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AN INTEGRATED APPROACH TO SPRAY COMBUSTION
MODEL DEVELOPMENT

by

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ABSTRACT

The major elements of an approach to the development of a more powerful spray combustion model is discussed. A model is sought that treats, in a numerically-efficient manner, unsteady, multidimensional, turbulent reacting flows with polydisperse, multicomponent sprays and properly accounts for transient droplet heating and vaporization, liquid-phase mass diffusion, and droplet drag and trajectory. Major advances are reviewed and important issues remaining for resolution are discussed.

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INTRODUCTION

There has been substantial progress in the theory of fuel droplet vaporization and in spray combustion theory over the past decade. Reviews of the research can be found in References 1 through 5.

It is appropriate now to begin to develop computer codes that can predict the behaviors of spray combustion flows where mutlicomponent, polydisperse liquid fuel sprays are burned. In particular, steady and unsteady multidimensional, recirculating flows must be analyzed. Account must be taken of the details of the transient heating of individual fuel droplets and of the fluid dynamics of the droplet interior and of the surrounding gas film since it affects the droplet heating and vaporization.

Resolution on a scale of a few microns may be required in order to resolve droplet behavior. Global dimensions of the combustor are typically of the order of ten to one hundred centimeters. This implies that the disparity of length scales can be five to six orders of magnitude. It is not possible therefore to resolve the problem by exact numerical solution. Rather, the droplet behavior must be modeled; essentially a sub-grid model is required. Even though only representative droplets in any neighborhood are to be considered, hundreds or even a thousand of these average droplets must be analyzed. Computational simplicity and speed are extremely important issues which must be addressed.

It is the purpose of this paper to indicate and to critique some of the key elements in the development of a physically-accurate and numerically-efficient computer code. Major advancements will be reviewed and remaining issues for further resolution will be outlined. Other spray models have, of course, been developed in the past and are well reviewed.[1,4,5] The

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discussion herein is significantly different in that an approach is needed that treats, in a numerically efficient manner, unsteady, multidimensional (including recirculating), turbulent reacting flows with multicomponent, polydisperse sprays and properly accounts for transient droplet heating and vaporization, liquid-phase mass-diffusion, and droplet drag and trajectory.

In the next section, a simplified droplet model is discussed. In order to calibrate that simplified model, an exact solution is required. Also, droplet drag coefficients must be determined before good trajectory predictions will result. These issues are discussed in the third section. Spray combustion in one-dimensional, two-dimensional, and axisymmetric configurations are examined in the fourth section. Some concluding comments are given in the final section.

SIMPLIFIED ALGORITHM FOR PREDICTION OF DROPLET VAPORIZATION

The fuel droplets in a combustion chamber are formed during the atomization process and move through an environment of hot gases. The magnitude of the relative velocity between the droplet and the gas implies that the Reynolds number, at least initially, is large compared to unity. A laminar boundary layer exists at the surface of the droplet in the gas moving past the droplet. The shear force at the droplet surface causes an internal circulation of the liquid in the droplet, typically with a boundary layer at the surface, an internal wake along the symmetry axis and a toroidal, nearly inviscid vortical core (see Figure 1). The fluid flow is established very quickly and can be considered as quasi-steady.

The high temperature environment means that the droplet vaporizes quickly and the droplet lifetime is comparable to the time required for a thermal wave

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to penetrate to the droplet interior. This rapid regression results in the highly transient nature of the problem. The internal circulation causes significant convective heating of the interior; conduction is still dominant in the direction normal to the liquid streamsurfaces.

The earlier theories[6,7,8] for convective transient heating and vaporization involved treatment of the quasi-steady laminar axisymmetric boundary layers in the gas and in the liquid at the surface by solving the governing two-dimensional partial differential equations by integral methods and numerical analysis. The vortex core analysis is simplified by the approximation that streamsurfaces are surfaces of uniform temperature and composition, although the values are time-varying. This high Peclet number approximation allows heat and mass diffusion only normal to streamsurfaces. A coordinate transformation to streamsurface coordinate yields a reduction of the axisymmetric, unsteady core diffusion problem to a one-dimensional, unsteady problem.

These earlier theories demonstrated that transient heating and vaporization and internal circulation are of critical importance and showed many interesting details about the phenomena. However, they were costly in terms of computer time. Most of the computer time was related to the two-dimensional resolution of the gas-phase boundary layer and of the liquid-phase boundary layer at the droplet surface. More recent efforts by Tong and Sirignano have resulted in a simplified algorithm for the calculation of transient droplet and vaporization. Through the use of approximate similar solutions, the gas-phase boundary layer was analyzed by a one-dimensional method[9,10,11,12]. In another analysis,[13] it was shown that certain details of the liquid boundary layer profile could be neglected, resulting in further simplifications.

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The simplified formulation assumes a Blasius profile in the gas-phase boundary layer governed by the following third order-equation

$$\frac{d^3 f}{d\eta^3} + f \frac{d^2 f}{d\eta^2} = 0 \qquad (1)$$

The boundary conditions are

(i) at $\eta = 0$, $\frac{df}{d\eta} = 0$

(ii) at $\eta = \infty$, $\frac{df}{d\eta} = 1$ $\qquad (2)$

(iii) at $\eta = 0$, $\frac{d^2 f}{d\eta^2} = -\frac{f}{B'}$

The heat flux into the liquid is given by

$$k_\ell \left. \frac{\partial T}{\partial y} \right|_{\ell s} = -Af(0) \left[\frac{h_e - h_s}{B'} - L \right] \qquad (3)$$

The mass flux due to vaporization is

$$\rho v)_s = -Af(0) \qquad (4)$$

The modified transfer number can be represented by

$$B' = \frac{Y_{fs}}{1 - Y_{fs}} \qquad (5)$$

Also, the velocity component in the major flow direction is proportional to the first derivative of the Blasius function f. η is the similarity

variable, A is a constant weighted over the spherical surface, h is enthalpy, T is temperature, k is thermal conductivity, Y_f is fuel vapor mass fraction, v is the velocity component normal to the surface, ρ is density, and L is latent heat of vaporization. The subscripts ℓ, s, and e refer to liquid, surface, and gas environment, respectively.

In standard fashion, the temperature and concentration profiles through the gas-phase boundary layer can be related to the velocity profile or, in other words, to the derivative of the Blasius function. So solution of the Blasius equation will quickly lead to solutions of the scalar properties. Note that a phase equilibrium condition relates Y_{fs} directly to T_s.

By numerical integration of the above equation, the Blasius function $f(n,B')$ is determined at the liquid-gas interface as a function of the modified transfer number B'. The mass vaporization rate per unit surface area is directly proportional to $f(0,B')$.

The particular value of B' depends upon heat flux into the liquid interior and surface temperature so that we see a strong coupling between the liquid and gas phase phenomena. We also begin to see the dangers of many analyses that neglect liquid heating or make assumptions about the surface temperature. A useful theory must allow the governing physics to determine fully the time-dependent value of B' and must not force some unnatural value of B' into the calculation.

