center of mass of the droplet), its velocity vector \( \mathbf{V}_{(i)}(t) \), and its radius \( R_{(i)}(t) \) \([R_{(i)}(t)>0]\). The position, velocity, and radius of a spray droplet are called the droplet properties, and the droplet property vector associated with each droplet is a seven-dimensional random vector. Additional droplet properties may be included as required, but they do not fundamentally alter the formulation, other than increasing the dimension of the space of droplet properties. The droplet properties associated with the \( i \)th droplet evolve by the following equations:

\[
\frac{d \mathbf{X}_{(i)}}{dt} = \mathbf{V}_{(i)},
\]

\[
\frac{d \mathbf{V}_{(i)}}{dt} = \mathbf{A}_{(i)},
\]

\[
\frac{d R_{(i)}}{dt} = \Theta_{(i)},
\]

where \( \mathbf{A}_{(i)} \) is the acceleration experienced by the droplet, and \( \Theta_{(i)} \) is the rate of radius change due to vaporization.

There are two ways in which the statistical properties of the ensemble of droplets can be characterized. These two approaches are similar to those used in kinetic theory, although there are subtle and important differences in their application to sprays. These differences, and their implications for the statistical representation of sprays, are described in Ref. 11. In kinetic theory terminology, one method is called the Liouville approach, while the other is termed the Klimontovich approach.

In the Liouville approach a fine-grained density function \( f'_{N_s=k}(t) \) which is conditional on the total number of droplets \( N_s=k \), is defined as...
The fine-grained Liouville density gives the density of spray systems (each composed of $N_v = k$ droplets) in the $7k$-dimensional phase space. The evolution of the ensemble of droplets given by Eqs. (1)–(3) implies an evolution equation for $f'_{[N_v = k]}(x, v, r, t)$ in the $7k$-dimensional phase space, which is called the Liouville equation. The standard approach in kinetic theory is to ensemble-average the fine-grained Liouville density to obtain the Liouville probability density in the $7k$-dimensional phase space. Marginal densities, which are defined on lower-dimensional phase spaces, may then be obtained by successively integrating the Liouville probability density, resulting in the well-known BBGKY hierarchy. The objective is to obtain a single-particle density on a seven-dimensional phase space in order to construct tractable models. However, in the case of sprays this approach is not as straightforward as in kinetic theory because an intermediate symmetrization procedure is required. This procedure is described in detail in Ref. 11. On the other hand, the Klimontovich approach provides an easier way to derive the spray equation from first principles.

In the Klimontovich approach the ensemble of droplets is characterized in a seven-dimensional position–velocity–radius space $[x, v, r]$ by a fine-grained density function $f'$ which is defined as

$$f'(x, v, r, t) = \sum_{i=1}^{N_v(t)} f'_i(x, v, r, t) = \sum_{i=1}^{N_v(t)} \delta(x - X_{(i)}(t)) \delta(v - V_{(i)}(t)) \delta(r - R_{(i)}(t)).$$

(5)

where $f'_i(x, v, r, t)$ is the fine-grained density function associated with the $i$th droplet, and is defined as

$$f'_i(x, v, r, t) = \delta(x - X_{(i)}(t)) \delta(v - V_{(i)}(t)) \delta(r - R_{(i)}(t)).$$

(6)

Note that $[X_{(i)}, V_{(i)}, R_{(i)}]$ are the Lagrangian coordinates of the $i$th droplet, whereas $[x, v, r]$ are the Eulerian coordinates of the position-velocity-radius phase space. [In this work we follow Williams’ terminology in denoting this space the “phase space,” but “phase” here should not be confused with its usage in the thermodynamic sense of liquid phase or gas phase.] The Klimontovich fine-grained density is not the same as its Liouville counterpart, which is clear from the very fact that it is defined on a different phase space. In the Klimontovich approach the fine-grained density function $f'$ represents the density of droplets in a seven-dimensional phase space. Since $f'$ is composed of delta functions it is not a smooth function in phase space.

The number of droplets in any region of phase space can be obtained by integrating $f'$ over that region. Since only droplets with nonzero radius belong to the spray system, if for convenience of notation we denote $r_+$ to be the positive $r$ axis ($r > 0$), then it is sufficient to integrate over regions only in $[x, v, r_+]$ space. If the number of droplets in any region $B_+$ in $[x, v, r_+]$ space is denoted $N_v(B_+; t)$, it is obtained by integrating $f'$ over the region $B_+$ such that

$$N_v(B_+; t) = \int_{B_+} f'(x, v, r, t) \, dx \, dv \, dr.$$

(7)

However, the statistical description of a spray in terms of $f'$ contains far more information than is necessary for engineering calculations. In order to obtain information concerning the average properties of the spray, it is advantageous to consider the ensemble average of $f'$. The ensemble average of $f'$ is denoted $f(x, v, r, t)$, and it defines the droplet distribution function (ddf):

$$f(x, v, r, t) = \langle f'(x, v, r, t) \rangle = \left( \sum_{i=1}^{N_v(t)} \delta(x - X_{(i)}(t)) \delta(v - V_{(i)}(t)) \times \delta(r - R_{(i)}(t)) \right).$$

(8)

When ensemble-averaging over a sum of fine-grained densities where the total number of such densities is itself a random variable, it is first necessary to condition on the total number taking a given value, before the ensemble-averaging operation can be taken inside the summation sign. Using standard conditioning arguments, the ddf can be written as

$$f(x, v, r, t) = \sum_{n=1}^{N_v} P[N_v(t) = n] \left( \sum_{i=1}^{n} \delta(x - X_{(i)}(t)) \times \delta(v - V_{(i)}(t)) \times \delta(r - R_{(i)}(t)) \right)$$

$$= \sum_{n=1}^{N_v} p_n \left( \sum_{i=1}^{n} f'_i(x, v, r, t) \right).$$

(9)

where $p_n(t)$ is the probability that $N_v(t)$, the total number of droplets at time $t$, is equal to $n$. [For a finite point process there exists a $K$ such that $p_n(t) = 0$, $n > K$, and therefore the series summation in the above equation does converge.]

In a previous paper on the statistical representation of sprays using point processes it was shown that the ddf can be written as

$$f(x, v, r, t) = \sum_{n=1}^{N_v} p_n f^{(n)}(x, v, r, t) = \sum_{n=1}^{N_v} p_n \sum_{i=1}^{n} f^{(n)}_i(x, v, r, t),$$

(10)

where $f^{(n)}(x, v, r, t)$ is the density of expected number of droplets in phase space (conditional on the total number of droplets being equal to $n$), and is given by $n$ times the single surrogate-droplet density $f^{(n)}_1(x, v, r, t)$. The above equation together with Eq. (9) leads to the identification of $f^{(n)}$ in terms of the sequence of droplet fine-grained densities $\{f'_i, i = 1, \ldots, n\}$ as

$$f^{(n)}(x, v, r, t) = \left( \sum_{i=1}^{n} f'_i(x, v, r, t) \right).$$

(11)

Note that in the above equation the ensemble-averaging operator is not taken inside the summation sign because, for reasons given in Ref. 11 we do not want to make the unnes-
essary assumption that the droplets are identically distributed. It also follows from Eqs. (10) and (11) that the single surrogate-droplet density, which is the same for all the identically distributed surrogate-droplets, is simply the arithmetic mean of \( f_i^{(n)} \):

\[
f_{i}^{(n)}(x,v,r,t) = \frac{1}{n} f_i^{(n)}(x,v,r,t) = \frac{1}{n} \left\{ \sum_{i=1}^{n} f_i^{(n)}(x,v,r,t) \right\},
\]

(12)
a result which was independently derived from the Liouville description in Ref. 11.

The temporal evolution of the ddf characterizes the evolution of the spray. When deriving an evolution equation for the ddf we need to account for temporal changes in both \( p_n(t) \) as well as in \( f_i^{(n)}(x,v,r,t) \). Since \( N_i(t) \) describes a finite point process where \( N_i \) takes integer values, there is no reason to assume that \( p_n(t) \) evolves continuously in time.

Let \( \delta f(t) \) be the change in \( f(x,v,r,t) \) over a small time interval \((t, t+\delta t)\) such that

\[
\delta f(t) = f(x,v,r,t+\delta t) - f(x,v,r,t).
\]

From Eq. (10) it follows that

\[
\delta f = \sum_{n=1}^{\infty} \left\{ \delta p_n(t) f_i^{(n)}(x,v,r,t) + p_n(t) \frac{\partial f_i^{(n)}}{\partial t} \right\},
\]

(13)
where

\[
\delta p_n(t) = p_n(t+\delta t) - p_n(t).
\]

It is important to note that \( \int_{[x,v,r]} \delta f \, dx \, dv \, dr \) is not zero, and \( f \) is not a conserved quantity. In fact \( \int_{[x,v,r]} \delta f \, dx \, dv \, dr \) represents the change in the expected total number of droplets in \( R \) over time interval \((t, t+\delta t)\). On the other hand, we can show that \( f_i^{(n)} \) should be conserved when integrated over the phase space because it is simply \( n \) times the single surrogate-droplet density conditioned on there being a total of \( n \) droplets in the flow at time \( t \). Therefore, the integral of \( f_i^{(n)} \) over phase space is a conserved quantity which is always equal to \( n \) such that

\[
\int_{[x,v,r]} f_i^{(n)} \, dx \, dv \, dr = n,
\]

and hence it follows that

\[
\frac{\partial}{\partial t} \int_{[x,v,r]} f_i^{(n)} \, dx \, dv \, dr = 0.
\]

(14)
Substituting the above equation into Eq. (13) and integrating over phase space tells us that the change in expected total number of droplets over the time interval \((t, t+\delta t)\) is given by

\[
\int_{[x,v,r]} \delta f \, dx \, dv \, dr = \sum_{n=1}^{\infty} n \, \delta p_n(t).
\]

In order to derive the ddf evolution equation we must first understand how \( p_n(t) \) changes with time. For the general spray problem \( p_n(t) \) changes due to inflow (or outflow) of droplets to (or from) the flow domain \( R \) in physical space, vaporization, or coalescence and breakup. The change of \( p_n(t) \) due to inflow/outflow or vaporization is associated with a nonzero flux of \( f_i^{(n)}(x,v,r,t) \) across the \( x \) and \( r=0 \) boundaries of phase space, respectively. Coalescence and breakup are not accounted for in this formulation for the sake of simplicity, although their inclusion is not intrinsically more difficult. However, the manifestation of coalescence and breakup in the evolution of \( f_i^{(n)} \) is fundamentally different because, unlike vaporization or inflow/outflow, these events are not associated with flux across boundaries of the phase space, but rather they appear as source terms in the interior of the phase space.

Prior to deriving the evolution equation for \( f_i^{(n)}(x,v,r,t) \) for the case when \( p_n(t) \) changes with time, we first derive the evolution equation for \( f_i^{(n)}(x,v,r,t) \) for the simpler case when \( p_n(t) \) does not change with time. In this case the flux of \( f_i^{(n)}(x,v,r,t) \) across boundaries in phase space is zero. Then we derive the expressions for \( \delta p_n(t) \) due to inflow/outflow or vaporization, in terms of the boundary fluxes of \( f_i^{(n)}(x,v,r,t) \). Since \( f_i^{(n)}(x,v,r,t) \) is a conserved quantity when integrated over phase space, additional source terms must appear in the evolution of \( f_i^{(n)}(x,v,r,t) \) to balance the nonzero probability fluxes at the boundaries of phase space that arise due to vaporization and inflow/outflow, for the case where \( p_n(t) \) changes with time. The physical interpretation of these source/sink terms in the evolution equation of \( f_i^{(n)}(x,v,r,t) \) is that they represent the required rescaling of \( f_i^{(n)}(x,v,r,t) \) as the probability of the population class \( n \) grows or dwindles due to nonzero fluxes of \( f_i^{(n)}(x,v,r,t) \) at the boundaries of phase space. Finally, we specify the source terms that must appear in the evolution of \( f_i^{(n)}(x,v,r,t) \), in terms of \( \delta p_n(t) \). This then leads to the desired general evolution equation for the ddf with vaporization and inflow/outflow.

