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NUMERICAL SOLUTION OF THE SPRAY EQUATION

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NUMERICAL SOLUTION OF THE SPRAY EQUATION *

Charles K. Westbrook

Abstract

The spray equation has been solved numerically using a statistical approach. The method has been applied to physical systems where all three space coordinates are independent, in an internal combustion engine with asymmetric liquid fuel injection. For physical configurations in which some degree of symmetry exists, the numerical model is simplified, at a considerable savings in computer time.

Difference equations are derived for the spray equation in one, two, and three dimensions. In three dimensions the equations are given in Cartesian and cylindrical coordinates. Quantities of physical interest which can be calculated from the droplet distribution function are defined. Coupling terms for use in combined spray-gas phase hydrodynamics models are derived, conserving the total mass, momentum, and energy of the two-phase system. The spray model is extended to allow for denser sprays in which the thin spray approximation is no longer valid.

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Introduction

The spray equation¹ describes the evolution of a distribution of liquid droplets in a gaseous medium. The spray equation is written in terms of a distribution function f , where $f(\vec{x}, \vec{v}, R, t) d\vec{x} d\vec{v} dR dt$ denotes the number of spherical droplets with radii in a range dR about R , in the time range dt about t , in the volume element $d\vec{x}$ about $\vec{x}$, and in the velocity range $d\vec{v}$ about $\vec{v}$. Thus we are dealing with the time evolution of droplets in a seven dimensional phase space. As noted, one idealization has been made in assuming that the droplets are spherical. The spray equation is then written

$$\frac{\partial f}{\partial t} + \frac{\partial(f\dot{R})}{\partial R} + \nabla_{\vec{x}} \cdot (f\vec{v}) + \nabla_{\vec{v}} \cdot (f\vec{F}) = S \quad (1)$$

where $\dot{R} \equiv dR/dt$ is the vaporization rate of droplets and may depend on R , $\vec{v}$, $\vec{x}$, t or any other variable, $\vec{F} \equiv d\vec{v}/dt$ is the external force on the droplets and may include gravity, aerodynamic drag, electromagnetic forces if the droplets have a charge, or other prescribed forces, and S is a generalized source and droplet interaction term. It can be seen that the spray equation is very similar to the Boltzmann Equation, with the addition of a term describing the change in particle size. We can simplify the spray equation by assuming that droplet interactions can be neglected. Among the processes thus removed from consideration are droplet fragmentation, including aerodynamic breakup, and droplet nucleation where two or more droplets could combine to make a larger droplet. Then the only method in which droplets change size is by evaporation, and the only way in which

they change speed or direction is through external forces. A second simplification which is generally made is to assume that the vaporization rate for a droplet depends only on the properties of the individual droplet and the surrounding gas medium. Collectively, the above simplifications can be reproduced if we assume that interdroplet separations are much larger than individual droplet radii. The result of these simplifications is the thin spray equation. An attempt is made in the last section of this paper to extend the model to some regions where the thin spray approximation is no longer valid.

In earlier papers^{2,3} the model to be described was applied to a specific configuration, a cylindrical, stratified charge engine chamber. However, the numerical details were not described in those papers, and other applications were not discussed at all. We will derive the difference equations used in present calculations in explicit and implicit forms and for a variety of coordinate systems. We will indicate those areas where more accurate difference schemes might be used if the added computational cost can be justified. Finally, we will describe some of the applications of the model in various forms which have been made to date.

Difference Equations

It can be seen immediately that the thin spray equation is a multidimensional, linear advection equation. It is also pertinent to note that if we expect to be able to handle a distribution function f in seven dimensions that we will need a lot of computer storage if we are to have any respectable resolution in each dimension. For example, 10 grid points in each dimension requires 10^7 words for f . For problems with some symmetry this size can be reduced, but it will still be necessary in most cases to compute with fairly coarse grids. As a result, it was decided that high order difference schemes were probably not warranted, and that a fast and simple difference scheme was desired. The prescription chosen was to use "upwind" or "donor cell" differencing in each dimension. It should be pointed out that this method is only first order accurate in each dimension⁴ and that a higher order scheme may be desirable for some applications.

We discretize each coordinate as ΔR , Δt , ΔX_1 , ΔX_2 , ΔX_3 , ΔV_1 , ΔV_2 , ΔV_3 . We will deal with each term in Eq. (1) separately. We will try to keep the notation as uncluttered as possible; we will write one difference equation for each cell in the seven-dimensional grid. Where subscripts are missing, we assume that the point in question refers to x_1^{j1} , x_2^{j2} , x_3^{j3} , v_1^{i1} , v_2^{i2} , v_3^{i3} , R_k . The time at which f is evaluated will depend on whether we choose the implicit or explicit form of the difference equations.

The time derivative is differenced directly;

$$\frac{\partial f}{\partial t} \rightarrow \frac{f(t^{n+1}) - f(t^n)}{\Delta t} \quad (2)$$

The vaporization term is written;

$$\frac{\partial(fR)}{\partial R} \rightarrow \frac{\dot{R}_{k+\frac{1}{2}} f(R_{k+1}) - \dot{R}_{k-\frac{1}{2}} f(R_k)}{\Delta R} \quad (3)$$

where $R_{k+1} > R_k$ gives the ordering for the R_k . This term is somewhat simpler than the remaining terms because the assumption that droplets can change size only through vaporization means that droplets move in this dimension in only one direction, in the direction of decreasing radius.

