

FUEL DROPLET VAPORIZATION AND SPRAY COMBUSTION THEORY

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Abstract—A critical review is presented of modern theoretical developments on problems of droplet vaporization in a high-temperature environment and of spray combustion. Emphasis is placed upon analytical and computational contributions to the theory with some mention of empirical evidence. Four areas of basic phenomena are discussed in some detail: (i) droplet slip and internal circulation, (ii) transient heating of the droplets, (iii) multicomponent fuel vaporization, and (iv) combustion and vaporization of droplet arrays, groups, and sprays. Various relationships amongst these phenomena are analyzed as well. Several other problem areas are given brief mention. Future directions are suggested.

NOMENCLATURE

a	Coefficient in Clausius–Clapeyron relationship	x, y	Coordinates in boundary layer on droplet
a, b	Major and minor axes of ellipsoidal shaped droplets	Y	Mass fraction
a, b	Coefficients {see Equations (22) and (23)}	z	Dummy variable
a, b	Sphere diameter and spacing between spheres in Section 5	α	Thermal diffusivity
A	Vortex strength	δ	Gas boundary layer thickness
B	Transfer number	ε	Reciprocal of Lewis number
B'	Transfer number modified to account for transient heating of droplet interior	η	Kolmogorov length scale
C_D	Drag coefficient	θ	Azimuthal position in droplet
C_v	Coefficient of specific heat at constant volume	λ	Thermal conductivity
d	Droplet diameter	μ	Viscosity
D	Mass diffusivity	v	Kolmogorov velocity
F	Friction force	ρ	Density
g_1, g_2	Functions defined in References [12] and [13]	τ	Shear stress
h	Enthalpy	τ_L	Characteristic droplet lifetime
I	Moment of inertia	ϕ	Mass fraction of decane in Fig. 7 also volume fraction of droplets in cloud
k	Droplet vaporization constant	τ, ϕ	Transformed coordinates for time and space in droplet interior
L	Latent heat of vaporization	v	Stoichiometric ratio
L'	Effective latent heat of vaporization {see Equation (19)}	ψ	Stream function coordinate
Le	Lewis number	ω	Vorticity
m	Droplet mass		
M	Droplet mass vaporization rate		
Nu	Nusselt number		
P	Pressure		
Pr	Prandtl number		
q	Heat flux		
Q	Energy value per unit mass of fuel		
r	Radial position in droplet		
r_c	Characteristic diffusion length in gas film surrounding a droplet in a cloud		
r_f	Flame position		
R	Droplet radius		
R_c	Droplet cloud radius		
Re	Reynolds number		
R^0	Gas constant		
s	Average spacing between centers of droplets in a group		
Sc	Schmidt number		
t	Time		
T	Temperature, also torque		
u	Gas velocity		
V	Droplet-gas relative velocity		
V_i	Droplet velocity		
w	Rotational velocity		

Subscripts

e	External or ambient
F	Fuel vapor property
g	Gas property
l	Liquid property
o	Initial condition
O	Oxygen property
r	Reference value
s	Droplet surface condition
∞	Ambient condition
i	Index for species
in	Initial value

1. INTRODUCTION

The theory of fuel droplet vaporization and spray combustion has been under development for several decades. During recent years, it has come to receive a large amount of attention. As new and heavier fuels become common, droplet vaporization in a liquid-fueled combustor becomes more significant as a rate-controlling factor.

This author is attempting here a critical review of modern developments in the theory of fuel droplet

vaporization and spray combustion. For that reason, four important limitations are placed upon the scope of this review. Firstly, in order to maintain a critical capability, the author limits the review to areas that he has carefully studied. Other areas are very briefly mentioned. Secondly, emphasis is placed upon publications of the last seven years or so. Furthermore, primary consideration is placed upon analytical and computational developments with very slight mention of experimental studies. Finally, the discussion centers on situations found in typical combustors where the gas temperatures are rather high and the gas is far from a fuel-vapor-saturated state so that regression rates of the liquid-gas interface are high.

It is assumed that the reader is aware of the classical fuel droplet vaporization theory as discussed in the textbooks by Williams,¹ Glassman,² Kanury,³ and Chigier.⁴ Classical droplet vaporization theory treats spherically-symmetric, quasi-steady, single-component, isolated droplets. It is on the relaxations of these features where modern developments are concentrating. In real combustors, the local field around a droplet is not spherically-symmetric but multidimensional; also, transient effects are extremely important. Real fuels are multicompositional with varying volatilities for the components. Droplets in a fuel spray are typically sufficiently close that they may not be treated as isolated from each other. This review will address the recent progress in treating these important theoretical issues. While substantial insight and understanding has been gained, it should not be inferred that the final solution is known; more work is required.

Section 2 contains a discussion of the effects of relative droplet-gas motion on the mechanics and dimensionality of the vaporizing droplet problem. Section 3 covers the issues of transient behavior of the droplet while Section 4 treats the real effects that occur with multicomponent fuels. Interaction between droplets in vaporizing fuel sprays is examined in Section 5. Finally, a brief mention of other important fuel droplet vaporization issues plus some summary statements are given in Section 6.

The reader is also recommended to examine previous reviews by Blazowski,⁵ Chigier,⁶ Williams,⁷ Sirignano and Law,⁸ Faeth,⁹ and Law.¹⁰ The issues that are emphasized in this review have not been covered in those previous reviews to a depth satisfactory to this author. Of course, other important issues are adequately discussed in those references.

2. DROPLET SLIP AND INTERNAL CIRCULATION

2.1. General Comments

Classical droplet vaporization theory describes a fuel droplet in a spherically-symmetric gas field. There, the only relative motion between liquid and gas involves radial convection due to vaporization. This model implies that droplets would travel through a combustion chamber at the gas velocity. Such an

implication could only be true, however, for very small droplets (certainly much less than thirty microns in diameter, for example). Since droplet mass is proportional to the cube of diameter and droplet drag is proportional to diameter squared, we can expect acceleration to be inversely proportional to the first power of diameter. Acceleration due to drag will always tend to decrease the relative velocity between gas and liquid. Of course, this tendency could be overcome in certain situations where the gas itself is accelerating due to pressure gradients and/or viscous stresses in such a manner so as to increase the relative velocity. In any event, the larger droplets will have a greater kinematic inertia.

The relative motion results in an increase of heat and mass transfer rates in the gas film surrounding the droplets; a thin boundary layer forms over the forward section of the droplet. This boundary layer also extends over a portion of the aft section. At sufficiently high Reynolds number (based upon relative velocity, droplet radius, and gas properties), separation of the gas flow occurs at the liquid interface. Since the liquid surface moves under shear, the separation phenomenon is not identical to separation on a solid sphere; for example, the zero-stress point and the separation point are not identical on a liquid sphere as they are on the solid sphere. The zero-stress points on the liquid sphere and the solid sphere occur at about the same point (110° to 130° measured from the forward stagnation point), but the separation point on the liquid sphere is well aft of that.

As mentioned above, the shear at the liquid surface causes a motion of the liquid at the surface. This liquid near the surface recirculates through the droplet interior so that an internal circulation results. The roughest approximation to this liquid motion is given by Hill's Spherical Vortex. As we shall see later, this results in a significant decrease in the characteristic lengths and times for liquid-phase heat and mass transfer. It does not, however, justify the so-called "rapid-mixing approximation" in which the characteristic times become zero.

Buoyancy effects on the gas film surrounding droplets scale with the third power of droplet diameter as compared to viscous effects; they are insignificant in practical combustors but can be important in certain laboratory experiments. Gravity effects on droplet trajectories also tend to be unimportant in high-mass-flow combustors but can be pertinent in certain fire-safety situations and in certain regions of furnace combustion chambers. Surface tension variations along the droplet surface due to surface temperature variations tend not to be significant. There is the possibility that surface active agents, present in the fuel via contamination, could cause surface tension variations. Generally, we assume that shear is continuous across the liquid-gas interface.

At high Reynolds number (a value in the hundreds), the inertial effects dominate the surface tension effects (a higher Weber number situation) and droplets break into smaller droplets. These droplets will have a

lower Reynolds number due to the decreased radius so that the implication is that a practical upper limit exists for droplet Reynolds number. One can show that the maximum Reynolds number decreases as relative velocity increases since Weber number is proportional to radius times the square of the relative velocity.

2.2. Evaluation of Reynolds Number Magnitude

Usually, the pressures and gas temperatures in a combustor are high leading to a large droplet Reynolds number. Consider, for example, the ambient gas pressure, density, temperature, and viscosity to be $p = 20$ atmospheres, $\rho_\infty = 0.7 \times 10^{-2}$ gm/cm³, $T_\infty = 1000^\circ\text{K}$, and $\mu = 0.4 \times 10^{-3}$ poise. With an initial droplet radius R_0 of 25 microns or greater, and an initial relative gas-droplet velocity of 25 m/s or greater, we may expect a Reynolds number (based upon radius rather than diameter) greater than 100. The implication is that a laminar high-Reynolds number boundary layer will exist over the droplet surface. Obviously, with atmospheric combustors, the density and, therefore, the Reynolds number, would be much smaller but this major conclusion about high Reynolds number is true for a very wide range of interest. The Reynolds number would increase as the ambient temperature decreases.

It can be shown that the Reynolds number remains high for most of the droplet lifetime in many typical situations. Yuen and Chen¹¹ have indicated that the drag data for vaporizing droplets can be correlated with the drag data for solid spheres if certain average viscosity in the boundary layer is employed for calculation of the Reynolds number. Let us consider, therefore, that $C_D = 12/Re$. (Note that many investigators would employ a $C_D = 24/Re$ where their Reynolds number is based upon diameter not radius.) This relationship for the drag coefficient is quite accurate for $Re = 1$ or less. It underestimates by a factor of 3 or so at $Re = 100$ but is still useful for the order of magnitude estimate that follows. The drag law is given by

$$m \frac{dV_l}{dt} = \frac{C_D}{2} \rho_g \pi R^2 |V|(-V) \quad (1)$$

where the mass of the droplet is

$$m = 4/3 \pi R^3 \rho_l$$

and V is the relative droplet velocity, V_l is the absolute droplet velocity, ρ_l is the liquid density, ρ_g is the gas density, and R is the droplet radius.

It follows that

$$\frac{dV_l}{V} = -\frac{9}{2} \frac{\rho_g}{\rho_l} \frac{|V|R}{Re} \frac{dR}{R^2} \quad (2)$$

The quantity $|V|R/Re$ will not change with time as velocity and radius change. For the representative values cited before, that constant will be of the order of 10^{-5} m²/sec. If the density ratio ρ_g/ρ_l is of the order

of 10^{-2} , it follows that the characteristic time for decrease of relative velocity is

$$\tau = R^2/k \quad (3)$$

where $k = O(10^{-7} \text{ m}^2/\text{sec})$ in our case. Now R^2 may be taken as an average or $R_0^2/2$. It may be considered that τ is about one millisecond.

The lifetime τ_L of this size droplet in a high-temperature environment with the relative velocity indicated will be about one millisecond also. Note further that, as the initial radius increases, the lifetime increases with a power somewhat weaker than the square due to a convective correction. That is, empirical evidence inferred from wetted porous spheres indicates that

$$\tau_L \sim R^2(1 + 0.3Pr^{1/3}Re^{1/2}). \quad (4)$$

So, for very low Reynolds numbers compared to unity, $\tau_L \sim R^2$ while, for high Reynolds numbers $\tau_L \sim R^{3/2}$. The velocity relaxation time τ will increase with R^2 as long as the drag law is obeyed. (The data of Yuen and Chen indicates that C_D decreases as Reynolds number increases up to a Reynolds number of about 1000). We may conclude that for initial droplet radii of twenty-five microns and greater, the time for velocity relaxation due to drag is comparable or greater than the droplet lifetime.

The change in droplet radius during the major portion of the droplet lifetime is not significant with regard to the determination of the order of magnitude of the Reynolds number. For example, as droplet mass decreases by a factor of eight (or about one order of magnitude), the radius only decreases by a factor of two. On account of the time scales for change in radius and relative velocity, the Reynolds number decreases by less than one order of magnitude during the period when most of the droplet mass vaporizes. Therefore, in many practical combustion situations, we may expect a laminar, high Reynolds number (of order 100) boundary layer to remain on the droplet for most of its lifetime. Since gas-phase Prandtl numbers are close to unity, the same conclusion can be made about the value of the gas Peclet number and the gas-phase thermal boundary layer. It should be understood that practical situations will also occur wherein the Reynolds number will be smaller, perhaps of order ten or less.

The velocities in the liquid phase associated with the internal circulation have been found by Prakash and Sirignano^{12,13} to be more than one order of magnitude lower than the relative gas-droplet velocity. However, the liquid density is two to three orders of magnitude greater than the gas density (depending upon the pressure level) so that, as a result, the liquid-phase Reynolds number, based upon droplet radius, liquid surface velocity, liquid density, and liquid viscosity is as large, or larger, than the droplet Reynolds number. Since the Prandtl numbers for ordinary liquids are of order ten, the liquid-phase Peclet numbers are very, very large compared to unity (of order 1000). We can expect a thin viscous layer and

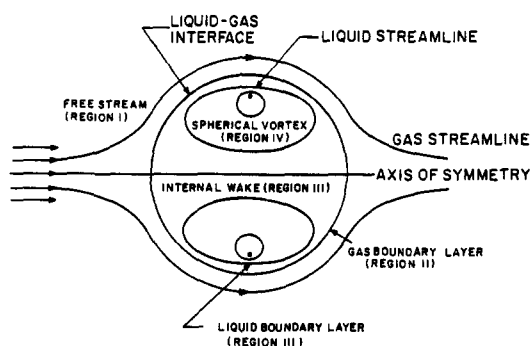


FIG. 1. Flow regions outside and within a fuel droplet at high Reynolds number.

a very thin thermal layer to exist in the liquid at the surface.

2.3. Discussion of Key Assumptions in Conceptual Model

The axisymmetric flow field within and around the droplet is depicted in Fig. 1 as including four major regions. Region I is the inviscid free stream of gas flowing over the droplet and outside of its wake as seen from a frame of reference moving with the droplet. Region II includes the gas-phase viscous boundary layer and near wake. Region III contains the liquid viscous layer and the liquid internal wake which is the zone along the axis of symmetry through which the liquid circulating out of the boundary layer passes. Region IV is the toroidal core region within the droplet that is rotational but nearly shear-free and is approximated as a Hill's spherical vortex.

Let us discuss the various assumptions implied by this model of a "slipping" droplet. Firstly, it is assumed that the droplet remains spherical; this has been shown by Lerner, *et al.*¹⁴ to be reasonable for hydrocarbon droplets with 400 microns diameter or less, and relative velocities of tens of meters per second. Obviously, the Weber number is a key parameter. Operation in the near critical region as discussed by Faeth⁹ would lead to a failure of the spherical assumption.

