Stochastic Spray Flow Models: A Review

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Abstract

Understanding and modeling multiphase flows is of primary interest in a wide variety of applications. Most theoretical and numerical models of multiphase flows can be placed into one of three categories: Eulerian-Eulerian, Lagrangian-Eulerian, or stochastic methods. With the Eulerian-Eulerian approach, a set of conservation equations is written for each phase, and the sets are coupled through their respective source terms. Typically, the spatial resolution of the Eulerian-Eulerian formulations is much larger than the interparticle spacing, and thus the discrete phase is treated as through it were a continuous medium with its own material properties. In the Lagrangian-Eulerian particle tracking framework, drops are injected into the gas and the drop trajectories are computed by numerically integrating Lagrangian equations of motion. Because of the large number of drops in a typical spray, computational parcels are often employed, where each parcel represents some number of individual drops. Probabilistic, or stochastic, methods generally involve the development of a probability density function (pdf) describing the random variables representing droplet properties, and the computation of the evolution of that pdf as the drops move through the gas phase, undergo secondary breakup, heat, and vaporize. This approach allows one to calculate general and/or detailed statistics about the spray drops and the gas phase at each point in the flow. This paper presents a survey of stochastic spray modeling frameworks that have appeared in the literature. A review of the spray equation provides a background to a more extensive discussion on specific modeling methods including assumed pdf's, maximum entropy moment closure, and particle methods. The assumed-pdf method is the simplest to implement but has the disadvantage that there is no guarantee the spray characteristics will always conform to the assumed form. The assumed forms may be anything from a delta function to an analytical expression approximating a well-known distribution function. The maximum-entropy method is perhaps the newest of the stochastic methods for determining the droplet pdf within a spray. With this method, a set of transport equations is solved for various moments of the pdf, which are in turn used to model the full pdf through a maximum entropy procedure. The final method is very similar to a Lagrangian droplet tracking method. Stochastic particles are tracked through the gas phase with the goal of indirectly obtaining the pdf. It differs from a conventional Lagrangian simulation in that the stochastic particles are notional and do not represent models of actual, physical drops, and the exchange terms between the discrete and continuous phases used in each approach generally differ in both functional form and physical interpretation. Examples are provided to highlight each stochastic modeling technique, as well as an examination of the advantages and disadvantages of each method.

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Introduction

Spray flows play an important role in many engineering applications. Examples include flows associated with liquid fuel injectors, industrial coating processes, and agricultural sprays. Following primary atomization, both the liquid and the gas phase continue to interact dynamically, exchanging mass, momentum, and energy. This interaction can have a significant impact, for example, on the combustion process inside a liquid rocket engine or on the coating produced by a spray application system. For this reason, it is necessary to have a full understanding of the physics of spray flows and to be able to accurately predict not only the distribution of the drops and their behavior, but also the dynamics of the gas phase, that is, the characteristics of the combined two-phase flow.

The research literature is replete with new ideas, approaches, and models of how to describe a multiphase flow. These models can generally be placed into three categories: Eulerian or two-continua, Lagrangian particle tracking, and stochastic methods. In the two-continua approach, a set of conservation equations is written for each phase, and the sets are coupled through their respective source terms. This is sometimes referred to as the Eulerian-Eulerian approach. Much of the work that has been done in this area has focused on modeling the effect the liquid phase has on the gas, such as turbulence modification. Typically, the spatial resolution of Eulerian-Eulerian formulations is much larger than the interparticle spacing, and thus the discrete phase is treated as though it were a continuous medium with its own material properties. This approach is not generally appropriate for sprays because droplet number densities in some regions of the flow can be too low for the continuum assumption to be valid, such as near the edge of a spray.

In the Lagrangian particle tracking approach, the gas phase behavior is typically predicted by solving the time-dependent, Reynolds-Averaged Navier-Stokes (RANS) equations with a suitable turbulence model and appropriate exchange terms. Drops are injected into the gas and the drop trajectories are computed by numerically integrating Lagrangian equations of motion. Because of the large number of drops in a typical spray and limited computer resources, computational parcels are often employed, where each parcel represents some number of individual drops. This approach has been effective at simulating spray flows in many applications, but requires detailed submodeling for the interphase exchange terms. Additionally, though the computational time required to compute the behavior of the drops is generally less than that required to predict the gas phase, the simulation can become computationally expensive if statistical information about the spray is desired due the large number of drops needed to achieve statistical convergence. Also, the Lagrangian equations represent a deterministic, and frequently stochastic, simulation of discrete events while the RANS equations represent a time-averaged description of the gas, and one could argue this represents a fundamental incompatibility in the way the two phases are treated. For instance, by time-averaging the Navier-Stokes equations, fluctuations and other short-term flow structures are smoothed out over the averaging period, and thus the interaction between these structures and the drops is not captured. On the other hand, the drop-tracking simulation represents a time-accurate calculation of multiple discrete events (i.e. the behavior of each tracked droplet). Though it is common practice to do so, to the author's knowledge it has not been proven that superimposing a time-accurate Lagrangian calculation over a time-averaged gas-phase calculation is fundamentally appropriate. A more compatible treatment of the combined two-phase flow might be to use a Large-Eddy Simulation (LES) with an appropriately-sized spatial filter to describe the gas phase with a Lagrangian tracking method to handle the drops. Direct Numerical Simulation (DNS) is another potential alternative for predicting the gas phase.

The third approach to spray modeling involves treating the droplet properties as random variables and constructing a probability density function (pdf) describing those variables from an ensemble of spray flows. The goal of the approach would then be to compute the evolution of that pdf as the drops move through the gas phase, undergo secondary breakup, heat, and vaporize. This approach allows one to calculate general and/or detailed statistics about the spray drops and the gas phase at each point in the flow. The purpose of this article is to review some of these statistical approaches and provide examples of their use in the literature. For brevity, only one or two examples of each approach are presented here. Additional discussion and examples can be found in Reference [1]. This work is not an exhaustive presentation of probabilistic models for spray flows, but rather represents a review of some of the most-prevalent approaches in the research literature.