The gas-phase analysis has now produced a function $f(0,B')$ that can be tabulated for a range of B' values. Through the use of similarity principles and the quasi-steady assumption, the two-dimensional, unsteady gas-phase equations have been reduced to a one-dimensional form. Upon integration of that ordinary differential equation, one function results that can be input in tabular form and may be considered as equivalent to an algebraic statement and

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therefore a "zero-dimensional" representation of the gas-phase has been developed.

The liquid hydrodynamic field is represented in terms of the classical Hill's spherical vortex and the liquid temperature and concentration are assumed to be uniform (but time-varying) along each streamsurface. This high Peclet number approximation allows conduction only normal to the streamsurface. The characteristic liquid heating length and heating time are thereby significantly reduced from the stagnant value.

The liquid phase heat diffusion equation has been shown to be approximately

$$\frac{\partial T}{\partial \tau} = \phi \frac{\partial^2 T}{\partial \phi^2} + (1 + C\phi) \frac{\partial T}{\partial \phi} \tag{6}$$

when ϕ is the normalized streamfunction and T is the liquid temperature. Note that

$$d\tau = \frac{b_1}{b_o} \frac{\alpha_\ell}{R^2} dt$$

and

$$C = C(\tau) = 2(\frac{R_o}{R})^{3/2} \frac{d}{d\tau} (\frac{R}{R_o})^{3/2} \tag{7}$$

The boundary conditions on (6) are given as

(i) at $\tau = 0$, $T = 0$

(ii) at $\phi = 0$, $\frac{\partial T}{\partial \phi} = \frac{\partial T}{\partial \tau}$ \hfill (8)

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(iii) at $\phi = 1$, $\dfrac{\partial T}{\partial \phi} = q_\ell$

In the above equations, t is the time variable, α_ℓ is the thermal diffusivity, R is the droplet radius, R_0 is the initial radius, σ_ℓ is the normalized heat flux at the surface, and b, and b_0 are constants.

On account of C, Equation (6) is nonlinear. However, C will be considered as slowly varying compared to T and will be taken as piecewise constant in our integration calculation. The approximately linear differential operator allows us to develop a Green's function and reduce the solution to an integral form whereby, via quadrature, the temperature at any point can be determined as a function of the heat flux at the liquid surface. In particular, an integral equation can result that relates the surface temperature to the surface flux. The Green's function or kernel function is given by

$$K(\tau,\phi) = \frac{\tau + F_s(0,C_o,\phi)}{G_s(0,C_o,1)} - \frac{1}{2}\frac{G_{ss}(0,C_o,1)}{G_s^2(0,C_o,1)}$$
$$+ \sum_{n=1}^{\infty} \frac{F(\lambda_n,C_o,\phi)}{\lambda_n G_s(\lambda_b,C_o,1)} e^{\lambda_n \tau} \tag{9}$$

where F and G are analytic functions of ϕ. The eigenvalues λ_n are determined by:

$$G(\lambda_n,C_o,1) = 0 \tag{10}$$

Now the temperature anywhere in the liquid may be determined as a function of the surface heat flux

$$T(\tau,\phi) = K(0,\phi)f(\tau) + \int_0^\tau f(x)\ \frac{\partial K(\tau-x,\phi)}{\partial \tau}\ dx \qquad (11)$$

where

$$f(\tau) = \frac{\partial T}{\partial \phi}\ \text{at}\ \phi = 1$$

In particular, at the surface, $\phi = 1$, we find that

$$T_s = \alpha \int_0^\tau f(x)\ dx + \sum_{n=1}^\infty \left[\beta_n \int_0^\tau f(x)\ e^{\lambda_n(\tau-x)}\ dx \right] \qquad (12)$$

where

$$\alpha = \frac{1}{G_s(0,C_o,1)}$$

$$\beta_n = \frac{F(\lambda_n C_o,1)}{G_s(\lambda_n,C_o,1)}$$

From the gas-phase analysis, we also have a relationship between the surface temperature and B' where B' does depend upon both surface temperature and surface heat flux. This allows for complete determination of the surface temperature and heat flux upon coupling with the liquid-phase solution. The solutions are numerical and time-dependent.

The integral equation at the surface can be replaced by the following system of ordinary differential equations. First we define

$$T_s = \sum_{n=0}^\infty g_n(\tau)$$

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where

$$g_o(\tau) = \alpha \int_0^\tau f(x) \, dx$$

and

$$g_n(\tau) = \beta_n \int_0^\tau f(x) d^{\lambda_n(\tau-x)} \, dx; \ n > 1$$

Then it follows that

$$\frac{dg_o}{d\tau} = \alpha \, f(\tau) \tag{13}$$

and

$$\frac{dg_n}{d\tau} = \lambda_n g_n(\tau) + \beta_n f(\tau) \ ; \ n > 1 \tag{14}$$

Note that by definition

$$g_n(0) = 0 \text{ for all } n > 0$$

The independent time variable in Equations (13) and (14) is a Lagrangian time so that an advantage of these equations is that they can be solved as we follow the vaporizing droplets through the spray combustor. As Figure 2 shows, less computer time is required for the ordinary differential equation system solution than for the direct numerical solution of Equation (6). The improved efficiency measured in CPU time occurs at any desired accuracy.

In the case of multicomponent fuels, liquid mass diffusion is of critical importance. The more volatile components will vaporize first from the surface

leaving the less volatile components as the dominant species in the vicinity of the surface. Liquid mass diffusion brings the volatile components to the surface for further vaporization. The vaporization rates of each component will change with time. In the latter part of the droplet lifetime, the vaporization rates of the less volatile components will become greater than the rates for the other components whose concentrations has decreased.

It is necessary to solve diffusion equations for n-1 of the n components in the liquid-phase. Species conservation equations for gas-phase fuel vapor components must also be solved. The same type of algorithms can be used here as were used in the solution f the temperature for the gas and the liquid. While interface conditions and diffusivity coefficients differ, the same type of differential operators are present. Details of the recommended methodology for multicomponent fuels are presented in References 11 and 12.

The results of Figure 3 show surface temperature and droplet diameter versus time. All quantities are normalized and nondimensional. The behavior is clearly seen to be highly transient and the danger of oversimplified assumptions about surface temperature is portrayed. Figure 4 shows the behavior of hexane as the more volatile component in a hexane-decane bicomponent mixture. A general decrease in surface mass fraction and component vaporization rate occurs with time due to mass diffusion control. A slight increase in the hexane surface mass fraction occurs late in the lifetime when the surface temperature becomes large enough to increase substantially the decane vaporization rate.

Figure 5 shows the variation of the coefficient C with time. Note that during the earlier part of the droplet lifetime, the assumption of slowly-varying C appears to be poor. Nevertheless, results for temperature, concentration, vaporization rate, and diameter, such as those shown in Figures

3 and 4, indicate essentially perfect agreement between our approximate solution and direct solution of the equations by finite-difference methods.

Some important differences exist between the results for different models of the liquid-phase heating. The most common approach in the literature is to assume uniform but time-varying temperature in the liquid, effectively, this means infinite liquid conductivity. Another model neglects the internal vortex and liquid circulation and assumes spherically-symmetric conduction. Figure 6 compares the simplified vortex model results with results from the other two models. The infinite conductivity model clearly is very poor. The spherical diffusion model predicts higher initial surface temperatures because it does not account for heat convected to the droplet interior from the surface. For the same reason, it underpredicts surface temperature later in the droplet lifetime.