$\dot{R}_{k+\frac{1}{2}}$ indicates that the vaporization rate is to be evaluated at $R = R_{k+\frac{1}{2}}$. In the cases to be described below, $\dot{R}$ is a function of R , $\vec{V}$, and $\vec{X}$, so $\dot{R}_{k+\frac{1}{2}} = \dot{R}(R_{k+\frac{1}{2}}, x_1^{j1}, x_2^{j2}, x_3^{j3}, v_1^{i1}, v_2^{i2}, v_3^{i3}, t)$. In Eq. (3), for the explicit case, $f(R_k) = f(R_k, t^n)$, while for the implicit case, $f(R_k) = f(R_k, t^{n+1})$. In the present formulation only uniform grids are considered, but non-uniform grids would replace ΔR with $(R_{k+\frac{1}{2}} - R_{k-\frac{1}{2}})$.

The spatial advection term, $\nabla_x \cdot (f\vec{V})$, depends mathematically on the coordinate system chosen, which in turn is often determined by the application desired. For rectangular Cartesian coordinates, we have

$$\begin{aligned} \nabla_x \cdot (f\vec{V}) \rightarrow & \frac{f(x_1^{j1+})v_1^{i1} - f(x_1^{j1-})v_1^{i1}}{\Delta x_1} \\ & + \frac{f(x_2^{j2+})v_2^{i2} - f(x_2^{j2-})v_2^{i2}}{\Delta x_2} + \frac{f(x_3^{j3+})v_3^{i3} - f(x_3^{j3-})v_3^{i3}}{\Delta x_3} \end{aligned} \quad (4)$$

The shorthand above describes the familiar situation for upwind differencing, namely

$$\begin{aligned}
 f(x_1^{j1+}) &= f(x_1^{j1}) & \text{if } v_1^{i1} &\geq 0 \\
 &= f(x_1^{j1+1}) & \text{if } v_1^{i1} &< 0 \\
 f(x_1^{j1-}) &= f(x_1^{j1-1}) & \text{if } v_1^{i1} &\geq 0 \\
 &= f(x_1^{j1}) & \text{if } v_1^{i1} &< 0 \quad \text{etc.}
 \end{aligned}
 \tag{4a}$$

The other common coordinate system for spray problems is a cylindrical coordinate system. In this system

$$\nabla_x \cdot (f\vec{v}) = \frac{\partial(fv_z)}{\Delta z} + \frac{1}{r} \frac{\partial}{\partial r}(rfv_r) + \frac{\partial(fv_\theta)}{rd\theta}$$

A conservative form for the difference equations in this system, with $x_1 = z$, $x_2 = r$, $x_3 = \theta$,

$$\begin{aligned}
 \nabla_x \cdot (f\vec{v}) \rightarrow & \left[\frac{f(z^{j1+})v_1^{i1} - f(z^{j1-})v_1^{i1}}{\Delta z} \right] \\
 & + \left[\frac{f(r^{j2+})r^{j2+\frac{1}{2}}v_2^{i2} - f(r^{j2-})r^{j2-\frac{1}{2}}v_2^{i2}}{\bar{r}_{j2} \Delta r} \right] \\
 & + \left[\frac{f(\theta^{j3+})w_3^{i3} - f(\theta^{j3-})w_3^{i3}}{\Delta \theta} \right]
 \end{aligned}
 \tag{5}$$

where $W_3 = \frac{V_\theta}{r}$, $r_{j2} = \frac{1}{2} (r^{j2+\frac{1}{2}} + r^{j2-\frac{1}{2}})$, and the criteria for choosing the appropriate spatial point for f depends on the signs of V_1 , V_2 , and W_3 as above.

The velocity space advection term, $\nabla_v \cdot (f\vec{F})$, is analogous to the spatial divergence term. For Cartesian coordinates, we find

$$\begin{aligned} \nabla_v \cdot (f\vec{F}) \rightarrow & \left[\frac{f(V_1^{i1+})F(V_1^{i1+\frac{1}{2}}) - f(V_1^{i1-})F(V_1^{i1-\frac{1}{2}})}{\Delta V_1} \right] \\ & + \left[\frac{f(V_2^{i2+})F(V_2^{i2+\frac{1}{2}}) - f(V_2^{i2-})F(V_2^{i2-\frac{1}{2}})}{\Delta V_2} \right] \\ & + \left[\frac{f(V_3^{i3+})F(V_3^{i3+\frac{1}{2}}) - f(V_3^{i3-})F(V_3^{i3-\frac{1}{2}})}{\Delta V_3} \right] \end{aligned} \quad (6)$$

Again, the centering of f , this time in velocity space, depends on the sign of F . To be specific, $F(V_1^{i1+\frac{1}{2}})$ will depend on a lot of quantities at each point, but its sign will usually depend on the sign of $(V_1^{i1+\frac{1}{2}} - U_1)$, where U_1 is the component of the local gas velocity parallel to $V_1^{i1+\frac{1}{2}}$. If this relative velocity is positive, the droplet will be decelerated, and $f(V_1^{i1+})$ will be replaced by $f(V_1^{i1+1})$, but if the relative velocity is negative then the droplet will be accelerated and $f(V_1^{i1+})$ will be replaced by $f(V_1^{i1})$. The same argument applies to the other components as well.

One Dimensional Symmetry

An earlier numerical model was used for the spray equation by Bracco^{5,6}, using a method which was time independent and limited to one dimensional symmetry, and applied to a liquid fuel rocket motor. The one dimensional time dependent version of our model was applied to this same problem and the results compared with those of Bracco. The time independent, or steady state, solution was achieved as the asymptotic solution in time of the time dependent solution, with the immediate result that the transient solution was also available. The results agreed very closely with the results of Bracco.