Starting from the definition of \( f_i^{(n)} \) [cf. Eq. (11)] and differentiating it with respect to time we have

\[
\frac{\partial f_i^{(n)}}{\partial t} = \frac{\partial}{\partial t} \left\{ \sum_{i=1}^{n} f_i^{(n)} \right\}.
\]

(15)
The evolution of the \( i \)th droplet by the set of droplet evolution equations [Eqs. (1)–(3)] implies an evolution equation for \( f_i^{(n)} \) in phase space [Eq. (A2) of Appendix A1], the detailed derivation of which is given in Appendix A1. Substituting the evolution equation for \( f_i^{(n)} \) into the above equation leads to the evolution equation for \( f_i^{(n)}(t) \):

\[
\frac{\partial f_i^{(n)}}{\partial t} = -\frac{\partial}{\partial x_k} \left[ v_{ij} f_i^{(n)} \right] - \frac{\partial}{\partial r_k} \left\{ \sum_{i=1}^{n} A_{k(i)} f_i^{(n)} \right\}
\]

\[
- \frac{\partial}{\partial r} \left\{ \sum_{i=1}^{n} \Theta_{ij} f_i^{(n)} \right\}.
\]

(16)
See Appendix A1 for details. We now define the following functions in phase space:

\[
\langle A_i^{(n)} \rangle_{x,v,r,t} = \frac{1}{f_i^{(n)}(x,v,r,t)} \left\{ \sum_{i=1}^{n} A_{k(i)} f_i^{(n)} \right\},
\]

if \( f_i^{(n)}>0 \),

(17)
and equal to zero otherwise, and

$$\langle \Theta^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle = \frac{1}{f^{(n)}(\mathbf{x}, \mathbf{v}, r; t)} \left\{ \sum_{i=1}^{n} \Theta_{(i)} f_{i}(\mathbf{x}, \mathbf{v}, r, t) \right\},$$

if $f^{(n)} > 0$, (18)

and equal to zero otherwise. Substituting these definitions into Eq. (16) we obtain the evolution equation for $f^{(n)}$ when there is no change in $p_n(t)$:

$$\frac{\partial f^{(n)}}{\partial t} = -\frac{\partial}{\partial \mathbf{x}} \left[ v \cdot f^{(n)} \right] - \frac{\partial}{\partial \mathbf{v}} \left\{ \langle A_{k}^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\}$$

$$- \frac{\partial}{\partial r} \left\{ \langle \Theta^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\}. \quad (19)$$

If we integrate Eq. (19) over $[\mathbf{x}, \mathbf{v}, r]$ space we get

$$\int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial f^{(n)}}{\partial t} d\mathbf{x} d\mathbf{v} dr = - \int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial}{\partial \mathbf{x}} \left[ v \cdot f^{(n)} \right] d\mathbf{x} d\mathbf{v} dr$$

$$- \int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial}{\partial \mathbf{v}} \left\{ \langle A_{k}^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\} d\mathbf{x} d\mathbf{v} dr$$

$$- \int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial}{\partial r} \left\{ \langle \Theta^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\} d\mathbf{x} d\mathbf{v} dr. \quad (20)$$

Each of the terms on the right-hand side of Eq. (20) is equal to zero if no changes in $p_n(t)$ are allowed. This is because either the “transport velocity” of $f^{(n)}$ in the phase space vanishes at the boundaries of the phase space (as is the case for the first and third terms), or $f^{(n)}$ itself vanishes at the boundaries of the phase space (as in the second term).

The expression for $\delta p_n(t)$ when $p_n(t)$ changes only due to vaporization is related to the outward flux of $f^{(n)}$ across the $r=0_+$ boundary of phase space as follows:

$$\delta p_n(t) = p_n(t) \langle \Theta^{(n)} | r=0_+; t \rangle f^{(n)}(r=0_+, t) \delta t. \quad (21)$$

(See Appendix A 2 for a detailed explanation.) Note that for vaporization $\langle \Theta^{(n)} | r=0_+; t \rangle$ is a negative quantity. Therefore vaporization results in a decrease of $p_n(t)$. The expression for $\delta p_n(t)$ when $p_n(t)$ changes only due to inflow or outflow of droplets at the boundary $S$ of the flow domain $\mathcal{R}$ in physical space is given in terms of the boundary flux of $f^{(n)}$ as follows:

$$\delta p_n(t) = - p_n(t) \int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial}{\partial \mathbf{x}} \left[ v \cdot f^{(n)} \right] d\mathbf{x} d\mathbf{v} dr \delta t. \quad (22)$$

(See Appendix A 4 for a detailed explanation.) The divergence theorem shows that the integral in the above equation represents the net outward flux of $f^{(n)}$ through the boundary $S$ of the flow domain $\mathcal{R}$, which has the effect of reducing $p_n(t)$.

Note that since the $p_n$ are probabilities they must always sum to unity such that

$$\sum_{n=1}^{N} p_n(t) = 1 - p_0(t), \quad (23)$$

where $p_0(t)$ is the probability that there are no droplets in the domain $\mathcal{R}$. Imposing the same requirement at time instant $t + \delta t$ implies that the changes in probability $\delta p_n(t)$ must satisfy the constraint

$$\sum_{n=1}^{N} \delta p_n(t) = p_0(t) - p_0(t + \delta t), \quad (24)$$

For many spray problems it is reasonable to assume that almost surely the flow domain $\mathcal{R}$ contains at least one droplet at initial time $t_0$, i.e., $p_0(t_0) = 0$. In this case the only physical processes that change $p_0$ from its initial value of zero are either complete vaporization of all droplets, or complete outflow of all droplets from the physical domain. For spray problems which are characterized by incomplete vaporization and incomplete outflow of all the spray droplets, the constraint on $\delta p_n(t)$ then simplifies to

$$\sum_{n=1}^{N} \delta p_n(t) = 0. \quad (25)$$

The requirement that $f^{(n)}$ be conserved [cf. Eq. (14)] necessitates the addition of source terms to the evolution equation [Eq. (19)] of $f^{(n)}$:

$$\frac{\partial f^{(n)}}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \left[ v \cdot f^{(n)} \right] + \frac{\partial}{\partial \mathbf{v}} \left\{ \langle A_{k}^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\}$$

$$\quad + \frac{\partial}{\partial r} \left\{ \langle \Theta^{(n)} | \mathbf{x}, \mathbf{v}, r; t \rangle f^{(n)} \right\} = S^{(n)}(\mathbf{x}, \mathbf{v}, r, t) + S_{io}^{(n)}(\mathbf{x}, \mathbf{v}, r, t). \quad (26)$$

The source term $S_v^{(n)}(\mathbf{x}, \mathbf{v}, r, t)$ arises as a result of vaporization, and the source term $S_{io}^{(n)}(\mathbf{x}, \mathbf{v}, r, t)$ arises as a result of inflow or outflow of droplets into the physical flow domain $\mathcal{R}$. These source terms are shown in Appendix A 3 and Appendix A 5 to be

$$S^{(n)}(\mathbf{x}, \mathbf{v}, r, t) = - f^{(n)}(\mathbf{x}, \mathbf{v}, r, t) \langle \Theta^{(n)} | r=0_+; t \rangle \times f^{(n)}(r=0_+, t), \quad (27)$$

$$S_{io}^{(n)}(\mathbf{x}, \mathbf{v}, r, t) = f^{(n)}(\mathbf{x}, \mathbf{v}, r, t) \int_{[\mathbf{x}, \mathbf{v}, r]} \frac{\partial}{\partial \mathbf{x}} \left[ v \cdot f^{(n)} \right] d\mathbf{x} d\mathbf{v} dr. \quad (28)$$

Substituting these source terms corresponding to vaporization and inflow/outflow into Eq. (19), we obtain the evolution equation for $f^{(n)}$ that accounts for changes in $p_n(t)$ due to vaporization and inflow/outflow to be
Substituting the above equation into Eq. (13) along with the expressions for $\delta p_n(t)$ for vaporization and inflow/outflow given by Eqs. (21) and (22), respectively, we obtain

$$\frac{\partial f}{\partial t} = \sum_{n=1} \int [u_{gf}^n] d\mathbf{x} d\mathbf{v} dr - \frac{\partial}{\partial \mathbf{x}_k} \left[ (A_k^n) \mathbf{x} \mathbf{v} r t f^n \right]$$

Substituting the above equation into Eq. (13) along with the expressions for $\delta p_n(t)$ for vaporization and inflow/outflow given by Eqs. (21) and (22), respectively, we obtain

$$\frac{\partial f}{\partial t} = \sum_{n=1} p_n(t) f^n \left\{ \left[ (A_k^n) \mathbf{x} \mathbf{v} r t f^n \right] - \frac{\partial}{\partial \mathbf{x}_k} \left[ (A_k^n) \mathbf{x} \mathbf{v} r t f^n \right] \right\}$$

and equal to zero otherwise, and

$$\langle A_k | \mathbf{x} \mathbf{v} r t \rangle = \frac{1}{f(\mathbf{x} \mathbf{v} r t)} \left\{ \sum_{n=1} p_n(t) (A_k^n) \mathbf{x} \mathbf{v} r t \right\}$$

and equal to zero otherwise. Substituting the above expressions into Eq. (30), then taking the limit as $\delta t \to 0$, and noting that the right-hand side is a continuous function of time results in the following familiar form of the spray equation:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \mathbf{x}_k} \left[ ((A_k^n) \mathbf{x} \mathbf{v} r t f^n) \right] + \frac{\partial}{\partial \mathbf{v}_k} \left[ ((A_k^n) \mathbf{x} \mathbf{v} r t f^n) \right]$$

$$= 0.$$  

A. Modeled ddf evolution equation

The conditional expectation terms $\langle A_k | \mathbf{x} \mathbf{v} r t \rangle$ and $\langle \Theta | \mathbf{x} \mathbf{v} r t \rangle$ are not closed at the level of the ddf, i.e., they are not completely determined by the ddf or its moments alone, since they may also depend on gas phase properties. This means that these conditional expectation terms must be modeled, and these models should in general depend on the gas phase properties. The specification of models for the unclosed terms in the spray equation results in a modeled ddf evolution equation:

$$\frac{\partial f^*}{\partial t} + \frac{\partial}{\partial \mathbf{x}_k} \left[ u_{gf}^n \right] + \frac{\partial}{\partial \mathbf{v}_k} \left[ A_k^* (\mathbf{x} \mathbf{v} r t) f^* \right]$$

$$+ \frac{\partial}{\partial r} \left[ \Theta^* (\mathbf{x} \mathbf{v} r t) f^* \right] = 0,$$

and its modeled counterpart Eq. (34) is the model for $f$ implied by the model specifications $A_k^*$ and $\Theta^*$. Expressing the modeled ddf evolution equation in this form clearly shows that the ddf approach defines a family of spray models, rather than just one single spray model. Later in this section, a particular class of this family of spray models will be described in detail. The specification of a particular spray model may impose additional restrictive assumptions that limit the regime of validity of the ddf approach. Therefore, prior to discussing any model specifics it is worthwhile to identify the conditions under which Williams' spray equation [and its modeled counterpart Eq. (34)] is a valid statistical representation of spray evolution.

B. Regime of validity of the spray equation

A detailed description of the mathematical basis of the ddf approach is given in Appendix B. The practical implica-
tions of the assumptions underlying this theory are given in Appendix B 1, and the salient points are briefly summarized here.

The point process model underlying the ddf approach makes only two assumptions concerning the spray. The first assumption, stated at the beginning of this section, is that each droplet be characterized by a characteristic size length scale, which in the case of spherical droplets is simply the droplet radius. At first this may seem to be problematic for regions of the spray where the liquid phase is present as nonspherical elements, rather than as fully dispersed droplets. From a purely representational standpoint however, even this does not pose serious difficulties since as long as the volume of such liquid elements can be defined, one can always associate with each liquid element a characteristic size length scale which is the radius of a spherical droplet of equal volume. The information concerning the shape of the nonspherical liquid element is lost in the process, and will have to be accounted for in the models. These implications are discussed later in the section.