There are certain shortcomings with the approach of Tong and Sirignano,[9-13] Prakash and Sirignano,[6,7] and Lara and Sirignano[9] as discussed above. Firstly, constant transport and thermal properties are employed. Secondly, the analysis is strictly correct only when the Reynolds number based upon relative velocity is sufficiently large to have a laminar boundary layer. Some attempts are underway to improve the situation. Abramzon and Sirignano[14] present an approach intended to cover a wider Reynolds number range and to treat variable properties.

EXACT SOLUTION OF THE TRANSIENT DROPLET HEATING AND VAPORIZATION PROBLEM

The simplified algorithm of the previous section is potentially very useful in spray combustion analyses. As already explained, a more detailed calculation would be very costly for a spray calculation wherein hundreds or

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even a thousand representative droplets must be considered. Nevertheless,
more new and useful information does result from more detailed calculations,
especially from "exact" finite-difference computations that minimize the
number of approximations.

The simplified method uses only boundary layer theory thereby providing
no information about the flow aft of the point on the droplet surface where
the shear stress goes to zero. The drag force on the droplet therefore cannot
be calculated from that method. The drag force, or equivalently, the drag
coefficient must be known in order to predict droplet trajectories and the
local vapor mixture ratio. The drag coefficient is expected to be very
different from that of an isothermal solid sphere due to a combination of
effects. Blowing due to droplet vaporization, variable properties due to
temperature and molecular weight gradients, apparent mass due to flow
acceleration or deceleration, and internal liquid circulation will each impact
the drag coefficient. Preliminary results from a number of investigators
indicate a reduction in drag coefficient from hard-sphere results. Nusselt
and Sherwood numbers also experience modification from hard-sphere results.

The exact solutions are also useful as a basis for comparison for the
simplified model. Since detailed experimental results do not exist, the exact
solutions give the most reliable information available about the flow field
within and around the droplets. The validity of various assumptions used in
the approximate models and the accuracy of those models can be evaluated
through the use of the exact models. since the exact solutions do not require
any limitation on Reynolds number, they cover the zero Reynolds number
(stagnant), low Reynolds number, and high Reynolds number (boundary layer)
domains while the simplified model discussed in the previous section is
limited only to the high Reynolds number domain. Other approximate solutions

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exist for the transient heating and vaporization in the stagnant case.

Dwyer, Sanders, and co-workers[15,16,17,18,19] have performed the most work on this subject. In a series of papers[16,17,19] assuming a uniform density gaseous media, they demonstrated certain interesting results. The internal circulation resulted in vortical streamsurfaces that did resemble those for Hill's spherical vortex. The internal circulation did affect the transient heating, especially at higher Reynolds numbers, and transient heating was very important to the droplet vaporization process.

The Reynolds number decreased with time due to deceleration of the droplet. For solid spheres, the drag coefficient increases as Reynolds number decreases. Their results with vaporization artificially eliminated do indicate a similar increase of the drag coefficient during the droplet lifetime. However, when vaporization occurred in accordance with the natural laws, the drag coefficient decreased with time, contrary to intuition. It is known that vaporization reduces friction drag due to the boundary layer blowing, but still the result must be considered as remarkable because it constitutes a qualitative difference and not just a quantitative difference when compared to solid sphere data.

The variable density case has been studied by Patnaik, et al[20] and the trend for the drag coefficient is the same generally but even more dramatic than in the constant density case. Figure 7 shows a typical result whereby droplet radius, mass, relative velocity, Reynolds number based upon relative velocity, and drag coefficient all decrease during the droplet lifetime. The rapid decreases of velocity and Reynolds numbers are especially notable. The vaporization rate first increases and then decreases during the droplet lifetime. The Nusselt number decreases during the droplet lifetime for both the constant density and variable density cases.

The above calculations that relate to decelerating droplets are made in a frame of reference fixed to the droplet. Since such a reference frame is non-Newtonian, a reversed D'Alembert force must be applied uniformly throughout the field. That is, at each time-step, there is a change in relative velocity between the free-stream and the droplet that occurs because of the change of velocity of the droplet due to the drag force. The droplet velocity is returned to zero in the frame of reference by deceleration of the flow field. Not just the free-stream velocity is decreased relative to the droplet, but is decreased relative to the droplet, but the whole gas flow field is reduced. It is important that the numerical adjustment of the velocity field is made at every point in the field at each time step to properly represent the reversed inertia force. It is clear from the constant density and the variable density calculations that the drag coefficient will depend upon a nondimensional acceleration or deceleration factor. (The standard parameter is an acceleration modulus.) The reversed inertia force will make the drag coefficient different from its steady-state value.

A general observation from the various calculations is that the transport within the droplet is convective-dominated in the early portion of the droplet lifetime. In the later part of the lifetime, the droplet relative velocity and the strength of the internal vortex have been reduced substantially so that internal conduction has increased in relative importance. This indicates that the simplified model of the previous section can be appropriate for the early lifetime but can become inaccurate for the later lifetime. Clearly, a more general simplified model is required. One approach is to use the vortex model of the previous section for a portion of the lifetime and then to switch to a spherically-symmetric conduction model later in the lifetime.

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The effect of burning in the gas film and wake of the droplet was considered by Dwyer and Sanders.[15] They treated an uncoupled gas-phase problem only but it is reasonable to believe that their conclusions will not change for the coupled gas-liquid problem. They found a thick flame raising questions about the validity of a d^2 law for stagnant droplets. For Reynolds numbers near 100, they found burning only in the wake with little heat feedback to the droplet.

It is reasonable to believe that the combined effects of droplet group behavior and high Reynolds number will limit the possibility of flames enveloping individual droplets in practical combustors. This is an important issue in the modelling of spray combustors since we must know whether or not to include the heat of combustion in the calculation of the transfer number B'. Without combustion in the boundary layer or near wake of the droplet, the value of B' would be lower.

Dwyer and Sanders[18] have examined the effect of pressure on the droplet vaporization, on the drag coefficient, and on the Nusselt number. They considered three cases at one, five, and twenty-five atmospheres, respectively. Reynolds numbers and Nusselt numbers decreased with time in all gases. Using a normalized time-scale independent of the pressure, they showed that Reynolds number decreased more rapidly and Nusselt number more slowly with time as pressure increased. Drag coefficients decreased with time for one and five atmospheres. The decrease was more rapid for one atmosphere. At twenty-five atmospheres, the drag coefficient increased with time.

The decrease in Reynolds number without mass transfer has been shown to result in an increase of the drag coefficient with time. Mass transfer tends to reduce the drag coefficient and mass transfer rates increase with time during the droplet lifetime. Apparently for one and five atmospheres, the

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increase in mass transfer rates more than compensates the decrease in Reynolds number. Therefore, the drag coefficient decreases with time. However for the largest value of pressure and gas density, the Reynolds number decrease is so rapid that even with increasing mass transfer rates, the droplet drag coefficient increases with time.

It is clear that an extensive parameter survey is needed to determine the drag coefficient as a function of the instantaneous Reynolds number, droplet acceleration modulus, and the instantaneous transfer number. Such numerical data would be critical input to a spray combustor analysis. The preliminary evidence cited above indicates that solid sphere data overpredicts the drag coefficient and thereby underpredicts the penetration of the droplets in a spray combustor.

