The Formulation of Spray Combustion Models: Resolution Compared to Droplet Spacing

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Formulations of the governing equations for burning air/fuel spray mixtures are discussed. The subsystem of equations describing liquid properties is formulated in three ways: Eulerian description, Lagrangian description, and probabilistic or distribution function description. The relationships among these approaches and the relative advantages and disadvantages are discussed. The reduction of numerical error, the ability to resolve multivalued solutions, and the ability to achieve resolution a scale smaller than droplet spacing lead to a preference of the Lagrangian method over the Eulerian method. However, when resolution is desired on a scale smaller than the average droplet spacing, the location of each droplet is known only in a statistical manner. The advantages of a probabilistic formulation in this case are evaluated.

I Introduction

The problem of spray combustion is of vital importance to practical combustors. It is mandatory to have reliable models of the relevant mechanical, physical, and chemical systems in order to achieve the predictive capability desired by the practicing combustion engineer and to acquire the understanding and insights sought by the combustion scientist.

In any review paper on the subject of spray combustion, complete coverage of the contributions cannot be presented on account of the limitations of times and expertise of any author. In this paper, which was an invited review at the 1984 ASME Winter Annual Meeting, the author does not even attempt to cover all material of interest to him since he has recently published an extensive review [1] on fuel droplet vaporization and spray combustion. Herein, the emphasis will be placed on the two-phase flow models that form the basis for computation.

An important factor for spray combustion calculations is the vaporization rate of individual droplets. Most of the existing work does not completely account for the effect of neighboring droplets on the rates of heat and mass transport and vaporization for any given droplet. There are two major ways in which these rates are affected. Firstly, the ambient gas properties just outside the film or boundary layer surrounding each droplet are affected by neighboring droplets since the gas exchanges mass, momentum, and energy with those droplets. Secondly, the Nusselt number or Sherwood number (or equivalently the characteristic length scales) is affected by the presence of the other droplets. The former phenomenon has been considered widely but the latter phenomenon has received limited attention [1-7]. The results of the spray calculations can be strongly related to the details of the vaporization model [8-15]. This is especially true in typical combustion situations where the ambient gas temperature is high and the vaporization rate is so high that droplet lifetimes and droplet heating times are of the same order of magnitude. It is noteworthy therefore that one should be very suspect of empirical spray vaporization based upon experimental data obtained in lower temperature ranges. The issues related to the vaporization rate of individual droplets will not be further discussed here.

In this paper, we shall discuss various approaches to formulating the system of differential equations that governs the spray and gas behavior in a coupled manner. Some comments will also be made about numerical methods of solution. The concept of treating the droplet properties as if they were continuous in the same domain as the gaseous properties will be discussed. This conceptual approach is useful when we are interested in resolving gas and liquid properties on a scale that is large compared to the average spacing between droplets. Here a droplet property at a point in space and time represents the average value over many droplets in a neighborhood of that point. An alternative approach is to track individual droplets and to calculate the properties for each droplet in the domain of interest. Obviously, this approach is useful when we are interested in resolution on a scale smaller than the average distance between droplets.

Several examples of such situations, where resolution must be finer than the droplet spacing, can be cited. Firstly, in the ignition of sprays by sources which are hot bodies or jets of hot gases, a thermal layer develops with time at the edge of the spray bordering the ignition source. Typically, the thermal layer reaches a thickness of a few millimeters at the end of the ignition time delay for a hydrocarbon fuel spray at atmospheric and near-stoichiometric conditions. For droplets of the order of 50–100 μm in diameter and near-stoichiometric mixtures, that thermal layer thickness is only a very few droplet spacings. A second example concerns a laminar flame propagation through a spray. For reasonably volatile fuels or for small droplets, the fuel vapor content in the mixture ahead of the flame can be sufficiently great to sustain a flame which would be a few millimeters in thickness. The droplets passing through this flame will heat and vaporize rapidly augmenting the combustion of the prevaporized fuel. Again, the thickness of the prevaporized fuel flame is a few droplet spacings so that fine-scale resolution with inherent unsteadiness is required. Another example involves group combustion of spray as defined by Chiu and co-workers [16-18]. In the limiting case of group combustion, a case of external sheath combustion results where only the droplets in a thin sheath or layer at the edge of a group of droplets are vaporizing. This layer regresses toward the interior of the sheath. Under proper conditions, this layer is only a few droplet spacings thick.

In each of the above examples, the results depend upon the initial conditions of the droplets including location, velocity, diameter, temperature, and composition. In a real spray these conditions will not be known exactly; only a distribution or probability function can be assigned. However, once we know the initial conditions for the droplets we can proceed to solve the problem in a deterministic fashion.