Another important assumption involves the axisymmetry of the flow field and the absence of droplet rotation. Rotation of the droplet would be caused by a torque on the droplet. Once the droplet is formed, the major cause of a torque would be a net moment due to friction forces on the droplet surface. Some asymmetry in the flow is necessary here to accomplish this since velocity gradients must exist in the approaching gas flow. The largest possible velocity gradients would be at the Kolmogorov scale in turbulent flow. This turbulent scale can be of the order of the droplet diameter (about 100 microns or so) in practical combustor situations. Estimates of the net torque and the perturbation in the friction force at the surface due to velocity gradients of this maximum amount indicate that: (i) the characteristic time for rotation of a solid

particle in the flow would be very large compared to the time of transit for an element of gas moving past the particle; and (ii) the fractional change in frictional force on the particle or droplet surface would be of the order of the reciprocal of the droplet Reynolds number. The process of estimation is presented in the Appendix. If a net torque were applied to a liquid, it is intuitively accepted by this author that the droplet would be induced to undergo an asymmetric internal circulation due to the shearing force imbalance rather than to rotate as a solid body. The basis for this belief is that moment of inertia of the liquid in the circulatory motion is significantly less than that associated with a solid-body-like rotation. The solid-body rotation model is a worst-case scenario, in some sense. In any event, conclusions (i) and (ii) above indicate that rotation or asymmetric circulation is not significant for droplets with the large Reynolds number under consideration here.

The same type of analysis can be employed to consider the effects of initial droplet rotation established during the formation or atomization process. The indication is that the net torque due to surface friction would oppose the rotation, which would be relaxed in the time required for the droplet to travel tens of diameters (but not hundreds of diameters). Again, droplet rotation does not seem very important.

Later, in Section 4, a brief discussion of the effects of the temporal change in the velocity field will be given. The conclusion, however, will be that the time-scale for even the most rapid turbulent fluctuation (those at the Kolmogorov scale) would be much longer than the residence time for flow past the droplet if the droplet Reynolds number is large compared to unity and if the Kolmogorov length scale is not smaller by an order of magnitude or more than the droplet diameter. Note that for small Kolmogorov length scales compared to droplet diameter, asymmetries in the flow due to that turbulent scale can be averaged and should become insignificant. It does seem that axisymmetry is a safe assumption.

Another assumption that should be discussed relates to the effect of surface regression upon the flow field. Basically, the reasonable argument is advanced that the residence time for a gas element flowing past the droplet and the circulation time for a liquid element in the droplet are orders of magnitude less than the droplet lifetime. The surface regression on those timescales is miniscule and can only result in very small perturbations to the flow field. The smallest length scales that we shall see in this problem will be the thicknesses of the heat and mass diffusion layers at the liquid surface. As long as a liquid element at the surface circulates very many times before the surface regresses that distance, our model will be reasonable. The assumption is best for the viscous layer, next best for the thermal layer, but weakest for the mass diffusion layer since the liquid Prandtl number is of order ten and the liquid Schmidt number is of the order of hundreds. In high-temperature environments,

such as combustors, the vaporization rate becomes so high that a fluid element in the boundary layer and internal-wake (Region III) will not circulate many times before the completion of vaporization; this assumption is rather weak, therefore, and its relaxation should be studied in the future.

Continuity at the liquid-gas interface would indicate that the surface velocity in the aft region of the droplet could be reversed on account of the existence of the near wake. Results of numerical calculations indicate that above a certain Reynolds number a small secondary vortex will exist at the aft region of the liquid sphere. The Hill's vortex model is oversimplified therefore, in that range where a secondary vortex must exist. Numerical results by Rivkind and Ryskin¹⁵ indicate that whenever the internal fluid (liquid) density is much larger than the external fluid (gas) density, the secondary vortex is quite small compared to the primary vortex. It follows that for our situation, the assumption of a single spherical vortex is reasonable as a first approximation.

Another important assumption is that the fluid motion in the droplet interior and in the gas-phase boundary layer is considered to be quasi-steady. The transient period for the establishment of the motion is quite small compared to the droplet lifetime. That characteristic time is the vorticity diffusion time given by the radius squared divided by the kinematic viscosity. Note that the time for heat diffusion across the droplet is much longer than the vorticity diffusion time by the factor of the Prandtl number while the mass diffusion time is longer by the factor of the Schmidt number. For a droplet vaporizing in a combusting environment, the droplet temperature and concentrations vary spacially through the droplet and behave in an unsteady manner.

In addition to the initial transient, some unsteadiness could result from vortex shedding in the gas from the droplet surface. Based on Strouhal number estimates, the frequency of shedding would be high compared to other phenomena in the droplet. Also, the vortex shedding, if it does occur, would only affect the aft side of the droplet, and should not perturb the gas boundary layer on the droplet through which most of the heat and mass transfer occurs. It is assumed, therefore, that any effect of vortex shedding averages to be negligible.

2.4. Droplet Drag Coefficient

As mentioned before, Yuen and Chen¹¹ have found that the droplet drag coefficient is very close to that for a solid sphere of the same diameter. The indications are that a balance exists between the decrease in friction drag and the increase in pressure drag due to the blowing effect associated with vaporization. They show, however, that the appropriate Reynolds number (to be employed in extracting the drag coefficient from the standard curve for a sphere) is based upon a certain "1 3" averaging rule for

weighting the free stream and the surface viscosity. In particular,

$$\mu_r = \mu_s + \frac{1}{3}(\mu_\infty - \mu_s) \quad (5)$$

where r , s , and ∞ subscripts indicate reference (averaged), surface, and ambient values, respectively. Note that if the most intense vaporization were on the aft surface of the droplet it is plausible that pressure drag would decrease and the conclusions of Yuen and Chen would not apply. This could occur with droplets that have wake flames.

The general results of Yuen and Chen were confirmed in the experiments of Lerner *et al.*¹⁴ who used the averaging principle for both density and viscosity. They also showed that the drag law could be applied to ellipsoidal droplets if the effective diameter D is taken as $(a^2b)^{1/3}$ where a and b are the major and minor axes, respectively, and their values are within 10% or so of each other. Note that the Reynolds number based upon the averaged reference values can be several times greater than a Reynolds number based upon free stream properties, increasing the likelihood of a high-Reynolds number boundary layer phenomenon.

The more recent experimental results are in disagreement with the results of Ingebo¹⁶ which were taken from spray measurements and therefore were marred by entrainment effects. Namely, an average droplet in a group of droplets will penetrate further into the gas than a single isolated droplet of the same size and initial velocity; the group of droplets will cause a significant motion of the gas affecting the relative gas-droplet velocity. It follows that the increased penetration of the droplets in the spray would give the appearance of a reduced drag coefficient when actually, it is the reduction in the relative velocity that decreases the drag. It is recommended that the Yuen and Chen drag coefficients be employed in calculations rather than the Ingebo results in the future since it is desirable to have a drag coefficient that relates to an individual droplet rather than to the global spray character. The entrainment effects would automatically be considered if the appropriate momentum balance were performed on both the gas and the liquid phases. It must be cautioned, however, that for dense spray regions, the effect of droplet spacing on the drag coefficient should be taken into account.

2.5. Internal Flow Field for Droplet

The stream function and the vorticity for the Hill's spherical vortex approximation to the internal circulatory flow in the droplet are given by:

$$\psi = -\frac{1}{2}Ar^2(R^2 - r^2)\sin^2\theta \quad (6)$$

and

$$\omega = 5Ar\sin\theta \quad (7)$$

where A is the vortex strength. The coordinate system and the stream surfaces are portrayed in Fig. 2.

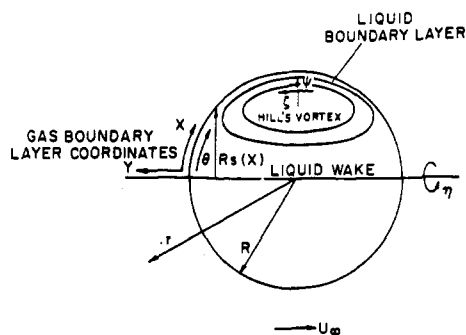


FIG. 2. Coordinate system for the circulating droplet problem.

It should be noted that the Hill's Spherical Vortex solution satisfies a linear partial differential equation even though it applies for liquid Reynolds number much greater than unity. In this sense, the solution is generally similar to the solutions for Poiseuille and Couette flows in that the inertial nonlinearities become identically zero. For this reason, a Stokes flow solution for the streamsurfaces in the droplet would be identical to the Hill's solution. Internal flows in droplets receive much discussion in the literature.^{12,13,39,46}

It should be understood that the particular value of the vortex strength will not be important provided that: (i) the circulation time in the droplet is shorter than other characteristic times; and (ii) the surface velocity is small compared to the relative gas-droplet velocity. (Both of these are reasonable assumptions in the practical high Reynolds number situations). It is fortunate that the vortex strength value is of secondary interest because the error in its calculation can be significant due to the variable viscosity due to large temperature differences through the boundary layers in the liquid and in the gas film.

3. TRANSIENT HEATING

Many authors^{8,12,13,14,17-33} have considered the effects of transient heating on fuel droplet vaporization. Most of the studies^{8,18,19,21-33} have dealt with spherically-symmetric vaporizing droplets but some have taken into account "slip" and internal circulation.^{8,12,13,14,17,19,20} The term "slip" is commonly employed to signify that the droplet is moving relative to the surrounding gas. It is somewhat confusing terminology since the no-slip condition still applies at the droplet surface. Nevertheless, the poor but conventional usage will be followed here. The primary effect of slip is to modify the heat exchange rate between the surrounding gas and the droplet while the primary effect of internal circulation is to modify the geometry, length, scale, and time scale, associated with the heat transfer within the liquid. Otherwise, the basic phenomenon is similar in both situations.

Heat is transferred from the hot gas to the liquid surface. Some of the heat from the gas will be required

to overcome the latent heat of vaporization while some is transferred to the interior. So, the liquid near the surface is warmest while the coolest region lies in the interior (with the precise location of this coolest region affected by internal circulation). Spatial and temporal gradients will exist in the liquid droplet with the surface temperature rising towards the boiling point in time and the droplet temperature field becoming more uniform in time. In typical combustor situations with the large vaporization rates involved, the period of transient heating is comparable to the droplet lifetime. The regression of the surface, therefore, can be a significant factor in the heating of the droplet; one must be careful before neglecting it.

3.1. Transient Spherically-Symmetric Vaporization

The earliest models¹⁻⁴ assumed that the droplet temperature was uniform and constant in time. Usually, they considered the temperature to be at the wet-bulb temperature which was calculated upon the assumptions that: (i) no heat was transferred to the droplet interior (all the heat from the surrounding gas went into vaporization); and (ii) equilibrium existed at the droplet surface (typically a Clausius-Clapeyron relationship was employed). Some investigators¹ assumed that the droplet temperature was at the boiling temperature so that the equilibrium condition was relaxed.

The resulting relationship for the mass vaporization rate M , and flame stand-off distance, heat transfer to the surface, and droplet lifetime in this totally quasi-steady situation are

$$M = 4\pi \left[\int_0^R \frac{dz}{\rho D z^2} \right]^{-1} \ln [1 + B] \quad (8)$$

$$r_f/R = \{\ln [1 + B]\} / \ln [1 + v Y_{O_2}] \quad (9)$$

$$q_g = ML \quad (10)$$

$$1 - R^2/R_0^2 = t/\tau_L \quad (11)$$

The equilibrium droplet temperature is determined by solution of the nonlinear relation:

$$\frac{1 + v Y_{O_2}}{1 - Y_{F_s}} = 1 + B \quad (12)$$

where

$$B \equiv \frac{h_\infty - h_s + v Q Y_{O_2}}{L} \quad (13)$$

and

$$Y_{F_s} = a e^{-L/R_0^2}$$

Note that (11) is a form of the well-known d^2 -law.

It has become understood that the liquid phase behaves in a very unsteady fashion during droplet vaporization. It can be easily verified that a transient heating time given as the ratio of the square of the droplet radius to the liquid thermal diffusivity is of the same order as the droplet lifetime. During the period of transient heating, assumption (i) above cannot

apply since heat is transferred to the interior. Since the gas-phase thermal and mass diffusivities are very large (except in near critical or supercritical domains of pressure and temperature) compared to the liquid diffusivity, the gas-phase behavior is typically considered to be quasi-steady.

In the first approach³⁴ to the transient heating problem, the authors relaxed the first assumption above but assumed that the temperature field in the droplet was uniform although time-varying. In particular, the heat transferred from the gas to the droplet surface was set by

$$q_g = ML + mC_v \frac{dT_l}{dt} \quad (14)$$

Implicitly, this statement assumes that the liquid thermal conductivity is infinite. Some authors^{8,21} have referred to this as a "rapid-mixing limit" approximation which results from the effects of internal circulation. Careful studies^{12,13,17,20} have shown that no such physical limit should be expected; this point will be further discussed in Section 3.2.

Generally, it is recognized to be more reasonable to consider a finite thermal conductivity in the liquid and to replace¹⁴ with the boundary condition

$$q_g = ML + q_l \quad (15)$$

to be placed upon the solution to the partial differential equation for spherically-symmetric heat diffusion in the droplet. The problem, of course, is complicated by the regressing or moving boundary. This approach is named the diffusion-limit model and should be considered as the most exact of the models for spherically-symmetric behavior.

Figures 3 and 4 (taken from Sirignano and Law⁸) compare temporal variations of the surface area and liquid temperature for the three models. Little difference (10% or so) is seen in the prediction of the droplet lifetime. The two models with surface temperature variation approach a d^2 -law behavior asymptotically. The liquid fuel here is *n*-octane; with less volatile fuels having higher boiling points, the approach to the asymptotic behavior would be slower and the differences between the models would be

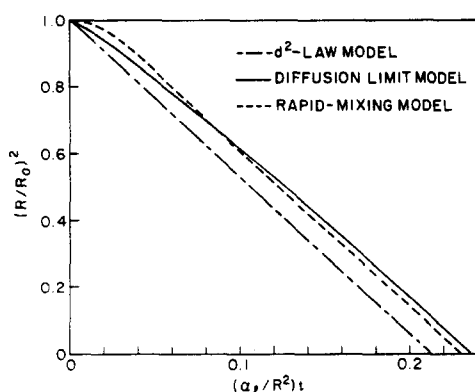


FIG. 3. Comparison of various models for spherically-symmetric vaporization (taken from Reference [8]).