The second assumption is that the spray droplet locations in physical space are characterized by a simple point process, which precludes the simultaneous presence of more than one spray droplet at any given location in physical space. This assumption is automatically satisfied by all sprays. A mathematical technicality (also described in Appendix B 1) requires that the definition of a conditional joint probability density function derived from the ddf needs special treatment in the case where the number density function takes delta-function jumps to account for the presence of fixed atoms in the point process in physical space.

The foregoing assumptions are not serious restrictions on the class of physical sprays that can be modeled using the ddf approach. This is of course quite different from claiming that the ddf constitutes an accurate model of these sprays in all flow regimes, or that the ddf even contains a representation of the important statistical characteristics of the spray that are needed to construct such an accurate model. These issues properly fall under the purview of a discussion on modeling, and are dealt with in the following subsections.

Finally, it is noteworthy that two assumptions that are commonly perceived as necessary to establish the validity of the spray equation, have not been used in this derivation. They are (i) the assumption of point particles and (ii) the dilute spray assumption.

1. **Point process vs point particle assumption**

The assumption of point particles is different from, and considerably more restrictive than, the assumptions required for modeling the spray as a point process. The point particle assumption requires that the size (radius) of the spray droplets be infinitesimal, or at least smaller than the Kolmogorov scale of the gas-phase flow. It is shown in this work that sprays with droplets of finite radius (which may be larger than the Kolmogorov scale of the gas-phase flow) can be modeled using the point process approach. In a subsequent discussion on model properties it is shown that specific forms of ddf spray models may impose restrictions on the size of the droplets, but these are nowhere as restrictive as the point particle assumption. In summary, the point particle assumption is unnecessary for the representation and modeling of sprays using the ddf approach, which admits droplets of finite size.

2. **Dilute spray assumption**

Another commonly held view is that the ddf approach is valid only for dilute sprays. The average liquid volume fraction is one measure (and by no means the only measure) of how dilute a spray is. The average liquid volume in a region \( A \) in physical space may be defined in terms of the ddf as

\[
\langle \theta(A,t) \rangle = \frac{1}{V_A} \int_A \theta(x,t) \, dx
\]

where

\[
\theta(x,t) = \int \frac{4}{3} \pi r^3 f(x,v,r,t) \, dv \, dr, \quad r > 0,
\]

is the density of average liquid volume in physical space. If \( V_A \) is the volume associated with region \( A \), then the average liquid volume fraction in region \( A \) is given by

\[
\frac{\langle \theta(A,t) \rangle}{V_A} = \frac{1}{V_A} \int_A \theta(x,t) \, dx,
\]

which reveals that if the average liquid volume density \( \theta(x,t) \) is uniform in the region \( A \) in physical space [i.e., the ddf \( f(x,v,r,t) \) is statistically homogeneous in \( A \)], then \( \theta \) is equal to the average liquid volume fraction. If \( f \) is statistically inhomogeneous in \( A \), then Eq. (37) states that the mean value of \( \theta(x,t) \) over the volume \( A \) is the average liquid volume fraction. It is important to note that there are other definitions of the average liquid volume fraction.

Because popular ddf models\(^5\) require that the average liquid volume density \( \theta(x,t) \) be negligible compared to unity, this version of the dilute spray requirement is mistakenly thought to apply to the ddf approach itself. In fact, the validity of the spray equation and the modeled ddf evolution equation [Eq. (34)] is not dependent on the average liquid volume density of the spray.

C. Modeling

For practical spray problems the solution to the spray equation is coupled to a gas-phase flow solver\(^5\) which is commonly a Reynolds-averaged Navier–Stokes (RANS) solver for single-phase turbulent flow with source terms added to represent the effect of the spray droplets. When the gas phase is represented by Reynolds-averaged fields, a class of deterministic models for the unclosed terms \( \langle A_k | x,v,r,t \rangle \) and \( \langle \theta | x,v,r,t \rangle \) may be written as follows:

Unclosed term Model

\[
\langle A_k | x,v,r,t \rangle: \quad A_k^F \{ \langle Q_k(x,t) \rangle \}, q(f(x,v,r,t),x,v,r,t).
\]
\[ \langle \Theta | x, v, r; t \rangle: \quad \Theta^*\{\langle Q_g(x,t) \rangle, q(f(x,v,r,t)), x, v, r, t \} \]  

where the models \( A^g \) and \( \Theta^* \) depend on \( \{ \langle Q_g(x,t) \rangle \} \) and \( q(f(x,v,r,t)) \). Here \( \{ \langle Q_g(x,t) \rangle \} \) represents the set of averaged fields from the gas-phase solution (which includes such fields as the turbulent kinetic energy and mean gas velocity), and \( q(f) \) is any simply computed function of the ddf. (A simply computed function is defined as a function that depends on the first few moments of the ddf, but is otherwise independent of the ddf.)

The dependence on \( q(f) \) is a general representation of the dependence that the modeled terms might have on quantities like the average liquid volume density in physical space, which can be expressed as a simply computed function of the ddf [cf. Eq. (36)].

D. Model properties

Knowing the exact relationship between the unclosed terms and the ddf [Eqs. (31) and (32)] enables us to deduce some important properties that models for the unclosed terms must satisfy. In addition, modeling of the unclosed terms using the functional forms given in Eqs. (38) and (39) restricts the regime of applicability of the ddf approach. These model properties, which provide important guidelines to modelers using the ddf approach, are detailed below.

1. Locality in physical space

The form of the models given by Eqs. (38) and (39) is local in physical space, i.e., the modeled term at \( x \) depends only on \( f(x,v,r,t) \) at the same physical location \( x \). Models that are local in physical space are strictly valid only if the characteristic length scale of variation \( l_f \) of the ddf \( f(x,v,r,t) \) in physical space, is always greater than a characteristic length scale \( r_c \) associated with the size of spray droplets. (For example, \( r_c \) may be defined such that with high probability (say 0.95) every droplet’s radius is less than or equal to \( r_c \).) This is because if the opposite situation were to prevail and \( r_c > l_f \), then surface phenomena such as vaporization occurring at a distance \( r_c \) from the physical location \( x \) would affect the evolution of \( f \) at \( x \). Clearly, such nonlocal effects cannot be represented accurately by a model that is local in physical space. On the other hand, if \( l_f > r_c \), then the spray is statistically homogeneous in a neighborhood \( l_f \) of \( x \), and a local model can be expected to be a reasonable representation of phenomena occurring at the droplet surface. In the limit of a statistically homogeneous spray the use of local models is fully justified.

Sprays which violate the restriction \( l_f > r_c \) can be represented using nonlocal models. The ddf approach can admit such nonlocal models as well, since the restriction \( l_f > r_c \) is not necessary to derive the spray equation. Such a model may have the form

\[ A^g_2(x,v,r,t) = \int D(y,v,r,t)K(x,y)\,d\,y, \quad (40) \]

\[ \Theta^*_2(x,v,r,t) = \int V(y,v,r,t)K(x,y)\,d\,y, \quad (41) \]

where \( D \) and \( V \) are functions representing drag and vaporization as surface phenomena occurring at a physical location \( y \), and \( K \) is a kernel function with compact support (say in a sphere of radius \( r_c \) centered at \( x \)) representing the nonlocal influence of phenomena occurring at \( y \), on \( f \) at \( x \).

2. Droplet interactions and nonlinearity

The expression for \( \langle A_2 | x,v,r,t \rangle \) in terms of droplet properties,

\[ \langle A_2 | x,v,r,t \rangle = \frac{1}{f(x,v,r,t)} \left\{ \sum_{\alpha=1}^{n} p_\alpha(t) \right\} \times \left\{ \sum_{i=1}^{n} A_{10}f_i(x,v,r,t) \right\} \]  

which is obtained by combining Eqs. (17) and (31), is useful in understanding the limitations of current models, and the assumptions underlying them. The commonly used KIVA drag model and its variants imply an \( A^g_2 \) that neglects drop–drop interactions, provided \( \theta(x;t) < \theta_{dil} \) [or more precisely \( \theta(x;t) < \theta_{dil} \), where \( \theta_{dil} \) is a threshold value of the average liquid volume fraction that characterizes the upper end of the dilute limit for statistically homogeneous sprays]. Since \( A^g_2 \) is a model for \( \langle A_2 | x,v,r,t \rangle \), this assumes that there exists a regime characterized by weak interactions between droplets, and that for \( \theta(x;t) < \theta_{dil} \) the effect of drop–drop interactions on \( \langle A_2 | x,v,r,t \rangle \) is negligible. (Since the same general argument holds for the vaporization term also, even though the actual threshold value of \( \theta(x;t) \) may be different for vaporization, only the acceleration term is discussed here.) The value of \( \theta_{dil} \) is somewhat arbitrarily chosen to be 0.1. This raises the following important question:

Is the characterization of the dilute spray regime by \( \theta(x;t) < \theta_{dil} \) sufficient to guarantee that all sprays that satisfy this condition also satisfy the weak-interaction condition, namely, that \( \langle A_2 | x,v,r,t \rangle \) is not affected by drop–drop interactions?

On physical grounds a necessary condition for the evolution of a droplet’s properties (in the sense of the individual droplet pdf of position, velocity, and radius) in the spray to be unaffected by the presence of other droplets can be quantified in terms of the distribution of the distance to the nearest-neighboring droplet (or its expected value), which is a second-order (or two-particle) statistic. A weak-interaction condition based on nearest-neighbor statistics might require that with high probability (greater than say 0.95) the distance to the nearest-neighboring droplet (normalized by a suitable droplet radius scale) be greater than a threshold value. Alternatively, a simpler weak-interaction condition might require that the mean normalized nearest-neighbor distance (again normalized by a droplet radius scale) should be greater than a threshold value. However, information concerning the distribution of nearest neighbors (or the mean value) is not known at the ddf level of description of the spray. In fact, it is easy to show that two sprays can have the same average liquid volume fraction, but very different distributions of nearest-neighbor distance. Given that the acceleration term
depends on the distribution of nearest-neighbor distance, and noting that sprays with the same ddf can correspond to different values of the acceleration term, leads us to conclude that sprays in the weak-interaction regime cannot be characterized on the basis of the ddf alone. It then follows that all sprays in the weak-interaction regime cannot be characterized on the basis of \( \theta(x;t) \) alone.

Another implication of the weak-interaction condition for sprays with a statistically homogeneous conditional joint pdf \( f_{y,n}^e(v,r|x;t) \) [which is defined by Eq. (50)] is that there may exist a linear regime \( \theta(x;t) \leq \theta_{\text{lin}} \) where \( \sum_{n \geq 1} |p_n(t) \times \sum_{i=1}^{n} A_{ki}(f_i^e(x,v,r,t)) \) varies linearly with \( n_i(x,t) \), the density of expected total number of droplets in physical space [see Eq. (49) for the definition of \( n_i(x,t) \)]. This then raises the following important questions:

1. Is there a class of sprays for which the linear-regime condition can be expressed more precisely than in terms of the existing dilute spray requirement?
2. What are the difficulties in generalizing these linear-regime conditions to sprays with statistically inhomogeneous \( f_{y,n}^e(v,r|x;t) \)?

One can consider marked point process models of sprays with statistically homogeneous conditional joint pdf \( f_{y,n}^e(v,r|x;t) \) [but spatially inhomogeneous \( n_i(x,t) \)], where the model parameters can be chosen such that the model matches measured spray statistics of both the average liquid volume fraction as well as the expected nearest-neighbor distance. One can then perform DNS of an ensemble of identically distributed droplets (EIDD) that are initialized using such a point process model, in order to directly quantify \( \sum_{n \geq 1} |p_n(t) \times \sum_{i=1}^{n} A_{ki}(f_i^e(x,v,r,t)) \). By varying the average liquid volume fraction in the point process model, this approach can also be used to determine the maximum value of the average liquid volume fraction corresponding to the upper limit of the linear regime for this EIDD. Since \( \langle A_4(x,v,r,t) \rangle \) depends on flow parameters other than \( \theta \) (such as the characteristic droplet Reynolds number, or the ratio of droplet relaxation time to characteristic gas-phase turbulence time scales), this limit would correspond to a surface in a multidimensional parameter space. This surface can be mapped out for parameter ranges of interest using DNS, which then defines the regime of validity of linear models for the EIDD. It is then reasonable to apply this linearity condition to the class of sprays that share the same underlying point process characteristics as the EIDD.