In Section II, we shall consider a two-continuum formulation wherein the gas properties and the droplet properties are

each described by equations in the Eulerian form. This Eulerian–Eulerian form is not useful when resolution is desired on a scale as small as or smaller than the average distance between droplets. In Section III, we examine an Eulerian–Lagrangian approach wherein the gas properties are formulated in an Eulerian manner and the droplet properties are given in a Lagrangian formulation. We shall see that such a formulation is useful over a wide range of resolution. However, when resolution over a very fine scale compared to average droplet spacing is required, the practical problem becomes probabilistic rather than deterministic since we do not know exactly where each droplet is at each instant of time. In Section IV, a probabilistic formulation and its relationships with other formulations are discussed. This method also allows for a wide range of resolution since the probability density function (pdf) can be considered to give the number of droplets found in the smallest volume of resolution when the scale of resolution is very large compared to the average distance between droplets. When the resolution scale is very fine, the pdf shall be considered as the probability of finding one droplet in that smallest volume. Usually, the pdf approach has been used as a basis for analysis which yields other formulations that are employed for final solution of the spray behavior. In Section V, we discuss direct solution using the probabilistic formulation in cases where resolution on a very fine scale is desired. Concluding remarks are given in Section VI.

II Eulerian–Eulerian Formulation

The describing equations for a vaporizing and reacting spray can be obtained by a standard control volume approach which accounts for the fluxes of mass, momentum, and energy for the gas phase and also for the liquid phase through entering and exiting the control volume. Unsteady storage terms in the volume, exchanges of mass, momentum, and energy between the phases, and effects of chemical reaction are considered in order to balance the equations. Species conservation equations are written for each of the gas-phase species via the same control volume approach. Under the assumption that coalescence and breakup of droplets are insignificant after the initial atomization period, droplet numbers are conserved and the control volume method yields a droplet number continuity equation. The continuity equations for droplet number density and for droplet distribution function in this paper are formulated such that droplets are counted even after the radius becomes negligible or zero. If compared to experimental data, renormalization is therefore necessary since only droplets of certain minimum radii can be counted experimentally.

The equations may be derived in one, two, or three space dimensions in a steady or unsteady form. The gas-phase and the droplet properties are considered to be continuous in space and time. This implies that the properties at any point are the average values over some neighborhood of that point. The size of that neighborhood is much larger than the average spacing between droplets. This averaging method allows for the superposition of a continuous gas field and a continuous liquid droplet field. The initial conditions could be specified in a locally monodisperse fashion. This means that at each point in space one initial droplet size is specified. Since the equations do not allow for multivalued solutions, the spray will remain locally monodisperse. If desired, a polydisperse spray may be represented by the superposition of several monodisperse sprays. This is equivalent to approximating a continuous size distribution function by several delta functions. When this is done, we must formulate equations for the conservation of mass, momentum, energy, and droplet number for each distinct class of droplet as determined by the initial size.

In our formulation, we shall examine a multidimensional, unsteady situation for a dilute spray. In this spray, the volume of liquid contained in a volume of the smallest resolution is very small compared to that volume. Realize that in a combustion situation the mass of air required is at least one order of magnitude larger than the mass of fuel required. Furthermore, except for near-critical or supercritical situations, the liquid density is one to three orders of magnitude greater than the gas density. We will not use a void fraction in the equations for this reason.

The droplet continuity equation becomes

$$\frac{\partial n^{(k)}}{\partial t} + \frac{\partial (n^{(k)} u_j{}^{(k)})}{\partial x_j} = 0 \qquad (1)$$

where $n^{(k)}$, $u^{(k)}{}_{ij}$, t, and x_j are the droplet number density, the droplet velocity component in the j direction, the time coordinate, and the spatial coordinate in the j direction, respectively. The superscript k represents the integer index for the class of droplets as determined by the initial size. For a monodisperse spray $k = 1$ while for a polydisperse spray $k = 1, 2, \ldots, N$ where N is chosen to give a reasonable fit to the distribution.

After some manipulation, the other conservation equations for the droplet properties will yield a droplet size equation, a droplet drag equation, and a droplet energy equation. The droplet size equation is

$$\frac{\partial R^{(k)}}{\partial t} + u^{(k)}{}_{ij} \frac{\partial R^{(k)}}{\partial x_j} = \frac{-\dot{m}_j{}^{(k)}}{4\pi (R^{(k)})^2 \rho_l} \qquad (2)$$

where $R^{(k)}$ is the instantaneous droplet radius, ρ_l is the liquid density, and $\dot{m}_j{}^{(k)}$ is the mass vaporization rate of a droplet. This rate is determined by some algorithm based upon a physical model of the behavior of the field in the liquid droplet and in the surrounding gas film. See [1, 8–15].