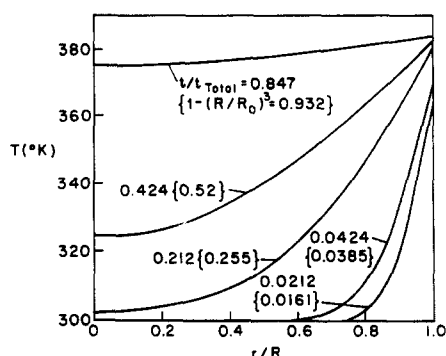


FIG. 4. Spatial variations in liquid temperature at various times for spherically symmetric vaporization (taken from Reference [8]).

greater. With the volatile fuel in Fig. 3, the greatest deviation from the d^2 -law behavior occurs during the initial heating transient.

Figure 4 shows that the temperature in the liquid has spatial gradients for most of the droplet lifetime and only approaches a uniform temperature towards the end of the lifetime as indicated by the record of the volume of liquid vaporized at each reported time. It is also seen that very little vaporization occurs during the initial period before the surface temperature is high.

In this case with a quasi-steady gas-phase and unsteady liquid phase, Eqs (8), (9), and (12) are modified to read

$$M = 4\pi \left[\int_0^R \frac{dz}{\rho Dz^2} \right]^{-1} \ln[1+B'] \quad (16)$$

$$r_t/R = \{\ln[1+B']\}/\ln[1+Y_{0\infty}] \quad (17)$$

$$B' = \frac{h_\infty - h_s + vQY_{0\infty}}{L'} \quad (18)$$

Also we have

$$L' = L + \frac{4\pi R^2}{M} \lambda_l \left(\frac{\partial T}{\partial r} \right)_{l,s} = L + \frac{q_l}{M} = \frac{q_g}{M} \quad (19)$$

whereby the amount of heat transferred into the liquid interior $q_l = 4\pi r^2 \lambda_l (\partial T / \partial r)_{l,s}$ is determined via the solution of the heat diffusion equation in the liquid.

$$\frac{\partial T_l}{\partial t} = \alpha_l \left(\frac{\partial^2 T_l}{\partial r^2} + \frac{2}{r} \frac{\partial T_l}{\partial r} \right) \quad (20)$$

Equation (15) still will hold. Obviously, the difference between the set of Eqs (8), (9), and (12) and the set (16), (17), and (18) involves the replacement of B and L by B' and L' .

In the determination of droplet lifetimes for low-boiling point fuels, the use of the d^2 -law gives a good first approximation. For higher boiling-point fuels, a more sophisticated approach is required. The vaporization rate per unit time during the droplet lifetime is often important information since it will determine vapor mixture ratio distribution with time (or with position when the droplets traverse a combustor). In that case, the d^2 -law would be inadequate

even for low boiling-point fuels such as octane and a more sophisticated approach would be needed.

As shown in Fig. 3, the infinite diffusivity model underpredicts the vaporization rate during the initial period and overpredicts the vaporization rate later in the lifetime. Since every unit of energy conducted into the droplet is distributed uniformly over the droplet in the infinite-diffusivity model, the surface temperature rise *per unit of energy exchanged* is less. This explains why the surface temperature is underpredicted initially by that model. However, since the difference between ambient temperature and surface temperature affects directly the heat conducted from the gas to the liquid, that model will overpredict the amount of heat transferred to the liquid during that initial period. This results eventually in a higher surface temperature for the latter portion of the lifetime.

This author recommends, whenever the additional computational complexity can be afforded, that the combustor modeller should employ the more exacting model, namely the diffusion-limit model. Note that a separate decision should still be made as to whether this diffusion-limit model should be spherically-symmetric, as discussed above, or should contain the effects of internal circulation, as will be discussed in the next subsection. Some of the issues concerned with the application of these models to spray combustor modelling will be discussed later in Section 5.

The effect of the regressing surface appears in two ways when the moving boundary heat transfer problem is transformed to a fixed boundary problem as shown by Law and Sirignano.¹⁸ Note, of course, that the vaporization rate is immediately related to the regression rate. Firstly, the vaporization rate can be seen to appear in the matching conditions for temperature and species mass fraction at the droplet-gas interface. This effect is never found to be negligible in combustion problems. Secondly, in the transformed problem, the vaporization rate (or the regression rate) appears within a radial convective term in the liquid heat diffusion equation. Law and Sirignano show that under some circumstances, this term can be neglected. It can be shown that this term is proportional to the factor

$$\frac{1}{\alpha_l} \frac{dr_s^2}{dt}$$

The radial liquid convective term can be neglected, therefore, for low vaporization rates but will be important for higher vaporization rates. Increases in the liquid diffusivity would tend to make this term less important. In general, the effect of this radial liquid convective term on the droplet lifetime is less significant than its effect upon the detailed temperature profiles in the liquid.

Seth, Aggarwal, and Sirignano³⁵ have shown that the neglect of the radial liquid convective term allows for a certain formulation of the transient heating in terms of an integral equation which is quite amenable

to application in a spray combustion model. More discussion on this point will occur in Section 5.

In some situations, it is desirable to relax the condition of a quasi-steady gas-phase. For example, in near-critical or supercritical ranges of pertinent thermodynamic parameters such as pressure and ambient temperature, the diffusivities of the liquid and of the gas could be comparable so that characteristic times for transient behaviors in the liquid and in the gas could be both comparable to the droplet lifetime.^{36,37} Another example would occur in the study of the relaxation to a quasi-steady gas phase. In reality, there is little or no vapor fuel in the gas film surrounding the droplet at the instant it is formed via atomization. However, a quasi-steady gas-phase assumption allows for fuel vapor to be present at the initial instant. The volume of the spherically-symmetric film surrounding the droplet is at least three orders of magnitude greater than the volume of the droplet itself since the gas film thickness is an order of magnitude greater than the droplet radius. This model forces the amount of fuel vapor to be comparable in order of magnitude to the amount of liquid fuel at the initial time. Of course, the higher the initial liquid temperature, the more significant is the error in this model. Even though the relaxation to quasi-steady conditions occurs rapidly, a major portion of the fuel vapor may vaporize during that relaxation period.^{29,31} On the other hand, if the initial droplet temperature is not too high, the amount of fuel vapor that would be present corresponding to that surface temperature could be very small compared to the amount of liquid fuel in the droplet. In such a case, it would be reasonable to follow the accumulation of fuel vapor in the film employing a quasi-steady model. See Law¹⁰ for further discussions. This effect could be significant in ignition and flame stability considerations. A final example would relate to extinction of flames around droplet, where obviously an unsteady phenomenon occurs in the film surrounding the droplet.^{28,30}

3.2. Transient Vaporization with Slip and Internal Circulation

The basic phenomena discussed in the previous sub-section still exist when slip and internal circulation are present. Important modifications will occur, however. The slip between the droplet and the surrounding gas leads to the formation of a boundary layer around the droplet with convective heating augmentation. The friction at the surface causes internal circulation which changes the geometry of the isotherms and the characteristic scales of liquid heating and, as we shall see in the next section, of liquid-phase mass diffusion.

The earliest empirical evidence of Ranz and Marshall³⁸ indicated that the Nusselt number and vaporization rate for quasi-steady vaporization from wetted porous spheres increase by a factor of $1 + 0.3 Pr^{1/3} Re^{1/2}$ due to convective effects. Here

Reynolds number is based upon the diameter and the relative velocity of the droplet, and gas density and viscosity while Prandtl number is based upon gas properties. It is seen that an increase in the Reynolds number will lead to increased rates of heat transfer, mass transfer, and vaporization and therefore, to a decreased droplet lifetime.

For very large Reynolds numbers compared to unity, the second term in the above factor is dominant and we can expect that Nusselt number and vaporization rate increase with the square root of Reynolds number. Since the vaporization rate for spherically-symmetric flow is proportional to droplet radius (from which the d^2 -law follows), the vaporization rate with the convective correction is proportional to radius to the three-halves power. From this statement, it follows that the droplet lifetime is proportional to the initial droplet diameter to the three-halves power for large Reynolds numbers.

The wetted porous sphere experiment, however, only simulates a droplet that has a uniform, steady droplet temperature at the wet-bulb temperature. The wetted sphere does not reproduce the real droplet effect of liquid-phase heat or mass transport and internal circulation. Those effects are not important for slowly-vaporizing droplets where the droplet lifetime is long compared to a characteristic time for transport in the liquid. In such a case, liquid diffusivity may be considered infinite and the details of the internal flow field are not important since the internal gradients of the scalar properties (such as temperature or concentration) go to zero.

For that reason, a porous wetted sphere experiment cannot simulate the situation for fuel droplets in combustors where the vaporization rates are sufficiently high that internal transport and, therefore, internal circulation, are interesting. The experiments of El Wakil *et al.*³⁴ also did not approach the range of high ambient temperatures and high vaporization rates so that their results are in agreement with those of Ranz and Marshall. We cannot recommend the use of results from porous wetted sphere experiments or from droplets vaporizing in low temperature environments in combustor analysis for the above reasons. In addition, there are some noteworthy modifications that should be made to the results of Ranz and Marshall and of El Wakil, *et al.*

Firstly, it has been shown by Lerner *et al.*,¹⁴ that the extension of the empirical $1/3$ averaging rule for the Prandtl and Reynolds numbers to the convective correction is necessary when large temperature differences exist across the gas film surrounding the droplet. Again, the Reynolds number based upon the average properties can be more than five times the number based upon ambient properties. The original experiments of Ranz and Marshall and El Wakil *et al.* did not have such large temperature differences.

Secondly, Sirignano¹⁹ has shown that the natural logarithm functional dependence upon the transfer number B is not correct and can, especially in an unsteady situation, produce serious error. The

dependence $\ln(1+B)$ results from the analysis of the spherically-symmetric, quiescent vaporizing droplet. In a quasi-steady situation, the value of B does not vary greatly over a range of typical hydrocarbon fuels in a combustion situation. Therefore, this dependence has never really been well-tested experimentally for convecting droplets (high Reynolds number) in a quasi-steady combustion environment since $\ln(1+B)$ has relatively small variation. However, as shown by Sirignano and Law,⁸ the effective transfer number can vary by an order of magnitude during the droplet lifetime when transient heating effects are properly considered. This implies that, for the convective situation, the proper functional dependence upon the effective transfer number becomes important. The $\ln(1+B)$ dependence simply cannot apply when a convective boundary layer exists over the droplet as demonstrated by recent theoretical developments.^{12,13,17,19,20} Its erroneous use in high Reynolds number situations becomes very serious as the unsteady effects (to be discussed shortly in this section and later in 4) become important when heating rates and vaporization rates are high.

For these reasons, a new approach to droplet vaporization with slip in a high-temperature environment became necessary. The problem cannot be viewed as a perturbation to the spherically-symmetric case when the droplet Reynolds number is high compared to unity. At best, we have an axisymmetric situation as discussed in Section 2.

Generally, we can safely assume that the gas-phase is quasi-steady even if the situation is near the critical thermodynamic conditions or the extinction domain (if a flame exists about the droplet). This quasi-steady behavior near the critical conditions or the extinction domain is not present in the spherically-symmetric case. The reason for the different behaviors is due to the large difference in the length scales for gas-phase diffusion. In the spherically-symmetric case, the gas film thickness is an order of magnitude greater than the droplet radius while in the high-Reynolds situation, the film thickness (or the boundary layer thickness) is much smaller than the droplet radius. Note that: (i) the characteristic time for diffusion is proportional to the diffusion length squared so that the difference between the above two cases becomes even more significant; (ii) the gas Prandtl and Schmidt numbers are of order unity so that the gas viscous, thermal and mass diffusion layers are all of the same approximate thickness and characteristic time; and (iii) the residence time in the boundary layer equals the diffusion time across the boundary layer.

The Prandtl number and Schmidt number for the typical hydrocarbon fuel are of order ten and order hundred, respectively. Due to the high liquid density, the Reynolds number and the Peclet numbers for the droplet interior will also be very large compared to unity. Two conclusions may be drawn from this order of magnitude analysis. Firstly, the transient time for heating and mass diffusion in the liquid phase can be quite long compared to the relaxation time for the

internal circulation to be established due to the large Prandtl and Schmidt numbers. Indications are that the heating time is comparable to and the mass-diffusion time is much longer than the droplet lifetime. Secondly, the large Peclet numbers demonstrate that thin boundary layers exist near the liquid surface.

At high liquid Peclet numbers, we expect that an axisymmetric thermal boundary layer exists near the liquid-gas interface; as the boundary layer flows away from the rear stagnation point, an internal wake forms. The thermal layer and thermal internal wake are thinner than the viscous layer and viscous internal wake of Region III in Fig. 1, but otherwise qualitatively similar. The toroidal core will be unsteady since heating is slow at large Prandtl number but may be assumed to be one-dimensional when cast in an optimal coordinate system as demonstrated by Prakash and Sirignano.^{12,13} The time required to circulate an element of liquid once around a stream surface is very small compared to other characteristic times (a consequence of high Peclet number). Within the core, therefore, the convection will tend to uniformize temperature (and also concentration) along the streamsurface although variations will exist across the streamsurfaces. Diffusion will then be normal to the streamsurfaces in the limit. Temperature variations and heat diffusion may be neglected along the streamsurface. Therefore the problem is recast in new orthogonal coordinates whereby one coordinate is constant along a stream-surface; the two-dimensional, unsteady problem is transformed to a one-dimensional unsteady problem. The unsteady core is qualitatively similar but slightly larger than the Hill's vortex core (Region IV, of Fig. 1).

Prakash and Sirignano^{12,13} analyzed the gas-phase boundary layer using an integral method to determine profiles for velocity, temperature, and species concentration. The integral method reduced the two dimensional, quasi-steady system of equations to a set of ordinary differential equations with the position along the droplet surface as the independent variable. These gas properties solutions were matched to the liquid boundary layer solutions. Those solutions were obtained via an extension of the analysis of Harper and Moore³⁹ that allowed for significant differences in the properties of the internal and external fluid. On account of the variation of properties along the interface, it is necessary that the liquid boundary layer solution be two-dimensional as considered by Harper and Moore and Prakash and Sirignano. The liquid boundary layer may be viewed as a relaxation zone or intermediate zone between the two-dimensional gas boundary layer and the one-dimensional core. Recent studies by Tong and Sirignano^{40,41} indicate that the assumption of uniform values of the properties at the surface and, consequently, a one-dimensional liquid boundary layer, can lead to acceptable approximate results. Prakash and Sirignano assumed the liquid boundary was quasi-steady since it was thin and the thermal inertia of that layer is small. Tong and

Sirignano⁴⁰ have shown that the thermal inertia effect in the boundary layer can be included without difficulty under the one-dimensional assumption and leads to a modest correction since the boundary layer is never infinitesimally thin. Basically, the one-dimensional unsteady core region is extended to the droplet surface and to the axis of symmetry.