Empirically establishing the existence of a regime of linear variation of \( \sum_{n \geq 1} |p_n(t) \times \sum_{i=1}^{n} A_{ki}(f_i^e(x,v,r,t)) \) with \( n_i(x,t) \) for EIDDs does not mean that mathematically this term is a linear function of \( n_i(x,t) \) for all sprays. Mathematically speaking, the linearity property results only if the acceleration (as well as position, velocity and radius) of each droplet is identically distributed, and the droplet ensemble has a symmetric Liouville pdf. It has been shown in Ref. 11 that in general sprays do not satisfy the conditions necessary for a symmetric Liouville pdf, whereas by definition the EIDDs do.

The linearity property forms the basis of the superposition principle. It is of interest to determine when the superposition principle holds for EIDDs, and for sprays. If two sets of EIDDs, denoted 1 and 2, are generated from the same marked point process [which results in the same statistically homogeneous \( f_{y,n}^e(v,r|x;t) \)], they will have the same second-order properties for the point process in physical space. Now if the individual component EIDDs satisfy \( \theta_1(x;t) \leq \theta_{\text{lin}} \) and \( \theta_2(x;t) \leq \theta_{\text{lin}} \) individually, and if the composite EIDD satisfies \( \theta_1 + \theta_2(x;t) \leq \theta_{\text{lin}} \), then we can expect \( \sum_{n \geq 1} |p_n(t) \times \sum_{i=1}^{n} A_{ki}(f_i^e(x,v,r,t)) \) for the composite EIDD to be the sum of \( \sum_{n \geq 1} |p_n(t) \times \sum_{i=1}^{n} A_{ki}(f_i^e(x,v,r,t)) \) of the component EIDDs. However, if \( f_{y,n}^e(v,r|x;t) \) is not the same for both component EIDDs, then even if they have the same underlying point process in physical space, the superposition principle fails. Of course, if the EIDDs are drawn from different point process models in physical space, their second-order (two-particle) statistics will in general be different [and may no longer satisfy the weak-interaction condition, and hence the linearity condition as characterized by \( \theta(x;t) \leq \theta_{\text{lin}} \), and the superposition principle is not guaranteed to hold for the composite EIDD. Since sprays are not necessarily EIDDs, it is easy to see why the superposition principle fails to hold for sprays in general.

The extension of linear models to sprays with statistically inhomogeneous \( f_{y,n}^e(v,r|x;t) \) will be an important and challenging area of research in ddf modeling of sprays.

3. Other issues in modeling the unclosed terms

In order to construct accurate physical models for \( \langle A_4(x,v,r,t) \rangle \) and \( \langle \Theta(x,v,r,t) \rangle \) in complex flows, it is first necessary to understand their behavior in simple canonical flows. Such information for modeling is usually available either from carefully controlled experiments, or from DNS. In the case of sprays it is difficult to accurately measure these unclosed terms in experiments, and controlling droplet parameters can also pose significant difficulties. On the other hand, in a DNS study of ensembles of identically distributed droplets in turbulent flow, parameters such as average liquid volume fraction or the initial radius pdf can be controlled. Therefore, advances in modeling may be anticipated from DNS of ensembles of identically distributed droplets. However, further study is needed in this area since there are unresolved issues concerning the validity of DNS initialized on the basis of single-point statistics, as well as the correct interpretation of such DNS results.11 It is important to note however, that any such DNS must actually calculate the drag on each droplet by solving the Navier–Stokes equations, and not assume any coupling models between the gas-phase and the droplets.

There are several difficulties associated with constructing accurate physical models for \( \langle A_4(x,v,r,t) \rangle \) and \( \langle \Theta(x,v,r,t) \rangle \). These unclosed terms depend on several physical parameters, as well as statistical descriptors of multiphase flow such as the average liquid volume density. Any model for these unclosed terms attempts to characterize their behavior in terms of a reduced set of parameters. The success of a model depends on a large extent on its ability to identify those parameters to which the unclosed terms are most sen-
sitive. Data from comprehensive tests of the sensitivity of the unclosed terms to all possible parameters of the problem is not yet available, but can be obtained by performing DNS of canonical multiphase flow problems. The task of modeling is made even more difficult by the fact that the sensitivity of the unclosed terms to problem parameters might change as the physical problem and its nondimensional flow parameters are changed.

In this section, some parameters that can be of importance in ddf modeling have been identified. However, in practical spray problems it is quite likely that parameters not identified in this study can also be important. Nevertheless, a rational approach to modeling requires that the influence of the parameters identified in this work be quantified and understood. A first step in this rational approach would be to determine the limit of the linear regime in terms of the average liquid volume density for the point process model described earlier in this section.

Another modeling issue is the loss of information associated with the ddf description of the spray. One of these has already been referred to, namely, the loss of information concerning the shape of the liquid elements. Another equally important issue is the loss of information arising from the decoupling of the two phases, and the validity of representing the influence of the spray droplets on the gas phase by the addition of source terms to the single-phase RANS equations. Further theoretical study is required to address the decoupling issue, and again DNS can be used to quantify the loss of information.

E. Particle method solution

In order to solve a general spray problem using the ddf approach, Eq. (34) for the modeled ddf is solved numerically with appropriate initial and boundary conditions on \( f^\# \), for a particular specification of the modeled terms \( A^\#_p \) and \( \Theta^\# \). This solution procedure is coupled to a gas-phase solver. The influence of the spray droplets on the gas phase is represented by the addition of source terms to the usual single-phase RANS equations.

The modeled ddf evolution equation [Eq. (34)] is a partial differential equation in a seven-dimensional space, whose direct solution by conventional finite-volume or finite-difference techniques is nontrivial, and computationally expensive. [Furthermore, if additional droplet properties, say \( p \) in number, need to be represented, then the modeled ddf evolution equation [Eq. (34)] is a partial differential equation in a \((7 + p)\)-dimensional space, and the computational cost is even greater.] For reasons of computational efficiency and ease of modeling, an alternative solution approach based on particle methods is commonly used to indirectly solve Eq. (34) in a computationally efficient manner. This solution approach is similar to particle methods used in the probability density function approach to modeling turbulent reactive flows, a thorough exposition of which is given by Pope.18 Most ddf-based spray codes are based on a particle method solution.

In a particle method solution of the modeled ddf evolution equation, an ensemble of \( N \) identically distributed computational particles is used to indirectly represent the modeled ddf \( f^\# \). With each computational particle \( i \) is associated a position vector \( \mathbf{X}^{(i)}_p \), velocity vector \( \mathbf{V}^{(i)}_p \), radius \( R^{(i)}_p \), and particle weight \( W^{(i)}_p \), such that the ensemble of computational particles approximates the modeled droplet distribution function \( f^\# \).

The properties associated with the \( i \)th computational particle evolve by a set of model evolution equations, an example of which is given by

\[
\frac{d\mathbf{X}^{(i)}_p}{dt} = \mathbf{V}^{(i)}_p , \tag{43}
\]

\[
\frac{d\mathbf{V}^{(i)}_p}{dt} = \mathbf{A}^{(i)}_p , \tag{44}
\]

\[
\frac{dR^{(i)}_p}{dt} = \mathbf{\Theta}^{(i)}_p , \tag{45}
\]

\[
\frac{dW^{(i)}_p}{dt} = \mathbf{\Omega}^{(i)}_p , \tag{46}
\]

where \( \mathbf{A}^{(i)}_p \) is the acceleration of the particle, \( \mathbf{\Theta}^{(i)}_p \) is the rate of change of particle radius due to vaporization, and \( \mathbf{\Omega}^{(i)}_p \) is the rate of change of particle weight.

Although particle methods are computationally efficient, they are an indirect solution to the modeled ddf evolution equation. Specification of the models \( \mathbf{A}^\#_p \) and \( \Theta^\# \) in the particle evolution equations implies a corresponding specification of the models \( A^\#_p \) and \( \Theta^\# \) for the unclosed terms in the modeled ddf equation [Eq. (34)], whose analytic form may or may not be derivable depending on the specifics of the particle model.

It is important to emphasize that the correspondence between computational particles and spray droplets is only at the level of the conditional expectations \( \langle A^\#_p | \mathbf{x}, \mathbf{v}, r, \tau \rangle \) and \( \langle \Theta^\# | \mathbf{x}, \mathbf{v}, r, \tau \rangle \). Computational particles in the particle method solution to the ddf are not representations of physical spray droplets, although this misidentification is widespread in the spray literature. A direct consequence of this observation is that there is no good reason to require that the properties of the computational particles evolve exactly like their droplet counterparts, i.e., Eqs. (43)–(45) need not evolve as Eqs. (1)–(3). In fact the assumption commonly encountered in many ddf-based spray models, namely, particle acceleration equals droplet acceleration, is as yet completely unjustified.

In Ref. 11 it is shown that the pdf resulting from the ddf is a weighted sum of surrogate-droplet pdf’s, where each surrogate-droplet pdf is in turn the arithmetic mean of the ensemble of corresponding single-droplet pdf’s. Therefore it is not merely desirable, but in fact necessary, to make a distinction between the particle acceleration \( \mathbf{A}^{(i)}_p \), and the droplet acceleration \( \mathbf{A}^{(i)}_p \), since they refer to different quantities that are not equal in general.

The principle of stochastic equivalence (see Pope19) tells us that two systems can evolve such that the individual realizations in each system are radically different, but the two may have identical mean values. Therefore, the system of computational particles can have different individual realizations from the physical droplets, and yet its implied condi-
tional expectation terms $A^*_e$ and $\Theta^*$ can match $\langle A_e | x, v, r; t \rangle$ and $\langle \Theta | x, v, r; t \rangle$. (The principle of stochastic equivalence also reveals that the mapping of particle models to $A^*_e$ and $\Theta^*$ is many-to-one, i.e., different particle models can result in the same $A^*_e$ and $\Theta^*$.) A direct corollary of the stochastic equivalence principle is that in addition to deterministic particle evolution models, one can also use stochastic particle models with random terms for the particle property evolution equations [Eqs. (43)–(46)]. (However, additional terms will appear in the modeled ddf evolution implied by such particle models.) Regardless of the nature of the modeled terms (deterministic or stochastic), particle methods can be employed to solve the modeled ddf evolution equation. The term “stochastic spray model” is an unfortunate misnomer attached to particle method solutions of the modeled ddf equation.

F. Summary

In this section the spray equation was derived and the unclosed terms identified. The regime of validity of the spray equation was established. Modeling issues were discussed and the commonly used particle method solution approach to the modeled ddf evolution equation was briefly described. In the next section certain properties of the ddf are explained with a view to establishing the basis for meaningful comparison of ddf model predictions to experimental measurements of spray properties.

III. THE DROPLET DISTRIBUTION FUNCTION

In this section some important properties of the droplet distribution function are described. The definition of the ddf given in Eq. (8) enables us to understand which statistical properties of the spray it characterizes. It is also shown at the end of this section that the ddf can be expressed as the product of two quantities: the intensity (or density of expected number of spray droplets in physical space), and the jpdf of velocity and radius conditioned on physical location. This “disintegration” of the ddf is useful in deriving an evolution equation for the intensity, which is the subject of the next section.

A technical detail which is important in the context of vaporizing sprays needs to be clarified at the outset to avoid ambiguities. The term “spray” or “spray droplets” is only used in reference to the dispersed phase (the nongaseous phase, typically the liquid phase) of the multiphase system. While this may seem to be an obvious fact, it is the root cause of prevailing ambiguity concerning the definition of the density of expected number of droplets in physical space, and its evolution equation which is derived in the following section. If the term “spray” refers only to the dispersed phase, this then implies that only the behavior of the ddf $f(x, v, r, t)$ in the domain of phase space defined by $r > 0$ characterizes the statistics of the spray droplets. This simply means that the behavior of the function $f(x, v, r, t)$ for $r \leq 0$ says nothing about the spray droplets, since by definition any “droplet” with radius $r \leq 0$ no longer belongs to the spray system. See Fig. 1. The behavior of $f(x, v, r, t)$ for $r \leq 0$ can be related to the interphase transfer terms which arise in the pdf description of multiphase flows.