Another important parameter, especially in dense sprays involves the effect of droplet spacing upon the droplet vaporization rate, the drag coefficient and the Nusselt number. Preliminary results[22] indicate that the vaporization rate, Nusselt number, and drag coefficient can be strongly affected by the proximity of other droplets. The flow field around two droplets in an axisymmetric configuration was calculated. Each droplet was artificially kept at constant Reynolds number. One droplet is aft of the other at a constant spacing. The calculations for the first (upstream) droplet are made neglecting the presence of the second (downstream) droplet. The wake solution of the first droplet then provides the upstream condition for the calculation of the flow around the second droplet.

Figure 8 shows that the drag coefficient generally decreases with time due to the increasing mass transfer effects. The drag coefficient is higher at the lower Reynolds number and is greater for the first droplet. It can be expected that the drag coefficient of the second droplet will be strongly

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dependent upon the distance between droplets. Further work on the effect of droplet spacing is required in the future.

Some interesting calculations are presented in Reference 23. The effects of variable properties are included and are shown to be of some importance. the utility of the analysis is limited because the study addresses only low values of the transfer number and the reversed inertia force is not properly considered. The conclusions that drag coefficient increases during the droplet lifetime is seriously misleading.

In summary, computational fluid dynamics provides a useful mechanism for the study of fuel droplet vaporization in spray combustion. Its potential has certainly been demonstrated and it should provide valuable inputs on drag coefficients, Sherwood numbers, and Nusselt numbers for spray analyses. The need for extensive parameter surveys to determine the dependence of drag coefficients and Nusselt numbers on transfer number, Reynolds number, Prandtl number, droplet spacing, and droplet acceleration modulus are required.

FLAME PROPAGATION AND FLAMEHOLDING STUDIES

In situations where droplet heating and vaporization are rate-controlling and ambient temperatures are sufficiently high that droplet lifetime is not long compared to droplet heating time, the details of the transient droplet thermal behavior are very important. It has been shown[24] that different vaporization models can produce significantly different results for local gaseous fuel-air mixture ratios. Three models were considered: infinite-conductivity, spherically-symmetric heat conduction, and heat conduction with high Peclet number internal circulation (vortex). Differences in mixture ratio were as high as 100% especially in the early vaporization period. These

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differences would dramatically affect predictions of flame stability and ignition.

On account of the significant sensitivity, it is necessary to employ the most accurate model in a given combustion situation. For zero or low Reynolds number based upon relative gas-droplet velocity, the spherically-symmetric droplet heating and vaporization model is recommended. When the droplet Reynolds number is large compared to unity, the vortex model is most appropriate. Only in the limit where droplet lifetime is much longer than droplet thermal time does the infinite conductivity model give accurate results. Note that all three models give the same result in that limit and also the limit is not interesting in combustion applications.

Eulerian-Lagrangian methods[1,2,3] have been utilized to study flame propagation[25,26] and flame holding[27] in various configurations. Transient droplet heating and vaporization were considered in each of these studies. Transient droplet behavior was also taken into consideration in a recent paper on ramjet combustion instability.[28]

A one-dimensional, unsteady analysis[25] of flame initiation and propagation in a closed volume showed many interesting results. The droplet number density was initially uniform but expansion of the burning gases and droplet motion due to drag caused subsequent stratification of the heterogeneous mixture. A hot wall at one end resulted in ignition and the propagation of a flame across the chamber. The fuel droplets do not completely vaporize as they are swept by the flame. This is especially time for larger droplets and less volatile fuels. The droplets vaporize in the hot gas behind the flame front and fuel vapor diffuses to the flame. Figures 9, 10, and 11 show that the advancing flame is actually a diffusion flame with fuel vapor and oxygen coming from opposite sides of the flame.

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Note that resolution is obtained on a scale smaller than the distance between droplets. Figure 10 shows local peaks of fuel vapor mass fraction at the droplet locations which are source points for the fuel vapor. The zone of chemical reaction in the diffusion flame is not large compared to droplet spacing so that resolution on this scale is absolutely necessary.

A two-dimensional, steady flame propagation analysis[26] considers parallel streams of droplets flowing adjacent to air streams that initially are cold. The domain is bounded by two walls, a hot wall and a cold wall, with heat conducting in a transverse direction across the flow. In the direction of flow, vaporization and mixing of fuel vapor with air occurs first. Then the combustible mixture ignites and as indicated by the schematic of Figure 12, a premixed-like flame propagates across the flow.

All of the droplets are not vaporized in this first flame-front; rather, vaporization continues beyond the front. All of the oxygen is not consumed in the first flame front, either. Diffusion flames are established around the droplet streams in the hot, oxygen-rich gases downstream of the premixed-like flame as shown in Figure 12. Fuel vapor mass fraction contours, shown in Figure 13, support the schematic description of Figure 12.

The results of References 25 and 26 together show that the simple concept of a flame sweeping a heterogeneous mixture and resulting in conversion of liquid fuel to gaseous products in a short distance is very seriously flawed. Except for very small droplets and very volatile liquids, the flame structure will be much more complex. Diffusion flame structures will arise. Transient droplet heating and motion due to droplet drag have been shown to be important factors in the model.

An axisymmetric, unsteady reacting heterogeneous flow in a center-body combustor has been analyzed.[27] A steady-state solution is found

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asymptotically in time via finite-difference techniques. Polydisperse and monodisperse sprays have been considered in the calculations. Transient droplet heating and vaporization are considered following the methodology outlined earlier in this paper. A Lagrangian calculation is made for droplet properties and an Eulerian calculation is employed for the gas properties.[2] A standard k, ε turbulence model is utilized.

Figure 14 shows droplet trajectories and size for a polydisperse spray calculation while Figure 15 indicates gas velocity magnitude and direction at the grid points of a nonuniform finite-difference mesh. It is seen that a double-vortex recirculation zone occurs behind the center-body; due to the momentum of the liquid spray originating from the center-body at the axis of symmetry, the inner vortex results. The smaller droplets in the spray tend to become bound in the recirculation zone while the larger droplets penetrate beyond the recirculation zone. Note that solid sphere drag data is employed, thereby overpredicting the drag coefficient and underpredicting the droplet penetration. In these calculations, the recirculation zone was predicted to be very fuel rich and turbulent transport of fuel vapors from the fuel vapor from the recirculation zone to the incoming air was also predicted to be very important. Improved drag coefficient calculations should decrease the importance of turbulent transport of fuel vapors and increase the relative importance of droplet penetration.

CONCLUDING REMARKS

An integrated approach to spray combustion modelling requires several types of analyses as key elements. Analysis of individual droplet behavior with the intention of developing an algorithm or a sub-grid model for

vaporization is required. An analysis to determine drag coefficients for use in droplet trajectory analysis is mandatory. Finally, a finite-difference analysis of the spray combustor, employing inputs from the droplet analyses, is required.

Numerically-efficient and physically-accurate algorithms for transient droplet heating and vaporization have been developed. Effects of internal liquid circulation have been carefully considered where appropriate. These models have successfully been applied to combustor calculations.