The one-dimensional, unsteady energy equation in the core has been derived in the following form

$$\frac{\partial T}{\partial \tau} = a(\tau, \phi) \frac{\partial^2 T}{\partial \phi^2} + b(\tau, \phi) \frac{\partial T}{\partial \phi} \quad (21)$$

where

$$a(\tau, \phi) = \frac{R_0^2 g_2(\phi)}{R^2 g_1(\phi)} \quad (22)$$

and

$$b(\tau, \phi) = \frac{R_0^2 g_2'(\phi)}{R^2 g_1(\phi)} + \frac{3}{g_1(\phi)R} \frac{dR}{dt} \int_0^\phi g_1(z) dz. \quad (23)$$

Note that τ and ϕ are nondimensional coordinates for time and stream-surface, g_1 and g_2 are known functions of ϕ which are also directly proportional to the vortex strength and are related to the details of the coordinate transformation. Appropriate boundary conditions, initial conditions and matching conditions have been applied to these equations. Namely, an initial uniform liquid temperature is assumed, the temperature at the vortex center is taken as a regular function of ϕ , and the heat flux through the liquid boundary layer from the gas is matched to the flux entering the core at its outer edge. See Prakash and Sirignano for details.

Certain interesting observations can be made even before the solution of the equation:

(i) The equation is a diffusion equation with variable coefficients. With no vaporization, the coefficients depend only on ϕ but in general they vary with both τ and ϕ .

(ii) The equation appears to be linear but, in actuality, a certain hidden nonlinearity is present. Namely, the regression rate dR/dt will depend upon surface temperature. Other nonlinearities due to the temperature-dependence of transport and thermodynamic properties could appear in a more exact analysis. One can, however, still take advantage of the apparent linearity in the analysis.

(iii) Since g_1 and g_2 are each proportional to vortex strength and since they or their derivatives only appear in ratio form, the coefficients a and b are independent of vortex strength. This implies that there is no such phenomenon as a "rapid-mixing limit". The diffusion equation (21) does not change form as vortex strength (or equivalently circulation) increases and no limiting condition results.

(iv) The characteristic length for diffusion is related to the shortest distance from the vortex center to the streamsurface coincident with the edge of the liquid boundary layer. If the edge of the layer were approximated as the surface of the droplet (an infinitesimally

thin layer), this distance becomes $R(1 - 1/\sqrt{2}) \sim 0.3R$. The characteristic length is about 30% of the characteristic length for liquid heating in the spherically-symmetric case. Since characteristic time is proportional to the square of the distance, the heating time is less than 10% of the corresponding time for the spherically symmetric case.

(v) In the limit of rapid regression rate (large dR/dt), the coefficient b becomes large resulting in the formation of a quasi-steady layer at the edge of the core whereby there exists an approximate balance between the second-derivative term and the pseudo-convective term in Eq. (21). The portion of the last term in that equation which contains the product of dR/dt and $\partial T/\partial \phi$ is named the pseudo-convective term because it becomes a convective term in a frame of reference fixed to the regressing droplet surface. The direction of the convection here is normal to the droplet surface. This boundary layer in this limit would amount to a relaxation zone that regresses into the interior of the droplet as rapid vaporization occurs; the core temperature would remain intact at the initial temperature until the relaxation zone arrives. This limit can only occur when the droplet lifetime is much shorter than the droplet heating time and has not been observed in practical situations at typical combustor temperatures and with typical fuels. The analog of this situation will be possible in the case of liquid-phase mass diffusion where a characteristic diffusion time can be much larger than the droplet lifetime. This point will be discussed in the next section. We would expect this relaxation zone appearing in this limit to overlay and to incorporate the boundary layer previously discussed as the relaxation zone between the two-dimensional gas-phase solution and the one-dimensional core solution.

When droplet slip is present, the droplet Nusselt number increases with the square root of the Reynolds number so that heat flux increases and droplet lifetime decreases. As mentioned in Point (iv) above, the characteristic heating time is less than that value for the non-slipping case but the heating time is independent of vortex strength (and implicitly Reynolds number for a fixed viscosity) at large vortex strength (or large Reynolds number). We already know that in the non-slipping, non-circulating case in a typical combustor environment with typical fuels, the droplet heating time and droplet lifetime are comparable. Note that here both scale with initial droplet radius squared. Coincidentally, for Reynolds numbers of the order of one hundred, both times are again comparable, although reduced from their values at zero Reynolds number. The heating time still scales with initial radius squared but the lifetime no longer does; in a quasi-steady situation, the lifetime can be shown to be proportional to initial radius squared divided by the square root of Reynolds number (effectively a radius to the three-halves power dependence). At lower Reynolds numbers, we may expect heating time to be shorter than lifetime so that a uniform temperature approximation could become reasonable. At

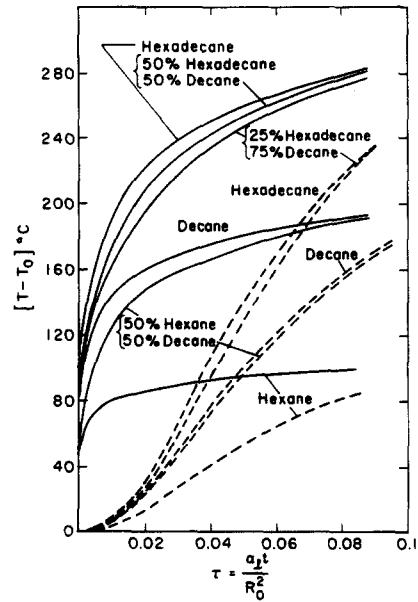


FIG. 5. Liquid temperature vs time for axisymmetric vaporization and a variety of fuels: $T_0 = 300^\circ\text{K}$ and ten atmospheres—surface temperature, $\theta = 90^\circ$; ---- vortex center temperature (taken from Reference [13]).

higher Reynolds numbers, lifetimes would become shorter and the rapid regression limit of Point (v) above would be approached; however, in practice, the Weber number tends to become large at high Reynolds number and droplets disintegrate into smaller droplets with decreased Reynolds numbers.

The solution of Eq. (21) has been obtained by finite-difference methods²⁰ and more recently approximate analytical solutions⁴¹ have been developed. The liquid-phase solutions are matched at every instant of time with the gas-phase solution. In addition to the integral methods^{12,13,20} for the gas-phase solution, other more expedient approximate solutions⁴² have been suggested.

Figure 5 shows the behavior of the surface temperature at 90° off the axis of symmetry and of the vortex center temperature for three different fuels of varying volatility. A non-dimensional time of 0.1 is about the droplet lifetime. It is seen that the transient period covers the droplet lifetime (especially for the least volatile fuels) since the temperature is continually rising. The surface temperature exceeds the center temperature so that spatial gradients are important. The boiling points are never reached; the maximum temperatures occur at the surface near the end of the lifetime and still are 80°C to 100°C below the boiling point (in these cases with ten atmospheres of pressure). Absolutely no justification can be found for a quasi-steady assumption.

Figure 6 shows radius to the three-halves power plotted vs time for three different fuels. The curvature or deviation from a linear relationship is a result of the transient behavior. With time, the behavior becomes closer to linear for all three fuels especially the more volatile *n*-hexane. These two last figures together

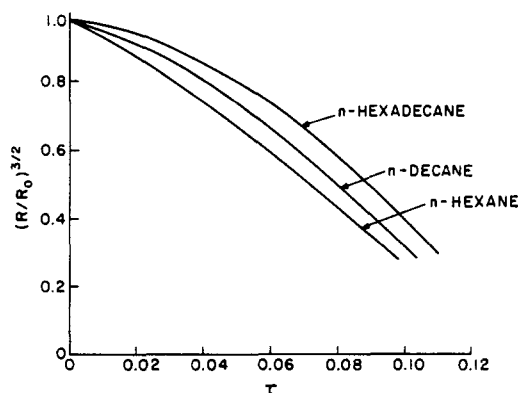


FIG. 6. Size variation vs time for three fuels with axisymmetric vaporization (taken from Reference [13]).

demonstrate that the less volatile fuels will undergo the more pronounced transient behavior but even the normal hexane fuel which is extremely volatile will have a transient behavior for much of its lifetime.

Some final comments about the validity of the "rapid-mixing approximation" are in order. The rapid-mixing concept is somewhat flawed; internal circulation does not reduce mixing time to a negligible amount. Through a change in characteristic length scale, internal circulation can reduce the mixing time by one order of magnitude at large vortex strength. However, that limit remains fixed as vortex strength increases so that the time never goes to zero even as strength becomes infinite. Since vortex strength is related to the degree of slip, Nusselt number and vortex strength increase together for a given droplet. So lifetime and mixing (or heating) time decrease together. Except for low (but not zero or very low) Reynolds number, uniform liquid temperatures will not result for droplet vaporizing in a combustor. Conceptually, it is not correct to relate the uniform-temperature limit to a rapid mixing due to internal circulation; it would be correct conceptually (but not practical for combustion applications) to relate the uniform-temperature limit to either the limit of infinite diffusivity or the limit of very slow vaporization (perhaps infinite latent heat of vaporization).

4. MULTICOMPONENT FUELS

Mass diffusion in the liquid phase is very slow compared to heat diffusion in the liquid and extremely slow compared to momentum, heat or mass diffusion in the gas film or compared to momentum diffusion in the liquid. In fact, the characteristic time for the liquid-phase mass diffusion based upon droplet radius is typically longer than the droplet lifetime. Nevertheless, this mass diffusion is of primary importance in the vaporization process for a multi-component fuel. At first, early in the droplet lifetime, the more volatile substances in the fuel at the droplet surface will vaporize leaving only the less volatile material that vaporizes more slowly. More volatile material still exists in the droplet interior and will tend

to diffuse towards the surface due to concentration gradients created by the prior vaporization. This diffusion is balanced by the counter-diffusion of the less volatile fuel components towards the droplet interior.

The result is that different components will have different vaporization rates and those rates can vary significantly during the droplet lifetime. Two limits exist in theory: (a) the rapid regression or zero diffusivity limit; and (b) the uniform concentration or infinite diffusivity limit. In practical combustion situations, the diffusion rate is finite but tending to be slow. The condition (a) could be interesting in some cases but condition (b) would only be interesting in non-combusting situations where the ambient gas temperature is low and the vaporization rate is low.

The rapid regression limit is one where a diffusion layer (of zero thickness in this limit) exists at the surface and regresses in a quasi-steady manner with the surface. There is a balance between normal (to the surface) convection and normal diffusion in this thin layer with the concentrations outside the layer (in the droplet interior) remaining uniform and constant with time at the initial values. A conservation of mass principle immediately yields the result that the vaporization rate for each component is proportional to its initial composition; e.g. for a 50% decane and 50% octane liquid fuel mixture, 50% of the mass vaporized per unit time is decane and 50% is octane in this limiting condition. The value of the concentration of each liquid component at the surface will be self-adjusting to whatever value is necessary to assume this vaporization rate. Obviously, the more volatile component (octane in this case) will assume a lower concentration value at the surface than its interior value while the less volatile substance (decane) will assume a higher value than its interior value. If the gas diffusivities of each of the components were identical the gas-phase concentrations at the surface would be proportional to the vaporization flux of each of the components which in turn is proportional to the initial concentration of the fuel.

In a low temperature environment, the droplet lifetime may be so long that diffusion can be considered to be fast and concentrations in the liquid may be assumed to be uniform but time-varying. Note that the required droplet lifetime for uniform concentration would be an order of magnitude greater than the necessary lifetime for the uniform temperature condition due to the large difference between diffusivities for heat and mass. Within this limit, another limiting condition of sequential vaporization of the components exists when the volatilities of the fuel components are very different from each other. In this limit, the most volatile component will first vaporize completely from the droplet with negligible vaporization of the other components; then the next most volatile component will completely vaporize without the vaporization of the other remaining components. The process continues until the least volatile substance vaporizes in sequence. The required com-

bination of low ambient temperature and widely varying volatility (say as measured by the boiling points) of the components makes this limit not very interesting in combustion. Furthermore, this argument indicates the danger of applying low temperature experimental results to predict behavior under combustion conditions.

The gas-phase Lewis number and Prandtl number are close to unity so that mass transfer, as well as heat and momentum transport, may be typified as quasi-steady. The individual fuel vapor components may diffuse at somewhat different rates and may react chemically at very different rates but no one has carefully investigated these effects for droplet vaporization in a combusting environment. Existing works^{17,18,26} tend to consider only a uniform diffusivity and a thin flame (or none at all).

4.1. Spherically Symmetric Diffusion

The concentration or mass fraction $Y_{i,i}$ of the i th species in the composition of the spherical liquid droplet obeys a diffusion equation of the spherically symmetric form:

$$\frac{\partial Y_{i,i}}{\partial t} = D_i \left(\frac{\partial^2 Y_{i,i}}{\partial r^2} + \frac{2}{r} \frac{\partial Y_{i,i}}{\partial r} \right) \quad (24)$$

This form is identical to that of the heat diffusion Equation (20) except that the mass diffusivity D_i is much smaller than the heat diffusivity α_i . This equation applies in the domain $t \geq 0$, $0 \leq r \leq R(t)$ so that we have a moving boundary problem. It may be transformed to a fixed boundary problem with the consequence that a convective term appears due to the surface regression. On account of the low diffusivity value, this convective term becomes much more important here than the corresponding term in the heat equation. The importance of this term is high-lighted in the above discussion of the rapid regression limit.

Landis and Mills²⁶ solved the coupled heat and mass transfer problem for vaporizing bi-component droplets. Pentane, hexane, and heptane were respectively mixed with octane. Their results indicate that batch distillation (both heat and mass diffusivities are taken to be infinite in this model) or infinite mass diffusivity models are highly inaccurate in predicting the results for vaporization rates of the individual components. The agreement between the more exact diffusion-controlled model and these over-simplified models appears to be slightly better at 600 K ambient temperature (low overall vaporization rate) than at 2300 K (high overall vaporization rate); but it is still quite poor. One might expect that the batch distillation model would improve slightly as the difference in volatilities of the two components increased. However, the paper does not address this point. For the heptane-octane mixture with 2300 K ambient temperature, the rapid regression limit appears to have been reached; a diffusion layer exists and each individual component vaporization rate is approximately proportional to its initial concentration. The

authors indicate that diffusion will not be as dominantly controlling for lower vaporization rates but will still be very important and the batch distillation model would not apply.

It is inferred that, the batch distillation model (or an infinite mass diffusivity model) should never be applied to a combustion situation since vaporization rates are too high. On the other hand, only at extremely high vaporization rates will the rapid regression limit apply. In general, it is advised to employ the finite diffusivity model whereby the diffusion equation is solved. However, care must be taken to resolve the fine structure near the surface that results from the small value of liquid mass diffusivity.

