A Comparison of Vaporization Models in Spray Calculations

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The effects of different gas- and liquid-phase models on the vaporization behavior of a single-component isolated droplet are studied for both stagnant and convection situations in a high-temperature gas environment. In conjunction with four different liquid-phase models, namely, d^2 law, infinite conductivity, diffusion limit, and internal vortex circulation, the different gas-phase models include a spherically symmetric model in the stagnant case and Ranz-Marshall correlation plus two other axisymmetric models in the convective case. A critical comparison of all these models is made. The use of these models in a spray situation is examined. A transient one-dimensional flow of an air-fuel droplet mixture is considered. It is shown that the fuel vapor mass fraction can be very sensitive to the particular liquid- and gas-phase models. The spherically symmetric conduction or diffusion limit model is recommended when the droplet Reynolds number is negligible compared to unity, while the simplified vortex model accounting for internal circulation is suggested when the droplet Reynolds number is large compared to unity.

Nomenclature

b_1,b_2 = constants in Eq. (19); $b_1 = 1.458\times10^{-5}$g/cm/s/K$^{0.5}$, $b_2 = 110.4$ K
C'_p = specific heat at constant pressure, cal/gm/K
D' = DD_c, gas diffusivity, cm^2/s
$f(B_k)$ = Blasius function used in Eqs. (15) and (A5)
H' = $HC'_pT'_c$, heat from the gas phase given to the liquid phase per unit mass of fuel vaporized, cal/g
L_c = length of the tube, cm
L' = $L\,C'_cT'_c$, heat vaporization, cal/g
L_r = L_c/r'_0, ratio of gas-phase characteristic length and the initial drop size
M'_f = $M_fM'_c$, molecular weight of fuel
M'_o = $M_oM'_c$, molecular weight of oxidizer
m'_k = $m_k\mu'_cr'_0$, vaporization rate, g/s
n'_k = n_k/L_c^2, number of droplets per unit cross-sectional area, 1/cm^2
p' = pp'_c, gas pressure, atm
r'_k = $r_kr'_0$, droplet radius, cm
T'_c = gas temperature at the tube entrance, K
T' = TT'_c, gas temperature
T'_k = $T_kT'_c$, droplet surface temperature
t' = tt'_c, time
t_r = $t_c/D'_c/L_c^2$, ratio of convection time to diffusion time in the gas phase
V'_c = gas velocity at the tube entrance, cm/s
V' = VV'_c, gas velocity, cm/s
V'_k = $V_kV'_c$, droplet velocity
x' = xL_c, axial coordinate, cm
X'_k = X_kL_c, droplet location
Y_{fs} = fuel vapor mass fraction at the droplet surface
Y_f = fuel vapor mass fraction
Y_o = oxidizer mass fraction
Y_N = neutral species mass fraction
Δx = spatial grid size
γ = ratio of specific heats
μ' = $\mu\mu'_c$, gas viscosity, g/cm/s
ϕ' = $\phi\phi'_c$, variable defined in Eq. (11)
ρ' = $\rho\rho'_c$, gas density
ρ'_k = liquid fuel density
ρ_r = ρ'_c/ρ'_k, ratio of initial gas-phase density and the liquid fuel density

I. Introduction

SPRAY vaporization and combustion studies are of primary importance in predicting and improving the performance of systems utilizing spray injection. Combustors, fire suppression, spray drying, and various forms of chemical power plants are typical examples of these systems. Often the vaporization of a droplet in the spray is affected by neighboring droplets. However, in spray combustion computations, it is assumed that the overall spray behavior can be obtained by summing behavior of individual isolated droplets surrounded by a gas phase that itself has varying properties. Even when the assumption that droplets behave as if they were isolated from each other is not satisfactory, the behavior of a single isolated droplet in an oxidizing environment will provide a fundamental input to the overall spray analysis.

Several models exist to represent the quasisteady behavior of the gas film or boundary layer surrounding the droplet. Also, various representations have been made of the transient behavior of the liquid phase. The purpose of this paper is to present two studies that are strongly coupled. First, an investigation is made of the impact of the various gas- and liquid-phase models on isolated droplet vaporization rates in a high-temperature environment. Second, the variation of the fuel vapor concentration in a fuel-air spray due to droplet model differences is evaluated. The accurate prediction of fuel-air mixture ratio, of course, is critical in a combustion situation. No chemical reaction is considered in the analyses but a high-temperature gas is considered; this is adequate to evaluate vaporization models for isolated droplets and sprays in combustion situations. Both steady and unsteady sprays are of interest in combustion. In this paper the more general unsteady case is studied.

In Sec. II, the effects of d^2 law, infinite conductivity, conduction limit, and vortex models on the vaporization behavior of a single-component droplet are studied. Both the stagnant and convective environments are considered. For the convective case, several models of the gas-phase boundary layer are studied. All these gas- and liquid-phase models are

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examined for three hydrocarbon fuels, namely, *n*-hexane, *n*-decane, and *n*-hexadecane. The use of different liquid-phase models in a spray vaporization situation is described in Sec. III, where a transient one-dimensional flow of an air-fuel droplet mixture in an open tube is considered. The effects of different droplet models on the fuel vapor mass fraction distribution in the tube are discussed in detail. An unsteadiness in the gas-phase properties, which is entirely due to the discrete droplet group locations, is also discussed. Conclusions are stated in Sec. IV.

II. Single-Droplet Vaporization

The basic droplet vaporization/combustion model for an isolated single-component droplet in a stagnant environment was given by Godsave[1] and Spalding.[2] Since then this model has been studied extensively both experimentally and theoretically. These studies have been reviewed by Williams,[3] Faeth,[4] and Law.[5] More sophisticated studies have also been reported. These consider the effects of relaxing the restrictions of the basic model. For example, the studies on the transient droplet heating models include the infinite conductivity model[6] and the conduction-limit model.[7] Law and Law[8] considered the variable gas-phase transport property effects. Hubbard et al.[9] considered the transient effects for the spherically symmetric case and concluded that the quasisteady gas-phase approximation yields small errors, at least for pressures below 10 atm. Their comparison with the constant transport property models using reference conditions indicated that the one-third rule gives the best agreement.

Basically, the existing literature on single-droplet vaporization can be classified into two major categories: spherically symmetric and axisymmetric. The different models in these two categories are discussed below.

Spherically Symmetric Models

d^2 Law Model

The most notable earlier work on droplet vaporization is by Godsave.[1] In that study, a quasisteady spherically symmetric model was used for both liquid and gas phases. The droplet temperature was assumed to be uniform and remained constant at its wet-bulb value. The properties in both the gas and liquid phases were assumed to be constant, together with Lewis number equal to unity. At the gas-liquid interface, it was assumed that the fuel vapor mass fraction was a function of the surface temperature given by some equilibrium vapor pressure equation such as the Clausius-Clapeyron relation. This theory gives the classic d^2 law and is the simplest possible model describing droplet vaporization. It should be noted that this model neglects the liquid-phase heat and mass transfer and is basically a gas-phase model. It does not consider some of the important physics and yields only a crude estimate of the droplet vaporization rate.