For convenience of notation, we denote $r_+$ to be the positive $r$ axis ($r > 0$). All spray statistics associated with the ddf can be expressed as integrals (over $[v, r_+]$ space) of the ddf $f(x, v, r, t)$. Requiring that the spray system be represented by the ddf $f(x, v, r, t)$ only for $r > 0$ is also consistent with particle method solutions to the spray equation (where “droplets” with $r \leq 0$ are not represented). Consequently, the equations arising from this requirement are not only physically meaningful, but are also useful in analyzing particle method solutions.

In Williams, the ddf $f$ is defined such that

$$f(x, v, r, t)dx dv dr$$

is called the probable number of spray droplets with positions in the interval $(x, x + dx)$, velocities in the interval $(v, v + dv)$, and radii in the interval $(r, r + dr)$ at time $t$. The term “probable number of droplets” in Williams’ definition of the ddf can now be interpreted in light of the definition of the ddf given by Eq. (8). It was shown in the preceding section that the number of droplets in any region in phase space is obtained by integrating $f'$ over that region [cf. Eq. (7)]. The ddf is defined to be the ensemble average of $f'$ [Eq. (8)]. Therefore it follows that if the expected number of droplets in a region $B_+$ of $[x, v, r_+]$ space is denoted $\langle N(B_+; t) \rangle$, it is obtained by integrating the ddf $f(x, v, r, t)$ over the region $B_+$ such that

$$\langle N(B_+; t) \rangle = \int_{B_+} f(x, v, r, t) dx dv dr.$$  \hspace{1cm} (47)

Therefore the term “probable number of droplets” in a region $B_+$ can be interpreted as denoting the expected number of droplets $\langle N(B_+; t) \rangle$ in that region.
If \( \langle N_s(t) \rangle \) represents the expected total number of spray droplets at time \( t \), then the droplet distribution function \( f(x,v,r,t) \) when integrated over the entire \( [x,v,r] \) space, must yield \( \langle N_s(t) \rangle \), such that

\[
\int_{[x,v,r]} f(x,v,r,t) \, dx \, dv \, dr = \langle N_s(t) \rangle.
\]

(48)

It is noteworthy that \( f \) does not possess the normalization property of a probability density function, since it does not integrate to unity over the space on which it is defined.

If the droplet distribution function is integrated over only \( [v,r] \) space, the density (in physical space) of the expected number of spray droplets \( n_s(x;t) \) is obtained:

\[
n_s(x;t) = \int_{[v,r]} f(x,v,r,t) \, dv \, dr.
\]

(49)

We denote the integral of this density over a region \( A \) in physical space by the quantity

\[
\langle N_s(A;t) \rangle = \int_A n_s(x;t) \, dx.
\]

(50)

where \( \langle N_s(A;t) \rangle \) represents the expected number of droplets in the region \( A \) in physical space.

It is shown in this paper that the ddf approach models the spray as a marked point process. \(^{13} \) The mathematical basis for this modeling approach is given in Appendix B. In the theory of point processes \( \langle N_s(A;t) \rangle \) is referred to as the mean measure of the point process in physical space. The density of the mean measure \( n_s(x;t) \), when it exists, is referred to as the intensity of a point process. If the spray is modeled as a marked point process, then the ddf can be expressed as the product of the intensity of the point process in physical space, and the jpdf of velocity and radius conditioned on physical location.

The jpdf of velocity and radius conditioned on physical location \( f_{VR}(v,r|x,t) \), is expressed in terms of the ddf as

\[
f_{VR}(v,r|x,t) = \begin{cases} f(x,v,r,t)n_s(x;t) & \text{if } r > 0, \\ 0 & \text{if } r \leq 0. \end{cases}
\]

(50)

(The reason why this conditional jpdf is not called an Eulerian jpdf is given in Ref. 11.) In the notation used for the conditional jpdf \( f_{VR}(v,r|x,t) \), variables such as \( v, r, \) and \( x \), which appear to the left of the semicolon in the argument list are measure space variables. (The reason why it is not appropriate to denote these as sample space variables is given in Ref. 11.) Variables such as \( t \), which appear to the right of the semicolon in the argument list, are parameter variables. Among the list of measure space variables, the variable \( x \) appears to the right of the vertical line \( | \) since it is the conditioning variable, and the superscript \( c \) serves to remind us that \( f_{VR}(v,r|x,t) \) is a conditional jpdf. In subsequent sections, for simplicity the adjective “conditional” is omitted when referring to \( f_{VR}(v,r|x,t) \), and it is understood that conditioning on \( x \) is implied by the superscript \( c \).

The theory of point processes shows that under certain conditions (detailed in Appendix B), \( f_{VR}(v,r|x,t) \) is the density of a probability measure. If \( f_{VR}(v,r|x,t) \) is integrated over \( [v,r] \) space it yields unity, and this is confirmed by Eqs. (50) and (49). It will be shown later that \( f_{VR}(v,r|x,t) \) obeys a conservative equation, and hence retains its unit normalization property for all time.

If \( Q_s \) is some smooth function of velocity and radius, then the mean field of \( Q_s \) is simply given by

\[
\langle Q_s(x;t) \rangle = \int_{[v,r]} Q_s(v,r)f_{VR}(v,r|x,t) \, dv \, dr.
\]

(51)

The mean field given by Eq. (51) is a useful mathematical idealization, but is inaccessible to experimental measurement since these measurements are necessarily made over some finite volume in physical space. However, experimental measurements can be related to the number-weighted mean of \( Q_s \) over a region \( A \) in physical space, which is denoted \( \langle Q_s(A;t) \rangle \), and is defined as

\[
\langle Q_s(A;t) \rangle = \frac{1}{\langle N_s(A;t) \rangle} \int_A n_s(x;t) \langle Q_s(x;t) \rangle \, dx.
\]

(52)

The global number-weighted mean of \( Q_s \) is denoted \( \langle Q_s(t) \rangle \), and is defined as

\[
\langle Q_s(t) \rangle = \frac{1}{\langle N_s(t) \rangle} \int_x n_s(x;t) \langle Q_s(x;t) \rangle \, dx.
\]

(53)

Using the definition of \( f_{VR}(v,r|x,t) \) in Eq. (50), the ddf can be written as the product of two quantities—namely, the intensity (or the density of expected number of spray droplets in physical space), and the jpdf of velocity and radius conditioned on physical location—such that

\[
f(x,v,r,t) = n_s(x;t)f_{VR}(v,r|x,t), \quad r > 0.
\]

(54)

IV. EVOLUTION OF THE SPRAY INTENSITY

Starting from the definition of the spray intensity \( n_s(x;t) \) given in Eq. (49), its temporal evolution may be written as

\[
\frac{\partial n_s(x;t)}{\partial t} + \frac{\partial}{\partial x} \int_{[v,r]} f(x,v,r,t) \, dv \, dr = \int_{[v,r]} \frac{\partial f}{\partial t} \, dv \, dr,
\]

(55)

where the differentiation with respect to time can be taken inside the integral sign since the measure space variables \( v \) and \( r \) are independent of \( t \).

Substituting for \( \partial f/\partial t \) from Eq. (33) and carrying out the required integrations results in the following evolution equation for the intensity \( n_s(x;t) \):

\[
\frac{\partial n_s(x;t)}{\partial t} + \frac{\partial}{\partial x} \left[ \langle V_k(x;t) \rangle n_s(x;t) \right] = \langle \Theta(x,r=0+) \rangle f_{DR}(r=0+) f_{VR}(v=0;\cdot) n_s(x;t).
\]

(56)

The detailed derivation of the final form of Eq. (56) starting from the ddf evolution equation Eq. (33), is given in Appendix C. The second term on the left-hand side of the above equation represents the transport of \( n_s(x;t) \) in physical space by the mean velocity at that physical location \( \langle V_k(x;t) \rangle \) which is defined as

\[
\langle V_k(x;t) \rangle = \int_{[v,r]} v \, f_{VR}(v,r|x;t) \, dv \, dr.
\]

(57)
The term on the right-hand side represents a sink in the density (in physical space) of expected number of droplets due to vaporization, and it appears because there is a finite flux of $f$ across the $r=0^+$ boundary in phase space. See Fig. 1. Since spray properties are characterized by $f(x,v,r,t)$ in $[x,v,r,\tau]$ space, the appearance of the sink term is consistent with our definitions, as well as with physical reality, that the density of the expected number of droplets in physical space must decrease for a vaporizing spray.

Previous derivations of the evolution equation for the density of expected number of droplets in physical space differ from Eq. (56) in that they have no sink term. The absence of this sink term implies a conservation of the expected total number of droplets (which is obtained by integrating the intensity over all physical space), and the intensity equation without the sink term closely resembles the mass conservation equation for the mass density of fluid flow. The only way to interpret the previously derived “conservative” equation for the density of expected number of droplets in physical space is to admit “droplets” of zero radius—which is neither physically realistic nor useful in understanding particle method solutions of the ddf equation. See Fig. 1. Furthermore, if one considers a complete representation of two-phase flows the interpretation based on “droplets” of zero radius is inadmissible—for now these “droplets” with zero radius are in the vapor phase and should be accounted for in the interphase transfer term.

In the sink term on the right-hand side of Eq. (56), the first factor $(\Theta|r=0^+,x,t)$ is the expected vaporization rate conditional on radius (and physical location $x$), evaluated at $r=0^+$, i.e.,

$$\Theta|r=0^+,x,t = [(\Theta|r,x,t)]_{r=0^+}.\]$$

The second factor $f_R^s(r=0^+|x,t)$ is the radius pdf, also evaluated at $r=0^+$, and the third factor is the intensity itself.

It is useful to consider a limiting case to understand the role played by each of these factors in the sink term. Consider an ensemble of immobile, vaporizing droplets which implies that $\langle V_R(x,t)\rangle$ is zero. The role of the conditionally expected vaporization rate $\langle\Theta|r=0^+,x,t\rangle$ is elucidated by the following example. Even if both the intensity field and the radius pdf are initially uniform in physical space (i.e., the ensemble of spray droplets is initially statistically homogeneous), a spatially nonuniform mean gas temperature field $\langle T_g(x,t)\rangle$ can generate spatial inhomogeneities in the intensity field at future time. This effect will manifest itself in the intensity equation if the conditionally expected vaporization rate is modeled as a function of the mean gas temperature at a given physical location, e.g.,

Unclosed \textit{term} Model

$$\Theta^s[(T_g(x,t)),r].$$

Since the mean gas temperature field is spatially nonuniform, this will result in a spatially inhomogeneously conditionally expected vaporization rate term. It is noteworthy that previous derivations of the intensity equation, which have no sink term and imply a conservation of the expected total number of droplets, are incapable of reproducing this important physical phenomenon.

V. EVOLUTION OF GLOBAL SPRAY PROPERTIES

The evolution of global spray properties, such as the expected total number of spray droplets $\langle N_s(t)\rangle$, and the expected total mass of the spray droplets $\langle M_s(t)\rangle$, as implied by the ddf evolution equation are now derived. First the evolution of the expected total number of spray droplets $\langle N_s(t)\rangle$ is derived from its definition in terms of the ddf [Eq. (48)] and the ddf evolution equation [Eq. (33)] given in the preceding section. Differentiating Eq. (48) with respect to time results in

$$\frac{\partial}{\partial t}\langle N_s(t)\rangle = \frac{\partial}{\partial t}\int_{[x,v,r,\tau]} f(x,v,r,t)dx\,dv\,dr$$

$$= \int_{[x,v,r,\tau]} \frac{\partial f}{\partial t} dx\,dv\,dr, \quad (58)$$

where the differentiation with respect to time can be taken inside the integral sign since both $x$, as well as the measure space variables $v$ and $r$, are independent of $t$.