Much work on the exact solution of the flowfields within and surrounding droplets has been performed. Drag coefficients for vaporization and decelerating droplets have been shown to be very different from those for isothermal, constant velocity, solid spheres. A more extensive parameter study is still required to provide useful input to spray combustor analyses. It should show the dependence of drag coefficient and Nusselt number upon mass transfer number, acceleration moduli, and inter-droplet spacing.

Spray combustion analyses have been performed and results presented for one-dimensional and two-dimensional, steady and unsteady flows with and without recirculation and with monodisperse and polydisperse sprays. Lagrangian droplet calculations and Eulerian gas-phase calculations have been made. The need for improved droplet drag coefficient data is a major limitation. Another limitation is the need for a droplet vaporization model that applies over a wide range of Reynolds numbers.

ACKNOWLEDGMENTS

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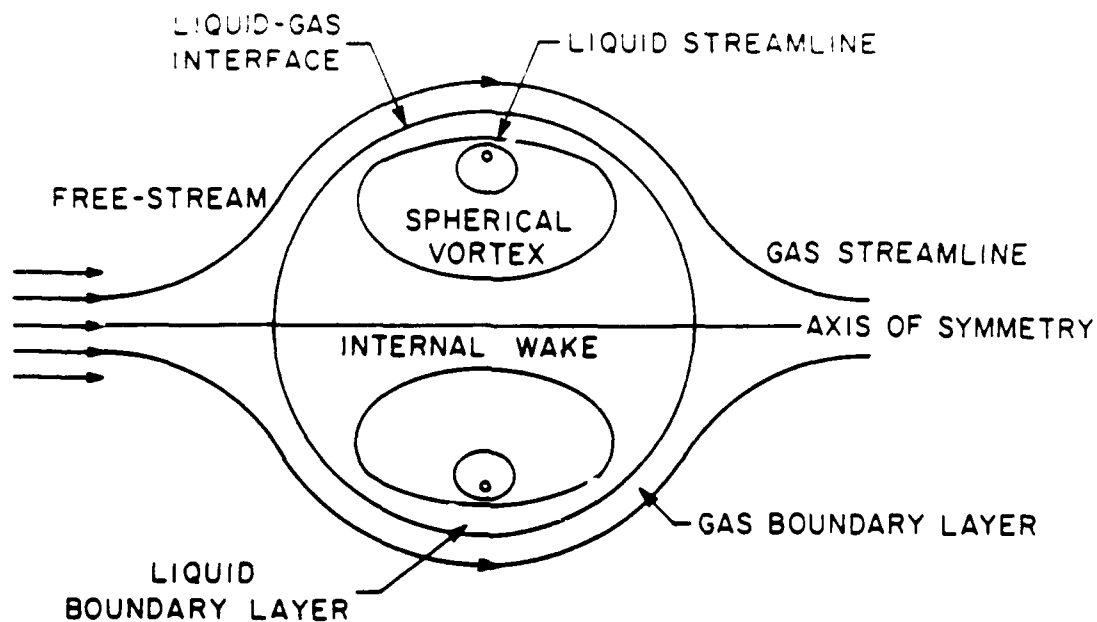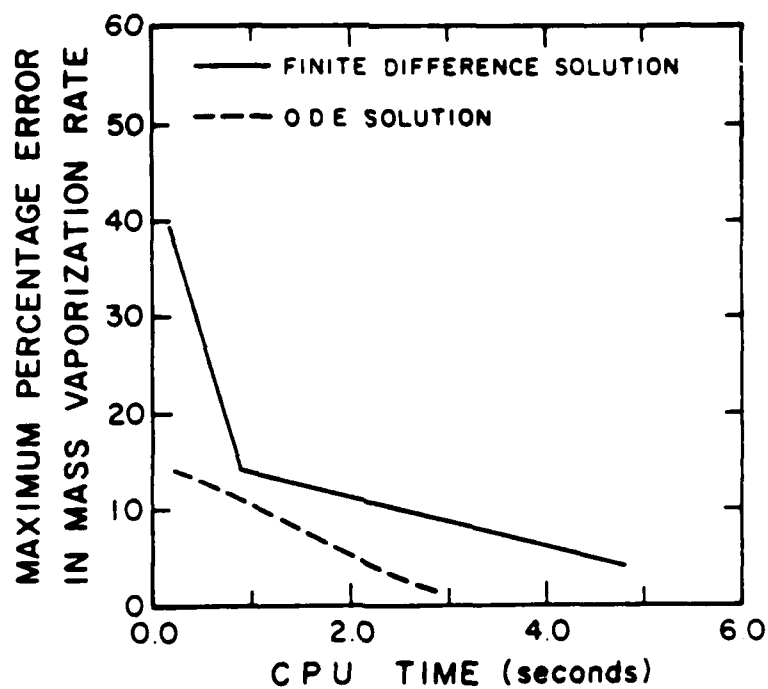
Figure 1. Vaporizing Convective Droplet
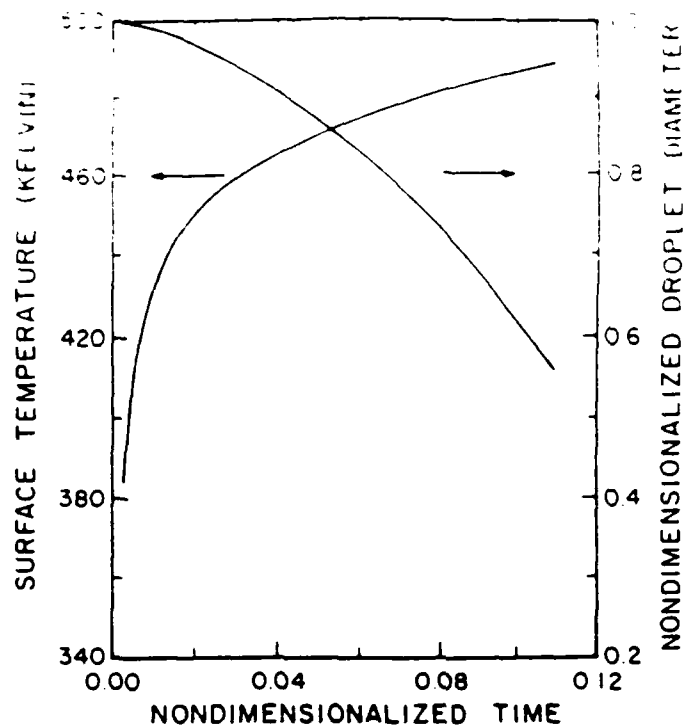

Figure 2. Maximum Percentage Error in Mass Vaporization
Rate Versus CPU Time Comparisons