Some of the resulting relationships are given below.

$$m/4\pi r\rho_g D = \ln(1+B) \tag{1}$$

$$B = \frac{C_{pg}(T_g - T_s)}{L} = \frac{Y_{fs}}{1 - Y_{fs}} \tag{2}$$

where m is the fuel mass vaporization rate, B the Spalding transfer number, L the latent heat of fuel, and Y_{fs} the fuel vapor mass fraction at the interface. Subscripts g and s denote gas phase and droplet surface, respectively.

Note that $Y_{fs} = Y_{fs}(T_s)$ is a function of surface temperature only. Therefore T_s and B can be determined by Eq. (2) and subsequently can be obtained through Eq. (1). For a given ambient condition, T_s and B are fixed in this model, Eq. (1) can be written as

$$\frac{\mathrm{d}r^2}{\mathrm{d}t} = k = \text{const} \tag{3}$$

which says that the radius squared (proportional to the droplet surface area) decreases linearly in time and hence this model is referred to as d^2 law model in the literature.

Infinite Conductivity Model

In a combustor the droplet is initially cold and heats up with time. Law[6] studied droplet combustion with rapid internal mixing where droplet temperature is spatially uniform but varying with time. It was found that droplet heating is a significant cause of the unsteadiness of droplet combustion and should be taken into account in any realistic analysis of unsteady droplet combustion phenomena. Basically, this model is the same as the d^2 law model except that the constant liquid-phase temperature assumption is relaxed and replaced by a uniform but time-varying temperature inside the droplet. The gas-phase model remains spherically symmetric and quasisteady.

Some authors believed that this uniform temperature limit was related to the rapid internal liquid circulation limit and, hence, is referred to as rapid mixing model. Sirignano[10] showed that even in the limit of high vortex strength, the internal liquid circulation can only reduce the characteristic length scale for diffusion by an order of magnitude. The rapid mixing limit can never exist. Rather, it would be conceptually more correct to think that the uniform temperature limit results from the infinite conductivity limit. Hence, it is more appropriate to call it an infinite conductivity model.

Equations (1) and (2) remain the same except that L is replaced by

$$L + \frac{1}{m}\left(\frac{4}{3}\pi r^3 \rho_\ell c_{p\ell}\right)\frac{\mathrm{d}T_\ell}{\mathrm{d}t}$$

The additional term accounts for the transient liquid droplet heating. Subscript ℓ denotes the liquid phase.

Conduction Limit Model

When the internal liquid motion is not significant, heat transfer inside the droplet will be controlled by thermal diffusion only. This will be a reasonable model for the stagnant case and represents the slowest heat-transfer limit.

The liquid-phase temperature variation is governed by the well-known heat diffusion equation,

$$\frac{\partial T_\ell}{\partial t} = \frac{\alpha_\ell}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_\ell}{\partial r}\right) \tag{4}$$

with the initial and boundary conditions

$$\begin{aligned} T_\ell(r,t) &= T_0(r) && \text{at } t=0 \\ \frac{\partial T_\ell(r,t)}{\partial r} &= 0 && \text{at } r=0 \\ k_\ell \frac{\partial T_\ell(r,t)}{\partial r} &= q_\ell(t) && \text{at } r=r_s(t) \end{aligned} \tag{5}$$

where $T_0(r)$ is the initial temperature distribution and $q_\ell(t)$ is the liquid-phase heat flux at the droplet surface.

Equations (1) and (2) remain essentially the same except that L is replaced by

$$L + \frac{1}{m}\left(4\pi r^2 k_\ell \frac{\partial T_\ell}{\partial r}\bigg|_{rs}\right)$$

The additional term accounts for the liquid-phase heat flux at the surface.

Since the droplet is vaporizing, the diffusion field has a moving boundary. Obviously this model is more complicated than the infinite conductivity limit model.

Droplet Vaporization with Convective Effects

In many practical situations, the droplet vaporizes in a convective gas field. The gas-phase convection influences the vaporization process in two ways. First, it increases the gasification rate as well as the heat-transfer rate between the phases. Second, it generates liquid circulation inside the droplet which increases the liquid-transfer rate. Note that at very high relative velocity, droplet deformation and shattering can occur. This situation is not considered in this paper. Semiempirical correlations[11] exist which account for the gas-phase convection by expressing the vaporization and interphase heat-transfer rates as a modification of the spherically symmetric case. Sirignano[10] analyzed the convective case through a combination of stagnation-point and flat-plate analyses and concluded that the convective case should not be treated by a correction on the spherically symmetric case. Prakash and Sirignano[12] analyzed the gas- and liquid-phase flowfields for a single droplet in a convective gas field. They considered a gas-phase boundary layer outside the droplet and a Hill's vortex in the droplet core with thin viscous and thermal boundary layers near the droplet surface and an inviscid internal wake near the axis of symmetry. Their results show that the infinite conductivity case is never realized and the characteristic liquid-phase heat diffusion time reduces (from the diffusion-limit case) by an order of magnitude. Their analysis, however, is too complicated and computer-time consuming to be included in spray calculations. Tong and Sirignano[13] simplified that analysis substantially by neglecting the thin boundary layer inside the droplet surface. The results of the simplified model are in close agreement with those obtained from the more exact analysis.[12]

Ranz-Marshall Model

Many investigators[4,5] suggested empirical correlations for vaporization rate in a convective field as a correction to the spherical symmetric case. The typical form of correlation is $m_{\text{convection}} = m_{\text{spherical}} f(Re,Pr)$, where $f(Re,Pr)$ is the correction factor. In the present study, the Ranz-Marshall correlation is examined, for which the factor $f(Re,Pr)$ is given by

$$f(Re,Pr) = 1 + 0.3\,Re^{1/2}Pr^{1/3} \tag{6}$$

Although this type of correlations is very simple, there is really very little theoretical justification for them. Moreover, these correlations are based on experiments conducted under quasisteady conditions. As mentioned previously, there is a transient droplet heating stage and during that period the quasisteadiness assumption for the liquid phase is invalid. Indeed, Sirignano[10] showed, through theoretical analysis, that a correlation of Ranz-Marshall type cannot predict the vaporization rate satisfactorily.