On the symmetry axis of the rocket motor, the spray equation droplet distribution is nearly one dimensional, depending only on the distance from the injector. In one dimension, the spray equation becomes

$$\frac{\partial f}{\partial t} + \frac{\partial(f\dot{R})}{\partial R} + \frac{\partial(fv)}{\partial x} + \frac{\partial(fF)}{\partial v} = S \quad (7)$$

The liquid droplets are injected at a low axial velocity into an air stream which is moving faster than the droplets. As a result, aerodynamic drag always accelerates the droplets and they all move down the chamber axis in one direction only. Since the droplets are also assumed to only evaporate, each term in Eq. (7) has one preferred direction and the choice of centering in the upwind difference form of Eq. (7) is unique and will not depend on position or time, this simplifying the notation in the difference equations. The difference equations in this system are then:

$$\begin{aligned} \frac{f(t^{n+1}) - f(t^n)}{\Delta t} + \left[\frac{f(R_{k+1})R_{k+\frac{1}{2}} - f(R_k)R_{k-\frac{1}{2}}}{\Delta R} \right] + v^{il} \left[\frac{f(x^{jl}) - f(x^{jl-1})}{\Delta x} \right] \\ + \frac{f(v^{il})F(v^{il+\frac{1}{2}}) - f(v^{il-1})F(v^{il-\frac{1}{2}})}{\Delta v} = S \quad (8) \end{aligned}$$

If explicit differencing is used, the difference equations for Eq. (8)

become:

$$\begin{aligned} f(t^{n+1}, R_k, x^{jl}, v^{il}) = f(t^n, R_k, x^{jl}, v^{il}) \left[1 + \frac{\Delta t}{\Delta R} \dot{R}_{k-\frac{1}{2}} - v^{il} \frac{\Delta t}{\Delta x} - \frac{\Delta t}{\Delta v} F(v^{il+\frac{1}{2}}) \right] \\ - \frac{\Delta t}{\Delta R} \dot{R}_{k+\frac{1}{2}} f(t^n, R_{k+1}, x^{jl}, v^{il}) + v^{il} \frac{\Delta t}{\Delta x} f(t^n, R_k, x^{jl-1}, v^{il}) \\ + \frac{\Delta t}{\Delta v} F(v^{il-\frac{1}{2}}) f(t^n, R_k, x^{jl}, v^{il-1}) + S \Delta t \quad (9) \end{aligned}$$

In this and most other applications, the source term S consists formally of a prescription of the injection process. In actual calculations the distribution function f is prescribed at the point representing the injector, rather than defining the source strength. The function S can be found, however, by solving Eq. (9) for S , with f given at the injector:

$$S = \frac{f_{inj}(t^{n+1}) - f_{inj}(t^n)}{\Delta t} + f_{inj}(t^n) \left[-\frac{R_{k-\frac{1}{2}}}{\Delta R} + \frac{v^{il}}{\Delta x} + \frac{F(v^{il+\frac{1}{2}})}{\Delta v} \right] \quad (10)$$

The total source rate is obtained by summing Eq. (10) over all droplet sizes and velocities.

Boundary conditions for Eq. (9) are included by imposing the known

physical constraints on the difference equations. If the largest allowed droplets have radius R_K , then $f(R_{K+1}) = 0$. The injector resides at $x^{j1}(j1=1)$. The maximum distance from the injector is at $j1 = J$, with $f(x^{j1}) = 0$ for $j1 > J$. If the droplets are always accelerated by the air stream, then they cannot move faster than the air velocity; therefore there is some maximum droplet velocity, v^I , such that $f(v^{I+1}) = 0$. Similarly, there is a minimum droplet velocity v^0 (zero in this case) such that $f(v^{I=-1}) = 0$. For this system of difference equations, it is possible to order the equations defined by Eq. (8) so that only one storage array is required for the distribution function f . This ordering will depend on whether Eq. (8) is explicit or implicit in time. As an example of this ordering, we can write the first few terms in Eq. (9). If $f(t^{n+1})$, with $K = 1$, $j1 = J$, and $il = I$ is calculated first all the terms required in Eq. (9) are still unchanged and the storage location for $f(t^n)$ can be over-stored with $f(t^{n+1})$. Then that value will not be needed again until the next time step. If Eq. (9) is solved in order of increasing K , decreasing $j1$, and decreasing il , then the one storage array can be used.

The implicit difference equations for Eq. (8) are

$$\begin{aligned}
 f(t^{n+1}, R_k, x^{j1}, v^{il}) & \left[1 - \frac{\Delta t}{\Delta R} \dot{R}_{k-\frac{1}{2}} + \frac{v^{il} \Delta t}{\Delta x} + \frac{\Delta t}{\Delta v} F(v^{il+\frac{1}{2}}) \right] \\
 & = - \frac{\Delta t}{\Delta R} \dot{R}_{k+\frac{1}{2}} f(t^{n+1}, R_{k+1}, x^{j1}, v^{il}) + v^{il} \frac{\Delta t}{\Delta x} f(t^{n+1}, R_k, x^{j1-1}, v^{il}) \\
 & + \frac{\Delta t}{\Delta v} F(v^{il-\frac{1}{2}}) f(t^{n+1}, R_k, x^{j1}, v^{il-1}) + f(t^n, R_k, x^{j1}, v^{il}) + S \Delta t \quad (11)
 \end{aligned}$$

The same boundary conditions apply as in the explicit case. As before, with a proper selection of the order in which the equations in Eq. (11) are solved, only one storage array is required. In this case, examination reveals that we must solve in the opposite order from the explicit case in each dimension, with decreasing K , increasing $i1$, and increasing $j1$.