The droplet drag equations are given as

$$\frac{\partial u_{l_i}{}^{(k)}}{\partial t} + u_{l_j}{}^{(k)} \frac{\partial u_{l_i}{}^{(k)}}{\partial x_j} = F_i{}^{(k)} \qquad (3)$$

where $F_i{}^{(k)}$ is the ith component of drag force on the droplet per unit mass of droplet. This drag can be modeled based upon some empirical evidence in the literature. (See [1].)

The liquid-phase energy equation may be formulated as

$$\rho_l \frac{\partial e_l{}^{(k)}}{\partial t} + \rho_l u^{(k)}{}_{ij} \frac{\partial e_l{}^{(k)}}{\partial x_j} = \frac{3}{R^{(k)}} \lambda_l \left(\frac{\partial T_l{}^{(k)}}{\partial r} \right)_s \qquad (4)$$

where $e_l{}^{(k)}$ is the average thermal energy per unit mass in the liquid. (Note that temperature gradients will exist in the liquid and the temperature variation can be determined by a solution of the heat diffusion in the liquid phase.) λ_l is a liquid thermal conductivity, $T_l{}^{(k)}$ is a liquid temperature, r is radial position in the droplet, and s is an index indicating a value at the droplet surface. The heat flux term should be taken as an average value over the surface.

The gas-phase continuity equation states that

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = \sum_{k=1}^{N} n^{(k)} \dot{m}_v{}^{(k)} \qquad (5)$$

where ρ and u_j are the gas density and gas velocity component in the j direction. The species continuity equations are written as

$$\frac{\partial}{\partial t} (\rho Y^{(l)}) + \frac{\partial}{\partial x_j} (\rho u_j Y^{(l)}) - \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y^{(l)}}{\partial x_j} \right)$$
$$= \sum_{k=1}^{N} n^{(k)} \dot{m}_v{}^{(k,l)} + \dot{w}^{(l)} \qquad (6)$$

Here $Y^{(l)}$ is the mass fraction of species l, D is a mass diffusivity (which is assumed to be the same for all species), $\dot{m}_v{}^{(k,l)}$ is the mass vaporization rate for the lth species (which is zero if that species is not one of the components of the fuel blend), and $\dot{w}^{(l)}$ is the mass chemical reaction rate for the lth species

(which is nonzero if that species is a reactant or a product).
Note that

$$\dot{m}_v^{(k)} = \sum_{i=1}^{\hat{N}} \dot{m}_v^{(k,i)} \qquad (7)$$

where $\hat{N}$ is the number of different species present. The $\hat{N}$ species equations can be summed to yield the continuity equation; therefore, only $N-1$ of the equations are independent.

The gas momentum equation can be formulated as:

$$\rho \frac{\partial u_i}{\partial t} + \rho u \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_u}{\partial x} = \sum_{k=1}^{N} n^{(k)} \dot{m}_v^{(k)}[u_{l_i}^{(k)} - u_i]$$

$$- \sum_{k=1}^{N} \frac{4\pi}{3} \rho_l [R^{(k)}]^3 n^{(k)} F_i^{(k)} \qquad (8)$$

Here p is the pressure and τ_{ij} is the viscous stress tensor.
The gas energy equation may be written as follows:

$$\rho c_p \frac{\partial T}{\partial t} + \rho u_j c_p \frac{\partial T}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) - \frac{\partial p}{\partial t}$$

$$= \sum_{k=1}^{N} \dot{w}^{(l)} Q^{(l)} - \sum_{k=1}^{N} n^{(k)} \dot{m}_v^{(k)}[h - h_s + L^{(k)}_{\text{eff}}] \qquad (9)$$

where T, c_p, λ, and h are the gas temperature, specific heat, thermal conductivity, and enthalpy outside of the gas films surrounding droplets. h_s is the gas enthalpy at the droplet surface; $Q^{(l)}$ is the energy released in combustion of the lth component (if that component is not a fuel, $Q^{(l)}$ is zero); and $L^{(k)}_{\text{eff}}$ is an effective latent heat of vaporization which accounts for the heat conducted into the surface of the droplet. This form of the energy equation is based upon a neglect of kinetic energy, viscous dissipation, radiation, and transport of energy via mass diffusion of species with different specific heats. Part of this heat is necessary for vaporization and the remainder is stored in the liquid interior.

It can be shown that

$$L^{(k)}_{\text{eff}} = L^{(k)} + 4\pi\lambda_l \left(\frac{\partial T_l^{(k)}}{\partial r}\right)_s (R^{(k)})^2 / \dot{m}_v^{(k)} \qquad (10)$$

where $L^{(k)}$ is a latent heat of vaporization for the fuel. For a single-component fuel, $L^{(k)}$ may be regarded as a constant independent of droplet size while for a multicomponent fuel, it depends upon the relative vaporization rates and the latent heat of each component. In that case, it implicitly can be time and size dependent. For proper evaluation of that heat flux, a droplet heating and vaporization model is required. See [1, 8–15].