Landis and Mills²⁶ also show that disruptive boiling or microexplosions are also possible since for certain regions of the droplet interior, the equilibrium vapor pressure of the more volatile component can exceed the ambient pressure. This is a very interesting phenomenon that may be important in multicomponent and/or emulsified spray combustion. The interested reader should seek the recent review by Law.¹⁰ Landis and Mills further suggest, in passing, that internal circulation would decrease the differences between the batch distillation model and the diffusion-controlled model because effectively the diffusivity is increased. In the next subsection, it will be demonstrated that their conjecture is not correct because the convective mechanism which causes the internal circulation, also increases the transport rates through the gas film and thereby increases the vaporization rate.

4.2. Liquid-Phase Mass Diffusion with Internal Circulation

Whenever droplet slip causes internal circulation, geometrical details of the situation will be modified but the same types of limiting behavior will exist. For liquid Peclet number (based upon mass diffusivity) of order unity, the convection will cause the diffusion problem to become axisymmetric and no longer spherically-symmetric as it was at zero Peclet number. However, at very high Peclet number, the convection is so fast that concentration becomes uniform along a streamsurface. Again, a one-dimensional problem, but now in a streamsurface coordinate system, will result.

The mass fraction $Y_{i,i}$ of species i in the liquid phase will be governed by the following equation

$$\frac{1}{\varepsilon} \frac{\partial Y_{i,i}}{\partial \tau} = a(\tau, \phi) \frac{\partial^2 Y_{i,i}}{\partial \phi^2} + b(\tau, \phi) \frac{\partial Y_{i,i}}{\partial \phi} \quad (25)$$

where $a(\tau, \phi)$ and $b(\tau, \phi)$ are defined in Eqs (22) and (23). The parameter ε is the ratio of the mass diffusivity to the thermal diffusivity (a reciprocal of the Lewis number) for the liquid and is typically quite small compared to unity. This equation has the exact same form as the heat diffusion equation (21) except for the coefficient of the time derivative term which reflects the very important difference between the

characteristic times for heat diffusion and for mass diffusion. Otherwise, the five points made following Eq. (21) would still apply to Eq. (25) and will not be repeated here.

Lara-Urbaneja and Sirignano²⁰ have solved this equation with the appropriate boundary, matching, and initial equations for multicomponent fuel droplet vaporization. Figure 5 shows the results for liquid temperature vs time at a position on the surface as compared to a position at the vortex center; various fuel combinations, of varying volatility are considered and an ambient pressure of ten atmospheres (and therefore elevated boiling points) is considered. It is seen that the behavior is transient and spatial gradients of temperature exist over the droplet lifetime for all mixtures considered. The degree of transient behavior decreases as the volatility of the mixture increases but even hexane demonstrates a very transient behavior. The boiling points of the fuels are never reached during the lifetime. In bicomponent mixtures, the heavier component seems to dominate the thermal behavior; i.e., the 25–75% mixture of hexadecane and decane (or the 50–50% of decane and hexane) behaves much more like pure hexadecane (or pure decane) than like decane (or hexane). The apparent reason for this behavior is that the more volatile component vaporizes quickly and most of the material near the surface consists of the heavier, less volatile component.

Figure 7 shows how liquid mass fraction for the more volatile species in a bicomponent mixture typically varies spatially and temporally. The species is depleted quickly near the surface and then diffuses from the interior to the surface. The characteristic diffusion time is clearly much longer than the droplet lifetime (about $\tau = 0.1$ here); the mass fraction is very nonuniform throughout the lifetime. The ambient gas temperature for this calculation is 1000 K, the pressure is ten atmospheres, and the initial mixture consists of 50% decane and 50% hexadecane. It is seen that the mass diffusion layer near the surface $\phi = 1$ thickens with time and does not remain as a thin layer near the surface; so this solution is not close

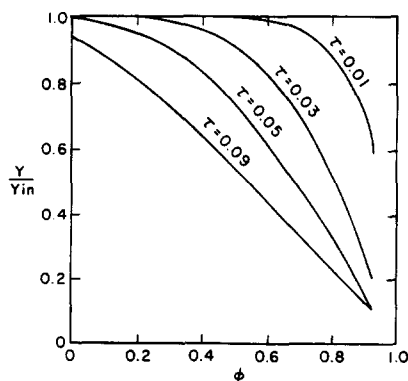


FIG. 7. Mass fraction of decane in an initial 50% decane-50% hexadecane mixture (taken from Reference [20]).

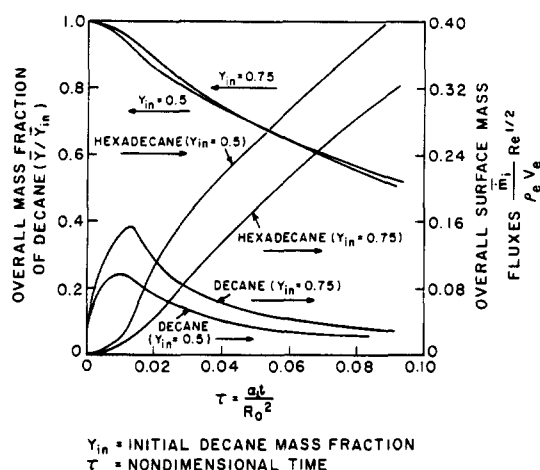


FIG. 8. Overall decane mass fraction and vaporization rates in decane-hexadecane mixtures Y_{in} = initial decane mass fraction, τ = nondimensional time (taken from Reference [20]).

to the rapid regression limit. It is conjectured that if 2300 K were taken as the ambient gas temperature and the mixture were heptane-octane as studied by Landis and Mills for spherical symmetry there would be qualitative agreement with their results. Namely, the higher ambient temperature (higher heat flux) and more volatile fuel would result in a sufficiently high vaporization rate to obtain the rapid regression limit.

It can be seen from Fig. 8 that the more volatile substance (decane) vaporizes early while the heavier substance (hexadecane) vaporizes later during the lifetime. Since a fuel droplet moves through a combustor, the implication is that certain regions will be relatively rich in the more volatile fuel vapors while other regions are relatively rich in the less volatile substance. Stratification of this type would have significant impacts on the characteristics of ignition, flame stability, and pollutant formation. In fact, these influences on those important combustion features are what provide the impetus for multicomponent vaporization studies.

The importance of the Soret and Dufour effects and the validity of the binary diffusion approximation with regard to liquid-phase mass diffusion in the droplet vaporization problem remain to be determined.

The concepts discussed in this section would have some application to the vaporization of emulsified fuels and coal (or carbon) slurries. These will not be discussed here in detail but rather the reader is recommended to the recent review by Law¹⁰ and to other interesting papers.^{43,44,45} This author will only comment that the theoretical issues related to emulsified fuel vaporization and to slurry vaporization seem very complex and relatively little of the interesting physics seems to have been characterized or modelled.

The phenomenon of microexplosions is an interesting possibility in miscible fuel mixtures and emulsified fuel mixtures. It has been observed in laboratory situations and could have practical impli-

cations.¹⁰ Although no evidence exists, it seems conceivable that slurries made from coal with volatile contents could also exhibit microexplosion behavior.

5. DROPLET ARRAYS, GROUPS AND SPRAYS

To this point in this review, we have discussed only isolated droplets. In practical situations, of course, many droplets are present in a spray and the average distance between droplets can become as low as a few droplet diameters. A typical droplet, therefore, will not behave as an isolated droplet; rather it will be strongly influenced by immediately-neighboring droplets and, to some extent, by all droplets in the spray.

The theoretical problem of droplet interactions has been approached in three ways: droplet array theory, droplet group theory, and spray theory. The distinct definitions are not universally accepted but this reviewer finds them very useful. In order to understand the distinctions, it must be visualized that a cloud or collection of droplets occupies a certain volume. This primary ambient gas conditions are defined as those conditions in the gas surrounding the cloud of droplets. Each droplet in the cloud has a gas film surrounding it. The local ambient conditions will be defined as the gas properties at the edge of the gas film but within the volume of the cloud. This definition becomes very imprecise when the gas films of neighboring droplets overlap; one can only cite that fact as evidence of conceptual weakness in the theory. In such a case, the local ambient conditions would be replaced by some average over the gas in the droplet neighborhood.

Three different new phenomena may be identified in the vaporization and burning of fuel droplet clouds or sprays:

(i) The primary ambient gas environment is strongly affected by the presence of droplets. Since typical combustors are finite in size, conditions in the gas surrounding a cloud of droplets will be coupled strongly to the gas and liquid properties within the cloud. The properties in the liquid-phase and in the gas film surrounding the droplet did not affect the ambient conditions in the isolated droplet studies but, in the realistic situation, the primary ambient gas temperature, momentum, and composition are strongly influenced by the presence of the droplets.

(ii) The local ambient environment is also affected by the droplets. This will directly affect the heat and mass transfer rates between individual droplets and the local gas environment. Vaporization rates will also be influenced.

(iii) The geometry and scale of the diffusion field surrounding each individual droplet will be affected. For example, we expect Nusselt number and the functional form of the relationship between vaporization rates and local ambient conditions would be affected by the droplet spacing. This functional relationship is named the vaporization law. Its limiting form will be that given for isolated droplets; see Eq.

(16). This effect of droplet spacing will also modify heat and mass transfer and vaporization rates.

It is seen that the second and third phenomenon each affect transfer rates. We would conjecture that a decrease in droplet spacing leads to an increase in local ambient fuel vapor concentration and a decrease in local ambient temperature. The implication is that this, by itself, would tend to decrease the heat and mass transfer rates. The third phenomenon should result in a decrease in the gas diffusion length scale as droplet spacing decreases. If r_c were the characteristic diffusion length in the gas film, the surface area through which diffusion occurs would be proportional to the square of r_c while the diffusion rate per unit surface area is inversely proportional to r_c . The net result is that the heat and mass transfer rates and (under diffusion control) the vaporization rate would be proportional to r_c . Here again the effect of a decrease in droplet spacing is to decrease the transfer and vaporization rates. The second and third phenomenon each would have the same qualitative effect as droplet spacing (or equivalently number density) vary.

A number of analyses have addressed the first phenomenon^{35,47-52} the second phenomenon^{35,47-65} and the third phenomenon,⁵⁹⁻⁶⁵ but no one analysis has addressed all three.

Some investigators⁵⁹⁻⁶⁵ have examined a few droplets in a well-defined geometry or a large number of droplets in a periodic configuration. Let us define these arrangements as droplet arrays. These arrays are artificial and contrived but can be very useful in obtaining information about the third phenomenon and, to some extent, about, the second phenomenon. Since the number of droplets in an array are typically small the impact on the primary ambient conditions are not significant and arrays are not useful to study the first phenomenon.

Another interesting approach taken by several investigators⁵³⁻⁵⁷ involves group vaporization and burning of droplets. The group combustion and vaporization theory takes the primary ambient conditions as given and proceeds to determine the local ambient conditions, droplet properties and vaporization rates. Droplet group theory is distinct (from array theory) in that a statistical description of droplet spacing (rather than a precise geometrical description) is employed. In particular, a number density of the droplets is considered. As a practical matter, group theory can deal with many more droplets than array theory. (An exception occurs when the array is geometrically periodic since then array theory can be used to analyze one cycle). Group theory is very useful in studying the second phenomenon but not useful in studying the first phenomenon since the primary ambient gas conditions are uncoupled and prescribed.

Array theory is conducive to the analysis of the third phenomenon but group theory is not; in group theory, the functional relationship between the local ambient conditions and the vaporization rate must be prescribed while in array theory it can be determined

by analysis. This is a consequence of the detailed field analysis of array theory vs the averaging or statistical approach of group theory. Array theory can be employed to determine the Nusselt number for a droplet in the array or to obtain the mathematical relationship between vaporization rate and local conditions; then the result of that analysis can be postulated as an input for a group theory analysis. The current analyses have not included the effect described here as the third phenomenon but rather considered only vaporization laws obtained for isolated droplets. No inherent limitation exists that prevents a better representation of the vaporization law for use in group theory.

Spray vaporization theory^{35,47-52,66-67} will be understood to be distinct from the theory of droplet array vaporization or the theory of droplet group vaporization in that the full coupling amongst the ambient gas properties, the local gas properties, and the droplet properties is considered. Again, a statistical or average representation of properties is made on account of the large number of droplets considered. The first and second phenomena are treated and analyzed. The effects of droplet spacing on Nusselt number and vaporization law can be included in spray theory so that the third phenomenon may be represented. However, no investigator has included that phenomenon in their model. Obviously, this is a serious neglect for dense sprays, i.e., sprays where the average distance between droplets is comparable to or less than the size of the gas film surrounding an average droplet.

5.1. Heating and Vaporization of Droplet Arrays

Two burning droplets of equal size were analyzed by Twardus and Brzustowski,⁵⁹ who employed a bispherical coordinate system to facilitate their analysis.

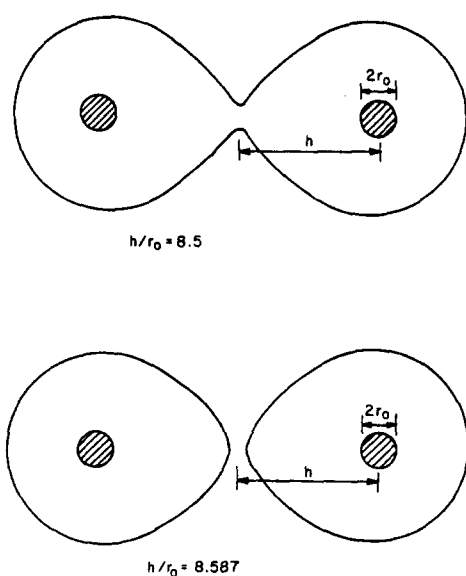


FIG. 9. Effect of droplet spacing on burning of two droplets (taken from Reference [59]).

Stefan convection and forced convection were not considered in the analysis. As shown in Fig. 9, there is a critical value of the ratio of the distance between droplet centers to the droplet radius, above which the droplets burn with two individual and separate flames and below which the two droplets burn with one envelope flame. The critical value depends upon the particular stoichiometry; for normal heptane, the value was found to be 17.067 by Twardus and Brzustowski. The vaporization rate remains diffusion-controlled and the rate of diffusion (and therefore the vaporization rate) decreases as the droplet spacing decreases. In the limit as the droplet contact, the vaporization becomes a factor of $\ln 2$ ($= 0.693$) of the value for two distant and isolated droplets.