The Spray Equation

Many statistical approaches to describing spray flows find their roots in what has come to be known as the spray equation [2-4]. The derivation of this equation begins with a restriction to single-particle statistics and to dilute sprays where the droplets are modeled as point-particles [5]. The parameterization of the spray must also be considered. A single drop can be described by any number of characteristics such as its size, velocity, and temperature. It is often sufficient to choose a relatively small set of characteristics that contains the important information about the drop. This

set of characteristics prescribes a state vector whose elements define the axes of a hyperspace through which the drop moves as it evolves. For example, if the chosen characteristics are the position in physical space and the diameter, then the drop's evolution may be described using a four-dimensional hyperspace whose axes are the three position coordinates *x*, *y*, *z*, and the diameter, ϕ. As the drop moves through physical space or as its size changes (e.g., it evaporates), its location in the hyperspace changes.

Under the preceding assumptions, a probabilistic description of the spray can be developed. Following Williams [2], one can define the unnormalized, single-particle density function for the spray $F(\bar{\alpha};t)$ such that $F(\bar{\alpha};t)d\bar{\alpha}$ is the probability of finding a particle with its state vector in the interval $d\bar{\alpha}$ about $\bar{\alpha}$ at any instant.* Letting $\bar{\alpha}=(\bar{x},\phi,\bar{v},T)$, a transport equation for $F(\bar{\alpha};t)$ (i.e. the spray equation) can be derived:

$$\frac{\partial F}{\partial t}+\nabla_x\cdot(F\bar{v})+\nabla_v\cdot(F\bar{a})+\frac{\partial}{\partial\phi}(F\Phi)+\frac{\partial}{\partial T}(F\Theta)=\dot{S}_2+\dot{S}_1+\dot{S}_0 \quad (1)$$

Eq. (1) describes the evolution of the single-particle probability density function $F(\bar{x},\phi,\bar{v},T;t)$ through joint physical, diameter, velocity, and temperature space and includes terms accounting for binary (two-body) collisions $\dot{S}_2$, unary (one-body) breakup and coalescence $\dot{S}_1$, and zero-body events $\dot{S}_0$ (such as nucleation and complete vaporization).

Because it is not an ordinary evolution equation, direct solution of Eq. (1) has not generally been viewed as a practical way of computing spray flows. The quantity of interest is transported not only through physical space, but also through diameter, velocity, and temperature space. A direct numerical solution requires a full discretization of this eight-dimensional hyperspace and vast computational resources. As an example, if the hyperspace were discretized such that there were 50 numerical cells in each of the eight coordinate directions, then the full computational mesh would consist of approximately 10^{14} grid cells, making data storage and computation time unfeasible.

Despite these difficulties, attempts have been made at a direct solution of the spray equation. The first attempt was made by Williams [3] who incorporated Probert's work on drop size distributions [6]. Williams looked at a steady, one-dimensional problem with no collisions or breakup. Temperature was not included (though the drops did evaporate), and the gas phase was not considered—the solution assumed that the gas-phase properties were known *a priori*. Bracco et al. [7] and Westbrook [8] attempted direct solutions to the spray equation, but showed that only a very coarse discretization of the phase-space was possible, leading to significant numerical errors [9].

Assumed PDF Transport

Perhaps the simplest method for calculating a droplet pdf is to assume its functional form and derive models for the parameters that characterize the assumed form. For example, consider a monodispersed spray where the droplet velocities are assumed to follow a Gaussian distribution, which is characterized by its mean and variance. One set of equations that might be used to describe the evolution of the mean and variance of the velocity could be [1]

$$\frac{\partial\langle v_k\rangle}{\partial t}+\langle\bar{v}\rangle\cdot\nabla\langle v_k\rangle=\langle a_k\rangle \quad (2)$$

$$\frac{\partial(\sigma_k^2)}{\partial t}+\langle\bar{v}\rangle\cdot\nabla(\sigma_k^2)=\frac{\partial\langle v_k^2\rangle}{\partial t}-2\langle v_k\rangle\langle a_k\rangle \quad (3)$$

where the brackets denote an ensemble average. The transient term on the right-hand side of Eq. (3) represents a source term for the velocity variance associated with the drop acceleration, and includes the second-order velocity moment, $\langle v_k^2\rangle$. To close the set of equations, the second-order moment can be related back to the variance:

$$\sigma_k^2=\langle v_k^2\rangle-\langle v_k\rangle^2 \quad (4)$$

The solution to this set of equations provides the droplet velocity mean and variance at each point in space and time. Substitution of these values into the expression for the assumed Gaussian distribution thus gives the evolution of the pdf. Similar equations could be derived for the drop size or other drop parameters. Of course, altogether different model equations for the mean and variance could also be developed.

The method can be further simplified. Because the pdf describing droplets is generally a joint function of position, size, velocity, and temperature (and possibly other parameters), even an assumed function containing each of these variables can be mathematically difficult to manage. As will be shown, it is a common practice to compute mean values for the velocity and temperature as a function of size and position, but assume that there is no dispersion about these mean values. This approach is equivalent to assuming the

* In the notation presented herein, variables which appear before the semicolon are those over which the density function is defined (the independent variables of the sample space), while those appearing after are parameters of the density function(variables on which it is conditioned).

marginal pdf's for velocity and temperature are delta functions centered on the means, and has the effect of eliminating higher-order moments from the governing equations. Because the delta function is typically only characterized by a mean value which is usually determined from the governing equations, additional equations are not required to describe its evolution.