Stability

The choice of the implicit or explicit form of the difference equations is determined, as usual, by stability requirements and the time steps desired. The implicit form is unconditionally stable, due to both the time centering and the upwind differencing. To examine the stability of the explicit scheme, we use the criterion derived for the simple advection equation in one coordinate and apply it to each coordinate in the spray equation. For the simple advection equation

$$\frac{\partial f}{\partial t} + \frac{u \partial f}{\partial x} = 0 \quad (12)$$

the condition for stability of the explicit scheme with upwind space differencing is:

$$\frac{u \Delta t}{\Delta x} \leq 1 \quad (13)$$

Similar analysis results in analogous expressions in each dimension for the spray equation, for explicit time differencing;

$$\frac{u\Delta t}{\Delta x} \leq 1$$

$$\frac{\dot{R}\Delta t}{\Delta R} \leq 1 \quad (14)$$

$$\frac{F\Delta t}{\Delta v} \leq 1$$

The largest term in this group of relations will determine the overall stability of the difference equations; the application being considered will determine the sizes of terms in Eq. (14) since droplet sizes, injection velocities, gas motion, and gas density all influence these terms. For the rocket injection problem the largest term is the $F/\Delta v$ term, the aerodynamic drag, which has a maximum of nearly 10^7 sec^{-1} for the fastest, smallest droplets. The largest values for the other terms are $\dot{R}/\Delta R \approx 10^6 \text{ sec}^{-1}$ and $u/\Delta x \approx 2 \times 10^3 \text{ sec}^{-1}$. For applications where the spray evolution must be followed for times much larger than about 10^{-4} seconds the implicit form will clearly be superior, particularly if only the steady state solution is required.

Three Dimensional Symmetry

In the general case it is not possible to use symmetry to simplify the equations. An example of this situation is the liquid fuel injector in an internal combustion engine, where the enclosed volume often has a somewhat complicated shape, the injector is placed in a non-symmetrical location, and the air motion in the chamber is swirling in some complicated way. For these and other similar cases the full three dimensional solution is needed.

The Cartesian difference equations can be written by analogy with the one dimensional case. The explicit result is formed by combining Eq. (2), Eq. (3), Eq. (4), and Eq. (6), with all terms on the right hand side evaluated at t^n . If we adopt the shorthand that $f = f(t^n, R_k, x^{j1}, y^{j2}, z^{j3}, v_1^{i1}, v_2^{i2}, v_3^{i3})$, and exceptions are noted by indicating only the argument that is different, then

$$\begin{aligned}
 & \frac{f(t^{n+1}) - f(t^n)}{\Delta t} + \frac{[\dot{R}_{k+\frac{1}{2}} f(R_{k+1}) - \dot{R}_{k-\frac{1}{2}} f(R_k)]}{\Delta R} \\
 & + v_1^{i1} \left[\frac{f(x^{j1+}) - f(x^{j1-})}{\Delta x} \right] + v_2^{i2} \left[\frac{f(y^{j2+}) - f(y^{j2-})}{\Delta y} \right] + v_3^{i3} \left[\frac{f(z^{j3+}) - f(z^{j3-})}{\Delta z} \right] \\
 & + \left[\frac{F(v_1^{i1+\frac{1}{2}}) f(v_1^{i1+}) - F(v_1^{i1-\frac{1}{2}}) f(v_1^{i1-})}{\Delta v_1} \right] + \left[\frac{F(v_2^{i2+\frac{1}{2}}) f(v_2^{i2+}) - F(v_2^{i2-\frac{1}{2}}) f(v_2^{i2-})}{\Delta v_2} \right] \\
 & + \left[\frac{F(v_3^{i3+\frac{1}{2}}) f(v_3^{i3+}) - F(v_3^{i3-\frac{1}{2}}) f(v_3^{i3-})}{\Delta v_3} \right] = S
 \end{aligned} \tag{15}$$

The terms x^{j1+} , etc. are defined as in the earlier descriptions, Eq. (4a). The implicit equations are defined in the same way, but all the terms in f are evaluated at t^{n+1} except the time derivative term noted as $f(t^n)$.

If the gas flow and droplet motion are known a priori, then the terms in Eq. (15) are known immediately. If, however, the gas flow varies with time and space, it is necessary to test the signs of F and V at each point. Since droplet radii only decrease, there is no ambiguity in the differencing of the vaporization term.

In cylindrical coordinates, the terms defined earlier are again combined with Eq. (5) instead of Eq. (4), with either explicit or implicit differencing used. Again, knowledge of the air flow and droplet relative velocities can simplify the testing in the actual computer program, but if necessary all of the tests must be included. In the paper cited earlier² on spray motion in a stratified charge engine an assumed gas motion was used, greatly simplifying the programming details. That model was somewhat simplified, but the above difference equations were used exactly as given.

The stability criteria in the explicit case are again found by analogy with the simplified Eq. (12). In the general case, the inequalities in Eq. (14) must be satisfied for each space and velocity coordinate, as well as for the vaporization rate term.

External Forces and Drag Equation

The force term F defined earlier is a composite of any and all relevant forces on each droplet. In most cases this includes aerodynamic drag as the droplet moves through the gaseous medium, and gravitational force. In a rotating coordinate system centrifugal force must also be included. In the general case any other forces can be included. For example, in some applications electrically charged droplets may be injected into an electromagnetic field, resulting in an additional force. In many cases it is possible to use order of magnitude estimates to simplify the force term, even eliminating some terms completely. A real consideration is often whether or not a term is comparable with diffusional terms inherent in the difference equations. Similarly, if the duration of the spray is short, small force terms may not have much effect on the droplet positions if the droplet velocities are large. For example, in the engine chamber injection mentioned earlier, drag terms, high droplet velocities, and high vaporization rates were sufficient to completely overwhelm both centrifugal and gravitational force terms which were therefore ignored.