Two important conclusions can immediately be seen. Firstly, spacing between droplets in typical fuel sprays will be smaller than this critical value. It is noteworthy that Chigier⁶⁸ has cited experimental evidence that droplets in combustors rarely burn in an isolated fashion; rather, a flame envelopes many droplets. Also, the interaction between (or effectively the merging of) the gas films surrounding droplets leads to a reduction in heat transfer, mass transfer, and vaporization rates. In the quasi-steady, non-convective situation considered, a d^2 -law for vaporization still exists but the coefficient is less than the value for an isolated droplet.

Labowsky⁶⁹ has been able to show that Stefan convection can be easily included via a transformation that reduced the mathematical form to that for slow vaporization. Laplace's equation for an array of droplets is then solved via a method of images. In the numerical example three droplets of equal size and temperature are arranged with their centers at the apices of an equilateral triangle. The theory is more general, however, and allows for an arbitrary number of particles of varying initial size and initial temperature. The quasi-steady assumption is made and thermodynamic equilibrium is assumed for the fuel vapor at the surfaces. The general conclusions are that: (i) vaporization rate is proportional to the vaporization rate for an equivalent isolated droplet times a corrective factor; (ii) the corrective factor decreases as droplet spacing decreases (obviously, it is unity for infinitely large spacing); and (iii) the droplet temperatures are independent of droplet spacing. (The last conclusion may be correct only under the assumption of unitary Lewis number since heat transfer and mass transfer have opposite effects on gas temperature.)

Some authors^{57,58} have studied arrays whereby the geometry is well defined but the droplets are considered to be monopole sources. Labowsky and Rosner⁵⁷ show that the difference in results between consideration of a continuous distribution of monopole sources of fuel vapor, and consideration of a discrete distribution of monopole sources, is not significant whenever the number of droplets in the cloud is large. The continuous distribution of sources is referred to as the continuum theory approach by

them but, with the terminology of this review, is a group combustion approach. The use of discrete sources is a first approximation within the realm of array theory. The fields around these monopole point sources are spherically-symmetric. On account of this neglect of higher-order terms that represent the deviation from spherical symmetry the third phenomenon cannot be treated by this approximation to array theory. In other words, the use of monopole sources in a well-defined array is somewhat pointless; once monopole sources are employed in large arrays, the effect of averaging the discrete sources locally to obtain a continuous source distribution does not have a significant effect on a scale larger than the average distance between droplets. It is recommended therefore, that one should use the group combustion (continuous or averaged) approach rather than monopole arrays. On a large scale, the resolutions are identical as shown by Labowsky and Rosner.⁵⁷ The monopole arrays can achieve a finer resolution on the small scale but could be quite inaccurate due to the neglect of the non-symmetric effects. If arrays are to be employed, a much better representation of the vaporizing droplet than a simple monopole should be used wherever possible and practical, to be consistent (that is, to make the finely-resolved features more believable). As previously mentioned, array analysis can provide insight to the small scale phenomena which should provide useful input to group analysis. For example, a Nusselt number relationship can be determined from array theory and then employed in a group theory.

The discussion on theories employing arrays with discrete monopole sources will be deferred until the next section on group vaporization and combustion of fuel droplets. For the reasons mentioned above, it is rational to separate array theories with monopole sources from the more exact representations of the local conditions around droplets.

It is noteworthy that no theory of vaporizing arrays or groups of droplets has yet considered the important

phenomena discussed in the previous sections. That is, forced convection and internal circulation, transient droplet heating, and liquid-phase mass diffusion for multicomponent droplets. Clearly, this will be a thrust area in the future due to its past neglect and its certain importance. Some work on heat and mass transfer to an array of non-vaporizing droplets with forced convection has been performed by Tal and Sirignano^{61,64} and Tal *et al.*^{62,63,65} These works are a precursor to work on vaporizing droplets; however, some interesting effects have already been observed that should be relevant to vaporizing droplets.

In these studies,⁶¹⁻⁶⁴ a cylindrical cell model has been employed to take advantage of the periodic structure of the array. Reynolds numbers are of the order of one hundred, based upon the diameter of the non-vaporizing sphere in the array of uniformly-sized-and-spaced spheres. The finite-difference calculations give excellent agreement with experimental results for drag coefficients (defined using local ambient conditions), indicating that drag increases as longitudinal (streamwise) and lateral (transverse) spacings decrease in identical fashion. This phenomena will be explained later. It has been shown that when the structure of the array is periodic, the problem for the flow field properties may be cast into a periodic form (although all properties are not exactly periodic, e.g. vorticity and temperature). Figures 10 and 11 taken from Ref. 62 show: (a) streamlines; (b) vorticity contours; and (c) isotherms for spheres in an array at two different spacings. Strong interaction between the flow fields surrounding neighboring droplets occurs when the droplet centers are less than two diameters apart. For example, at $Re = 100$ with droplets in tandem in the flow stream, the recirculation zone aft of the first sphere would make contact with forward portion of the next sphere.

Table 1 shows typical results for the friction drag coefficient, pressure drag coefficient and total drag coefficient. A calculation with three spheres in tandem confined laterally within a cylindrical cell (contrived

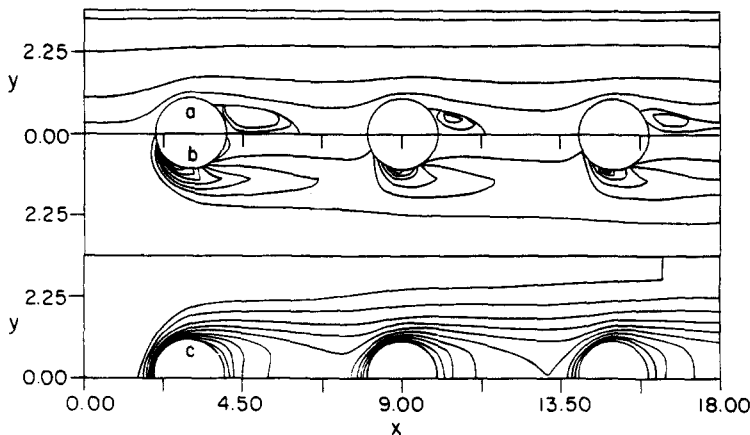


FIG. 10. Stream function (a), vorticity (b), and isotherm (c) contours for three spheres in a cell with spacing of 1.5 diameters, $Re = 100$, $Pr = 1$ (taken from Reference [62]).

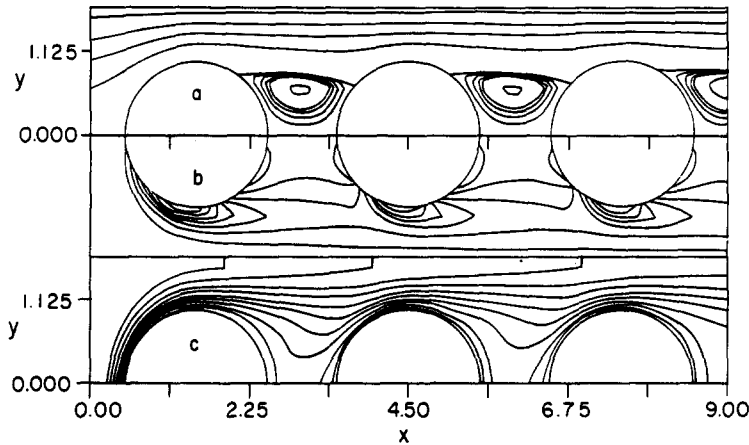


FIG. 11. Stream function (a), vorticity (b), and isotherm (c) contours for three spheres in a cell with spacing of 3.0 diameters, $Re = 100$, $Pr = 1$ (taken from Reference [62]).

to represent the periodic structure in the lateral direction) is compared to a periodic cell with one sphere (contrived to represent periodicity of the array structure in both lateral and streamwise directions). Results for a single unconfined sphere are also indicated.

Table 2 indicates that heat transfer to each sphere decreases as the position of the sphere becomes further downstream of the first sphere. This effect is due to the decrease in gas temperature as it flows downstream. This can be seen when we define the Nusselt number based on the primary ambient conditions (the inlet conditions to the cell of the first sphere). If we define the Nusselt number based upon the local ambient conditions (inlet conditions at each cell) the Nusselt number becomes approximately constant after the first sphere; its value here is greater than in the first definition but still less than the value for an unconfined sphere.

The same studies produced Table 3 which show that Nusselt number depends upon lateral (or transverse) spacing in one way and upon longitudinal (or streamwise) spacing in an opposite way. As lateral spacing decreases in the array, the flow field accelerates and Nusselt number increases; as longitudinal spacing decreases, droplets are protected by the wakes of other droplets and Nusselt number decreases. Note that the friction drag coefficient is expected to increase as lateral spacing decreases and the pressure drag should increase as longitudinal spacing increases due to accelerated flow over the individual sphere (a venturi effect). With lateral and longitudinal spacing identical in the array, the drag increases as spacing decreases and exceeds the drag for an unconfined sphere. However, the Nusselt number decreases as spacing decreases and is below the value for an unconfined sphere.

Two spheres in tandem were studied for inter-

TABLE 1. Drag coefficients of spheres in cylindrical cells ($Re = 100$, $b/a = 1.5$)

Type of solution	C_{Dr}			C_{Dp}			C_D		
	1st,	2nd,	3rd	1st,	2nd,	3rd	1st,	2nd,	3rd
3 spheres in cell	0.966,	0.692,	0.677	0.977,	0.693,	0.671	1.964,	1.385,	1.349
Periodic	0.673			0.657			1.330		
Unconfined	0.675			0.639			1.314		

TABLE 2. Values of Nusselt number in cylindrical cells ($Re = 100$, $b/a = 1.5$)

Type of solution	Nu	Remarks
3 Spheres in a cell	1st, 2nd, 3rd 7.644, 4.765, 4.061	Nu based on inlet to first sphere
	1st, 2nd, 3rd 7.644, 6.151, 6.270	
Periodic	5.935	
Unconfined	7.910	

TABLE 3. Average Nusselt number values for the second of three spheres in a cell, $Re = 100$, $Pr = 1$

Lateral spacing	Longitudinal spacing	Nu
1.5	1.5	4.765
1.06	1.5	5.708
1.5	1.35	4.594
1.5	1.2	4.372

mediate Reynolds number using bispherical coordinates.⁶⁵ The general qualitative conclusions are similar to those obtained by Twardus and Brzustowski for the zero Reynolds number case. Namely, transport rates decrease as spacing decreases. However, with a mean flow, the two spheres are not identical in their transport characteristics; the upstream sphere has a higher Nusselt number than the downstream sphere but both values are reduced from that for an isolated or unconfined sphere.

Tal and Sirignano⁶⁴ have shown by numerical calculations that internal circulation for a liquid droplet in the vicinity of other droplets can still be well-approximated by a Hill's spherical vortex. The implication is that the approach used to study transient heating and multicomponent vaporization for isolated droplets may still be followed for droplets in sprays. The effect of the droplet interactions can be properly represented through the drag coefficient and Nusselt number for the gas film. While the coupling between gas and liquid phases will change the quantitative behavior of the liquid, there seems to be no qualitative change in liquid behavior due to interaction amongst droplets.

The preliminary evidence indicates that transport rates and vaporization rates will be reduced from the values for isolated droplets for two reasons. Firstly, the local ambient environment is affected by the presence of droplets in the neighborhood. The droplets cool the environment, thereby decreasing heat transfer to the droplet, and supply fuel vapor to the environment, so that mass transport also decreases. These two effects may be expected to increase as droplet number density increases or equivalently (for a given droplet size) spacing decreases. Secondly, the Nusselt number based upon local ambient conditions will be less than the corresponding value for an isolated droplet and will decrease as spacing decreases.

5.2. Group Vaporization and Combustion

In this section, we shall discuss representations of vaporization of clouds where the precise position of each droplet is not important and only such average quantities as droplet number density (or, equivalently, the average distance between droplets) are important. Theories⁵³⁻⁵⁷ that employ continuum representations of droplets as distributed monopole sources of fuel vapor are included herein. Also included are representations⁵⁷⁻⁵⁸ of droplets as discrete monopole

sources with such a high number density of droplets that the distinction between discrete and continuum representations is not very significant.

Two major shortcomings can be cited in the existing theories. Firstly, the theories do not account for the fact that the Nusselt number and the vaporization law for each droplet will depend upon the spacing between droplets (with one exception to be mentioned later). Secondly, the theories are quasi-steady and do not consider transient droplet heating or unsteady gas-phase conduction across the clouds. Since the time scale for droplet heating and the time and length scales for conduction across the cloud can be large, these types of unsteadiness can be profound. With this in mind, the present theories should be viewed as a base for further studies rather than as complete theories.

The most interesting results of these theories is that certain distinct regimes of combustion have been discovered: isolated droplet combustion, internal group combustion, external group combustion and sheath combustion. The particular regime of operation will be determined by droplet number density, the primary ambient conditions, droplet radius, and fuel volatility. Chemical kinetics is, of course, an important factor as well, but it is typically considered to be quite fast.

Chiu and co-workers⁵³⁻⁵⁵ have provided an extremely interesting approach to group combustion. They consider a quasi-steady vaporization and diffusion process with infinite kinetics and show the importance of a group combustion number given by

$$G = 3(1 + 0.276Re^{1/2}Sc^{1/3})LeN^{2/3}(R/s)$$

where Re , Sc , Le , N , R , and s are the Reynolds number, Schmidt number, Lewis number, total number of droplets in the cloud, instantaneous average droplet radius, and average spacing between the centers of the droplets. This number G increases with Reynolds number, Prandtl number, and the size of the cloud (measured in droplet numbers) while it decreases with increasing Schmidt number and spacing between droplets.

The value of G has been shown to have a profound effect upon the flame location and distributions of temperature, fuel vapor, and oxygen. Four types of behavior are found: for large G numbers, external sheath combustion occurs, then as G is progressively decreased, external group combustion, internal group combustion, and isolated droplet combustion occurs. These regimes are identified in Fig. 12. Isolated droplet combustion involves a separate flame enveloping each droplet. Typically a group number of less than 10^{-2} is required. Internal group combustion involves a core within the cloud where vaporization is occurring with the core totally surrounded by a flame. Outside of the core, each droplet is enveloped by individual flames. This occurs for G values above 10^{-2} and somewhere below unity. As G increases, the size of the core increases. When the single flame envelopes all droplets, we have external group combus-

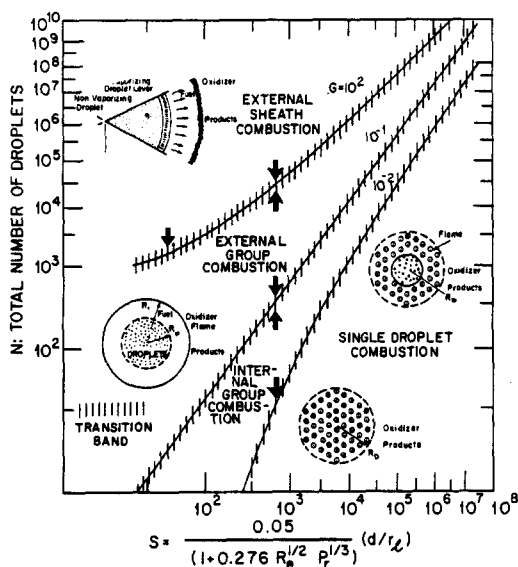


FIG. 12. Effect of group number on type of spray combustion (taken from Reference [55]).

tion. This phenomenon begins with G values close to order unity so that many industrial burners and most gas turbine combustors will be in this range. With external group combustion, the vaporization rate of individual droplets increases with distance from the center of the core. At very high G values (above 10^2), only the droplets in a thin layer at the edge of the cloud are vaporizing. This regime has been called external sheath combustion by Chiu and co-workers.