An ideal gas law may be written as

$$p = \rho R T \qquad (11)$$

where the gas "constant" R depends upon the local mixture composition.

The above-described model is based upon diffusion governed by Fick's Law and laminar flows. Generalizations for other situations have been presented in the literature. The chemical rate terms may be modeled here via single-step or multistep kinetics as preferred. The formulation also assumes that the time for energy and mass transport across the gas film surrounding a droplet is negligible.

Equations (1) through (4) represent $4N$ equations governing the liquid properties $n^{(k)}$, $R^{(k)}$, $u_{l_i}^{(k)}$, and $e_l^{(k)}$. Of course, since equation (3) is a vector equation, we really have $6N$ scalar equations. Equation (4) is, however, never actually employed in the form presented. In the special case where droplet temperature is assumed to be uniform in the droplet, we consider that $e_l^{(k)}$ is directly proportional to $T_l^{(k)}$ and that the heat flux term on the right-hand side of equation (4) is not

represented in terms of a temperature gradient at the surface but rather as the difference between the heat flux coming from the gas to the surface and the rate of energy conversion associated with the vaporization process. In general, for combustion applications where heating rates are rapid, the uniform temperature model is not recommended. In the case where temperature gradients in the droplet are taken into account, it is not useful to evaluate $e_l^{(k)}$ which is the average liquid thermal energy per unit mass. Therefore, equation (4) is not employed. Rather, the equations governing energy transport in the film surrounding the droplet and in the liquid interior are solved as discussed in [1, 8–15].

Equations (5), (6), (8), and (9) represent a subsystem of 5 + $(\hat{N} - 1)$ partial differential equations governing scalar gaseous properties. They can be solved numerically via finite difference schemes on an Eulerian mesh by explicit, implicit, block implicit, or split operator techniques. In general, the problem has many time and space scales and it is difficult to give a general preferred method for integration. Note that in the one-dimensional case with low flow Mach number, the momentum equation (8) may be replaced by a uniform pressure assumption. In confined flows, the pressure may still be time varying. An example of this type of calculation is given in [19].

The subsystem of equations governing the droplet properties is also solved numerically by finite difference schemes on an Eulerian mesh. The numerical scheme might introduce artificial diffusion into the results. Although the same effect may be present with the gas properties, it is less severe there since it is superimposed upon real diffusion effects. Since no physical diffusion of liquid properties occurs (the behavior is totally hyperbolic), artificial or numerical diffusion is more bothersome there. An example of a troublesome situation is one where a sharp boundary exists between a region where fuel spray and gas occur and a region where only gas exists. Numerical errors could lead to a diffusion of liquid properties across these boundaries.

In this two-continuum approach, droplet properties represent averages in neighborhoods so that only single-valued solutions should be allowed. In practice, however, multivalued solutions are possible and interesting. This occurs when we have two or more clouds of droplets (all in the same class as determined by initial size), with each cloud following different paths which cross in space and time. Realize that, since the droplets are small in size compared to the average spacing between droplets, the droplet clouds may cross paths with each other with no or negligible collisions. In general, the droplets in different clouds will have different properties such as size and temperature, even if initially they were of the same size and same temperature. Therefore, the two or more clouds on intersecting paths should have different temperatures, different diameters, and different velocities. Such physically meaningful multivalued solutions are lost due to a combination of the averaging of properties and the large numerical diffusion which occurs when the two clouds approach each other creating large gradients of the averaged properties. Note that most finite difference schemes are designed to provide unique solutions to partial differential equations and would automatically suppress multivalued evolutions.

The two-continuum approach is not able to resolve phenomena on the scale of the droplet spacing since averaging occurs over a distance that is large compared to that spacing.

On account of these problems with an Eulerian–Eulerian formulation, the approach of the next section becomes worthy of attention.

III Eulerian–Lagrangian Formulation

An alternative approach [20–22] has received attention in recent years. The gas-phase subsystem of equations (5)–(11) remains the same as in the previous section. The droplet prop-

erties are no longer governed by equations (1)–(4), however. Instead, ordinary differential equations are written which describe the change in droplet properties along the droplet path.

We have the choice of following every individual droplet which is representative of a fixed number of droplets in a neighborhood. It is assumed here that initial conditions are continuous so that any droplet which begins in the neighborhood of some given droplet remains in the neighborhood of that droplet as they both move. On account of this type of calculation which involves a fixed number of droplets, there is no need to develop an equation for the conservation of droplet numbers; droplet numbers are automatically conserved.

It is necessary to track the droplets as they move. The trajectory is given by

$$\frac{dx_{li}^{(k)}}{dt} = u_{li}^{(k)} \tag{12}$$

where $x_{li}^{(k)}$ is the position of the center of the droplet in the kth size class. In general, the paths will not pass through mesh points for the Eulerian calculation of the gas-phase properties.