With spherical droplets and the assumptions in the thin spray approximation, it is often sufficient to use the drag equation with Stokes' drag coefficient. The drag equation is written

$$\vec{F} = \frac{3C_D \rho}{8R\rho_L} |\vec{u} - \vec{v}| (\vec{u} - \vec{v}) \quad (16)$$

where C_D is the drag coefficient, $\vec{u}$ is the gas velocity, $\vec{v}$ is the droplet velocity, ρ_L is the liquid specific gravity, ρ is the gas density, and R is the droplet radius. For a sphere of constant radius in a non-burning atmosphere, Stokes' drag equation can often be used, with

$$C_D = \frac{24}{Re} \quad (17)$$

where Re is the Reynolds number

$$Re = \frac{2R\rho}{\mu} |\vec{u} - \vec{v}| \quad (18)$$

and μ is the liquid viscosity coefficient. In a medium where forced convection affects the droplet drag, a correction term can be added⁷

$$C_D = \frac{24}{Re} (1 + 0.15 Re^{0.687}) \quad (19)$$

Another correction term can be added if the droplets are evaporating^{8,9} to define the overall drag term:

$$C_D = \frac{24}{Re} \frac{(1 + 0.15 Re^{0.687})}{(1+B)} \quad (20)$$

It should be pointed out that these correction terms to the Stokes' drag equation are derived by correlating theoretical expressions with experiments and depend ultimately on the exact details of the experiments.

The fuel used, the gas medium, relative velocities, and other factors

all are involved; one must be careful in using correlations which have been derived for a different class of applications. It is at least clear that the fluid dynamics assumptions leading to the Stokes' drag coefficient are not satisfied in most combusting liquid sprays, so it is not unreasonable to expect that correction terms would improve theoretical agreement with experiments. As in most cases the final decision on whether or not to include correction terms and what form they should have rests on comparisons with actual experiments. For many applications Stokes' drag coefficient is satisfactory.

Vaporization Rate

The vaporization of a spherical liquid droplet is affected by two major processes. In a completely stagnant air flow a droplet will evaporate at a rate which will depend upon the droplet radius and whether or not the gaseous fuel is burning. Relative motion between the gas medium and the droplet will enhance the evaporation rate through forced convection. The amount of enhancement depends on the droplet Reynolds number as well as other terms. The resulting vaporization rate expression, originally proposed by Ranz and Marshall¹⁰ is

$$\dot{R} = -\frac{k}{8R} (1 + 0.3Re^{1/2} Pr^{1/3}) \quad (21)$$

where Pr is the Prandtl number,

$$Pr = \frac{4\gamma}{9\gamma-5} \quad (22)$$

and γ is the specific heat ratio of the fuel. Part of the temperature and density dependence included in the vaporization rate constant k has been included by Bracco⁵ by redefining Eq. (21),

$$\dot{R} = -\frac{k^*}{8\rho R} (1 + 0.3Re^{1/2} Pr^{1/3}) \quad (23)$$

In the same paper, Bracco discusses other forms proposed for $\dot{R}$ by a variety of investigators, under a variety of operating conditions. Again, these

correlations and others like them are derived for one set of conditions which may or may not obtain in another application. Care must be exercised in using them in any application.

Expectation Values

It is often necessary to evaluate certain average values for the spray distribution. Just as in conventional statistical mechanical calculations, the average value of a quantity h is defined

$$\bar{h}(t) = \frac{\int_{\vec{v}} \int_{\vec{x}} \int_R h(\vec{x}, \vec{v}, r, t) f d^3x dR d^3v}{\int_{\vec{v}} \int_{\vec{x}} \int_R f d^3x dR d^3v} \quad (24)$$

Other quantities can be defined at each point as appropriate sums or integrals over the velocity and size dimensions. Of particular interest is the condensed phase density ρ_c :

$$\rho_c(\vec{x}, t) = \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L f d^3v dR . \quad (25)$$

Another quantity of interest is the total vaporization rate $\dot{m}$:

$$\dot{m}(\vec{x}, t) = \int_{\vec{v}} \int_R 4\pi R^2 \dot{R} \rho_L f d^3v dR . \quad (26)$$

The total mass vaporization rate $\dot{m}(t)$ is found by

$$\dot{m}(t) = \int_{\vec{x}} \dot{m}(\vec{x}, t) d^3x . \quad (27)$$

The total amount of mass that has been vaporized up to time t , $M(t)$, is found from

$$M(t) = \int_0^t \dot{m}(t') dt' . \quad (28)$$

Similarly, another quantity of frequent interest is the total amount of mass which has vaporized at a point $\vec{x}$ up until time t , $M(\vec{x}, t)$, which is defined

$$M(\vec{x}, t) = \int_0^t \dot{m}(\vec{x}, t') dt' . \quad (29)$$

Therefore, we see that we can also redefine

$$M(t) = \int_{\vec{x}} M(\vec{x}, t) d^3x \quad (30)$$

Coupling to Gas Equations

The gas phase parameters, particularly the density and velocity components, can be specified in any one of several ways. In experiments where the gas properties are known in advance and are either constant with time or change with time in some known way, those values can be used in the evaluation of vaporization rates and drag terms. This situation is not often the case, however, with the result that the gas phase and liquid phase properties are closely coupled together. If the changes in the gas properties cannot be ignored, then the overall conservation equations for both phases must be solved.