The greatest advantage of this method is its simplicity. It does not require stochastic simulation to construct the pdf, and provided that models to describe transport of mass, momentum, and energy between the liquid and gas phases are incorporated, the equations form a fully closed set. One need not be concerned with the moment hierarchy problem where the derivation of a transport equation for one moment results in the introduction of a new, higher-order moment. Furthermore, most pdf's of interest have only one or two parameters that characterize them, keeping the equation set relatively small.

The primary drawback of this approach is that there is no guarantee that the spray will always conform to the assumed distribution throughout its evolution. To illustrate this, assume that the drop diameter distribution of three size classes (small, medium, and large) within some volume is initially described roughly by a truncated Gaussian. If all the drops move with the same velocity, the truncated Gaussian would continue to describe the size distribution. It is possible, however, that the drops in the medium size class are moving faster than both the larger and smaller drops. So long as there are no velocity or number density gradients, again the size distribution would not change. But now imagine there is a positive velocity gradient with the medium-sized drops as shown in Figure 1. The mediums drops will leave the volume faster than like-sized drops will enter (Figure 2). The size distribution will be characterized by a peak in the large and small drops and a trough in the medium drops. The truncated Gaussian will have been lost. A similar situation occurs if all the drops are moving with the same velocity, but there is a positive gradient in the mean number density of the medium drops. More drops of this size will leave than enter (Figure 3). The example can be easily extended to include drop properties other than the diameter. These examples demonstrate how a pdf may not always conform to an assumed shape as the spray develops. Nevertheless, the simplicity of the approach has resulted in several models based upon it.

Laurent and Massot [10-12] considered a poly-disperse spray, but assumed no velocity dispersion in developing their kinetic and Eulerian multi-fluid models. Their work focused on a comparison between the sectional approach of Tambour [13,14] and an Eulerian sampling approach, restricting their development to dilute sprays where collisions, breakup, and coalescence were negligible. They reproduced the sectional equations of Greenberg et al. [15] while simultaneously extending them to include temperature in the sample space. Laurent and Massot began with the same probability density function for the droplets as in Eq. (1), but discretized the size axis into sections such that the n^{th} section was defined as $\phi_n \le \phi < \phi_{n+1}$. The authors assumed that the pdf could be represented as the product of five independent pdf's for the various droplet characteristics (size, temperature, and three components of velocity),

$$F\left(\vec{x},\phi,\vec{v},T;t\right) = \lambda_n\left(\vec{x},\phi;t\right)\psi_n\left(T-\left\langle T\right\rangle_n\right)\prod_{k=1}^{3}\varphi_n\left(v_k-\left\langle v_k\right\rangle_n\right) \quad (5)$$

A Gaussian distribution centered on zero was assumed for the function $\varphi_n\left(v_k-\left\langle v_k\right\rangle_n\right)$. The spray equation was used to derive transport equations for the expected number density, velocity, and enthalpy within a given section. Of relevance here, the equation for the expected velocity is

$$\frac{\partial}{\partial t}\left(\lambda_n\left\langle\vec{v}\right\rangle\right)+\nabla_x\cdot\left(\lambda_n\left\langle\vec{v}\right\rangle\left\langle\vec{v}\right\rangle+\lambda_n\underline{\underline{P}}\right) +\frac{\partial}{\partial\phi}\left(\lambda_n\left\langle\Phi\vec{v}\right\rangle\right)=\lambda_n\left\langle\vec{a}\right\rangle \quad (6)$$

where λ_n is the expected drop number density in the n^{th} section. The term under the divergence operator is the sum (multiplied by the section expected number density) of the dyadic product of the average velocity plus a diagonal tensor $\underline{\underline{P}}$ representing the dispersion of velocity about the mean in all directions. This tensor is illustrative of the moment-hierarchy problem common with moment methods. In this case, $\underline{\underline{P}}$ represents a second-order moment. To avoid the need to model the dispersion term, Laurent and Massot assume there is no velocity dispersion, which is to assume $\left\langle v_k^2\right\rangle=\left\langle v_k\right\rangle^2$. The vaporization term $\left\langle\Phi\vec{v}\right\rangle$ presented a similar problem, as it was desired to equate this term to $\left\langle\Phi\right\rangle\left\langle\vec{v}\right\rangle$. To this end, the authors also assumed no temperature dispersion about the mean drop temperature. These assumptions are equivalent to assuming the velocity and temperature pdf's are delta functions centered on the mean values:

$$F\left(\vec{x},\phi,\vec{v},T;t\right) = \lambda_n\left(\vec{x},\phi;t\right)\delta\left(T-\left\langle T\right\rangle\right)\delta\left(\vec{v}-\left\langle\vec{v}\right\rangle\right) \quad (7)$$

Assuming a single characteristic velocity (or temperature) for a section has implications on the

resulting solution, as Laurent and Massot demonstrate. They described a vaporizing spray consisting initially of only two drop sizes, with the larger-size drops (Class A) moving slower than the smaller drops (Class B). Because of their slower velocity (and thus longer residence time in the vaporization region), as the drops from Class A evaporate, their average size approaches the average size of the evaporating drops in Class B. Eventually, the average drop sizes in both classes are equal, defining a new Class C. The velocities of all the drops in Class C are averaged to determine the characteristic velocity of the class. Having assumed no velocity dispersion, this average velocity is henceforth taken to be the velocity of all drops in Class C, even though the drops actually have different velocities stemming from the average velocities of the initial Classes A and B. Laurent and Massot demonstrated the computed error by comparing their results to those of a conventional sampling method where each drop (or drop packet) is individually tracked. The results clearly show differing mass-averaged velocities computed by the sectional approach using a delta function and the sampling method. This example suggests that a no-dispersion assumption is not appropriate where drops of the same size but different velocities interact. Flows involving recirculating droplets (for example) would be poorly modeled under such a restrictive assumption.