The droplet radius is governed by

$$\frac{dR^{(k)}}{dt} = \frac{-\dot{m}_v^{(k)}}{4\pi(R^{(k)})^2\rho_l} \tag{13}$$

This is essentially equivalent to equation (2) except that a Lagrangian time derivative is taken.

The droplet velocity is given by the relationship

$$\frac{du_{li}^{(k)}}{dt} = F_i^{(k)} \tag{14}$$

while the droplet thermal energy can be calculated via

$$\rho_l \frac{de_l^{(k)}}{dt} = \frac{3}{R^{(k)}} \lambda_l \left(\frac{\partial T_l^{(k)}}{\partial r}\right)_s \tag{15}$$

Note that equation (12) not only gives the droplet path but it also describes the characteristic direction for the first-order hyperbolic partial differential equations (2), (3), and (4). We may view equations (12)–(15) as describing a method of characteristics whereby integration occurs along the characteristic paths.

The integration of these ordinary differential equations along the trajectories or characteristic lines avoids numerical diffusion which would result from upwind differencing of the spatial derivatives in the hyperbolic equations (1)–(4). One must be careful, however, in interpolation between the Lagrangian mesh and the Eulerian mesh. This interpolation is necessary because the droplet equations and the gas equations are strongly coupled due to the exchange of mass, momentum, and energy and the characteristic paths, in general, pass between rather than through the Eulerian mesh points. The interpolation scheme should be second order accurate in order to avoid errors of the same magnitude as the numerical diffusion which has been eliminated [21].

When resolution is desired on a scale large compared to the spacing between droplets, each characteristic is representative of many droplets. The characteristics along which droplet calculations are made should be chosen so as to be separated by a distance of the same order of magnitude as the Eulerian mesh size for the gas property calculations. In this case, characteristics may cross, implying multivalued solutions, without significant collisions between droplets.

In the case where resolution is desired on a scale small compared to the spacing between droplets, a calculation of equations (12)–(15) is performed for each droplet. Obviously, a limited number of droplets can be considered in accordance with computer resources. The Eulerian mesh size for the gas property calculations is taken to be small compared to the droplet spacing. The approximation is made that the droplets

provide point monopole sources of mass, momentum, and energy so droplet diameter and varying vaporization rate over the droplet surface are not taken into account. Typically, no more than one droplet center and usually none exists in any cell defined by the Eulerian mesh points. The source terms are distributed via linear interpolation at the two, four, or eight rectangular mesh points (for one, two, or three dimensional calculations) that define the edge of the cell containing a droplet. Realize that if two droplet paths cross in these calculations, a collision is implied (unless the mesh size is much larger than a droplet diameter).

The Eulerian–Lagrangian approach can be used either in a case where the droplet properties are viewed as a second continuum superimposed upon the gas field or in a case where droplets are considered as discrete particles which are individually tracked. In the former case, the Lagrangian calculations are a method of characteristics and resolution is expected on a scale that is large compared to the droplet spacing. In the latter case, resolution is expected on a scale that is small compared to droplet spacing. In the intermediate case where mesh size and average droplet spacing are of the same order of magnitude, the droplet properties cannot be viewed as continuous but the error associated with discrete particle calculation is large; for example, the crossing of droplet paths does not necessarily imply collision since resolution has been lost in the calculation.

IV Probabilistic Formulation

It is sometimes convenient to define a droplet number distribution function or, in other words, a droplet number probability density function. This function $f(x, t, R, v, e_l)$ depends upon spatial position x, time t, droplet radius R, droplet velocity v, and droplet thermal energy e_l. f is a function of time plus eight scalar properties; we consider an infinitesimal eight-dimensional volume as $dV = dx\, dv\, dR\, de_l$, and $f\,dV$ is the number of droplets in the infinitesimal volume located at x, v, R, and e_l at the instant of time t.

When the desired resolution of the liquid and gas properties is sufficiently coarse so that the volume of a cell in a numerical mesh would contain very many droplets, we can view the droplet properties as continuous. At the other extreme where very fine resolution is required, most cells will not contain a droplet at some particular instant of time. The exact location of the individual droplets will not be known in a practical spray situation. The function f should be viewed as the probability of finding a droplet in a unit volume of eight-dimensional space.

When resolution is required on a large scale, averaging over many droplets is useful. Among other things, this averaging eliminates unsteadiness on the scale of the spacing between droplets; if no large-scale unsteadiness is present, the average properties will behave in a steady fashion. However, when fine-scale resolution is required, averaging is not useful and the unsteadiness on the scale of droplet spacing is inherent. For example, the motion of droplets through the gas is unsteady on the fine scale since at one instant of time a droplet may be at some position and at a later instant, the droplet has moved and gas exists at the same position. With averaging on the coarse scale, both droplet properties and gas properties will exist at any point at any time and this type of unsteadiness is not resolved.