25

Figure 3. Surface Temperature and Droplet Diameter
Versus Time Comparisons (Decane)
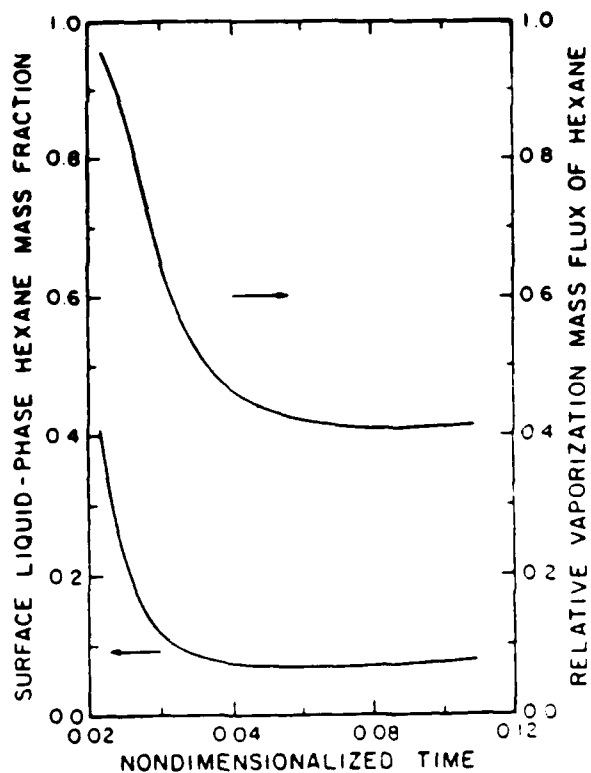
Figure 4. Surface Liquid-Phase Mass Fraction and Relative
Vaporization Mass Flux of Hexane Versus Time
Comparisons (Lewis No.=10)

26
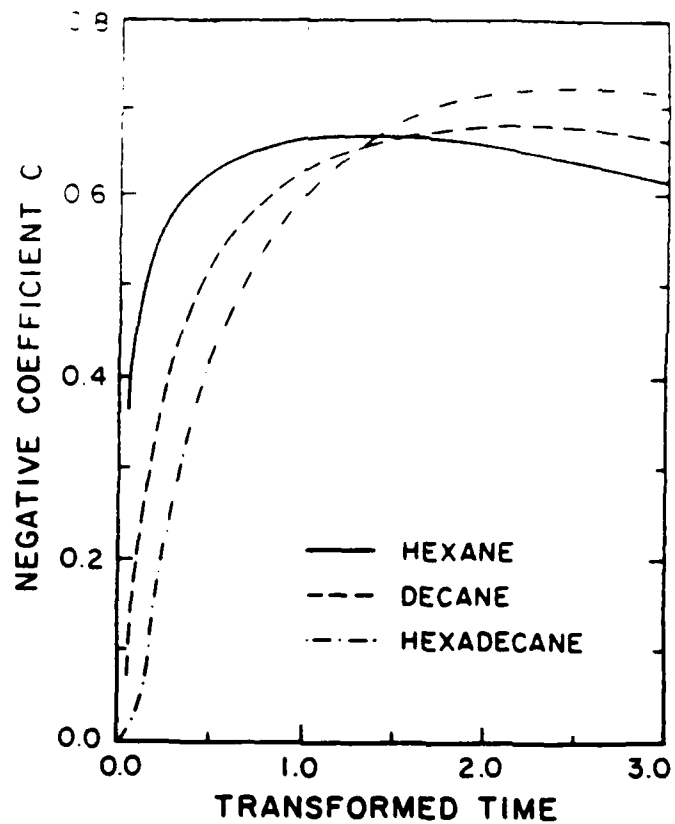
Figure 5. Negative Coefficient C Versus Time Comparisons
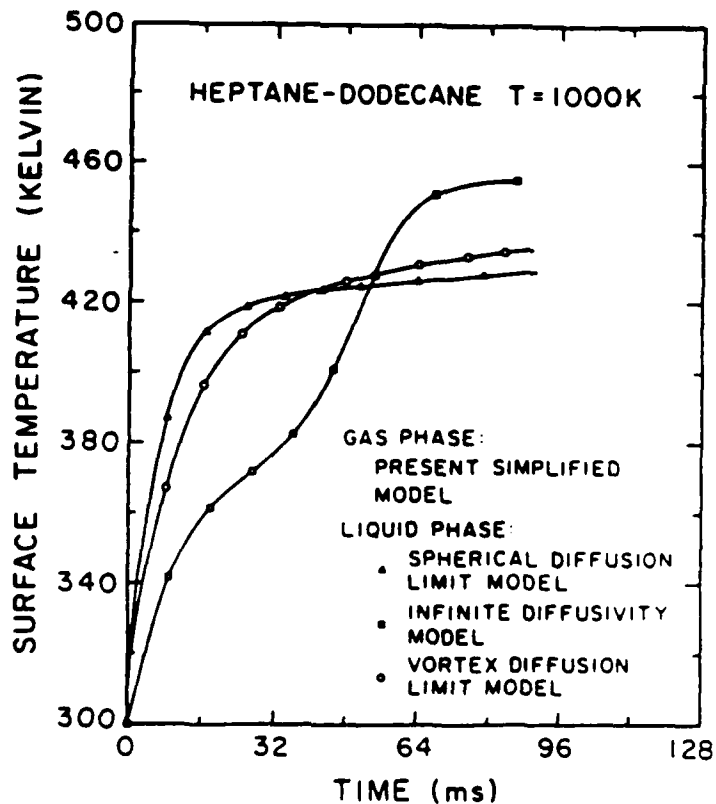
Figure 6. Surface Temperature Versus Time Comparisons

27
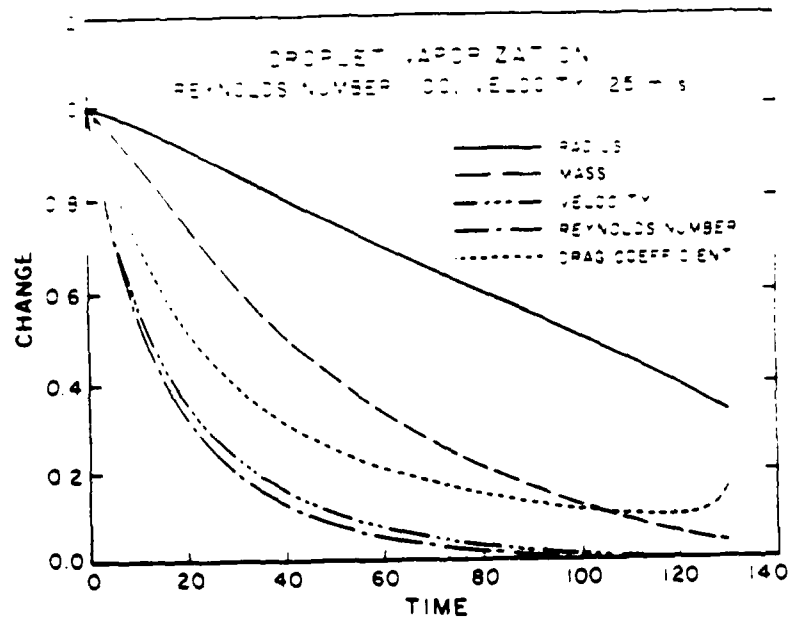
Figure 7.   Overall Droplet Behavior
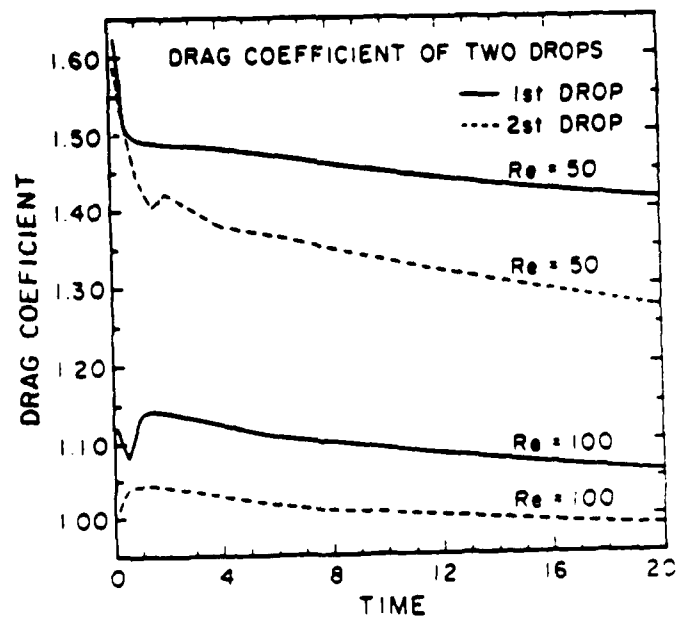
Figure 8.   Drag Coefficient