A second example of the use of an assumed pdf is the work of Beck and Watkins [16-21]. The purpose of their work was to provide an efficient model for a polydisperse spray by deriving equations for the first four moments of the droplet size distribution function. Their analysis began be defining $F = F(r;\vec{x},t)$ [*] and with the derivation of the liquid-phase mass, momentum, and energy transport equations [16]:

$$\tfrac{4}{3}\pi\frac{\partial}{\partial t}\left(\rho_l\left\langle r^3\right\rangle\right)+\tfrac{4}{3}\pi\frac{\partial}{\partial x_k}\left(\rho_l\left\langle r^3\right\rangle U_{3k}\right)=-S_m \quad (8)$$

$$\begin{aligned}&\tfrac{4}{3}\pi\frac{\partial}{\partial t}\left(\rho_l\left\langle r^3\right\rangle U_{3k}\right)\\&+\tfrac{4}{3}\pi\frac{\partial}{\partial x_j}\left(\rho_l\left\langle r^3\right\rangle U_{3k}U_{3j}\right)+U_{3i}S_m\\&=\tfrac{4}{3}\pi\frac{\partial}{\partial x_j}\left[\rho_l\left\langle r^3\right\rangle\sigma_v\nu_l\left(\frac{\partial U_{3k}}{\partial x_j}+\frac{\partial U_{3j}}{\partial x_k}\right)\right]\\&-S_{U_k}\end{aligned} \quad (9)$$

$$\begin{aligned}&\tfrac{4}{3}\pi\frac{\partial}{\partial t}\left(\rho_l\left\langle r^3\right\rangle E_l\right)\\&+\tfrac{4}{3}\pi\frac{\partial}{\partial x_k}\left(\rho_l\left\langle r^3\right\rangle E_l U_{3k}\right)+E_l S_m\\&=\tfrac{4}{3}\pi\frac{\partial}{\partial x_k}\left[\rho_l\left\langle r^3\right\rangle\sigma_v\nu_l\frac{\partial E_l}{\partial x_k}\right]-S_E\end{aligned} \quad (10)$$

E_l is the total energy of the droplets, σ_v is a coefficient attributable to Melville and Bray [22], and S_m, S_{u_i}, S_E are source terms due to evaporation, momentum exchange, and heating, respectively. U_{ik} is the k^{th} component of the i^{th}-moment-averaged liquid velocity, given by

$$U_{ik}=\frac{1}{\left\langle r^i\right\rangle}\int_0^\infty Fr^iU_k\,dr \quad (11)$$

Thus, U_{3k} is the k^{th} component of the liquid volume-averaged velocity. To derive Eq. (9), it was assumed that differences between individual droplet velocities and the mass-averaged velocity were small for large drops, and thus the product of these velocity differences were negligible. This essentially imposed an assumption of no velocity dispersion about the mass-averaged velocity, similar to the no-velocity-dispersion assumption imposed by Laurent and Massot. The difference, however, is that unlike the pdf employed by Laurent and Massot, this did not constitute an assumption on the droplet distribution function in the work of Beck and Watkins since velocity was not a parameter of their distribution function, only radius. Transport equations for addi-tional moment-averaged velocities took the form

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\left\langle r^i\right\rangle U_{ik}\right)+\tfrac{4}{3}\pi\frac{\partial}{\partial x_j}\left(\left\langle r^i\right\rangle U_{ik}U_{ij}\right)\\&+\frac{\partial}{\partial x_j}\left[\left\langle r^i\right\rangle\left(U_{3k}-U_{ik}\right)\left(U_{3j}-U_{ij}\right)\right]\\&+U_{3k}B_i+U_{ik}\left(S_i-B_i\right)\\&=\frac{\partial}{\partial x_j}\left[\left\langle r^i\right\rangle\sigma_v\nu_l\left(\frac{\partial U_{ik}}{\partial x_j}+\frac{\partial U_{ij}}{\partial x_i}\right)\right]-S_{U_{ik}}\end{aligned} \quad (12)$$

where B_i represents a droplet breakup source term and S_i is a source term dependent upon the particular radius moment (e.g. collision).

Beck and Watkins proposed that enough information about the droplet size distribution could be obtained by solving the transport equations for the distribution's first four moments. To do this, a function would have to be determined that approximates the size

[*] The authors did not explicitly state the dependence on $\vec{x}$ and t, but the context makes clear the dependence exists.

distribution function and have its first four moments match the distribution function, a task the authors noted is "non-trivial." The authors also discussed concerns of stability in the numerical solution scheme. These concerns arose because the moment-averaged velocities associated with each of the four moments can vary substantially at the spray's edge. All these difficulties could be overcome (or at least significantly reduced), they argued, by employing a two-moment scheme rather than solving for four moments.

A Rosin-Rammler volume distribution was chosen as a reference function

$$V(r) = \left(\frac{2}{\langle r \rangle^2} \right) r \exp\left[-\left(r / \langle r \rangle \right)^2 \right] \qquad (13)$$

To approximate this function, Beck and Watkins chose the following analytically integrable function:

$$f(r) = \frac{16r}{r_{32}^2} \exp\left[-\frac{4r}{r_{32}} \right] \qquad (14)$$

where r_{32} is the Sauter mean radius (SMR). The authors showed that they could obtain values for the SMR by solving the transport equations for $\langle r^2 \rangle$ and $\langle r^3 \rangle$. This provided enough information to evaluate the assumed pdf, Eq. (14), from which the other two moments λ and $\langle r \rangle$ could be obtained through integration.