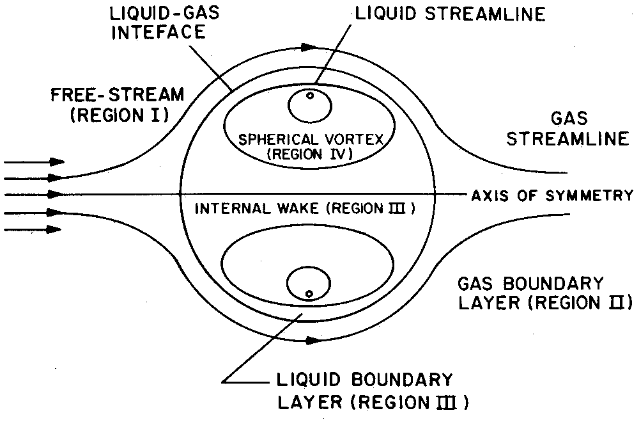

Fig. 1 Flow regions outside and within a fuel droplet at high Reynolds number.

Prakash and Sirignano's Axisymmetric Model

Recently, Prakash and Sirignano[12,14] studied the problem of transient liquid droplet vaporization in a hot convective environment. They first[14] studied liquid internal circulation and droplet heating and later[12] developed a gas-phase boundary-layer analysis and coupled it to the previous liquid-phase analysis. Basically, they used a two-dimensional axisymmetric model (valid for a droplet Reynolds number large compared to unity) and divided the problem into several physical regions as shown in Fig. 1. These regions were outer inviscid gas flow, gas-phase boundary layer, liquid-phase boundary layer, internal liquid wake, and inviscid liquid core. Because of the relatively high Reynolds number and high Peclet number, the boundary-layer approximation was used in their analysis for both the momentum and the energy transfers in both the gas and liquid phases. The outer inviscid gas flow was treated as steady potential flow around a sphere with no flow separation. The gas and liquid-phase boundary layers were both treated as quasisteady for both momentum and energy transfer while, for the liquid core, the momentum transfer was treated as quasisteady and the energy transfer was considered transient. This model, named as Prakash and Sirignano's model herein, has been included in the single-droplet study. It should be mentioned that this model, although quite detailed, uses an algorithm that is too cumbersome to be included in a complete combustion analysis. Simplifications, taking into account the important physics, are needed.

In Prakash and Sirignano's analysis, there is a thin thermal boundary layer near the droplet surface which is coupled to the thermal core in the matching region. The thermal boundary layer which allows for the heat flux to adjust from two-dimensional behavior along the droplet surface to one-dimensional behavior along the boundary layer and thermal core matching region was treated as quasisteady. The importance of the thermal boundary layer and the quasisteadiness assumption have been reviewed recently by Tong and Sirignano.[13] The results of that study show that, unless the thermal boundary layer is very thin (very large Peclet numbers), the thermal inertia term is important and quasisteadiness assumption for that layer is invalid. The results also tend to suggest that the elimination of the thermal boundary-layer representation and the assumption that the thermal core solution is valid up to the droplet surface may still give solutions with an acceptable degree of accuracy. It should be noted that while the thermal boundary-layer formulation is two dimensional, the thermal core formulation is one dimensional. Hence, the removal of the thermal boundary-layer will simplify the problem tremendously. With the elimination of the thermal boundary layer and the assumption that the thermal core solution is valid up to the droplet surface, Tong and Sirignano[13] subsequently simplified the thermal core solution. Their simplified liquid-phase model is included in this study.

Tong and Sirignano's Axisymmetric Model

Tong and Sirignano[15] further developed a one-dimensional gas-phase model. They simplified the axisymmetric convective analysis in the gas phase by representing the heat- and mass-transfer rates by an optimum average for the stagnation point region and the shoulder region of a droplet. The results from coupling this simplified gas-phase model to their simplified liquid-phase model which was obtained earlier are in reasonably good agreement with the results of the more detailed model of Prakash and Sirignano. The gas-phase model has been employed in the spray calculations reported in Sec. III.

Results and Discussions on Single-Droplet Vaporization

Liquid fuel droplets initially at 300 K vaporizing in 1000 K, 10 atm pressure fuel-free environment is used to study the various gas- and liquid-phase models. Hexane, decane, and hexadecane droplets of initial radius of 0.00476 cm are considered. The physical properties are the same as those in the Prakash and Sirignano's analysis.[12]

The results for the stagnant case are given in Figs. 2 and 3. The gas-phase model is quasisteady and spherically symmetric. Three different liquid-phase models, namely, the d^2 law, the conduction limit, and the infinite conductivity limit are compared. Since the existence of a vortex in a stagnant environment cannot be realized conceptually, it is excluded for comparison. One would think that if the vortex model were included, it would be in between the infinite conductivity and conduction limits. This indeed can be shown to be true. Figures 2 and 3 show the temporal variation in the surface temperature and surface area, respectively. The physical time t is nondimensionalized by using the liquid thermal diffusivity α_ℓ and the initial droplet radius r_0 as $\tau = t/(r_0^2/\alpha_\ell)$. For the d^2 law model the surface temperature is at the wet-bulb temperature and remains constant while the surface area regresses linearly in time. The d^2 law serves as an asymptotic limit for the other two models. This is reflected in Fig. 2 where the surface temperature of the other two models approaches the wet-bulb temperature, and in Fig. 3 where the curves become more linear.

Since the d^2 law neglects the initial transient droplet heating, the droplet vaporizes much faster than the other two models. The difference is bigger for the heavier fuels which have higher boiling temperatures and, hence, a longer transient heating period. Conversely, the conduction limit and the infinite conductivity limit have about the same droplet lifetime. Note that these two limits intersect each other. Since the droplet temperature is uniform in the infinite conductivity limit, the surface temperature increase per unit of energy absorption is less. Consequently, the fuel vapor mass fraction at the droplet surface is lower, which leads to lower vaporization rate. On the other hand, the difference between the ambient and surface temperatures, which relates directly to the heat-transfer rate to the liquid, is higher. This eventually results in a higher surface temperature and faster vaporization rate during the latter portion of the lifetime for the infinite conductivity model. Note that the wet-bulb temperatures in these calculations are considerably lower than their corresponding boiling temperatures of the fuels. The effect of the different liquid-phase models on the interior liquid temperature is quite significant and, therefore, the conduction limit model, which is considered to be exact, should be used if detailed temperature distribution inside the droplet is needed. The infinite conductivity model may be useful in the low ambient temperature case when the droplet lifetime is long. The d^2 law model, which gives poor agreement with the conduction limit model, is oversimplified and should be discarded.