If we assume conservation of droplet numbers and consider a sufficiently dilute spray so that droplet collisions are negligible, the following evolution equation may be derived

$$\frac{\partial f}{\partial t} + \frac{\partial(v_j f)}{\partial x_j} + \frac{\partial(F_j f)}{\partial v_j} + \frac{\partial(\dot{R}f)}{\partial R} + \frac{\partial(\dot{e}_l f)}{\partial e_l} = 0 \tag{16}$$

where the superscript dot denotes a time derivative. If we relate the divergence term to the rate of change of a small volume ΔV in eight-dimensional space, we have

$$\frac{1}{\Delta V}\frac{d(\Delta V)}{dt}=\frac{\partial v_j}{\partial x_j}+\frac{\partial F_j}{\partial v_j}+\frac{\partial \dot{R}}{\partial R}+\frac{\partial \dot{e}_l}{\partial e_l}$$

and therefore by combination with equation (16), we find

$$\frac{\cdot}{\cdot}(f\Delta V)\equiv\left(\frac{\partial}{\partial t}+v_j\frac{\partial}{\partial x_j}+F_j\frac{\partial}{\partial v_j}+\dot{R}\frac{\partial}{\partial R}+\dot{e}_l\frac{\partial}{\partial e_l}\right)f\Delta V=0 \tag{17}$$

This equation states that the number of droplets $f\Delta V$ remains constant along the trajectory in eight-dimensional space.

Integration of equation (16) and its moments will lead to equations (1)–(4). It is useful to define the droplet number density

$$n^{(k)}=\iiint f^{(k)}dv\,dR\,de_l \tag{18}$$

Here and later, integration with respect to the three velocity components and the thermal energy is performed over the infinite ranges of values. Note that we have a different distribution function $f^{(k)}$ for each class of droplet; the kth class of droplets is the set of all droplets with initial radius between $\zeta^{(k-1)}$ and $\zeta^{(k)}$ where $\zeta^{(0)}$, $\zeta^{(1)}$, etc., is a monotonically increasing sequence. The average initial radius for the kth class will be between the values of $\zeta^{(k-1)}$ and $\zeta^{(k)}$. The vaporization will lead to droplet radius of the kth class decreasing below $\zeta^{(k-1)}$ toward zero; the limits of integration with respect to radius are $\cdot$ and $\zeta^{(k)}$ for the kth class of droplets.

We also define the average droplet velocity

$$\langle u_{l_i}{}^k\rangle=\frac{\iiint v_i f^{(k)}dv\,dR\,de_l}{n} \tag{19}$$

Here $\langle\ \rangle$ implies an average over a large number of droplets. Similarly, we define

$$\langle F_i^{(k)}\rangle=\frac{\iiint F_i f^{(k)}dv\,dR\,de_l}{n} \tag{20}$$

$$\langle \dot{R}^{(k)}\rangle=\frac{\iiint \dot{R} f^{(k)}dv\,dR\,de_l}{n} \tag{21}$$

$$\langle R^{(k)}\rangle=\frac{\iiint R\,f^{(k)}dv\,dR\,de_l}{n} \tag{22}$$

$$\langle \dot{e}_i^{(k)}\rangle=\frac{\iiint \dot{e}_i f^{(k)}dv\,dR\,de_l}{n} \tag{23}$$

$$\langle e_i^{(k)}\rangle=\frac{\iiint e_i f^{(k)}dv\,dR\,de_l}{n} \tag{24}$$

We can interpret equation (16) as governing $f^{(k)}$ for each value of k. Integration of (16) with use of the definitions (18) and (19) leads to an equation governing droplet number density for each value of k

$$\frac{\partial n^{(k)}}{\partial t}+\frac{\partial}{\partial x_j}(n^{(k)}\langle u_{l_j}^{(k)}\rangle)=0 \tag{25}$$

This equation is essentially identical to equation (1). They strictly identical when the variations of f^k with respect to initial values of R, v_i, and e_l are represented by delta functions. If the ranges $\Delta\zeta=\zeta^{(k)}-\zeta^{(k-1)}$ are sufficiently narrow, and if at any x position at the initial time both e_l and v_i correlate well with R, the distinction has no practical significance. By a good correlation we mean that each narrow initial size a narrow range of e_l values and a narrow range of v_i values associated with it. For our purposes, we disregard the differences, eliminate the use of the averaging symbol $\langle\ \rangle$, and regard the two equations as identical.

Now, if we multiply equation (16) by v_i and integrate the resulting moment equation, we find an equation essentially equivalent to equation (3). In addition to the neglect of differences such as mentioned above, we neglect effects of the

order of the dot product of $v_i-u_{l_i}{}^{(k)}$ with itself. This error is insignificant if droplets in the same initial size range do not vary widely in their initial velocity; a correlation of initial size and initial velocity is implied.