The authors tested their model in three cases: high-pressure narrow-angle sprays, low-pressure wide-angle full-cone sprays, and hollow-cone sprays. Each case was tested against corresponding experimental data [23-25]. Beck and Watkins reported that, in comparison with the experimental data, their model predicted excellent spray-penetration results and a good radial distribution of droplet sizes, including the prediction of the collapse of the hollow-cone spray. However, the radial mass-flux distributions were not accurately predicted, perhaps attributable to the first-order discretization scheme or a non-uniform mass distribution at the liquid nozzle exit.

Maximum Entropy

In general, the shape of the droplet pdf is not known *a priori*, yet moments of the pdf are required to utilize a particular spray model. In the previous section, the approach of assuming a functional form for the pdf was discussed. These forms may be anything from a delta function to an analytical expression approximating a well-known distribution function. Further, the pdf may encompass a single random variable such as size, or several such variables. Returning to the spray equation, one could even develop a model where $F(\bar{\alpha};t)$ is assumed. However, as discussed earlier, the essential problem with the assumed-pdf approach is that there is no guarantee that the spray will always conform to the assumed distribution throughout its evolution.

Though one might not be able to describe it easily, and it may change significantly as the flow evolves, $F(\bar{\alpha};t)$ has some functional form at all times. That form, even for the most general pdf, can be described by the complete set of moments for the distribution. The value of each moment affects the shape of the distribution in some way, but a change in each higher-order moment affects the shape in a less drastic way than a change in the next lower-order moment. The maximum entropy approach provides a means for modeling the droplet pdf using any number of low-order moments. The primary assumption associated with this method is that the lowest-order moments—the means, the variances, the co-variances, etc.—carry sufficient information to reasonably approximate the shape of the distribution function.[*] Once the function has been approximated, it can be integrated to provide any higher-order moment of interest.

Consider a discrete, single-random-variable probability distribution function, $p(x_i) = \left[p_1(x_1), p_2(x_2), \ldots, p_n(x_n) \right]$. Shannon's entropy is defined as [26]

$$S = -\sum_{i=1}^{n} p(x_i) \ln p(x_i) \qquad (15)$$

For a continuous probability density function $f(x)$, this definition can be extended to

$$S = -\int f(x) \ln f(x)\, dx \qquad (16)$$

The idea behind the maximum entropy principle is to find the probability distribution function that maximizes Shannon's entropy subject to constraints [27]

$$\int_a^b f(x)\, dx = 1 \qquad (17)$$

and

$$\int_a^b f(x) A_r(x)\, dx = \langle A_r \rangle, \quad r = 1, 2, \ldots, m \qquad (18)$$

[*] This assumption follows from recognizing that a representation of a pdf by its moments comes about by taking the Fourier transform of the pdf to obtain its characteristic function. Expanding the exponential in the kernel of this function in a power series yields a characteristic-function expansion, the coefficients of which are the moments of successively higher order of the original pdf.

where *a* and *b* represent the upper and lower bounds, respectively, of the random variable *x*, $\langle A_r \rangle$ is a moment of $f(x)$, and *m* is the number of such moment constraints. Jaynes [28] showed that an infinite number of probability distribution functions are consistent with a set of known constraints (i.e. known moments), but the one that should be chosen is the one with maximum entropy. If a distribution function with less entropy were used, it would imply the existence of some additional knowledge. However, since all the available knowledge was applied in the form of constraints, no additional knowledge could exist, and thus it would be inappropriate to choose any distribution function other than the one with maximum entropy. This maximization can be accomplished using the method of Lagrange multipliers, which leads to [29]

$$f(x) = \exp\left[-\beta_o - \sum_{r=1}^{m} \beta_r A_r(x)\right] \tag{19}$$

where the β's are the Lagrange multipliers which must be determined numerically [30]. Eq. (19) represents the most unbiased pdf possible within the given constraints. The method is immediately extendable to multivariate pdf's [27].

The maximum entropy approach has been used extensively in spray modeling applications, but mostly to describe the result of primary atomization [31-35]. For atomization, the constraints might be related to the mass, momentum, and energy of a slug of fluid that must be conserved through the breakup process, as well as a normalization constraint. The predicted pdf would describe the size and/or velocity distribution of the resulting drops which in turn might be used in a droplet tracking scheme. This differs from using the maximum entropy procedure to determine the droplet pdf at each spatial location within an evolving spray flow, an approach that is not as well-represented in the literature.

Archambault et al. [36-39] applied this method to a quasi-one-dimensional spray problem using $F = F(\bar{x}, \bar{v}, \phi, T; t)$. Moment constraints were placed upon the mean and mean-squared axial velocity, the mean-squared transverse velocity, and the mean and mean-squared temperature. Collision, breakup, and vaporization were neglected. The authors developed transport equations for each of the moment constraints by integrating Eq. (1) with no source terms. The quasi-one-dimensional nature of the flow eliminated mean velocities and variations of averaged quantities in the transverse directions. The authors also discretized the diameter axis to avoid numerical issues associated with the inverse dependence of the drag terms on the diameter, leading to a set of moment transport equations for each section. With these assumptions, the governing equations for the discrete phase reduced to [37]

$$\frac{\partial \lambda_n}{\partial t} + \frac{\partial\left(\lambda_n \langle v_x \rangle_n\right)}{\partial x} = 0 \tag{20}$$

$$\frac{\partial\left(\lambda_n \langle v_x \rangle_n\right)}{\partial t} + \frac{\partial\left(\lambda_n \langle v_x^2 \rangle_n\right)}{\partial x} = \frac{\lambda_n}{\Delta\phi_n}\langle a_x \rangle_n \tag{21}$$

$$\frac{\partial\left(\lambda_n \langle v_x^2 \rangle_n\right)}{\partial t} + \frac{\partial\left(\lambda_n \langle v_x^3 \rangle_n\right)}{\partial x} = 2\frac{\lambda_n}{\Delta\phi_n}\langle a_x v_x \rangle_n \tag{22}$$