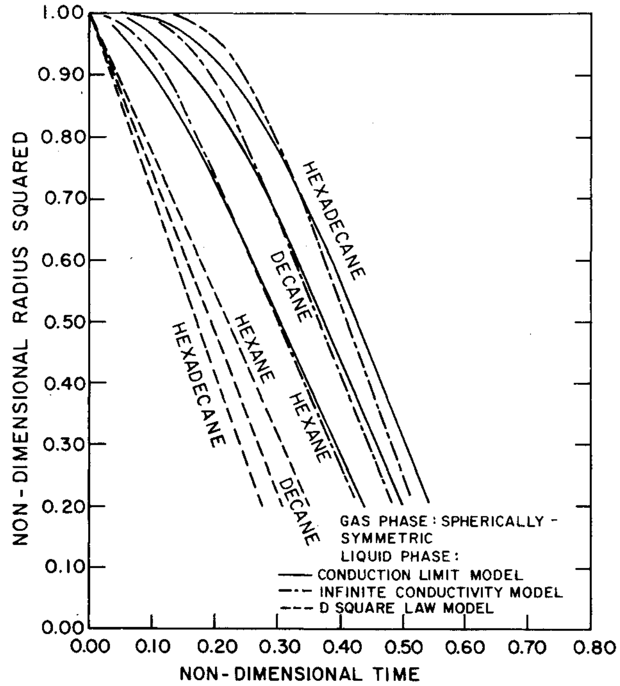

Fig. 3 Nondimensional radius square vs time comparisons.

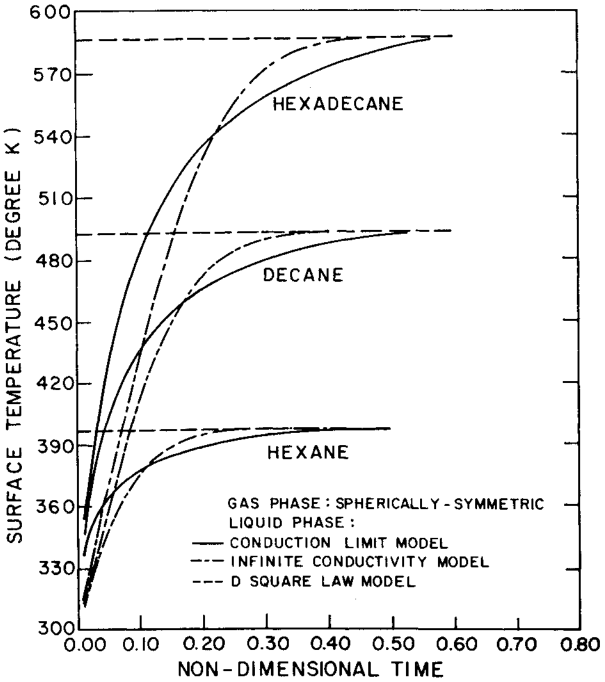

Fig. 2 Surface temperature vs time comparisons.

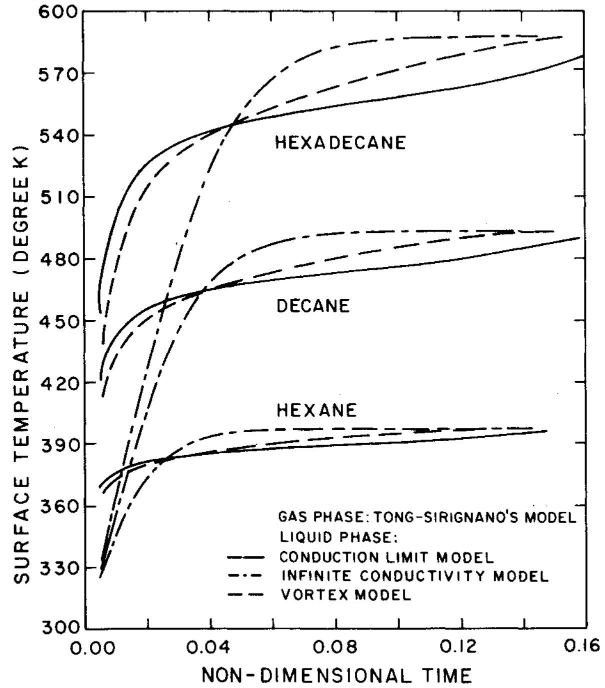

Fig. 4 Surface temperature vs time comparisons.

The results for the convective case are given in Figs. 4-7. In these calculations, the Reynolds number (based on droplet diameter) is initially 200 and decreases with the diameter as the droplet vaporizes. The relative velocity is 2500 cm/s and is assumed to be constant throughout. In reality the relative velocity will be reduced by the drag force; this is considered later in the spray vaporization case.

Although Prakash and Sirignano's model is the most detailed and should be considered the most exact, it is quite cumbersome to be included in a complete spray analysis. Instead, Tong and Sirignano's model and the simplified vortex model, which have been shown[15] to give close agreement with Prakash and Sirignano's results, are used as reference model in the figures.

Figures 4 and 5 show the results of the various liquid-phase models. The d^2 law does not exist in this convective case. Again, the conduction and infinite conductivity limits intersect due to the same reasoning as in the stagnant case. The vortex model lies in between the other two models as expected. Note that the droplet lifetime is considerably shorter than that in the stagnant case. In the convective case, $(r/r_0)^{3/2}$ regresses asymptotically linearly with time and is used in Figs. 5 and 7. Figure 5 shows that, for the heavier fuel, the percentage variation in droplet lifetime can depend quite significantly on the liquid-phase model.

Figures 6 and 7 show the effects of the different gas-phase models. The Ranz-Marshall correlation overpredicts the vaporization rate and underestimates (for decane) the surface temperature. As indicated by Sirignano,[10] this type of correlation has very little theoretical justification and cannot give satisfactory results. The present study supports Sirignano's qualitative analysis. Tong and Sirignano's model appears to be in good agreement with the more detailed model of Prakash and Sirignano.

The simplified vortex model applies to a situation where 1) the streamfunction patterns are described reasonably well by a Hill's spherical vortex pattern, and 2) the circulation time is very short compared to other characteristic times. Hill's spherical vortex can be obtained when the nonlinear inertial terms in the momentum equation can be neglected compared to other terms. This can occur at low Reynolds number via an order-of-magnitude argument. Fortuitously, in similar fashion to Couette flow or Poisseuille flow, the inertial terms go identically to zero so that the streamfunctions are valid even at higher Reynolds number. The very short circulation time or very high vortex strength implies a very high Peclet number for the liquid (upon comparison of diffusion time to circulation time). Since Prandtl number is of order ten, a high Reynolds number is implied. For low Reynolds number, the heat conduction will occur in a two-dimensional fashion, both normal and tangent to the streamsurfaces. This complicates the application of a simplified model to a low Reynolds situation. The gas-phase models are also limited to high Reynolds numbers, since thin boundary layers are considered. Therefore, for several reasons, additional modeling is required if the low Reynolds number case is to be considered.