Labowsky and Rosner⁵⁷ have found similar results. They use a different terminology; their "incipient group combustion" is internal group combustion and their "total group combustion" is external group combustion. They use a quasi-steady continuum approach similar to that of Chiu and co-workers. As discussed in the previous sub-section earlier, they also use a superposition method with discrete monopole sources. This has the advantage of giving the details of the flame shape, or the field around each droplet; however, since the monopole approximations produces errors on that fine scale, this is a very questionable advantage. The authors do not advocate the non-continuum approach but rather were interested in gaining insight through comparison.

Labowsky and Rosner⁵⁷ also show that the Thiele Modulus $(3\phi)^{1/2} R_c/R$ is an important parameter in the determination of the onset of internal group combustion. Here ϕ is the volume fraction of droplets and R_c is the radius of a spherical cloud of droplets. The square of that factor $3\phi R_c^2/R^2$ is a Damkohler number, as stated by the authors. Although the authors do not indicate it, this Damkohler number can be readily shown to be equal to $3N^{2/3}R/s$; so that it equals the group combustion number of Chiu⁵³⁻⁵⁵ for the case of zero Reynolds number and unitary Lewis number.

Correa and Sichel⁵⁶ perform an asymptotic

analysis for large G values and obtain external sheath combustion results that agree well with those of Chiu and co-workers. A " d^2 -law" based upon cloud size is obtained in this quasi-steady sheath limit. They do raise concerns about whether the quasi-steady formulation will apply for lower values of G .

Kerstein and Law⁶⁹ have recently presented an interesting model of group combustion based upon percolation theory. The presentation contains no quantitative results for profiles, vaporization rates, and flame locations so that it is quite difficult to evaluate their contribution. However, they do seem to be attempting to represent the third phenomenon mentioned at the beginning of the section. Also, as we shall discuss later in the next subsection, there does seem to be a need for new approaches based upon stochastic methods.

All the approaches to group combustion theory have been based upon infinite chemical kinetic rates. Obviously, finite rates should produce significant quantitative differences. Only Chiu has introduced a convective effect into his model; he uses an *ad hoc* extension of the empirical correction for single droplets. This procedure could be improved in the future.

5.3. Finite difference calculations of vaporizing and combusting sprays

As mentioned earlier, spray combustion is distinct from group combustion in that it includes a strong coupling with the gas flow surrounding the cloud. In the group combustion approach the primary ambient conditions were specified and therefore passive to the vaporizing cloud of droplets. In a real combustor, especially with recirculation of the flow, conditions in one domain are not passive to conditions in other domains. Furthermore, boundary conditions are more complicated than simple specifications of distant quantities; combustors are finite in size and inflow, outflow, and wall conditions must be specified.

The existing approaches to spray combustion adapt a continuum approach whereby point properties for both gas and liquid are considered to be averages over neighborhoods that include many droplets. Therefore, properties are not resolved on the scale of the distance between droplets. Furthermore, the addition of gas due to vaporization is represented as a distributed monopole source; that is, the effect of neighboring droplets on the Nusselt number, or vaporization law, are not taken into account.

A probability distribution function can be created for the droplets in the spray.¹ A multidimensional, first-order, partial differential equation governs the function. The method of characteristics for this partial differential equation solutions yields a system of ordinary differential equations which describe the droplet position and properties as a function of the Lagrangian time following the path of any given droplet. In this representation, a droplet with any given set of properties has a certain possibility of existing. On the other hand, one can integrate the

equation over droplet diameter and velocity spaces to obtain a system of partial differential equations governing the average properties of the droplets. It is these equations, that deal with the average properties, which are generally used in spray combustion analysis. Understand that these averaged equations are first order and can be solved by the method of characteristics as well. Here the characteristics would be the particle path of an average droplet in a cluster of droplets rather than the path of an individual droplet. In analogy to the kinetic theory of gases, the same droplets do not have to remain in a given cluster as they travel through the combustor.

Since the gas-phase properties in a spray are normally taken as averages over a scale larger than the average distance between droplets, it seldom makes sense to treat the droplets on a finer scale. For that reason, we consider a cluster of droplets. If we discuss an individual droplet in a spray, it is implied therefore that we mean the average droplet in some cluster in the neighborhood of a given point. There are situations, however, where the interesting physical scale is comparable to the average distance between droplets. For example, Aggarwal and Sirignano^{70,71} have studied the problems of laminar spray flame structure and ignition of sprays where the interesting structure is on a fine scale. We shall discuss these later.

The spray combustion problem is sufficiently complicated that numerical integration of partial differential equations is required. Finite-difference methods have been frequently employed. Finite-element methods are feasible but have not been utilized for spray combustion problems. Two major approaches have been followed in the finite-difference calculations. In one approach,^{35,47,66,67} the same basic Eulerian numerical mesh is involved for both gas-properties calculations and liquid-properties calculations. In the other approach,⁴⁸⁻⁵¹ different integration methods and meshes are engaged for each of the two subsystems of equations. An Eulerian mesh is taken for the gas properties and a Lagrangian mesh is taken for the liquid properties.

The second method is realized to have some inherent advantages. The Lagrangian mesh eliminates the numerical diffusion which can enter through an Eulerian scheme for the droplet equations. Of course, if the gas equations are still Eulerian, errors due to numerical diffusion can still result there. Furthermore, the two mesh calculations require interpolation between the meshes since gas and liquid properties are strongly coupled. If the interpolation process is too crude, Aggarwal, *et al.*⁴⁹ have shown that errors of the same (first) order as the diffusion error have been eliminated. In particular, the droplet properties should not be averaged over the numerical cell as suggested by Ducoz⁵⁰ and Gosman⁵¹ but rather a linear interpolation should be made.

Another advantage to the second method is that it is better suited to deal with multivalued solutions of droplet properties. Since a droplet path in the calculations actually represents the path of an average

droplet in some cluster and since the average distance between droplet centers in the cluster can be at least several droplet diameters, the probability of droplet collision even when paths cross is quite small and collisions can be neglected. The implication of crossing paths is that more than one value of droplet properties can exist at a given point in space and time.

The hybrid Eulerian-Lagrangian method also offers the obvious advantage of allowing different numerical techniques to be employed for the gas-phase subsystem and for the liquid-phase subsystem of equations. This means that a great degree of procedural optimization with saving in computer costs may occur. Typically, the Lagrangian subsystem for the droplets may be solved by higher order Runge-Kutta schemes, for the ordinary differential equations; apply along the path of the characteristics. Aggarwal *et al.*⁴⁸ have studied implicit, block implicit, explicit, and operator-splitting methods for the gas-phase equations; the equations are sufficiently stiff due to the vaporization source terms that a relatively small time-step is usually required. This means that explicit methods are generally superior to implicit or block implicit methods for these types of equations with volatile fuels. The equations do not seem to be so stiff, however, that the additional complications of operator splitting are worthwhile.

Results of unsteady, constant volume, one-dimensional spray combustion calculations by Seth *et al.*³⁵ using an Eulerian mesh are shown in Figs 13 through 17. The constant cross-sectional area tube is closed at both ends and ignition occurs at the left end. At the initial time, hot products exist in a small region in that end; heat transferred from these hot products to the neighboring combustible mixture causes a flame to be established. In the figures, it is shown that a flame propagates from the left to the right. The theory is able to predict the liquid droplet velocity, size, number density, temperature and concentration as functions of position and time. The initial droplet size, number density, and temperature are uniform through the closed chamber. The droplets and gas are initially quiescent; once the flame begins to propagate, the expanding gases cause the droplets to move. Since the initial spray is not saturated, vaporization occurs ahead of the flame resulting in a time-varying mixture-ratio in the gas ahead of the flame. Another cause of unsteadiness occurs in the constant-volume case due to the temporally-increasing (but spatially uniform) pressure. Not all of the liquid fuel vaporizes before the flame front passes the droplets; the vaporization behind the propagating results in additional fuel vapor that burns in a diffusion flame. The diffusion flame is approximately stationary and causes a further increase in temperature as shown in Fig. 13. The temperature increase ahead of the flame is the net result of compressive heating and some cooling due to vaporization. The distinction between the propagating laminar heterogeneous flame and the diffusion flame is most clearly seen by examination of the fuel vapor and oxygen concentrations in Figs 14 and 15.

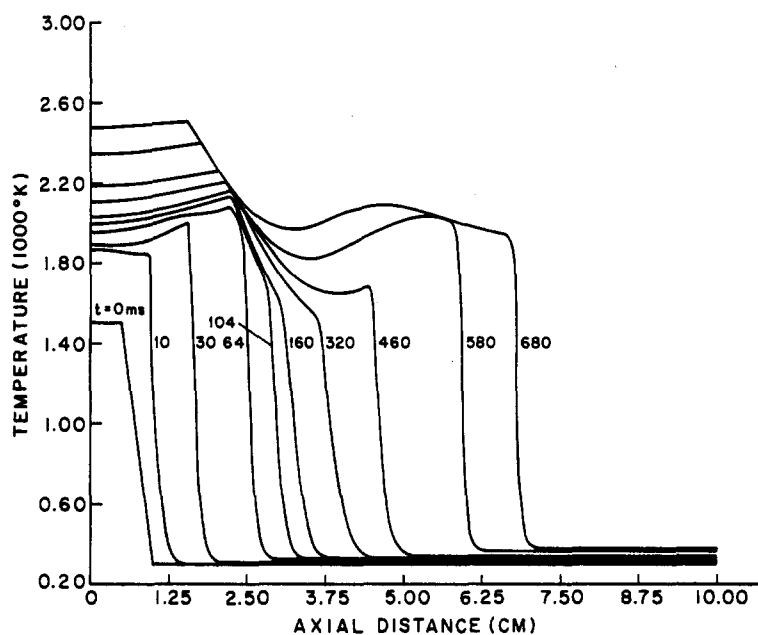


FIG. 13. Gas temperature variation with position and time for one-dimensional monodisperse spray flame propagation (taken from Reference [35]).

Figures 13 through 15 contained results for a monodisperse spray. A polydisperse spray may be approximated by the superposition of several monodisperse sprays. For example, Figs 16 and 17 contain results for a bidisperse spray calculation. The smaller droplets are seen to vaporize more quickly and to be dragged by gas motion more readily. The gas motion is primarily caused by the expansion of the gases during the combustion process. The above spray calculations

accounted for transient heating of single-component fuel droplets via a Ranz-Marshall correction to a spherically-symmetric droplet model. Spatial variations in the droplet interior temperature during transient heating were analyzed following an integral equation procedure developed by Law and Sirignano.¹⁸ The kernel of the integral and the surface heat flux are expanded in a series so that one partial differential equation (actually an ordinary differential

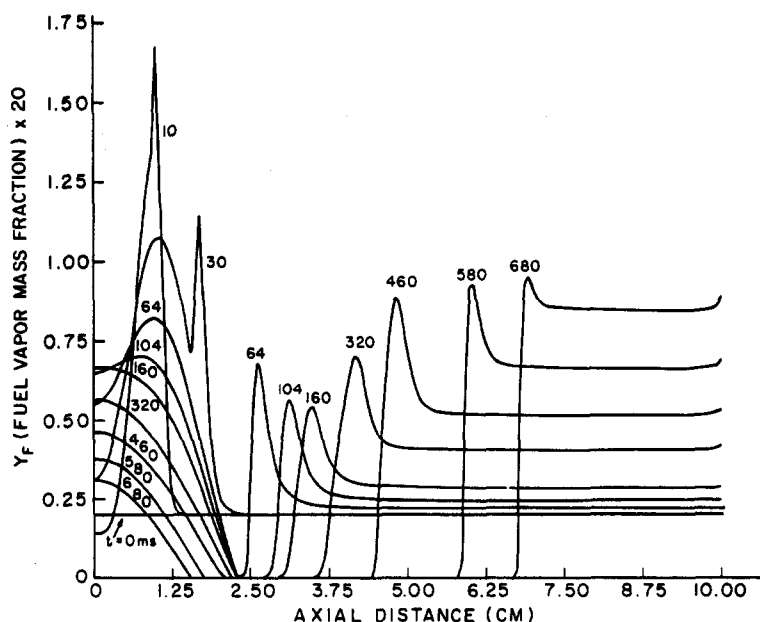


FIG. 14. Fuel vapor mass fraction variation with position and time for one-dimensional monodisperse spray flame propagation (taken from Reference [35]).

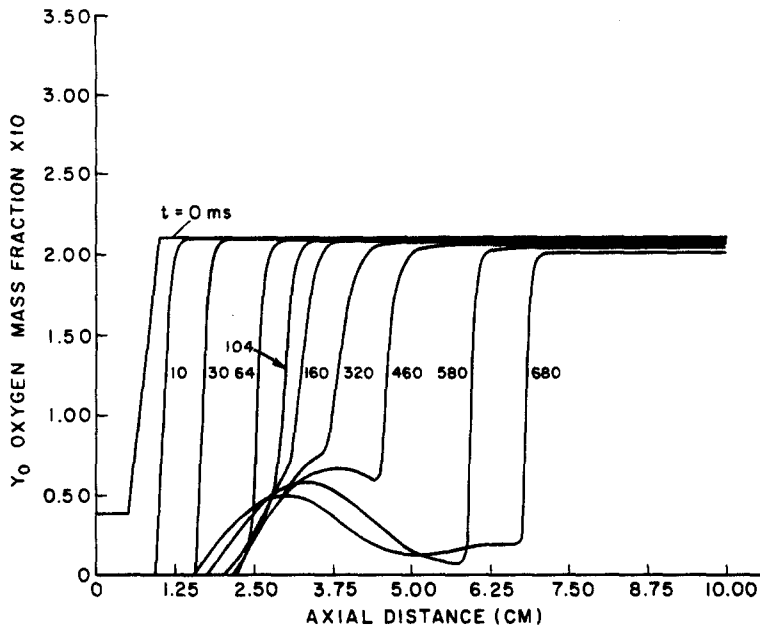


FIG. 15. Oxygen mass fraction variation with position and time for one-dimensional monodisperse spray flame propagation (taken from Reference [35]).

equation in a Lagrangian frame of reference) is constructed for each term in the series. For reasonable accuracy, this approach is superior to the solution of a finite-difference representation of the heat diffusion equation in the droplet interior. As mentioned earlier, the surface temperature and the instantaneous vaporization rate are quite sensitive to the droplet heating model. For this reason, the additional complications required in order to account for spatial variations of interior temperature are deemed to be necessary.