$$\frac{\partial\left(\lambda_n \langle v_y^2 \rangle_n\right)}{\partial t} + \frac{\partial\left(\lambda_n \langle v_x v_y^2 \rangle_n\right)}{\partial x} = 2\frac{\lambda_n}{\Delta\phi_n}\langle a_y v_y \rangle_n \tag{23}$$

$$\frac{\partial\left(\lambda_n \langle T \rangle_n\right)}{\partial t} + \frac{\partial\left(\lambda_n \langle T v_x \rangle_n\right)}{\partial x} = \frac{\lambda_n}{\Delta\phi_n}\langle \Theta \rangle_n \tag{24}$$

$$\frac{\partial\left(\lambda_n \langle T^2 \rangle_n\right)}{\partial t} + \frac{\partial\left(\lambda_n \langle T^2 v_x \rangle_n\right)}{\partial x} = 2\frac{\lambda_n}{\Delta\phi_n}\langle T\Theta \rangle_n \tag{25}$$

where Θ is the heating rate. Eqs. (20)–(25) are coupled through the source terms to equations describing the gas phase. While the moments appearing in each of the time derivative terms in the governing equations are the constraint variables being sought, the moments in the convective terms are determined through the maximum entropy procedure and those in the terms on the right-hand side of the equations were modeled as functions of the gas phase properties.

Solutions to Eqs. (20)–(25) were compared to results from a corresponding Lagrangian drop tracking simulation, and the authors reported excellent agreement in the statistically steady regions. In those regions where steady statistics had not been achieved, statistical results for the Lagrangian simulation were noisier, but still compared well with the general trend of the maximum entropy solution.

One of the advantages suggested by Archambault et al. is the savings in computational time the maximum entropy approach provides in comparison to a Lagrangian simulation. Because the maximum entropy pdf was part of the solution procedure, it was possible to integrate the pdf to obtain any statistic of interest. To compute moments in a Lagrangian simulation, one must post-average sampled data, the amount of which depends on the level of statistical detail desired. This post-averaging process can be time-intensive. Considering that a large-scale spray may have millions

of drops, Archambault et al. argued that computing detailed statistics from a Lagrangian simulation is prohibitively time consuming, but the maximum entropy solution avoids this complication.

There are disadvantages to the maximum entropy approach as well. As the number of sections, droplet properties, or moment constraints increases, so too does the number of governing equations. This increases the numerical complexity of the problem, making solutions more difficult to obtain. Further, the maximum entropy approach as currently developed is not capable of handling multimodal pdf's. Because the maximum entropy procedure seeks to provide the widest, most-unbiased pdf possible within the provided constraints, the usual results are single-modal functions. It is not clear what additional constraints are needed to achieve multimodal pdf's. It appears that additional progress must be made with this approach to accurately predict intersecting sprays with significantly different properties or sprays with recirculating flow.

Particle Method

The particle method for solving the spray equation differs from the previously described methods in two important ways. First, whereas the assumed pdf and maximum entropy approaches are Eulerian-based methods, the particle method is Lagrangian-based. The trajectories of computational particles (not individual drops) are determined through Lagrangian equations of motion representing each of the dimensions of the hyperspace described by the spray equation. As with the other approaches, the gas phase is typically modeled with the RANS equations and the two phases are coupled through source terms. The second important difference is that the particle method provides an *indirect* solution to the spray equation. As discussed above, the high-dimensionality of the spray equation makes it infeasible to discretize the equation and obtain a direct numerical solution. Instead, an ensemble of computational particles is used to represent the pdf, and as these particles evolve in space and time, the pdf can be reconstructed at each point in the flow through a weighted-average of the particle properties and number density. This approach is sometimes referred as a Monte Carlo method.

Consider N computational particles, each with specified size, velocity, and temperature properties. The number of particles must be sufficiently large so as to minimize scatter in the data and provide statistically meaningful results. Initially, each particle is randomly weighted according to a specified distribution function at the point where the particles are introduced into the computational domain. If each property of each particle represents a point on an axis of the hyperspace described by the pdf, then each of those properties evolves according to a Lagrangian equation of motion along the associated axis. For instance, the properties of the i^{th} particle will evolve consistent with

$$\frac{d\bar{x}_i}{dt} = \bar{v}_i \tag{26}$$

$$\frac{d\bar{v}_i}{dt} = \bar{a}_i \tag{27}$$

$$\frac{d\phi_i}{dt} = \Phi_i \tag{28}$$

$$\frac{dT_i}{dt} = \Theta_i \tag{29}$$

The rate of change terms on the right-hand side of Eqs. (26)-(29) must be modeled and typically provide the means for coupling to the gas phase. After each time step that the particles are evolved, the pdf can be reconstructed at each point in the flow. For example,

$$F\left(\phi,\bar{v},T;\bar{x},t\right) = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N}\delta\left(\phi_i-\phi\right)\delta\left(\bar{v}_i-\bar{v}\right)\delta\left(T_i-T\right) \tag{30}$$

If the pdf is being sought in a stochastically steady region of the flow, it is sufficient to run the simulation long enough to model many "flow-through" times such that each statistical sample is reasonably independent of all other samples. However, for unsteady flows, multiple simulations, each representing one realization of the ensemble of spray flows, must be conducted to obtain converged statistics at each instant in time.

It must be emphasized that the computational particles used in this method are separate and distinct from the individual drops comprising the spray. The computational particles are conceptual in nature and do not represent real drops. Neither actual droplets nor droplet packets are being tracked. This distinction becomes important when modeling the terms on the right-hand side of Eqs. (26)–(29), and it is common to find this distinction overlooked in the spray modeling literature. For instance, as Subramaniam [40] points out, it is unclear whether it is reasonable to assume that the model for the acceleration term in Eq. (27) is the same as a model describing the acceleration of a single, real drop.