The results indicate that the droplet heating and vaporization are essentially unsteady for most of their lifetimes, particularly for the heavier fuel. For a detailed analysis, Prakash and Sirignano's model is recommended, but

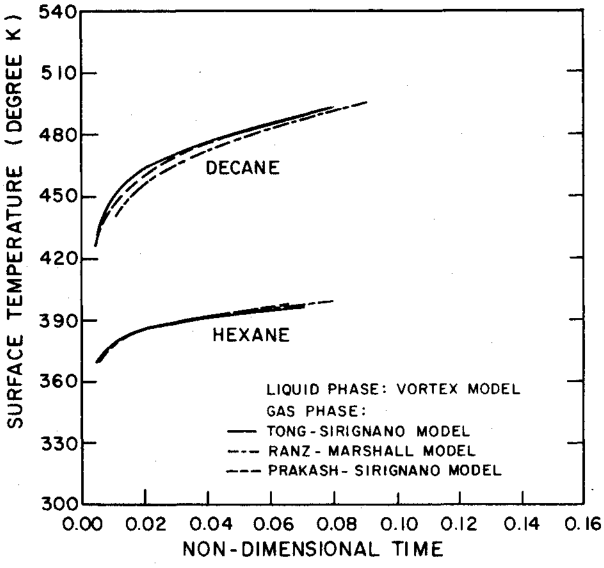

Fig. 6 Surface temperature vs time comparisons.

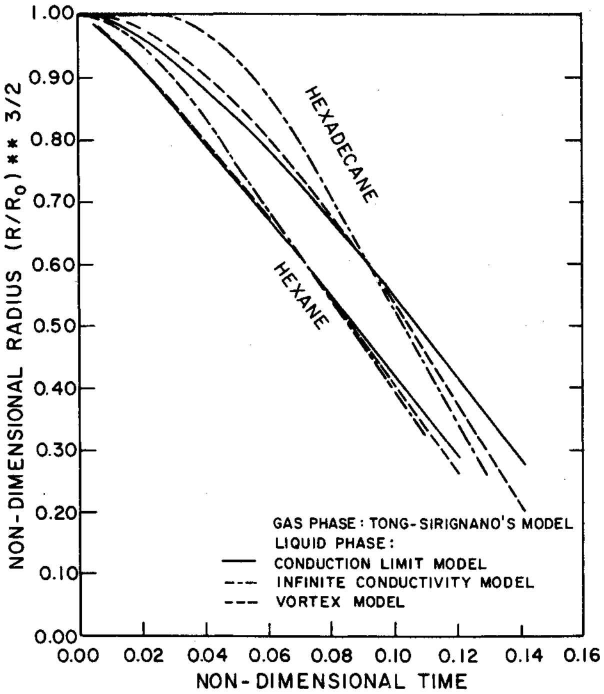

Fig. 5 $(R/R_0)^{3/2}$ vs time comparisons.

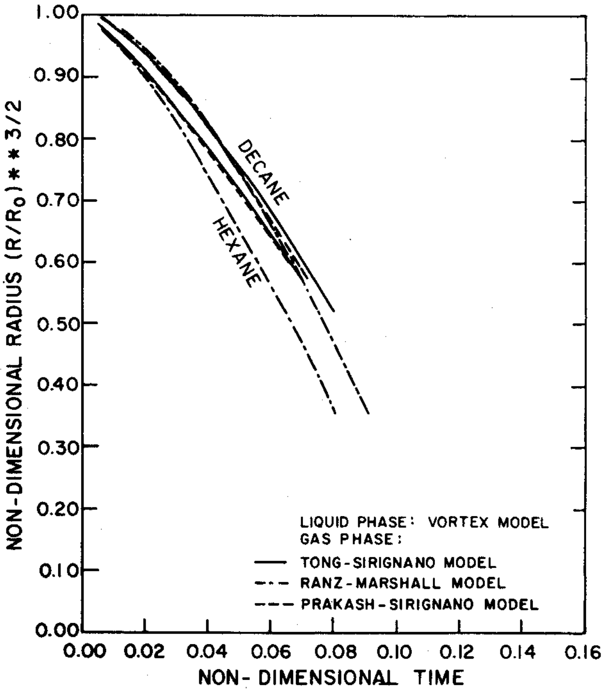

Fig. 7 $(R/R_0)^{3/2}$ vs time comparisons.

for more practical application, Tong and Sirignano's model with the simplified vortex model would be useful.

III. Spray Vaporization Study

In the spray vaporization problem, a one-dimensional transient flow of air and fuel droplets in an open tube is considered, where the motion and vaporization of a monodispersed spray in a laminar, hot gas stream are studied. The purpose is to examine the effects of different liquid-phase models on the bulk vaporization characteristics as well as on the gas medium. The different liquid-phase models considered are the infinite conductivity, the conduction limit, and the vortex models. The different convective models for the gas phase are the Ranz-Marshall correlation and the model of Tong and Sirignano. The physical situation consists of a continuous laminar flow of hot air in an open tube. The gas-phase properties initially in the tube and later at the tube entrance are prescribed. The injection of fuel droplets is intermittent. One group of droplets is injected every given time interval. The number of droplets in a group (or with a characteristic) represents the number of droplets per unit cross-sectional area. That is, the spacing between droplet groups is precisely the spacing (in the flow direction) between individual droplets. The grouping of the droplets eliminates only the effect of droplet spacing in the transverse direction. The constancy of the frequency of injected droplets is, of course, artificial, but will not affect any of the qualitative results of this paper. The frequency of injection and initial droplet velocity depends on the overall fuel-to-air ratio in the tube, the mass flow of air, droplet spacing, and droplet diameter at the tube entrance. The prescription of the overall fuel-to-air ratio, the droplet diameter, and the droplet velocity at the entrance yields the value of the droplet number density. The droplet spacing in the axial direction and the number of droplets per unit cross-sectional area are so adjusted as to provide initially an isotropic droplet spacing in a unit cube. Initially a high relative velocity is provided between the two phases. As a droplet group moves in the hot gas stream it accelerates. At the same time, the droplets heating and vaporization is taking place. The spray processes influence the state of the gas, i.e., the gas phase is continuously retarded, cooled, and enriched with fuel vapor.The gas-phase properties are also being influenced by the upstream convection. All of these gas- and liquid-phase processes are modeled by a system of unsteady, one-dimensional equations. The gas phase is represented in Eulerian coordinates, whereas the liquid phase is represented in Lagrangian coordinates. The governing equations in nondimensional form are given as follows.