28
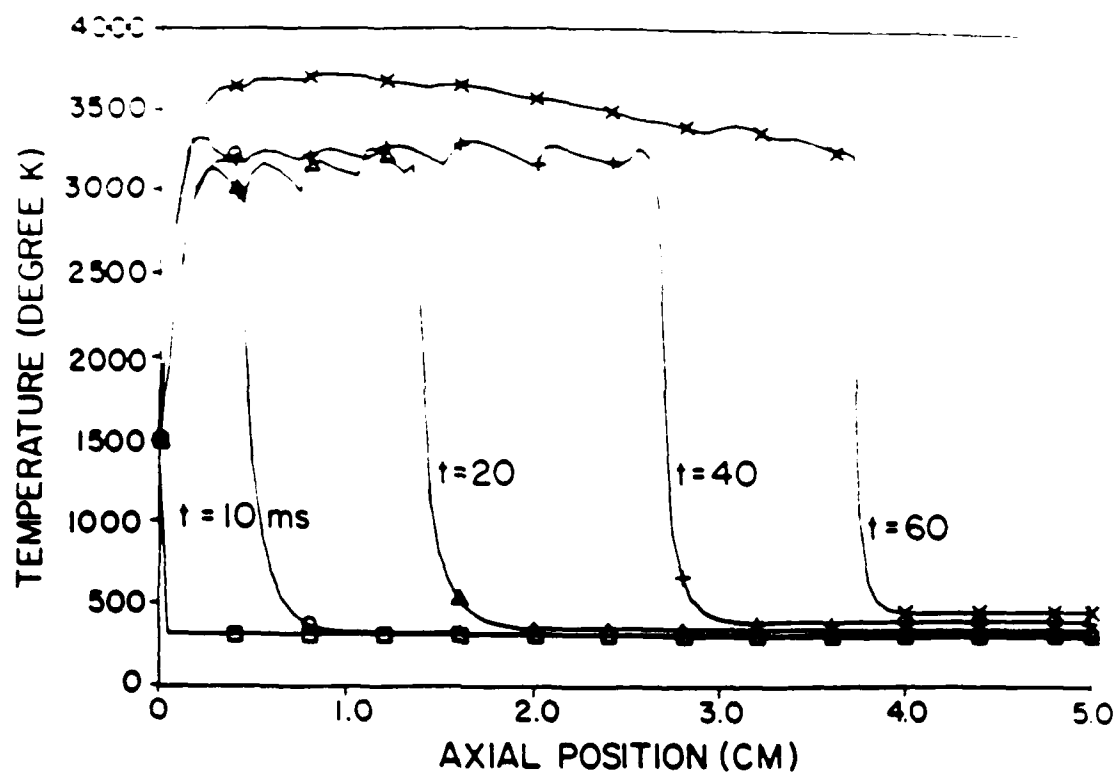
Figure 9. Gas Temperature VS Axial Position
at Different Times
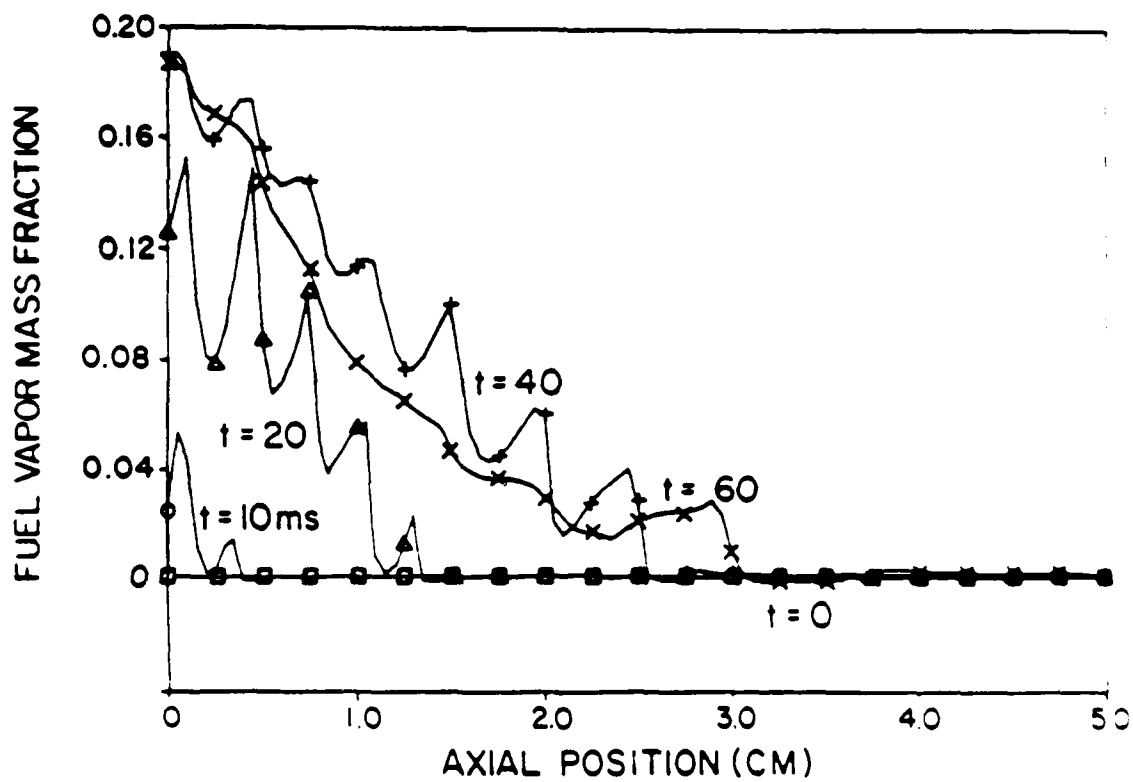
Figure 10. Fuel Vapor Mass Fraction VS
Axial Position at Different Times