Substituting for $\partial f/\partial t$ from Eq. (33) and carrying out the required integrations (see Appendix D for details) results in the following evolution equation for the expected total number of spray droplets:

$$\frac{\partial}{\partial t}\langle N_s(t)\rangle = -\int_{\mathcal{R}} \frac{\partial}{\partial r} \left[(V_R(x,t))n_s(x,t)\right]dx$$

$$+ \langle\Theta|r=0^+,t\rangle f_R^s(r=0^+,t) \langle N_s(t)\rangle. \quad (59)$$

The divergence theorem shows that the first term on the right-hand side of the above equation is simply the net flux of expected number of droplets into $\mathcal{R}$ (the flow domain in physical space), and the second term is defined by the relation

$$\langle\Theta|r=0^+,t\rangle f_R^s(r=0^+,t)$$

$$= \frac{1}{\langle N_s(t)\rangle} \int_{\mathcal{R}} \langle\Theta|r=0^+,x,t\rangle f_R^s(r=0^+,x,t) n_s(x,t) \, dx, \quad (60)$$

where the overbar represents the fact that the quantity has been weighted by the intensity $n_s(x,t)$.

The total expected spray mass $\langle M_s(t)\rangle$ is defined as

$$\langle M_s(t)\rangle = \int_{[x,v,r,\tau]} \frac{4}{3} \pi r^3 \rho_s f(x,v,r,t) \, dx \, dv \, dr, \quad (61)$$

where $\rho_s$ is the liquid density. Using the disintegration of the ddf in terms of the intensity and the pdf of velocity and radius, the total expected spray mass may also be written as

$$\langle M_s(t)\rangle = \int_{[x,v,r,\tau]} n_s(x,t) m_s(x,t) \, dx, \quad (62)$$

where $m_s(x,t)$ is the mean mass field as a function of physical space, and is given by the relation

$$m_s(x,t) = \int_{[v,r,\tau]} \frac{4}{3} \pi r^3 \rho_s f_R^s(v,r|x,t) \, dv \, dr. \quad (63)$$

The evolution of the expected total spray mass as implied by the ddf evolution is
\[
\frac{\partial \langle M_s(t) \rangle}{\partial t} = -\frac{4}{3} \pi \rho_l \int \left( \frac{\partial}{\partial x_k} \left\{ (R^2 V_k(x,t)) n_s(x,t) \right\} \right) \, dx \\
+ \langle N_s(t) \rangle + \frac{4}{3} \pi \rho_l \left( \langle R^4 \Theta \rangle_{r=0+} \right) f^c_{VR}(r=0+) \\
+ 3 \langle R^4 \Theta(t) \rangle,
\]
where
\[
\langle R^4 \Theta(x;t) \rangle = \int_{[r,r_\text{+}]} I^{\text{E}}(\Theta|x,v,r;t) f_{VR}(v,r|x;t) \, dv \, dr,
\]
and the overbar represents intensity-weighted global averages as in Eq. (60). In Eq. (64), the first term on the right-hand side represents the net flux of expected mass of droplets into the flow domain \( R \), the first term in braces on the right-hand side represents the change in the expected total mass of spray droplets due to the flux of the ddf across the \( r=0+ \) boundary (corresponding to the vaporization sink term in the intensity evolution equation), and the second term represents the change arising from the evolution of the mean volume field (corresponding to the radius evolution equation).

VI. EVOLUTION OF THE VELOCITY-RADIUS PDF

Starting from the definition of the jpdf given in Eq. (50), and substituting the evolution equations for the ddf [Eq. (33)] and the intensity [Eq. (56)], results in the following evolution equation for \( f_{VR}(v,r|x;t) \):
\[
\frac{\partial f_{VR}(v,r|x;t)}{\partial t} + \frac{\partial}{\partial x_k} \left[ v_k f_{VR}(v,r|x;t) \right] \\
+ \frac{\partial}{\partial v_k} \left[ \langle A_k|x,v,r,t \rangle f_{VR}(v,r|x;t) \right] \\
+ \frac{\partial}{\partial r} \left[ \langle \Theta|x,v,r,t \rangle f_{VR}(v,r|x;t) \right] \\
= f_{VR}(v,r|x;t) \left\{ \frac{\partial \ln n_s(x,t)}{\partial x_k} \left( V_k(x,t) - v_k \right) \right\} \\
+ f_{VR}(v,r|x;t) \frac{\partial \langle V_k(x,t) \rangle}{\partial x_k} \\
- f_{VR}(v,r|x;t) \langle \Theta \rangle_{r=0+} f^c_{VR}(r=0+) |x;t|.
\]
The terms on the left-hand side of Eq. (65) represent the temporal evolution term and the transport of \( f_{VR}(v,r|x;t) \) in physical, velocity, and radius space, respectively.

A convenient simplification of the right-hand side terms, which is obtained by substituting Eq. (56), enables Eq. (65) to be rewritten as
\[
\frac{\partial f_{VR}(v,r|x;t)}{\partial t} + \frac{\partial}{\partial x_k} \left[ v_k f_{VR}(v,r|x;t) \right] + \frac{\partial}{\partial v_k} [\langle A_k|x,v,r,t \rangle f_{VR}] \\
+ \frac{\partial}{\partial r} [\langle \Theta|x,v,r,t \rangle f_{VR}] \\
= -f_{VR} \frac{D \ln n_s(x,t)}{Dt}.
\]
where
\[
\frac{D \ln n_s(x,t)}{Dt} = \frac{\partial \ln n_s(x,t)}{\partial t} + v_k \frac{\partial \ln n_s(x,t)}{\partial x_k}.
\]

Both forms of the velocity-radius jpdf evolution [Eqs. (65) and (66)] preserve the normalization property of \( f_{VR}(v,r|x;t) \) for all time, i.e.,
\[
\int_{[v,r_\text{+}]} \frac{\partial f_{VR}(v,r|x;t)}{\partial t} \, dv \, dr = 0.
\]
See Appendix E for details. The right-hand side in Eq. (66) represents the source term in the jpdf evolution equation that is necessary to preserve the jpdf’s normalization property at all time.

VII. NUMERICAL CONVERGENCE ISSUES

When using a numerical implementation of a ddf-based spray model to simulate a spray problem, it is important to ensure that the results are numerically converged. It has already been noted that difficulties in obtaining numerically converged results using the KIVA spray model have partly motivated this study. In this section some of the numerical resolution requirements imposed by the coupled spray-gas equation system are investigated. The numerical requirements associated with the number of computational particles are specifically not considered in this work because even the convergence of the particle method solution to the spray equation has not been rigorously established. Therefore, only the numerical parameters associated with the space-time grid are considered here.

In spray computations it is useful to distinguish between two types of convergence: strong convergence, which guarantees pointwise convergence of the coupled spray-gas equation system in physical space; and weak convergence, which ensures convergence of number-weighted mean quantities integrated over a volume of physical space. It is hypothesized that the resolution requirements imposed by the weak convergence criterion are likely to be far less computationally demanding than those arising from the requirement of strong convergence. Furthermore, satisfying the weak convergence criterion is sufficient for most engineering calculations. Methods to test weak convergence are outlined, which should provide useful guidelines to users of ddf-based spray models.

A. Strong convergence

Obtaining a solution to a ddf-based spray model involves solving the coupled spray-gas equation system. If \( \langle Q_g(x,t) \rangle \) represents a mean gas-phase quantity that is solved by the RANS solver, its evolution equation can be cast in the generic form
\[
\frac{\partial \langle Q_g(x,t) \rangle}{\partial t} = \langle \dot{R}_g(x,t) \rangle + \langle \bar{R}_g(x,t) \rangle,
\]
where \( \langle \dot{R}_g(x,t) \rangle \) is the mean source term arising from the gas-phase terms in the evolution equation for \( \langle Q_g \rangle \), and \( \langle \bar{R}_g(x,t) \rangle \) is the mean source term arising from the spray
pressed in terms of these length scales as

The minimum spatial resolution requirement can be ex-

However, the strong convergence requirement is very likely

the computational capabilities of today’s supercomputers.

calculations, while also being easier to satisfy using modest

proposed, which is more likely to be useful for engineering

mean spray source terms

variation of the ddf

The theory of stochastic point processes is used to estab-

is the volume

spray source terms is denoted $l_g(x)$, and is defined as the minimum (over all mean gas-phase flow quantities and over all time) of the length scales $l_g(R_g(x,t))$ associated with each source term arising from the gas-phase, such that

There are two length scales that can be associated with

the spray. The first length scale characterizes the scale of

variation of the ddf $f(x,v,r,t)$ and is denoted $l_g(x)$. The

second length scale characterizes the scale of variation of the

mean spray source terms $\langle R_g(x,t) \rangle$. It is denoted $l_s(x)$, and

may be defined as the minimum (over all mean spray source

terms and over all time) of the length scales associated with

each mean spray source term, such that

The minimum spatial resolution requirement can be ex-

pressed in terms of these length scales as

$h_m(x) \leq \min\{l_g(x), l_s(x), l_f(x)\}$.

Numerical convergence studies show that this resolu-
tion requirement is onerous, and satisfying this requirement
for realistic three-dimensional engine calculations is beyond
the computational capabilities of today’s supercomputers.

However, the strong convergence requirement is very likely

not necessary (although sufficient) for the purposes of engi-

neering calculations. An interesting observation is that even

if pointwise convergent solutions are generated, these could

not be directly compared to experimental measurements,

since pointwise experimental measurements of the intensity

or the velocity-radius jpdf (or moments thereof) are impos-

sible. Therefore, a different criterion for convergence is now

proposed, which is more likely to be useful for engineering

calculations, while also being easier to satisfy using modest

computational resources.

B. Weak convergence

In engineering calculations of sprays we are usually in-

terested in number-weighted mean spray properties which

are obtained by integrating the intensity-weighted mean

spray property over some volume in physical space. A spray

property is some smooth function $Q_s(x,v)$ of the droplet

properties. If $Q_s$ is the spray property, and $V_m$ is the volume

in physical space corresponding to a region $R_m$, then the

number-weighted mean spray property $\langle Q_s(R_m) \rangle$ is writ-

ten as

\[ \langle Q_s(R_m) \rangle = \frac{1}{n_s(R_m)} \int_{R_m} n_s(x,t) Q_s(x,t) \, dx. \]  

Similarly the mean gas-phase flow fields can be integrated

over the same volume to obtain

\[ \langle Q_g(R_m) \rangle = \int_{R_m} Q_g(x,t) \, dx. \]  

The weak convergence criterion requires that for a specified

set of volumes $V_m(x,k=1,\ldots,K)$, a specified set of spray

properties $\{\langle Q_s(R_m) \rangle\}$, and a specified set of gas-

phase flow quantities $\{\langle Q_g(R_m) \rangle\}$ converge with respect to

numerical parameters associated with the space-time grid.

Note that the specified set of spray properties does not nec-

essarily have to include the spray source terms. Since the

weak convergence criterion depends on a characteristic vol-

ume parameter $V_m$, there exists a continuous family of con-

vergence criteria indexed by this parameter.

The upper limit of the volume parameter $V_m$ is of course

the entire physical volume occupied by the system. This cor-

responds to the minimal requirement expressed by the weak

convergence criterion. When the number-weighted mean

spray property $\langle Q_s(R_m) \rangle$ is evaluated at the upper limit of

$V_m$ (over the entire physical volume), it represents a global

spray property such as the expected total mass of the spray

droplets. One of the minimal requirements expressed by the

weak convergence criterion is that the global spray properties

such as the expected total number of droplets $\langle N_s(t) \rangle$, and

the expected total mass of the spray droplets $\langle M_s(t) \rangle$, should

be numerically converged.

At the lower limit the volume $V_m$ could be the measure-

ment volume associated with a measurement technique. In

the limit of infinitesimal $V_m$, the weak convergence require-

ment becomes identical to the strong convergence require-

ment. In general, while strong convergence implies weak

convergence, the converse is not true. For finite $V_m$, the

weak convergence criterion does not guarantee that the

coupled spray-gas equation system is pointwise numerically

converged. The choice of the volume parameter $V_m$ will de-

pend on the application, the length scales associated with the

measurement volume (if comparisons with experiments are

desired), and the available computational resources.