Table 1 Values used in the computation

Parameter	Value
Fuel	*N*-decane
Liquid density, ρ'_k	0.773
Initial drop radius, r'_0	50 μm
Initial drop temperature, T'_k	300 K
Number of drops per unit cross-sectional area, N'_k	400 cm^{-2}
Drop spacing in the axial direction, d'_s	0.05 cm
Gas velocity at the tube entrance, V'_c	1000 cm/s
Drop velocity at the tube entrance, V'_k	0.1 V'_c
Tube length, L_c	10 cm
Pressure, p'_c	10 atm
Gas temperature at the entrance, T'_c	1000 K
Temporal step size, $\Delta t'$	10^{-5}s
Spatial step size, $\Delta x'$	0.1 cm
Specific heat at constant pressure, C'_p	0.25 cal/g/K
Molecular weight of fuel, M'_f	142.3 g/mole
Molecular weight of oxidizer, M'_o	32.0
Boiling temperature of the fuel at 1 atm, T'_{bn}	447.3 K
Heat of vaporization, L'	86.5 cal/g
Gas constant, $R'_{\rm gas}$	2.8393 atm cm^3/g/K

Gas-Phase Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho V) = S_\rho \tag{7}$$

$$\frac{\partial Y}{\partial t} + V\frac{\partial Y}{\partial x} - t_r D\frac{\partial^2 Y}{\partial x^2} = S_Y \tag{8}$$

$$Y = Y_f, Y_o, \phi \tag{9}$$

$$Y_N = 1.0 - Y_f - Y_o \tag{10}$$

$$\phi = T p^{(1-\gamma)/\gamma} \tag{11}$$

$$\rho = p^{(1/\gamma)}/\phi \tag{12}$$

Liquid-Phase Equations

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \tag{13}$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}t} = \{\rho_r L_r^2 t_r\}\left\{\frac{3}{16}\frac{C_D \mu Re_k (V - V_k)}{S_k}\right\} \tag{14}$$

$$\frac{\mathrm{d}S_k}{\mathrm{d}t} = -2\{\rho_r L_r^2 t_r\}(1 + 0.3 Re_k{}^{0.5})\, \ell n(1 + B_k) \tag{15}$$

for Ranz-Marshall correlation model

$$\frac{\mathrm{d}S_k}{\mathrm{d}t} = -2\{\rho_r L_r^2 t_r\}\left[\frac{2}{\pi} Re_k\right]^{0.5} f(B_k)$$

for Tong-Sirignano model

$$S_k = r_k^2 \tag{16}$$

$$C_D = \frac{24}{Re_k}\left(1 + \frac{Re_k^{2/3}}{6}\right) \tag{17}$$

$$Re_k = \frac{2}{t_r L_r}\frac{r_k \rho}{\mu}|V - V_k| \tag{18}$$

$$\mu = \mu(T'_{\rm ref}) = \frac{1}{\mu_o}\left[\frac{b_1 T'^{3/2}_{\rm ref}}{b_2 + T'_{\rm ref}}\right] \tag{19}$$

where

$$T'_{\rm ref} = {}^1\!/_3\, T' + {}^2\!/_3\, T'_k \tag{20}$$

The source terms in the gas-phase equations result from the coupling between the two phases. These are given in the Appendix. It should be noted that a transformation, as given by Eq. (11), has been employed. This transformation is useful for a constant-volume situation.[16] However, it has been retained here (a constant-pressure case) for the sake of generality.

In nondimensionalizing the gas-phase equations, the length scale is the length of the tube, and the velocity scale is the gas velocity at the tube entrance. The time scale is determined by these two scales. The gas-phase properties are nondimensionalized by using the respective properties at the entrance. For the liquid-phase equations, the droplet location, velocity, and surface temperature are nondimensionalized by the gas-phase length, velocity, and temperature scales, respectively. The droplet radius is nondimensionalized by the initial droplet radius. The above nondimensionalization gives rise to three additional dimensionless groups, t_r, L_r, and ρ_r; t_r is the ratio of convective time to diffusion time in the gas phase, L_r the ratio of gas-phase length scale and initial drop radius, and ρ_r the ratio of initial gas-phase density and liquid density.

The important assumptions made in writing these equations are that the gas pressure is constant, radiative heat transfer is negligible, the species diffusion follows Fick's law with equal mass diffusivities for each pair, the specific heat at constant pressure is constant, and the gas-phase Lewis and Schmidt numbers are unity. In addition, the product ρD $(=\mu)$ is assumed constant. It is noteworthy, however, that in the calculation of liquid-phase properties μ is considered a function of temperature as given by Sutherland correlation.[17] As indicated in Eq. (19), a reference temperature is used for the calculation of μ and the reference temperature is obtained by the one-third rule as recommended by Sparrow and Gregg.[18]

The drag coefficient is evaluated by using an expression as proposed by Putnam.[19] The evaluation of Reynolds number for the drag coefficient is based on the freestream density and viscosity evaluated at the one-third reference state. This follows the recommendation of Yuen and Chen.[20] In the calculations the Reynolds number for each droplet varies with time due to changes in size, relative velocity, and local conditions. It should also be noted that the effect of relative droplet-gas velocity on the vaporization rate [see Eq. (15)] has been treated by a semiempirical correlation,[11] as well as by an axisymmetric model.[15]

The Solution Procedure

A hybrid Eulerian-Lagrangian numerical scheme is used to calculate the gas- and liquid-phase properties at the $(n+1)$th time level from the values known at the nth time level. First, a second-order accurate scheme is employed to interpolate the gas-phase properties from the Eulerian locations (fixed-grid points) to the Lagrangian (or droplet) locations. The scheme uses the gas-phase properties at two grid points x_i and x_{i+1} and gives the corresponding properties at a Lagrangian location X_k, where X_k is between x_i and x_{i+1}. Using these gas-phase properties, the droplet surface temperature is then calculated. For the infinite conductivity model it involves the solution of an ordinary differential equation for each droplet group. For the conduction limit and vortex models a partial differential equation needs to be solved. The details have been discussed in Sec. II. Knowing T_k for each droplet group, other droplet properties (X_k, V_k, r_k) can be obtained by solving Eqs. (13-16). A second-order Runge-Kutta scheme is used for this purpose. It should be noted, however, that there is some loss of accuracy due to the fact that the gas-phase properties are not updated in the Runge-Kutta scheme. Using the new liquid-phase properties, the source terms as given in the Appendix can be evaluated at the Lagrangian locations. Then a second-order accurate scheme is used to distribute these source terms from a Lagrangian location to the two neighboring gas-phase locations. Using these source terms, the gas-phase properties $(Y_f, Y_o$, and $\phi)$ at the $(n+1)$th time level are obtained by solving Eq. (8). An explicit finite difference method is used for this purpose. The gas temperature and gas density are then obtained by using Eqs. (11) and (12). Finally, the gas velocity is obtained from an integral form of the continuity equation (7). It is worth emphasizing that, in the present case, the gas-phase convection term dominates the diffusion term. Therefore, an upwind difference scheme[21] is employed for the convection term. It also should be noted that an explicit method was found to be the most efficient for reacting two-phase flow.[21] However, an implicit method may be more efficient for the present vaporizing case without combustion since the equations may not be as stiff.