This author believes that we are now ready to consider droplet internal circulation with axisymmetric droplet vaporization models and multicomponent fuels with liquid-phase mass diffusion in spray

combustion calculations. In fact, this has already been accomplished for a one-dimensional unsteady, two-phase flow. Two-dimensional calculations⁴⁷⁻⁵¹ of course, have already been made for vaporizing sprays but these calculations have not yet included the most sophisticated representations of transient droplet heating and vaporization. Three-dimensional calculations seem possible if the appropriate computer is available to the researcher. It is believed that useful design tools for spray combustors will begin to emerge over the next few years. At this point, however, the predictions can only be expected to be qualitatively correct rather than exact.

There are some situations where the average

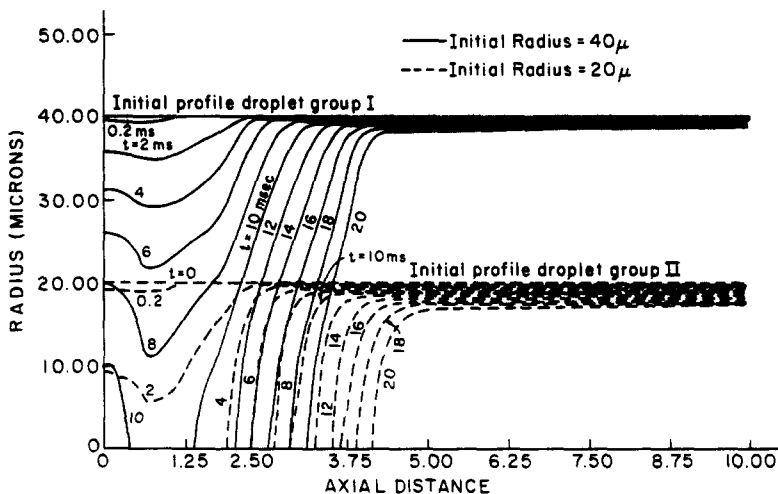


FIG. 16. Droplet radius variation with position and time for one-dimensional bidisperse spray flame propagation (taken from Reference [35]).

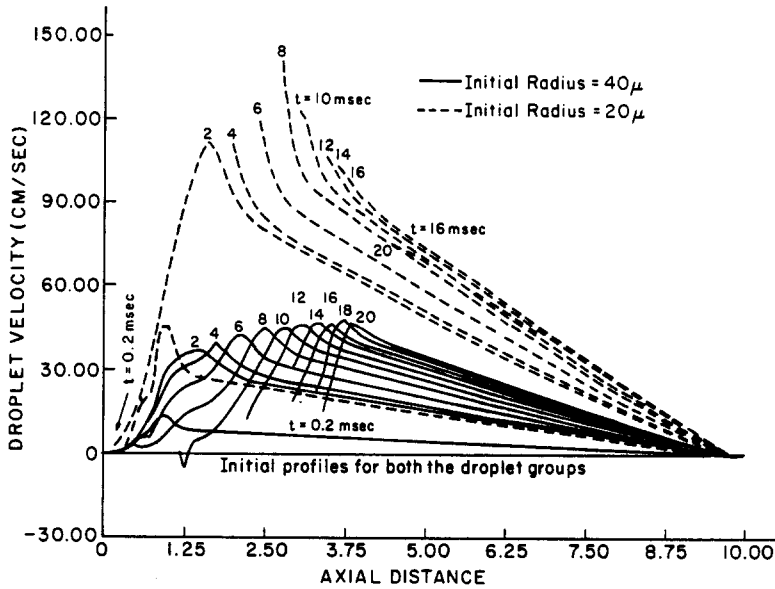


FIG. 17. Droplet velocity variation with position and time for one-dimensional bidisperse spray flame propagation (taken from Reference [35]).

distance between droplets will be comparable to the interesting physical scale. Here we can proceed with a deterministic calculation whereby each droplet is followed in the calculation and average droplet properties are not employed.^{70,71,72,73} In Fig. 18, the results of a one-dimensional unsteady spray calculation, wherein individual droplets are tracked, are presented. Fuel droplets and hot air with fuel vapor are moving from left to right with the gas moving at a greater speed. Vaporization occurs so that fuel vapor mass fraction increases with time and with downstream distance from the entry point. As fuel vapor is created, it diffuses away from the droplet in both

directions and also convects with the gas stream; the local peaks in the mass fraction shown in Fig. 18 occur at the instantaneous droplet position for this reason. If we were interested in resolving the structure on the scale of the average distance between droplets, this waviness in the solution must be considered. If we are only interested in a larger scale structure, we can integrate away the waviness and may track a cluster of droplets. (Note that for near stoichiometric mixtures for typical hydrocarbon fuels with droplets about 100 μm in diameter and atmospheric condition, the average spacing is a few millimeters). The gradual decay of fuel vapor mass fraction in the direction of the flow occurs since the gas velocity is greater than the droplet velocity in this case. Also, three different models have been examined and the comparison is made in Fig. 18. The effects of internal circulation are shown in the "vortex" model while the other two models consider: (i) spherical conduction without circulation and with finite conductivity; and (ii) infinite conductivity. It is seen that the vortex model, with a characteristic diffusion time between the other two models has results that lie between the results of the other two models. Furthermore, the fuel vapor mass fractions differ by as much as a factor of about two, especially near the point of inflow. These differences can be significant in flame stability considerations.

The practical problem is that the initial conditions for each droplet are not known precisely; only average conditions or distribution functions are known. Clearly, some uncertainty must exist with respect to the exact location or the exact size of a droplet throughout its history. A shortcoming exists, therefore, with the deterministic approach for this type of problem. Recent theoretical findings⁷² demonstrate

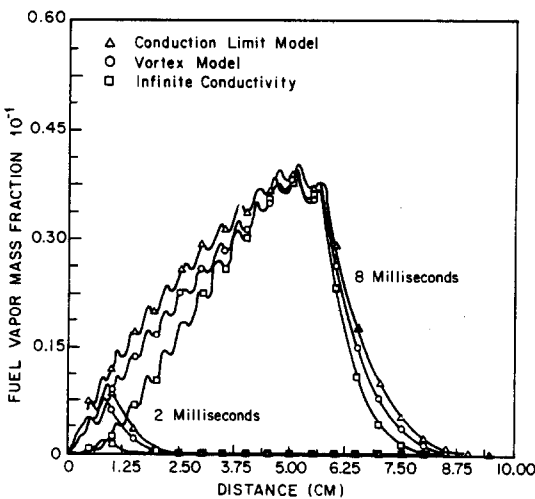


FIG. 18. Fuel vapor mass fraction variation with distance and time for a vaporizing, non-reacting spray with structure resolved on the scale of the distance between droplets (taken from Reference [73]).

that ignition energies for sprays should be probabilistic rather than deterministic. The thermal layer around typical ignition sources can be of the same order as the average distance between droplets in a spray. The variation of the exact location of a droplet within the thermal layer will affect the ignition process; however, we cannot prescribe a droplets location with any certainty to a better resolution than a few average inter-droplet spacing lengths. A new approach may be required to analyze and to understand spray ignition.

O'Rourke and Bracco⁷⁴ have modelled sprays where the average distance between droplets is small and comparable to droplet size. Collisions and coalescence of droplets are considered. The model is based upon theoretical and empirical evidence from several independent studies.

6. CONCLUDING REMARKS

In the previous four sections, several major aspects of fuel droplet vaporization in a high-temperature environment and spray combustion have been discussed. The importance of relative droplet-gas motion has been explained in terms of its impact on droplet trajectory and vaporization rate. The heating and vaporization rates are seen to be very unsteady in typical situations so that the classical quasi-steady formulation is unsatisfactory. The complexities of multicomponent vaporization are analyzed and a highly-transient process is revealed. It is the author's belief that these areas are now rather well understood compared to other areas of fuel-droplet vaporization and spray combustion science. Certainly, the next generation of combustion textbooks and reference books should not be allowed to proceed with the oversimplified and naive representations of fuel droplet vaporization and burning that are contained in the present books.

Some very exciting developments have occurred over the last decade in group combustion and spray combustion theory. Much still remains to be accomplished. The interaction between droplets in a spray has not yet been fully explained. The inclusion of multicomponent fuel behavior, transient heating, and extension to three dimensions remains to be completed. This problem area strikes the author as a very important challenge to the theoretical and computational community.

Other important theoretical problem areas have not been discussed in any real detail in this paper. Their importance should, however, be stressed. One key area that remains virgin territory for the researcher involves the interaction of turbulent eddies with fuel droplets. The range of turbulent length scales in the spectrum of a typical combustor reaches, at the lower end, the droplet diameter range. The impact on droplet trajectory has been studied somewhat but the relationship with heating and vaporization rates is very uncertain. This author in a recent workshop⁷⁵

presented certain conjectures and suggestions that were intended to stimulate research on the subject.

The vaporization processes for emulsions and slurries remain to be modelled in a convincing fashion.⁷⁶⁻⁹¹ An important issue here involves the detail of the atomization process; for example, we know very little about the distribution function for the number of particles in a slurry droplet. The inclusion of radiative heating of the droplets is mandatory for use in many practical combustors.⁹²⁻⁹³ Near-critical and super-critical behavior deserves further study.⁹⁴⁻⁹⁶ In the spherically symmetric situation, the gas-phase heating time becomes long near the critical point. However, if relative motion exists, a thin gas boundary layer is present and the gas heating time is equal to a residence time which is independent of gas density (other than through its effect on relative motion). Studies of pollutant and soot formation in group combustion and spray combustion situations should be encouraged as well.⁹⁷⁻¹¹⁸ Other important subject areas are the ignition of sprays¹¹⁹⁻¹³¹ and the development of diagnostic methods.¹³²⁻¹⁵⁸

Other interesting recent papers, not previously mentioned herein, cover the areas of: detonations and shocks,¹⁵⁹⁻¹⁶³ buoyancy, convective effects, and drag,¹⁶⁴⁻¹⁷⁰ atomization and injection,¹⁷¹⁻¹⁷⁸ droplet vaporization theory,¹⁷⁹⁻¹⁹¹ multicomponent fuel droplet vaporization and fuel characterization,¹⁹²⁻¹⁹⁷ droplet arrays and droplet interactions,¹⁹⁸⁻²⁰⁹ aerodynamics effects and flame stabilization,²¹⁰⁻²¹⁶ related two-phase flows,²¹⁷⁻²²⁰ flame propagation,²²¹⁻²²³ flash vaporization,²²⁴⁻²²⁵ practical applications,²²⁶⁻²³⁴ spray modelling,²³⁵⁻²⁵⁵ spray measurements and experiments.²⁵⁶⁻²⁶⁷

Acknowledgements—This author wishes to acknowledge the National Science Foundation, the Department of Energy, the Army Research Office, and the Air Force Office of Scientific Research for their research support of his efforts in this area over the past seven years. He also benefited from the generosity of United Technologies Research Center since he entered the problem area in 1973-74 while on sabbatical leave and serving as their Research Fellow. The many colleagues (including both students and more senior collaborators), with whom research on the subject has been performed, have contributed significantly to the author's understanding of the subject. Miss Lisa Papalia is acknowledged for her assistance in typing and editing this manuscript. Lynn Sirignano is acknowledged for her assistance in the literature search.

APPENDIX—EFFECT OF FLUCTUATING TORQUE ON DROPLETS

We expect a balance between the inertial terms and the friction along the droplet surface so that

$$\frac{d(\rho u^2)}{dx} \sim \frac{\partial \tau}{\partial y} \sim \frac{\tau}{\delta} \quad (A1)$$

where δ is the gas boundary layer thickness and is the order of $R Re^{1/2}$, note that the wiggly sign again implies that quantities are of the same order of magnitude. Since the relevant arc length along the

surface is of the order of the droplet radius, we can say that

$$\rho u^2 \sim \tau \frac{R}{\delta} \sim \tau Re^{1/2} \quad (A2)$$

Whenever a fluctuation occurs, the axisymmetry can be lost and a difference in the velocity and the stress is found across the droplet. It is expected from Eq. (2) that these differences Δu and $\Delta \tau$ must be related by

$$2\rho u \Delta u \sim Re^{1/2} \Delta \tau \quad (A3)$$

If Δu is dictated by a fluctuating turbulent eddy at the Kolmogorov scale, it follows that

$$\Delta u \sim v/\eta \sim v/R \quad (A4)$$

where it has been assumed that the eddy size η is of order of the droplet size. Furthermore, the friction force F will be given by

$$F \sim \tau R^2 \quad (A5)$$

so that the net friction force ΔF due to the fluctuation in velocity is

$$\Delta F \sim R^2 \Delta \tau \quad (A6)$$

and the torque on the droplet is

$$T \sim R \Delta F \sim R^3 \Delta \tau. \quad (A7)$$

Combination of (3), (4) and (7) yields

$$T \sim \rho u v Re^{-1/2} R^2. \quad (A8)$$

Now the moment of inertia of the droplet I will be of the order of $\rho_l R^5$ so that the acceleration

$$w \sim \frac{T}{I} \sim \frac{\rho}{\rho_l} u v Re^{-1/2} R^{-3} \quad (A9)$$

or

$$w \sim \frac{\rho}{\rho_l} \frac{u^2}{R^2} Re^{-3/2} \sim \frac{\rho}{\rho_l} Re^{-3/2} \frac{1}{t_{res}^2} \quad (A10)$$

where t_{res} is the residence time for an element of gas flowing past the droplet. If we consider the angular acceleration w to be roughly constant with time and if we define the time for one rotation as t_{rot} , we may obtain from (10) that

$$\frac{t_{rot}}{t_{res}} \sim \left[\frac{\rho_l}{\rho} \right]^{1/2} Re^{3/4} \gg 1 \quad (A11)$$

(1) through (5) will yield that

$$\frac{\Delta F}{F} \sim \frac{2}{Re} \quad (A12)$$

(11) and (12) support the conclusions of Section 2.3 concerning the largeness of the droplet rotational time and the smallness of the fractional change in the friction force.

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