Perhaps the best-known example of the particle method is its representation in various versions of the KIVA flow solver [41,42]. KIVA is a widely-used tool for solving chemically reacting flows involving sprays, particularly in the internal combustion research community. [43-46] In addition to the standard random

drop property variables, the pdf modeled in KIVA also includes the random variables denoting the deviation from sphericity y and the time rate of change of that deviation $\dot{y}$. This leads to a transport equation for the pdf $F(\bar{x},\bar{v},\phi,T,y,\dot{y};t)$:

$$\frac{\partial F}{\partial t}+\nabla_x\cdot\left(F\bar{v}\right)+\nabla_v\cdot\left(F\bar{a}\right)+\frac{\partial}{\partial\phi}\left(F\Phi\right) + \frac{\partial}{\partial T}\left(F\Theta\right)+\frac{\partial}{\partial y}\left(F\dot{y}\right)+\frac{\partial}{\partial\dot{y}}\left(F\ddot{y}\right)=\dot{S}_2+\dot{S}_1 \tag{31}$$

KIVA has the ability to model multiple injectors. At each injector, the particle velocity magnitude and temperature are uniform and specified, and the injection angle is uniformly distributed about the spray axis and between the specified minimum and maximum spray cone angles. The injected drops are assumed to be perfect spheres, and a dimensionless amplitude and dimensional frequency are specified to provide a value for $\dot{y}$. The size of each particle is the only variable randomly determined at the injector based on a χ-squared distribution, and the number of drops associated with each particle is determined such that the mass of each particle is the same.

Subramaniam and O'Rourke [47] however reported that the particle method as implemented in KIVA-3 has problems associated with numerical convergence that are unrelated to the physical modeling. Convergence tests conducted while modeling spray penetration length into a gas flow provided results with statistically-significant grid dependence, irrespective of the grid resolution. Motivated by these findings, Subramaniam conducted a study investigating the convergence requirements for the particle method [40] wherein he identifies both strong and weak convergence criteria. Strong convergence is associated with ensuring convergence of the spray/gas governing equations at each point in the domain, and requires spatial and temporal resolution of the smallest scales of the flow. Weak convergence is associated with convergence of mean quantities (for both spray and gas) integrated over a given volume in the domain. Strong convergence is the more stringent criterion, however weak convergence is generally sufficient for engineering applications.

To demonstrate the convergence issues, Pai and Subramaniam tested the particle method (as implemented in KIVA-3) for an ensemble of vaporizing, non-mobile, statistically homogeneous drops [48]. An analytic solution was obtained for this problem which served as the basis for comparison to the numerical results. When the computational particles were uniformly sampled from the initial pdf, KIVA properly reproduced the analytic solution. The authors noted however that this sampling method is inefficient since there could be many computational particles associated with small droplet radii which do not contribute much to the overall spray mass. More commonly, larger radii are preferentially sampled to reduce the number of droplets per computational particle while maintaining the same number of particles and overall spray mass in the system [49]. However, this preferential sampling method led to deviations from the analytic solution both because the criterion for when a droplet completely vaporizes (when the droplet's radius falls below 10% of its initial radius) was incorrect, and because implementation of the preferential sampling technique used in KIVA-3 does not well-represent the pdf near $r = 0$. This suggests that while the preferential sampling technique may be more efficient, uniform sampling may be more accurate.

Summary

Three distinct probabilistic approaches for modeling spray flows have been reviewed and examples of their use in the literature provided. The first approach involves assuming a functional form for the pdf describing spray drop properties. This method is relatively simple to implement but has the disadvantage that it will poorly-predict the spray flow in regions where the droplet properties do not conform to the assumed pdf. The maximum-entropy method is perhaps the newest of those reviewed here for determining the droplet pdf within the spray, though it has been more extensively used for predicting a resulting droplet pdf after primary atomization. With this method, a set of transport equations is solved for various moments of the pdf, which are in turn used to model the full pdf through a maximum-entropy procedure. The final method is very similar to a Lagrangian droplet tracking method. Stochastic particles are tracked through the gas phase with the goal of indirectly obtaining the pdf. It differs from a conventional Lagrangian simulation in that the stochastic particles are notional and do not represent models of actual, physical drops, and the exchange terms between the discrete and continuous phases used in each approach generally differ in both functional form and physical interpretation.

Nomenclature

A_r	a function of random variables
$\bar{a}$	drop acceleration
E	total energy
F	single-drop probability density function, including position as a random variable
f	single-drop probability density function, excluding position as a random variable

N	number of drops or number of sections (bins)
$\underline{\underline{P}}$	dispersion tensor
p	a generic discrete probability distribution function
r	drop radius
r_{32}	Sauter mean radius
Re_ϕ	Reynolds number based on drop diameter
S	Shannon's entropy
$\dot{S}_o$	source term associated with complete drop vaporization or nucleation
$\dot{S}_1$	source term associated with drop breakup and coalescence
$\dot{S}_2$	source term associated with drop collision
T	drop temperature
t	time
U	moment-averaged liquid velocity
$\vec{u}$	gas-phase velocity
V	volume
$\vec{v}$	drop velocity
$\vec{x}$	position vector
x, y, z	position vector components
y	drop sphericity
$\dot{y}$	time rate of change of drop sphericity

Greek Variables

$\vec{\alpha}$	drop state vector
β	Lagrange multiplier
δ	Dirac delta function
Θ	drop heating rate
λ	expected drop number density
ν	kinematic viscosity
ρ	material density
σ	drop velocity standard deviation
σ^2	drop velocity variance
Φ	drop vaporization rate
ϕ	drop diameter
ψ	drop temperature probability density function
φ	drop velocity probability density function

Subscripts

g	gas phase
i	sample index
j, k	vector component index
l	liquid phase
n	section or bin index
x, y	Cartesian coordinate components