Discussion of Results

The effects of using different liquid-phase models on the bulk spray and gas-phase properties are now discussed. The various values used in the computation are listed in Table 1. The criterion used in selecting these values was to consider a spray vaporization situation with a moderate gas-phase convection for the droplets. The selected values provide an initial Reynolds number (based on the relative velocity and

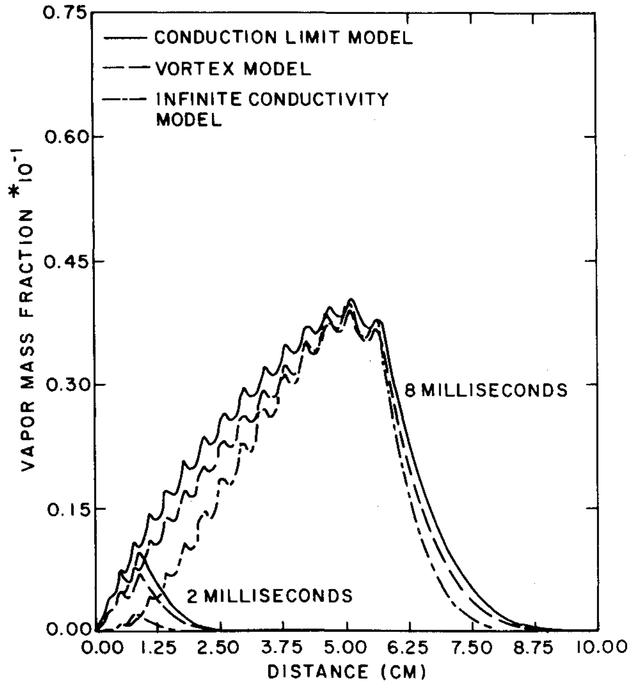

Fig. 8 Fuel vapor mass fraction vs distance at various times for different liquid-phase models.

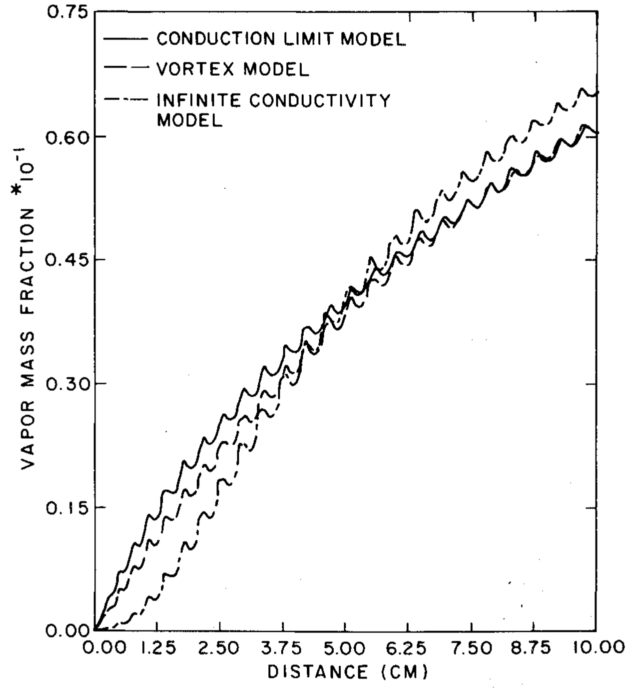

Fig. 9 Fuel vapor mass fraction vs distance at 16 ms for different liquid-phase models.

Table 2 Properties of the first droplet group for different liquid-phase models

t, ms	X_k', cm	r_k/r_0	$(r_k/r_0)^3$	T_k', K	V_k', cm/s
		Conduction limit model			
0	0	1.000	1.000	300.0	100.0
2	0.885	0.961	0.887	445.0	590.0
4	2.272	0.902	0.734	453.3	773.1
6	3.916	0.842	0.597	458.1	861.2
8	5.691	0.781	0.476	462.2	909.2
10	7.540	0.716	0.367	465.9	937.2
12	9.433	0.648	0.272	469.1	954.5
		Infinite conductivity model			
0	0	1.000	1.000	300.0	100.0
2	0.889	0.994	0.982	412.5	587.6
4	2.257	0.948	0.852	459.4	758.2
6	3.869	0.867	0.652	471.8	845.0
8	5.615	0.779	0.473	474.5	897.1
10	7.445	0.692	0.331	475.0	930.3
12	9.328	0.604	0.220	475.1	951.6
		Vortex model			
0	0	1.000	1.000	300.0	100.0
2	0.885	0.973	0.921	438.1	588.0
4	2.264	0.920	0.779	452.6	767.5
6	3.895	0.858	0.632	460.6	854.7
8	5.658	0.791	0.495	465.6	903.4
10	7.496	0.721	0.375	468.8	932.7
12	9.382	0.648	0.272	470.9	951.3

drop diameter) of 113 and a droplet residence time of about 12.5 ms. During this time 80% of the droplet mass is vaporized. The effects of different liquid-phase models on the bulk gas-phase properties are presented in Figs. 8-10. Figures 8 and 9 indicate that the choice of a particular droplet heating model can influence the fuel vapor distribution in the tube significantly, especially in the early vaporization period. This can have a profound effect on the subsequent combustion process in a practical situation. The maximum difference between the fuel vapor mass fraction values is as much as 100% between the conduction limit and the infinite conductivity models. As Fig. 9 indicates, the conduction model initially (up to a distance of 5 cm) predicts the highest fuel vapor mass fraction, whereas the infinite conductivity model predicts the lowest. At later times the situation is reversed. The vortex model results are always in between those of the other two models. The difference in the fuel vapor distribution is a direct consequence of the difference in the droplet surface temperature values for the three models. As discussed in Sec. II, the conduction limit model initially predicts the highest droplet surface temperature and, therefore, the fastest vaporization rate, whereas the infinite conductivity model predicts the lowest surface temperature and the slowest vaporization rate. As also discussed in Sec. II, this behavior is reversed at later times.

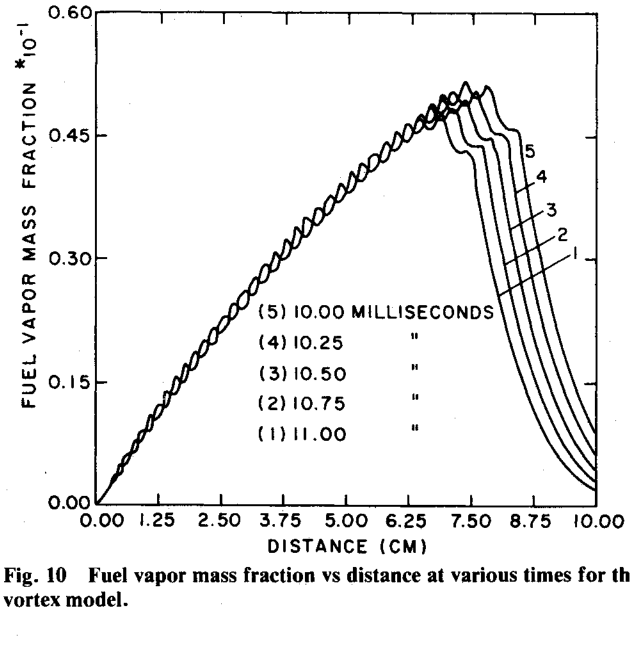

Fig. 10 Fuel vapor mass fraction vs distance at various times for the vortex model.