29
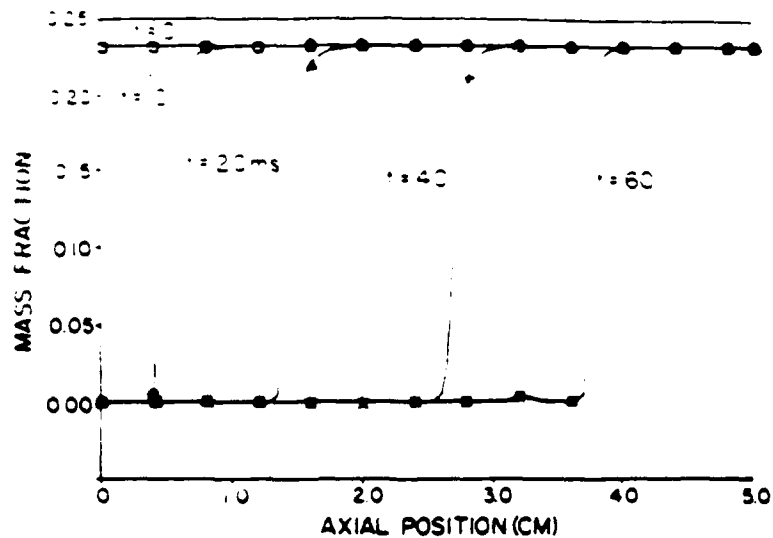
Figure 11. Oxygen Mass Fraction VS Axial
Position at Different Times
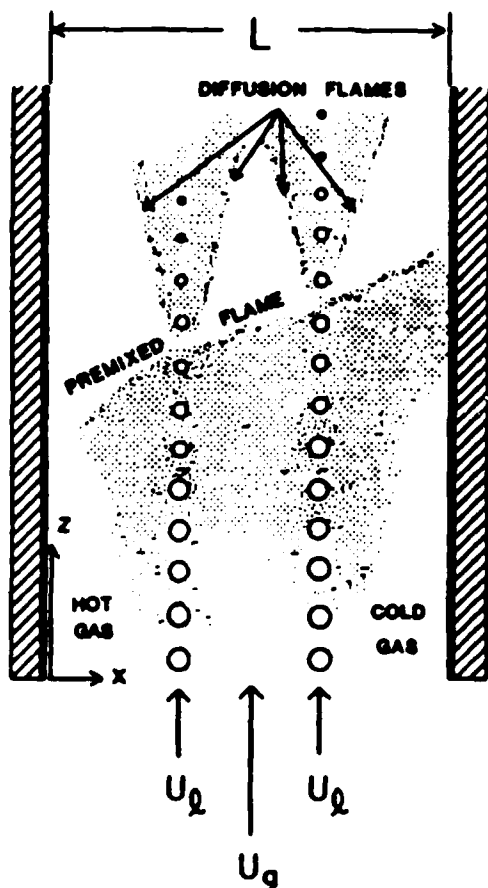
Figure 12. Vaporization, Ignition, and
Combustion of Two Parallel
Fuel Droplet Streams
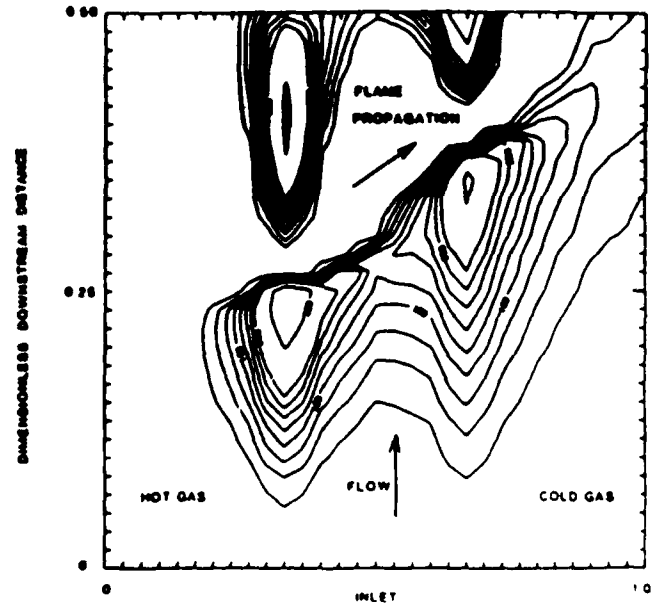
Figure 13. Fuel Mass Fraction
Contours

30
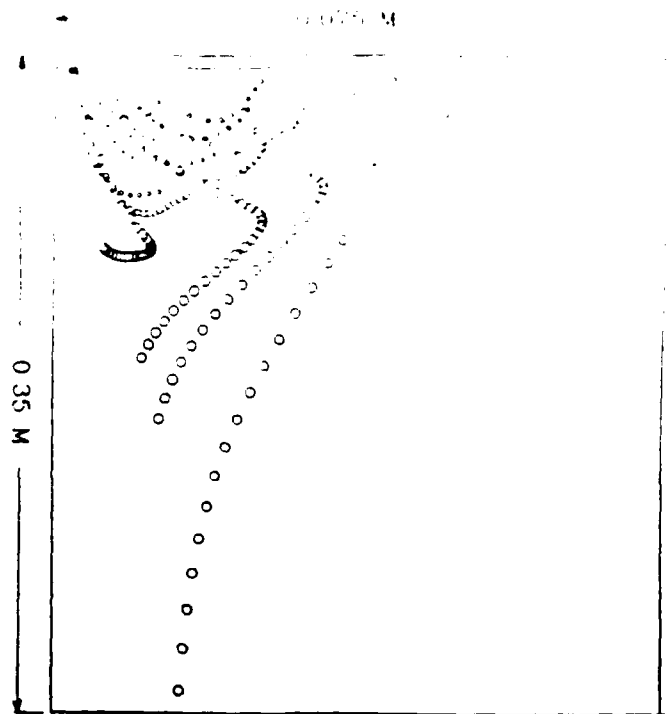
Figure 14.   Droplet Trajectories in Polydisperse
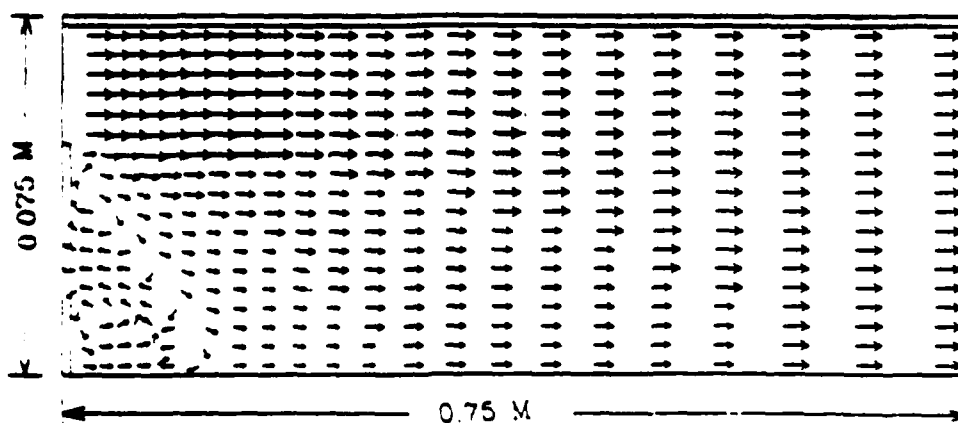Spray with Recirculating Flow

Figure 15.   Gas Velocity in Recirculating Flow
with Polydisperse Spray

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