VIII. SUMMARY AND CONCLUSIONS

The theoretical foundations of the droplet distribution

function approach to spray modeling are established. The

evolution of the ddf is derived from first principles using a

novel approach. It is shown that the ddf is the density of

expected number of droplets in phase space.

The theory of stochastic point processes is used to estab-

lish the existence of a disintegration of the ddf in terms of a

spray intensity, which is the density in physical space of the

expected number of spray droplets, and the joint pdf of ve-

locity and radius conditional on physical location. The evo-


dr. This system of gas-phase equations has to be solved

in conjunction with the ddf evolution equation [Eq. (33)] in

which models for the conditionally expected acceleration and

vaporization rate have been specified. Each mean source

term in this coupled equation system has a characteristic

length scale and time scale associated with it. In order to

obtain numerically converged solutions the space-time grid

must to be fine enough to resolve the smallest characteristic

scales.

For example, the minimum requirements on the spatial

grid resolution $h_m(x)$ imposed by these characteristic scales

can be estimated as follows. The characteristic length scale

associated with the gas phase source terms is denoted $l_g(x)$,
olution equation of the spray intensity and the conditional jpdf of velocity and radius, as implied by the ddf evolution equation, are derived.

The intensity equation derived in this study contains a sink term that is absent in other works, and which is essential to represent inhomogeneities that arise as a result of a spatially inhomogeneous mean gas temperature field. Criteria for establishing numerical convergence of computed solutions to the ddf equation are proposed, which should be useful in evaluating the convergence properties of ddf-based computational models of sprays. The study also provides insight into what constitutes a meaningful comparison of ddf model predictions with experimental data.

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APPENDIX A: DETAILS OF THE SPRAY EQUATION DERIVATION

1. Evolution equation for \( f^{(n)} \) when \( p_n \) is constant

Differentiating Eq. (6) with respect to time results in

\[
\frac{\partial f^{(n)}_i}{\partial t} = \left[ -V_{ki}(t) \frac{\partial}{\partial x_k} \left[ \delta(x-X_{ki}(t)) \delta(v-V_{ki}(t)) \delta(r-R_{ki}(t)) \right] \right. \\
- A_{ki}(t) \frac{\partial}{\partial x_k} \left[ \delta(x-X_{ki}(t)) \delta(v-V_{ki}(t)) \delta(r-R_{ki}(t)) \right] \\
- \Theta_{ki}(t) \frac{\partial}{\partial r} \left[ \delta(x-X_{ki}(t)) \delta(v-V_{ki}(t)) \delta(r-R_{ki}(t)) \right].
\]  
(A1)

where \( V_{ki}(t) \) represents the velocity of the \( i \)th droplet along Cartesian coordinate \( k \), \( A_{ki}(t) \) represents the acceleration of the \( i \)th droplet along Cartesian coordinate \( k \), and we have used the chain rule and the following identity:

\[
\frac{\partial}{\partial a} f(a-b) = -\frac{\partial}{\partial b} f(a-b).
\]

Then substituting the relation

\[
a \cdot \delta(a-b) = b \cdot \delta(a-b),
\]

leads to

\[
\frac{\partial f^{(n)}_i}{\partial t} = -V_{ki}(t) \frac{\partial}{\partial x_k} \left[ f^{(n)}_i \right] - A_{ki}(t) \delta(x-X_{ki}(t)) \delta(v-V_{ki}(t)) \delta(r-R_{ki}(t)) \\
\times \left[ \frac{\partial}{\partial r} \Theta_{ki}(t) \delta(x-X_{ki}(t)) + \frac{\partial}{\partial r} \left[ \Theta_{ki}(t) \delta(x-X_{ki}(t)) \right] \\
\times \delta(v-V_{ki}(t)) \delta(r-R_{ki}(t)) \right].
\]  
(A2)

Starting from the definition of \( f^{(n)} \) and differentiating it with respect to time we have

\[
\frac{\partial f^{(n)}}{\partial t} = \frac{\partial}{\partial t} \left( \sum_{i=1}^{n} f_i^{(n)} \right) = \sum_{i=1}^{n} \frac{\partial f_i^{(n)}}{\partial t},
\]  
(A3)

where it should be noted that the droplets are still not assumed to be identically distributed. Substituting Eq. (A2), into the above equation, and taking the derivatives with respect to the phase-space variables outside the summation sign for each term results in

\[
\frac{\partial f^{(n)}}{\partial t} = -\frac{\partial}{\partial x_k} \left[ V_k f^{(n)} \right] - \frac{\partial}{\partial v_k} \left[ \sum_{i=1}^{n} A_{ki}(t) f_i^{(n)}(x,v,r,t) \right] \\
- \frac{\partial}{\partial r} \left[ \sum_{i=1}^{n} \Theta_{ki}(t) f_i^{(n)}(x,v,r,t) \right].
\]  
(A4)

2. Change in \( p_n(t) \) due to vaporization

We now derive the expression for \( \delta p_n(t) \) when \( p_n(t) \) changes only due to vaporization. The change in \( p_n(t) \) is related to \( f^{(n)}(x,v,r,t) \) since the two do not evolve independently of each other. In fact, since in the class of spray problems under consideration the only way \( p_n(t) \) can evolve in time is if there is a nonzero flux of \( f^{(n)} \) across the boundaries of phase space, we can relate \( \delta p_n(t) \) to the boundary flux of \( f^{(n)} \) as follows:

\[
\delta p_n(t) = -p_n(t) \int \frac{\partial}{\partial r} \left[ \left\langle \Theta^{(n)} \right\rangle(x,v,r,t) f^{(n)}(x,v,r,t) \right] dx dv dr dt.
\]  
(A5)

If there is no inflow/outflow and \( p_n(t) \) changes only due to vaporization, then \( \delta p_n(t) \) is related to the outward flux of \( f^{(n)} \) across the \( r = 0 \) boundary of phase space as follows:

\[
\delta p_n(t) = p_n(t) \left\langle \Theta^{(n)} \right\rangle(r = 0) f^{(n)}(r = 0) dt.
\]  
(A6)

Note that for vaporization \( \left\langle \Theta^{(n)} \right\rangle(r = 0) \) is a negative quantity. Therefore vaporization results in a decrease in \( p_n(t) \).

3. Vaporization source term

Now require that \( f^{(n)} \) be conserved since it must always integrate to \( n \) over phase space:

\[
\int_{[x,x,r,r]} \frac{\partial f^{(n)}}{\partial t} dx dv dr dt = 0.
\]  
(A7)

This necessitates the addition of a source term in the evolution equation of \( f^{(n)} \) such that we have

\[
\frac{\partial f^{(n)}}{\partial t} + \frac{\partial}{\partial x_k} \left[ V_k f^{(n)} \right] + \frac{\partial}{\partial v_k} \left[ \left\langle A^{(n)}_k \right\rangle(x,v,r,t) f^{(n)} \right] \\
= -\frac{\partial}{\partial r} \left[ \left\langle \Theta^{(n)} \right\rangle(x,v,r,t) f^{(n)}(r=0) + S^{(n)}_v(x,v,r,t) \right].
\]  
(A8)

The source term \( S^{(n)}_v(x,v,r,t) \) arises as a result of vaporization. Since the physical interpretation of the vaporization source term is that it is the rescaling of \( f^{(n)}(x,v,r,t) \) to account for the nonzero boundary flux, it must be proportional to \( f^{(n)} \), and of the form

\[
S^{(n)}_v(x,v,r,t) = S^{(n)}_v(t) f^{(n)}(x,v,r,t).
\]  
(A9)

Applying the integral constraint of Eq. (A7) reveals that

\[
S^{(n)}_v(t) = -\left\langle \Theta^{(n)} \right\rangle(r=0) f^{(n)}(r=0) dt.
\]  
(A10)
4. Change in \( p_n(t) \) due to inflow/outflow

We now derive the expression for \( \delta p_n(t) \) when \( p_n(t) \) changes only due to inflow or outflow of droplets at the boundary \( \mathcal{S} \) of the flow domain \( \mathcal{R} \) in physical space. We can relate \( \delta p_n(t) \) to the boundary flux of \( f^{(n)} \) as follows:

\[
\delta p_n(t) = -p_n(t) \int_{[x,v,r]} \frac{\partial}{\partial x_k} [v J f^{(n)}] d\mathbf{x} d\mathbf{v} dr \delta t. \tag{A11}
\]

5. Inflow/outflow source term

The requirement that \( f^{(n)} \) be conserved necessitates the addition of a source term in the evolution equation of \( f^{(n)} \) such that we have

\[
\frac{\partial f^{(n)}}{\partial t} + \frac{\partial}{\partial x_k} (A_{k}^{(n)} | \mathbf{x}, \mathbf{v}, r, t) f^{(n)} + \frac{\partial}{\partial r} (\Theta^{(n)} | \mathbf{x}, \mathbf{v}, r, t) f^{(n)} = - \frac{\partial}{\partial x_k} [v J f^{(n)}] + S_{io}^{(n)} (\mathbf{x}, \mathbf{v}, r, t). \tag{A12}
\]

The source term \( S_{io}^{(n)} (\mathbf{x}, \mathbf{v}, r, t) \) arises as a result of inflow and outflow of droplets to or from the flow domain in physical space. Since the physical interpretation of the inflow/outflow source term is that it is the rescaling of \( f^{(n)}(\mathbf{x}, \mathbf{v}, r, t) \), it must be proportional to \( f^{(n)} \), and of the form

\[
S_{io}^{(n)} (\mathbf{x}, \mathbf{v}, r, t) = S_{io}^{(n)} (t) f^{(n)}(\mathbf{x}, \mathbf{v}, r, t). \tag{A13}
\]

Applying the integral constraint of Eq. (A7) reveals that

\[
S_{io}^{(n)} (t) = \int_{[x,v,r]} \frac{\partial}{\partial x_k} [v J f^{(n)}] d\mathbf{x} d\mathbf{v} dr. \tag{A14}
\]

APPENDIX B: MATHEMATICAL BASIS FOR THE ddf APPROACH

The ddf approach is based on the theory of point processes, which is a theory that enables us to build models for a random distribution of points in a space. Such models can be used to characterize diverse physical phenomena such as: the positions and times of earthquakes in a region, or the locations of stars in space. A clear exposition of the theory of point processes may be found in Daley and Vere-Jones (DVJ).\(^{13}\) As well as Resnick.\(^{22}\) Since there are frequent references to results from the text by Daley and Vere-Jones, these will be denoted DVJ preceded by the appropriate page number.

For point process models of sprays it is reasonable to assume that the total number of spray droplets is finite with probability 1. Such point processes are called finite point processes. In fact, it can be shown rigorously that if \( \mathbf{Y} = (y_1, \ldots, y_n) \) is a random vector with components in a \( d \)-dimensional Euclidean space \( \mathcal{X} \) (each component \( y_i \) takes values in a space \( \mathcal{X} \)), and formally this constitutes a mapping from a probability space into the \( n \)-fold product space \( \mathcal{X}^n \), then the counting function

\[
N_\lambda (A) = \#\{ i : y_i \in A \},
\]

which is defined on a set \( A \) in \( \mathcal{X} \), defines a point process (p. 201, DVJ). Taking the space \( \mathcal{X} \) to be the three-dimensional Euclidean physical space, this establishes that the locations of spray droplets in physical space \( \{ \mathbf{X}_i, i = 1, \ldots, N_\lambda \} \) do generate a point process in physical space.

When modeling physical systems as point processes, it is often useful to assign "tags," or marks, to the points which characterize the point process. In the case of the spray droplets it is useful to assign the properties of velocity and radius as marks to the points characterized by the droplet position.