Multiplication of equation (16) by R and integration leads to an equation approximately equivalent to equation (2). If the initial droplet diameter and the initial droplet velocity are not widely varying and do correlate well, the approximation is good; in the limit where the distribution function becomes a delta function, the two equations are exact. Similarly, e_l is multiplied by equation (16) and the resulting equation can be integrated to yield an equation approximately equivalent to equation (4). These two equations become identical as the distribution function becomes a delta function.

The characteristics for equation (17) are

$$\frac{dx_i^{(k)}}{dt}=v_i^{(k)} \tag{26}$$

$$\frac{dv_i^{(k)}}{dt}=F_i^{(k)} \tag{27}$$

$$\frac{dR^{(k)}}{dt}=\dot{R}^{(k)}=-\frac{\dot{m}^{(k)}}{4\pi(R^{(k)})^2\rho_l} \tag{28}$$

$$\frac{de_l^{(k)}}{dt}=\dot{e}_l^{(k)}=4\pi(R^{(k)})^2\lambda_l\left(\frac{\partial T_l^{(k)}}{\partial r}\right)_s \tag{29}$$

Realize that averaging of these equations via integration over many droplets yields equations similar to equations (12)–(15). As the distribution function $f^{(k)}$ goes to a delta function, the two sets of equations become exactly identical. Otherwise, the two sets have important differences that are self-evident.

In the case where resolution is desired on a scale smaller than the droplet spacing, integration of equations (26)–(29) describes the path along which some probable number of droplets will move through eight-dimensional space. Note that equation (16) or equivalently the system of equations (26)–(29) is deterministic in nature with no randomization effect present. The initial conditions for those equations will be random in practical situations but once conditions are specified, the droplets will behave in a deterministic fashion. Equation (16) is different, therefore, from the Boltzmann equation for the kinetic behavior of gases where the collision term provides a randomizing effect that usually makes the solutions independent of the detailed initial conditions. In the droplet case, the solution to (16) is strongly dependent on initial conditions. Randomization effects may occur with sprays in special situations that we shall not consider. One example is the case where turbulent fluctuations in the gas cause a dispersion of the droplets. Another special situation is the case of very small droplets where Brownian motion is important.

The distribution function that has been formulated here is somewhat more general than what exists in the literature. In particular, the dependence on the droplet thermal energy has been included. Since droplet heating strongly affects vaporization rate which affects droplet size and, in turn, influences droplet drag and trajectory since trajectory and heating are related via a varying gas environment, we see that a strong coupling exists. While the inclusion of thermal energy is important, the present approach is limited. The extension to a more exact description is obvious.

Whenever droplet heating is sufficiently rapid tempertaure gradients will occur in the droplet interior. It is then necessary to solve a heat diffusion equation in the liquid. Although the partial differential equation is linear, the boundary condition at the regressing droplet surface causes the problem to be nonlinear. Numerical integration of the diffusion equation has been performed but a more efficient approximate method is recommended [14, 19, 27, 28]. A Green's function is

developed via eigenfunction expansion; then the partial differential equation in the droplet interior is transformed to an integral equation for the droplet surface temperature. The coefficients multiplying the eigenfunction in the expansion are time-varying and from the integral formulation, a system of ordinary differential equations governing these coefficients is developed. In the solution of these first-order ordinary differential equations, marching with Lagrangian time occurs along the droplet trajectory. e_l would be now eliminated as a dependent variable. It would be replaced by the number of coefficients in the eigenfunction expansion required for convergence of that expansion.

The use of such coefficients would increase the number of terms in equation (16). In principle, an infinite number of terms is required in an eigenfunction expansion but, in practice, a finite number will suffice. Likewise equation (29) would be replaced by a set of ordinary differential equations governing the coefficients along the characteristic paths. Note that the extension of variables to account for droplet temperature would also imply that equations (4) and (15) would each be replaced by a set of equations governing the coefficients.

Another generalization of the distribution function and of equation (16) can be made for the case of multicomponent fuels. Here the composition of the droplets becomes relevant; the composition varies spatially as well as temporally. It is necessary to solve an equation for mass diffusion in the liquid phase. An eigenfunction approach can also be made for this effect with an extension of the number of the independent variables for the distribution function and of the number of characteristic equations.

V   Droplet Spacing and Probabilistic Behavior

An equation governing the droplet number distribution function, such as equation (16), has typically been used via integration of moments to obtain other equations governing average liquid properties; it generally is not employed directly to solve for the distribution function. However, in an emerging set of problems, there is an interest in dealing with phenomena that must be resolved on a scale as small as or smaller than the average spacing between them. It is useless and, in fact, counterproductive to seek average properties by integrating over a scale large compared to the droplet spacing. Rather, we must treat directly equation (16), or equivalently, equations (26)–(29).