Superscripts

i	order of moment

Symbols

$\nabla_x = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$	spatial gradient operator
$\nabla_v = \frac{\partial}{\partial v_x} + \frac{\partial}{\partial v_y} + \frac{\partial}{\partial v_z}$	velocity gradient operator
$\langle \cdot \rangle$	ensemble average operator

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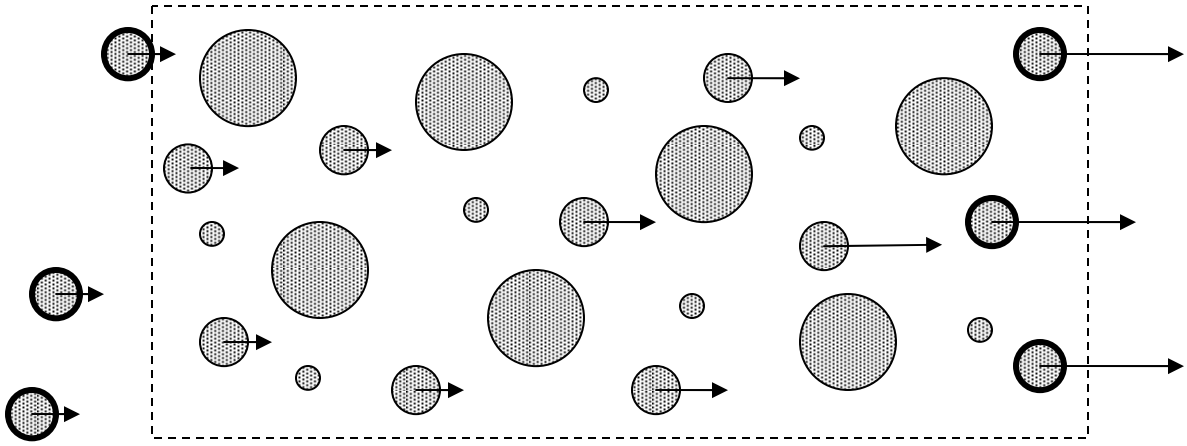

Figure 1. Drop flow through volume with velocity gradient on medium-sized drops in a volume at time t

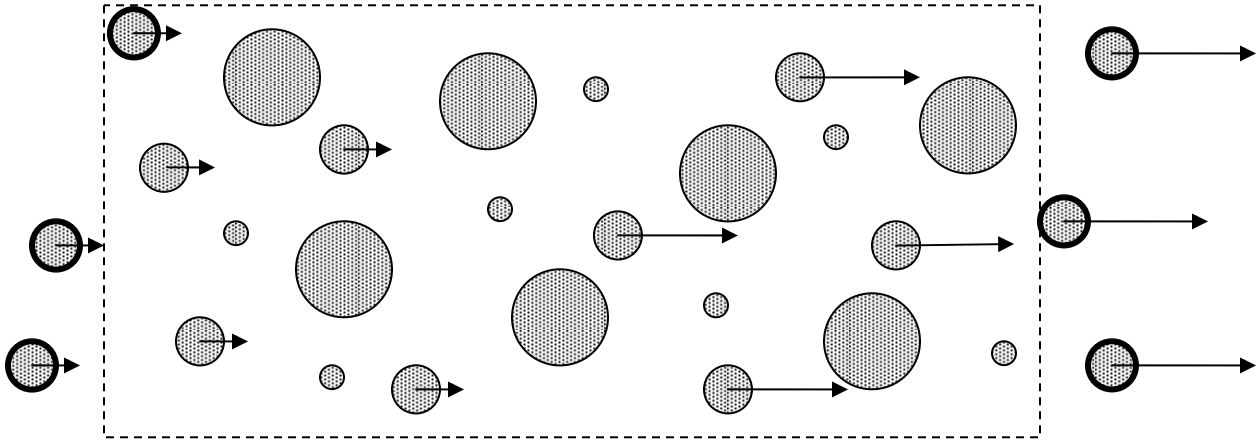

Figure 2. Drop flow through volume with velocity gradient on medium-sized drops in a volume at time $t+\Delta t$

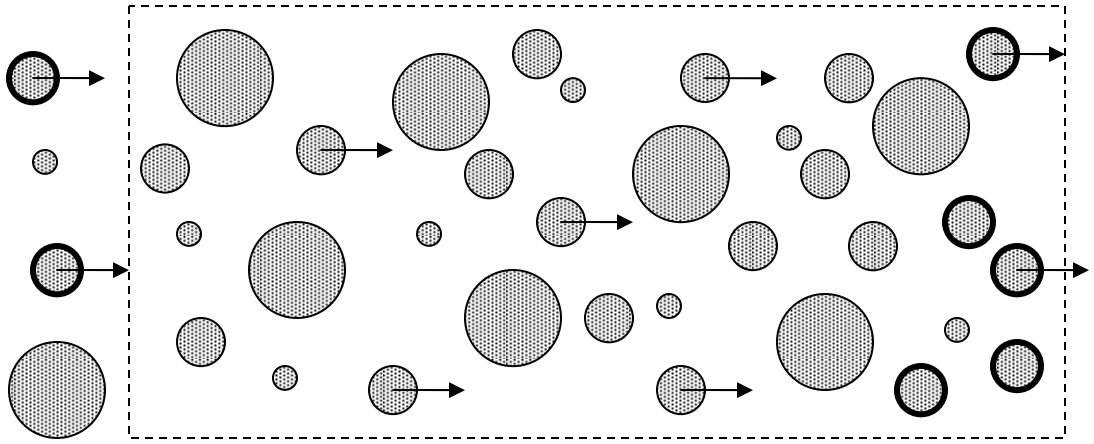

Figure 3. Drop flow through volume with number density gradient on medium-sized drops in a volume at time *t*