A convenient way of coupling the two phases together when both must be included in a problem uses a form of operator splitting. The basic strategy of this method is the following: the spray equation is solved for one time step Δt , assuming that the gas density and velocity components are fixed. Then the amount of mass that has vaporized during that time step in each spatial grid interval is added to the gaseous mass already in that grid space, increasing the gas density at each point. The amount of momentum in each dimension that has been lost by the droplets during the time step is then added to the gas phase material, changing the gas velocity in that direction. If the momentum of the droplets has increased, the gas phase velocity is decreased. In both cases, the total momentum of the gas and liquid phases combined is conserved. In this way the effects of drag and gas entrainment by the spray can be evaluated, and the total mass and momentum conservation equations can be satisfied. To

conserve the total energy, the change in total energy of the droplet distribution can be calculated and the energy of the gas corrected to balance that change. Finally, the gas phase conservation equations can be solved independently of the spray equations.

Qualitatively, this splitting has the important effect of simplifying the computational procedure. Multidimensional hydrodynamic models are already exceedingly intricate without the complicating feature of coupling to the droplet equations. The disadvantage of the splitting is that if the coupling between liquid and gas phases is rapid, if the drag terms are large and there is a lot of gas entrainment, or if the evaporation is very rapid, then it will be necessary to pay a price computationally through a reduced time step.

With the qualitative features discussed above, we will describe analytically the coupling terms and how they should be evaluated. The mass loss term of the droplets (and therefore the mass source term to the gas phase) can be defined in two ways. In the limit of small grid spacings in time, droplet radius, and position, the two expressions reduce to the same formula. In terms of the vaporization rate $\dot{R}$, the mass loss rate is given by

$$\dot{m}(\vec{x}, t) = \int_{\vec{V}} \int_R 4\pi R^2 \dot{R} \rho_L f d^3v dR . \quad (26)$$

Another way to find the total mass loss rate within a given spatial cell is to add the contributions to the total mass in the cell ΔVol

$$\dot{m}(\vec{x}, t^{n+1}) = \left[\frac{\rho_c(\vec{x}, t^n) \Delta Vol + \left(\frac{\text{Net mass flux}}{\text{into } \Delta Vol} \right) - \rho_c(\vec{x}, t^{n+1}) \Delta Vol}{\Delta t} \right] \quad (31)$$

With the definition in Eq. (31), the total conservation of mass is assured, since the mass flux terms cancel identically at each zone interface. The expression in Eq. (26) is often easier to evaluate, so the choice between Eq. (26) and Eq. (31) is a qualitative one, depending on how important exact mass conservation may be for the chosen application.

Momentum deposition is evaluated in two analogous ways. The component of drag in the x-direction is F_x , so the momentum deposition rate is

$$\dot{P}_x(\vec{x}, t) = \frac{d}{dt} P_x(\vec{x}, t) = \frac{d}{dt} \left[\int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L v_x f d^3v dR \right] \quad (32)$$

$$\dot{P}_x(\vec{x}, t) = \int_{\vec{v}} \int_R \left[\frac{4\pi}{3} R^3 F_x \rho_L f + v_x \frac{4\pi}{3} \rho_L \frac{d(R^3 f)}{dt} \right] d^3v dR \quad (33)$$

Equivalently, we specifically evaluate the droplet momentum in the x-direction, assuming that any change during the time step has been imparted to the gas.

$$\dot{P}_x(\vec{x}, t^{n+1}) = \left[\frac{P_x(\vec{x}, t^n) + \left(\frac{\text{net momentum flux}}{\text{into volume } \Delta Vol} \right) - P_x(\vec{x}, t^{n+1})}{\Delta t} \right] \quad (34)$$

The momentum at the point $\vec{x}$ is given by

$$P_x(\vec{x}, t) = \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L v_x f d^3v dR \quad (35)$$

so to evaluate the momentum flux across a boundary it is necessary to combine Eq. (35) with the appropriate values of the function f . This will depend on the spatial differencing being used. A convenient quantity is the following;

$$\Delta f = f^n + \frac{v_1 \Delta t}{\Delta x} f_{j1-1} - \frac{v_1 \Delta t}{\Delta x} f_{j1} + \frac{v_2 \Delta t}{\Delta y} f_{j2-1} \quad (36)$$

$$- \frac{v_2 \Delta t}{\Delta y} f_{j2} + \frac{v_3 \Delta t}{\Delta z} f_{j3-1} - \frac{v_3 \Delta t}{\Delta z} f_{j3} - f^{n+1}$$

This term Δf has been written assuming that v_1 , v_2 , and v_3 are all positive. A more general form for Δf would include the proper indexing depending on the signs of v_1 , v_2 , and v_3 as discussed in Eq. (4). An even more general form for Δf would include the terms generated by whatever spatial differencing scheme has been used. Only the spatial gradient terms are to be included in Δf in Eq. (36). With Δf we can rewrite Eq. (31),

$$\dot{m}(\vec{x}, t) = \frac{1}{\Delta t} \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L \Delta f d^3v dR \quad (37)$$

and rewrite Eq. (34),

$$\dot{P}_X(\vec{x}, t) = \frac{1}{\Delta t} \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L v_X \Delta f d^3v dR \quad (38)$$