The formal definition of a marked point process (p. 204, DVJ) may be paraphrased as follows. A marked point process \( N_{\mathcal{X} \times \mathcal{K}} (\cdot) \), with positions in a \( d \)-dimensional Euclidean space \( \mathcal{X} \) and marks in a \( p \)-dimensional Euclidean space \( \mathcal{K} \), is a point process on the product space \( \mathcal{X} \times \mathcal{K} \), with the additional property that the marginal process of locations \( \{ N(A) \} \) is itself a point process, for all reasonable sets \( A \) in \( \mathcal{X} \).

A (reasonable set is a member of the Borel \( \sigma \)-field generated by open spheres of \( \mathcal{X} \)). The marginal process is denoted \( N_{\mathcal{X}} (\cdot) \). It is important to note that not all point processes on product spaces \( \mathcal{X} \times \mathcal{K} \) are marked point processes.

The ddf approach models the spray as a marked point process in the phase space (which is the product space generated by the position space \( \mathcal{X} \) times the velocity-radius mark space \( \mathcal{K} \)), with velocity and radius as marks, and the point process of droplet locations in physical space as the marginal process \( N_{\mathcal{X}} (\cdot) \). Furthermore, the marginal process of droplet locations must be a simple point process. The marginal point process \( N_{\mathcal{X}} (\cdot) \) is simple when

\[
P\{ N_\lambda (\{ \mathbf{x} \}) = 0 \text{ or } 1 \{ \text{all } \mathbf{x} \} \} = 1.
\]

In other words, only two events are possible at any physical location \( \mathbf{x} \): either a droplet is located there, or there is no droplet there. Another way to describe a simple point process, is as one without multiple points.

On every reasonable set \( A \) in \( \mathcal{X} \), a set function \( \mu_\lambda (A) \) can be defined which represents the expected number of points from the point process \( N_{\mathcal{X}} \) contained in set \( A \), such that

\[
\mu_\lambda (A) = E (N_\lambda (A)), \tag{B1}
\]

where \( E \) represents the expectation. The set function \( \mu_\lambda (A) \) is called the expectation measure, and for the finite point process \( N_\lambda \) this measure is finite for all bounded sets \( A \) (p. 39, DVJ), i.e., \( \mu_\lambda \) is a boundedly finite measure. If the expectation measure is absolutely continuous with respect to the Lebesgue measure, then it can be written as the integral of a density \( n_\lambda (\mathbf{x}, t) \) such that

\[
\mu_\lambda (A) = \int_A n_\lambda (\mathbf{x}, t) d\mathbf{x}. \tag{B2}
\]

For a simple point process the density of the expectation measure is the same as the intensity, and therefore it is appropriate to call \( n_\lambda (\mathbf{x}, t) \) the intensity of the point process \( N_{\mathcal{X}} \).

Similarly, a boundedly finite expectation measure for the marked point process \( N_{\mathcal{X} \times \mathcal{K}} \) can also be defined as

\[
\mu_{\mathcal{X} \times \mathcal{K}} (A \times B) = E (N_{\mathcal{X} \times \mathcal{K}} (A \times B)), \tag{B3}
\]

where \( A \) and \( B \) are reasonable sets in \( \mathcal{X} \) and \( \mathcal{K} \), respectively.
An extension of the existence theorem for regular conditional probabilities on product spaces, to the case of boundedly finite measures, shows that if \( \mu_{X \times K} \) is absolutely continuous with respect to \( \mu_X \), then the following disintegration is valid:

\[
\mu_{X \times K}(A \times B) = \int_A \mu_K(B|x)n_s(x;t)dx.
\]  

(B4)

Furthermore, since the definition of the marginal process \( N_s(\cdot) \) requires that

\[
\mu_X(A) = \mu_{X \times K}(A \times K),
\]

it follows that \( \mu_K(B|x) \) is in fact a probability measure. If \( \mu_K(B|x) \) is also absolutely continuous with respect to the Lebesgue measure in \( K \), then Eq. (B4) may be written as

\[
\mu_{X \times K}(A \times B) = \int_A \left[ \int_B f^v_{VR}(v,r|x,t)dv dr \right] n_s(x;t)dx.
\]  

(B5)

The above equation may be recast in the following more familiar form

\[
EN_{X \times K}(A \times B) = \int_A \int_B f(x,v,r,t)dv dr dx,
\]  

(B6)

\[
f(x,v,r,t) = f^v_{VR}(v,r|x,t)n_s(x;t).
\]  

(B7)

The existence of the droplet distribution function, and its definition as the density of expected number of droplets in phase space, follows from Eq. (B6). The disintegration of the ddf into the intensity and the pdf follows from Eq. (B7).

**Practical implications of assumptions.** The assumptions made in establishing the mathematical basis of the ddf approach impose certain restrictions on the class of sprays that may be modeled with this approach. The practical implications of these restrictions are now examined.

1. **Simple point process assumption.** The simple point process assumption precludes the presence of more than one spray droplet at any given location in physical space. This assumption is naturally satisfied by all practical sprays of interest.
2. **Absolute continuity of \( \mu_X \) with respect to Lebesgue measure.** One consequence of this assumption is that it precludes the presence of fixed atoms in the process \( N_s(\cdot) \). A fixed atom for this process is a point in physical space where there is a positive probability of a spray droplet recurring over a whole family of realizations. An example might be the physical location of an intrusive measurement device in a spray of electrically charged droplets which has the property of attracting the spray droplets. As such this is not a serious restriction, since even if there are fixed atoms, these can be incorporated in the model by adding delta functions to the intensity \( n_s(x;t) \).

In summary, the underlying assumptions do not impose serious restrictions on the class of physical sprays which are capable of being modeled using the ddf approach.

**APPENDIX C: DERIVATION OF THE INTENSITY EVOLUTION EQUATION**

Starting from Eq. (55) and substituting for \( \partial f/\partial t \) from Eq. (33) results in

\[
\frac{\partial n_s(x,t)}{\partial t} = -\int_{[v_r,+\infty]} \frac{\partial}{\partial x_k} [v_{sf}] dv dr - \int_{[v_r,0]} \frac{\partial}{\partial u_k} [\mathcal{A}_k(x,v,r,t)f] dv dr - \int_{[v_r,0]} \frac{\partial}{\partial r} [\mathcal{T}[x,v,r,t]f] dv dr.
\]  

(C1)

Using the independence of the phase-space variables and substituting Eq. (54), the first term on the right-hand side of Eq. (C1) can be written as

\[
-\frac{\partial}{\partial x_k} \int_{[v_r,+\infty]} [v_{sf}] dv dr = -\frac{\partial}{\partial x_k} \langle V_k(x;t) \rangle n_s(x;t).
\]

After substituting Eq. (54) the second term on the right-hand side of Eq. (C1) can be written as

\[
-n_s(x;t) \int_{[v_r,0]} \left[ \left( [\mathcal{A}_k(x,v,r,t)]_{v=+\infty} - [\mathcal{A}_k(x,v,r,t)]_{v=-\infty} \right) dr \right] = 0.
\]

which follows from the assumption that the term \( \langle A_k(x,v,r,t) \rangle f^v_{VR}(v,r|x,t) \) vanishes at the velocity boundaries of the phase space.

After substituting Eq. (54) the third term on the right-hand side of Eq. (C1) can be written as follows:

\[
-\int_{[v_r,+\infty]} \frac{\partial}{\partial r} [\mathcal{T}[x,v,r,t]f] dv dr
\]

\[
= -\int_{[v_r,+\infty]} \frac{\partial}{\partial r} [\mathcal{T}[x,v,r,t]f^v_{VR}(v,r|x,t)n_s(x;t)] dv dr
\]

\[
= -n_s(x;t) \int_{[v_r,0]} \frac{\partial}{\partial r} \left[ \int_{[v] \left[ \mathcal{T}[x,v,r,t]f^v_{VR}(v,r|x,t) \right] dv \right] dr
\]

\[
= -n_s(x;t) \int_{[v_r,0]} \left[ \int_{[v] \left[ \mathcal{T}[x,v,r,t] \right] dv \right] \times f^v_{VR}(v,r|x,t) dr
\]

\[
= -n_s(x;t) \int_{[v_r,0]} \left[ \int_{[v] \left[ \mathcal{T}[x,v,r,t] \right] dv \right] \times \delta(r|x,t) dr
\]

\[
= \mathcal{T}[x=0+,v|t]f^v_{VR}(r=0+,x,t)n_s(x;t).
\]

**APPENDIX D: DERIVATION OF THE EVOLUTION OF GLOBAL SPRAY PROPERTIES**

Starting from Eq. (58) and substituting for \( \partial f/\partial t \) from Eq. (33) results in
\[ \frac{\partial N_s(t)}{\partial t} = - \int_{[x,v_r]} \frac{\partial}{\partial x_k} [v_k f] \, dx \, dv \, dr \\
- \int_{[x,v_r]} \frac{\partial}{\partial t} [(A_k(x,v,r,t)f)] \, dx \, dv \, dr \\
- \int_{[x,v_r]} \frac{\partial}{\partial x_k} [(\Theta(x,v,r,t)f)] \, dx \, dv \, dr. \]  

(D1)

Substituting the expression for the ddf from Eq. (54), and using similar arguments as in the intensity equation derivation concerning the behavior of the integrated terms at the phase-space boundaries, it can be shown that the first term on the right-hand side of Eq. (D1) is

\[ - \int_\mathbb{R} \frac{\partial}{\partial x_k} [(V_k(x;t)) n_s(x;t)] \, dx, \]

the second term is zero, and the third term can be rewritten starting from its form in Appendix C as

\[ \int_{[x]} \langle \Theta \rangle |r = 0_+; x(t); t \rangle f_R^s(r = 0_+; x(t)) \, dx \]

\[ = \langle N_s(t) \rangle |\Theta |r = 0_+; t \rangle f_R^s(r = 0_+; t). \]

**APPENDIX E: VERIFICATION OF THE NORMALIZATION-PRESERVING PROPERTY OF THE jpdf EVOLUTION**

Using Eq. (66) we may write

\[ \int_{[v_r]} \frac{\partial f_{VR}(v_r|x;t)}{\partial t} \, dv \, dr \\
= - \int_{[v_r]} f_{VR}^s \left( \frac{\partial \ln n_s(x;t)}{\partial t} + v_k \frac{\partial \ln n_s(x;t)}{\partial x_k} \right) \, dv \, dr \\
- \int_{[v_r]} \left\{ \frac{\partial}{\partial x_k} [v_k f_{VR}^s] + \frac{\partial}{\partial v_k} [(A_k(x,v,r,t)f_{VR}^s)] \right\} \, dv \, dr \\
- \int_{[v_r]} \left[ \frac{\partial}{\partial r} [\Theta(x,v,r,t)f_{VR}^s] \right] \, dv \, dr. \]  

(E1)

Performing the various integrations and making the usual assumptions concerning the behavior of terms at phase-space boundaries, the above equation may be simplified to

\[ \int_{[v_r]} \frac{\partial f_{VR}^s(v_r|x;t)}{\partial t} \, dv \, dr \\
= - \left( \frac{\partial \ln n_s(x;t)}{\partial t} + \langle V_k(x;t) \rangle \frac{\partial \ln n_s(x;t)}{\partial x_k} \right) \\
- \left\{ \frac{\partial \langle V_k(x;t) \rangle}{\partial x_k} \right\} + \left[ \langle \Theta(x,r = 0_+; t) f_R^s(r = 0_+; x(t)) \rangle \right]. \]  

(E2)

The intensity evolution equation may be rewritten as

\[ \frac{\partial \ln n_s(x;t)}{\partial t} + \frac{\partial \langle V_k(x;t) \rangle}{\partial x_k} + \langle V_k(x;t) \rangle \frac{\partial \ln n_s(x;t)}{\partial x_k} \\
= \langle \Theta(x,r = 0_+; t) f_R^s(r = 0_+; x(t)) \rangle. \]  

(E3)

if each term in Eq. (56) is divided by \( n_s(x;t) \). Substituting Eq. (E3) into Eq. (E2) shows that the evolution of \( f_{VR}^s(v_r|x;t) \) as given by Eq. (66) does indeed guarantee that the normalization property of \( f_{VR}^s(v_r|x;t) \) holds for all time.