A need is seen, therefore, for a theoretical/computational approach to this probabilistic problem. There are two general approaches that might be developed. At this point, the more straightforward approach is to solve a large number of deterministic problems where different sets of initial conditions are employed in each calculation. The probability density function associated with each set of initial conditions provides a weighting factor on the results of all the calculations. With this weighting factor, the statistical results can be developed.

A second approach would involve direct solution of equation (16) coupled with the solution of equations (5)–(11) governing the gas phase. Since the droplet properties have a probabilistic character, the source terms in equations (5), (6), (8), and (9) related to droplet vaporization and drag will also have a probabilistic character. Therefore, the gas properties which are solutions to these equations will have a probabilistic character and will depend upon an extended set of independent variables in the same fashion as the droplet distribution function depends upon these variables. It is felt that it is better to proceed with the former approach and to accept the tradeoff in favor of lower dimensionality at the expense of more but less extensive calculations.

Suppose, as an example, we were interested in the ignition of a monodisperse fuel spray which at the initial time is stagnant and is placed in contact on one side with a hot planar surface. A one-dimensional unsteady analysis of this situation

has been performed [23]. It has been found that the ignition delay and the minimum ignition energy are very sensitive to the initial distance from the hot wall of the droplet nearest to the wall. This is the result of many deterministic calculations for different initial droplet locations x_0. As a result of this set of deterministic calculations, we can deduce the ignition delay time

$$\tau_{ig} = \tau_{ig}(x_0)$$

Now, say we also know that the probability of having the initial condition between the values of x_0 and of $x_0 + dx_0$ is $f(x_0)dx_0$. Then the probability for the ignition delay to have a value between τ_{ig} and $\tau_{ig} + d\tau_{ig}$ is given by

$$P(\tau_{ig})d\tau_{ig} = \Sigma f(x_0(\tau_{ig}))dx_0$$

where a summation is taken since more than one value of x_0 may exist for a given value of τ_{ig}. It follows that the probability function for ignition delay can be related to the probability function for location of the nearest droplet to the ignition source by the formula

$$P(\tau_{ig}) = \Sigma f(x_0(\tau_{ig})) \frac{dx_0}{d\tau_{ig}} (\tau_{ig})$$

Obviously, it is convenient to invert the function $\tau_{ig}(x_0)$ to obtain $x_0(\tau_{ig})$. This method exemplifies the first approach described above.

The interesting result is that the ignition delay and also the minimum ignition energy will not have precise values for a given mixture ratio as they do for a gaseous mixture. Rather, ranges of values exist and we can represent the ignition delay and the minimum ignition energy in a statistical manner for a spray. Therefore, the statistical results are of practical engineering value.

More work is required in order to apply these concepts to a wider range of problems. Also, in addition to the statistical variation in droplet location, the variations in droplet size, velocity, and temperature can be taken into account in future studies.

VI   Concluding Remarks

The three formulations of equations describing the liquid properties have been presented and the relationships among them with relative advantages and disadvantages have been discussed.

In situations where resolution is desired only on a scale that is large compared to the average spacing between droplets, the Lagrangian formulation of the droplet equation is superior to the Eulerian formulation. The advantages are that numerical error is more easily reduced and the ability to resolve multivalued solutions is maintained in the Lagrangian method. The probabilistic formulation is not directly useful on this scale but serves as a basis for developing other formulations. Examples of cases with coarse resolutions where deterministic Lagrangian or Eulerian calculations have been useful are presented in [19–25].

In other situations where the droplet spacing is as large as or larger than the resolution scale, the Eulerian formulation governing average droplet properties is not useful. The Lagrangian formulation only remains useful when applied to individual droplets rather than to the average droplet in some cluster of droplets. That is, on this scale, the Lagrangian method should be used as a method of characteristics for the hyperbolic equation (16) which governs the probability density function rather than as a method of characteristics for the hyperbolic system of equations (1)–(4) which govern the average droplet properties. At this point, it seems more convenient to solve equation (16) indirectly by a method of characteristics, as represented by equations (26)–(29), than to solve it directly. If some randomizing effect such as turbulent motion entered equation (16) this last conclusion might change.

An interesting approach that employs a gas concentration pdf for spray analyses can be found in [26]. The pdf discussed in that paper is different from the pdf discussed herein, however, in that we are dealing with liquid properties in this paper.

The equations presented herein could be generalized to account for temperature and composition gradients in the liquid droplet interior. The major conclusions above are not expected to change under those conditions but the system of equations will become more complex.

The errors associated with the formulation of the equations (Eulerian or Lagrangian) governing average droplet properties become greater as the correlation between initial droplet diameter and other droplet properties decreases. That is, the averaged equations are most accurate when the droplets in some narrow range of initial droplet size and spatial location also have narrow ranges of initial velocity and thermal energy.

Acknowledgments

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