These are the most convenient forms for actual computations. The energy content of the spray distribution must include the kinetic and internal energy of the droplets. Also, the heat of vaporization of the liquid must be included, since the gas loses that energy in order to vaporize the droplets. The total energy in the droplets is thus

$$\epsilon(\vec{x}, t) = \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L \left[\frac{v^2}{2} + \int_{T_0}^T C_v dT' \right] f d^3v dR \quad (39)$$

Using Eq. (36), the total energy rate deposited to the gas can be written

$$\begin{aligned} \dot{\epsilon}(\vec{x}, t) = & \frac{1}{\Delta t} \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L \left[\frac{v^2}{2} + \int_{T_0}^T C_v dT' \right] \Delta f d^3v dR \\ & - \lambda \dot{m}(\vec{x}, t) \end{aligned} \quad (40)$$

where λ is the heat of vaporization of the liquid, in energy per unit mass. The temperature T_0 is an arbitrary reference temperature and C_v is the liquid specific heat, which may be a function of temperature. A first approximation for Eq. (40) might be to neglect the changes in droplet temperatures.

A further quantity which must be conserved in problems with swirl is angular momentum. This can be defined for the spray

distribution as

$$L_{\theta}(\vec{x}, t) = \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_c r v_{\theta} f d^3v dR \quad (41)$$

where V_{θ} is the tangential droplet velocity component and could be replaced by $v_{\theta} = rw$. The variable r is the radial space coordinate. Then the angular momentum deposition to the gas is

$$\dot{L}_{\theta}(\vec{x}, t) = \int_{\vec{v}} \int_R \frac{4\pi}{3} R^3 \rho_L r v_{\theta} \Delta f d^3v dR \quad (42)$$

Other quantities can be defined as needed. For example, with a multi-component fuel, separate conservation equations for each component would be defined to give the mass source rate in the gas phase for each species.

Injector Correlations

In this model it is very important to be as accurate as possible in specifying the distribution function at the injector, f_{inj} . This is because the problem as defined is a combination initial value and boundary value problem, where all values are eventually determined by the given value at the injector. The injection process is modelled by giving f_{inj} for the grid interval that represents the physical injector.

The injector droplet distribution function is generally written as a separable function of droplet size and velocity. This assumption is made to simplify the function, although there is considerable reason to expect that this function is in fact not separable. Stated mathematically, this gives

$$f_{inj} = f_1(R)f_2(\vec{v})f_3(\vec{x})f_4(t) \quad . \quad (43)$$

In most cases, $f_4(t)$ is a step function, set to 1 if the injector is on, set to 0 if the injector is off. Other alternatives could include a sinusoidal variation;

$$f_4(t) = 1 - \sin wt \quad . \quad (44)$$

The spatial term $f_3(\vec{x})$ is set to 1 for those points which represent the physical injector, and 0 for all other points.

The remainder of f_{inj} consists of two terms which determine the

droplet size distribution and velocity distributions. In actual injectors, these distributions are coupled. Large droplets are usually closer to the average velocity of the entire distribution than are the smaller droplets. As a result, what is done is to use the velocity distribution of the larger droplets, since these comprise most of the mass of the total spray. Part of the answer to this dilemma is that experimental data on velocity and size distribution correlations are not available. This leaves a lot of freedom in choosing the form to be used for f_{inj} , with the final decision based on how well the results match experiments. In most of the applications of the model to date, separability of f_{inj} into $f_1(R)f_2(\vec{v})$ has been assumed.

The form for $f_2(\vec{v})$ has usually been chosen as

$$f_2(\vec{v}) = - \left[\frac{(v_1 - v_{10})}{d_1} \right]^2 - \left[\frac{(v_2 - v_{20})}{d_2} \right]^2 - \left[\frac{(v_3 - v_{30})}{d_3} \right]^2 \quad (45)$$

where v_{10} , v_{20} , v_{30} , d_1 , d_2 , and d_3 are chosen to give the desired shape to the distribution. In the case of a single hole nozzle in an engine chamber² in cylindrical coordinates it was convenient to choose

$v_{10} = v_0$, $v_{20} = v_{30} = 0$, giving a centrally peaked jet along the chamber axis. The spread of the spray in the radial direction was determined by the choice of d_2 . For a pintle nozzle, both v_{10} and v_{20} would be non-zero, giving a hollow cone.

Velocity correlations can be introduced into $f_2(\vec{v})$ if desired.

One such correlation is motivated by a desire to confine the spray to a given solid angle about the spray axis. No droplets are permitted outside

the spray cone angle α . It can be seen from Eq. (45) above that since the velocity components are decoupled, some droplets may have small values of v_1 and large values of v_2 . If we are to restrict the droplets to a cone of angle α , where

$$\tan \alpha = \frac{v_2}{v_1} \quad (46)$$

can choose $f_2(\vec{v})$ as

$$f_2(\vec{v}) = e^{-\left[\frac{(v_1 - v_{10})}{d_1}\right]^2} g(v_2) e^{-\left[\frac{(v_3 - v_{30})}{d_3}\right]^2} \quad (47)$$

where

$$g(v_2) = \begin{cases} e^{-\left[\frac{(v_2 - v_{20})}{d_2}\right]^2} & v_2 \leq v_1 \tan \alpha \\ 0 & v_2 > v_1 \tan \alpha \end{cases} \quad (48)$$

Other correlations are of course possible and may improve agreement with experiments. The real problem here is that definitive experiments on droplet velocity distributions at or near an injector are extremely difficult, largely due to the fact that the spray thickness in that region generally precludes optical access. Very recent diagnostic techniques¹¹, particularly LDV, appear to offer some hope in this area. Even beyond this level, velocity-radius correlations are also needed.

Droplet size distribution functions are generally expressed in a

form introduced by Nukiyama and Tanasawa¹²

$$f_1(R) = aR^p e^{-bR^n} \quad (49)$$

where four parameters a , p , b , and n are available for experimental evaluation. Several functions derived from Eq. (49) are discussed by Tishkoff and Law¹³. The most common form used is called the Nukiyama-Tanasawa distribution, and is derived from Eq. (49) by setting $p = 2$ and $n = 1$,

$$f_1(R) = aR^2 e^{-bR} \quad (50)$$

Experimental correlations are still needed to evaluate the remaining parameters a and b .

The entire distribution function at the injector requires an overall normalization. This is generally accomplished by requiring that the numerical flux of liquid through the injector is equal to the known experimental flux. The flux of liquid through the injector $\dot{W}_f$ is calculated from

$$\dot{W}_f = \int_S (\rho_c \vec{v}) \cdot \hat{n} dS \quad (51)$$

where $\hat{n}$ is the unit normal to dS , the surface through which the spray is passing into the chamber. The integral in Eq. (51) can be evaluated by a combination of analytical and numerical steps, made possible or at least simpler by the choice of a separable function for f_{inj} in Eq. (43).

Extension To Thick Sprays

The model as described is properly applicable only to thin sprays. In practice this means that each droplet behaves as if it were physically unaware of the presence of other droplets and is affected only by gas properties. Of course, since all other droplets affect the gas properties which then affect individual droplets, there is a coupling between droplets, but only through the gas parameters. If we wish to extend the model to conditions where droplets are closer together than the 10-20 diameter separations implied by the thin spray approximation, we will need to modify some of our treatments.

It should be pointed out here that what is proposed is an intermediate approach using the thin spray model but with some simple modifications. In theory, as the spray becomes less thin, different physical processes become important, including droplet nucleation, coalescence, collisions, continuous liquid bodies, and a very complex two-phase flow. Because that problem is intractable or at least exceedingly difficult to solve, we adopt the point of view that perhaps it is possible to stretch the thin spray model somewhat beyond its formal limits and deal with some additional applications.

In a gaseous medium with closely spaced droplets we would expect that the relative velocity between gas and droplets would approach zero due to the increased effect of momentum transfer to the gas, entrainment. We would also expect that the gas between the droplets would become rich in vapor from droplets which are vaporizing. Whether or not the gas

would actually become saturated is difficult to say, but some effect should be evident. These two effects would be noticed when the average inter-droplet spacing reached some low value, perhaps 3-5 times the droplet diameters. A simple approximation to the behavior of the drag and vaporization rate expressions might be that they range monotonically from their maximum values for isolated droplets, the very thin case, to zero in the limit of very closely packed droplets. For simplicity, let us then define scaling functions for those expressions in terms of ρ_c , which is a convenient measure of how closely the droplets are spaced. For example

$$\begin{aligned} F' &= F \Theta_1 \\ \dot{R}' &= \dot{R} \Theta_2 \end{aligned} \tag{52}$$

where Θ_1 and Θ_2 are the scaling terms. Possible expressions for either scaling function might be

$$\Theta = \left[1 - \frac{\rho_c}{\rho_L d} \right]^n \tag{53}$$

or

$$\Theta = \exp \left(-\frac{\rho_c}{\rho_L d} \right) \tag{54}$$

In these expressions the parameters d and n can be chosen to produce the best fit to experimental data. In Eq. (53) the function Θ is assumed to

have a minimum value of zero for $\rho_c \geq \rho_L d$, with $n \geq 1$.

As an example of the use of the above scaling functions in a spray where the thin spray assumption is not valid, let us examine vaporization rates calculated with and without scaling. The spray droplet distribution used in both cases was taken from a calculation of an axisymmetric spray injected into an internal combustion engine chamber². Scaling was done with Eq. (54), with $d = 0.01$. Contours of constant vaporization rate with no scaling are shown in Fig. 1. Without scaling, the contours representing the highest vaporization rates are at the center of the spray cone where the condensed phase density is largest. From Fig. 2, showing contours of constant condensed phase density, it is clear that the spray is certainly not thin near the center of the spray cone. Application of the scaling Eq. (54) to the same spray droplet distribution produces vaporization rate contours shown in Fig. 3, in which the contours representing the highest vaporization rates are now at the perimeter of the central spray cone, in an annular region surrounding the dense portion of the spray. Experience and some experimental data¹¹ suggest that the vaporization rate in a thick spray will be highest at or near the periphery of the thick portion of the spray, although very little relevant experimental data are available.

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FIGURE 1

Vaporization rates without scaling. In the central cross-shaded region $\dot{m} \geq 0.8 \text{ gm/cm}^3\text{-sec}$. In the next single-shaded region $\dot{m} \geq 0.5 \text{ gm/cm}^3\text{-sec}$. In the unshaded region, $\dot{m} \leq 0.5 \text{ gm/cm}^3\text{-sec}$.

FIGURE 2

Condensed phase density. The contours are very nearly the same at this time, 0.1 msec. after injection begins, for both the scaled and unscaled cases.

FIGURE 3

Vaporization rates with scaling, $d = 0.01$. As in Fig. 1, in the cross-shaded region $\dot{m} \geq 0.8 \text{ gm/cm}^3\text{-sec}$, in the single-shaded region $\dot{m} \geq 0.5 \text{ gm/cm}^3\text{-sec}$, and in both unshaded regions $\dot{m} \leq 0.5 \text{ gm/cm}^3\text{-sec}$.

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