The fuel vapor mass fraction profiles in Figs. 8 and 9 exhibit an oscillatory and undulating behavior. This is due to the periodic nature of the droplet injection process which causes a finite droplet spacing in the streamwise direction. Thus the period of this oscillation is the same as the time interval between two subsequent injections. This is clearly illustrated in Fig. 10. As this figure indicates, the profiles overlap after every 0.5 ms, which is the time interval between two subsequent injections. This unsteady gas-phase behavior, which is entirely due to the spray discretization, should be kept in mind in spray modeling. A continuous drop in the gas temperature occurs in the downstream direction and is indicative of the continuous cooling of the gas phase due to droplet heating and vaporization. The difference in the gas temperature distribution due to the different liquid-phase models is not as significant as that in the fuel vapor distribution. This is due to the fact that the spray heating and vaporization constitute only a small heat loss in the overall gas-phase heat budget. An oscillatory behavior in the gas temperature profiles occurs again due to the intermittent droplet injection process. This intermittency is prescribed exactly in our idealized calculation. In a practical situation it may not be so well defined and perhaps should be taken as random. That is, the distance between droplets as they flow into the domain of interest will not be fixed as they are given in this calculation but rather will be distributed about some average value.

If random injection rather than orderly injection had been chosen, the oscillatory behavior in the fuel-vapor concentrations would not have been eliminated. Droplet spacing would vary from droplet pair to droplet pair so that the wavelength or period would no longer be constant in a random injection case but the fundamental oscillatory phenomenon would still be present.

The effect of different liquid heating models on the droplet properties is illustrated in Table 2. The properties of the first droplet groups, i.e., the location, the nondimensional radius, the surface temperature, and the velocity, are given as functions of time for the three models. The difference in the surface temperature, droplet radius, and droplet volume values for the three models is very similar to that discussed in Sec. II. The conduction limit model predicts the highest droplet velocity, whereas the infinite conductivity model predicts the lowest value. This occurs since the conduction limit model initially predicts the fastest vaporization rate, the smallest drop size, and, consequently, the highest droplet acceleration. It should be noted, however, that the difference in the droplet velocities for the three models is quite small.

The effect of different convective models is presented in Fig. 11. It should be noted that the model of Tong and Sirignano is valid only when the Reynolds number is large compared to unity; as indicated by Eq. (15), this model predicts a vaporization rate, which is proportional to the square root of the Reynolds number. For this reason, initial droplet radius of 100 μm is used for these calculations. This gives a value of 226 for the initial Reynolds number. Figure 11 shows that the Ranz-Marshall correlation overpredicts the vaporization rate as compared to that given by the axisymmetric model. This behavior is consistent with the one observed for the single-droplet case in the previous section. Since the Ranz-Marshall correlation predicts a higher vaporization rate and, therefore, a higher heat loss from the gas phase, it gives lower gas temperatures than those given by the correlation. It is also important to note that at very small Reynolds number, our model predicts an unacceptably small vaporization rate. Consequently, the model should have the capability to switch from the Tong and Sirignano model to some valid low Reynolds number model as the Reynolds number becomes small. This is presently under investigation.

IV. Conclusions

The most common vaporization models have been compared for fuels of varying volatility in a high-temperature environment. Both isolated droplet and spray vaporization have been studied. The use of the d^2 law or the infinite conductivity model (sometimes named the rapid mixing model) has been shown to be very inadequate. For spherically symmetric vaporization (no relative gas-droplet motion), the conduction limit model for transient heating is recommended. In practical situations where a relative gas-droplet motion exists, the simplified vortex model of Tong and Sirignano is recommended when the droplet Reynolds number based on relative velocity is high compared to unity. That model compares well with the more detailed model of Prakash and Sirignano and predicts well the effects of the laminar gas-phase boundary layer over the droplet and the internal circulation in the droplet.

The spray calculations indicate an inherent unsteadiness due to the intermittent character of a spray. This unsteadiness will be interesting whenever we wish to resolve structure on the scale of the average distance between droplets.

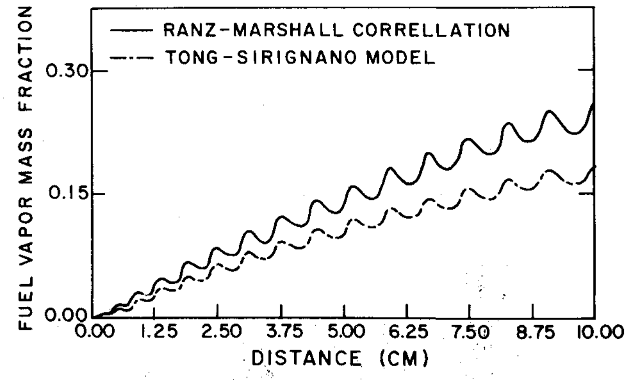

Fig. 11 Fuel vapor mass fraction vs distance at 16 ms for different gas-phase models.

Appendix

The source and sink terms in gas-phase equations (7) and (8) are given as follows:

$$S_\rho = \frac{t_r}{L_r}\frac{1}{\Delta x}\sum_k m_k n_k \tag{A1}$$

$$S_{Yf} = \frac{1}{\rho} S_\rho (1 - Y_f) \tag{A2}$$

$$S_{Yo} = -\frac{1}{\rho} S_\rho Y_o \tag{A3}$$

$$S_\phi = -\frac{S_\rho}{\rho p^{\gamma-1}}\left\{H + T - T_k\right\} \tag{A4}$$

$$m_k = 4\pi r_k \mu (1 + 0.3 Re_k^{0.5} \ell n (1 + B_k)$$

for the Ranz-Marshall correlation

$$= 4\pi r_k \mu \left\{\frac{2}{\pi} Re_k\right\}^{0.5} f(B_k)$$

for the Tong-Sirignano model (A5)

$$B_k = T - T_k / H \tag{A6}$$

$$H = \frac{(1 - Y_{fs})(T - T_k)}{Y_{fs} - Y_f} \tag{A7}$$

$$Y_{fs}^{-1} = 1 + \frac{M'_a}{M'_f}(x_{fs}^{-1} - 1) \tag{A8}$$

$$x_{fs} = \frac{p'_n}{p'}\exp\left[\frac{L'M'_f}{R'}\left(\frac{1}{T'_{bn}} - \frac{1}{T'_k}\right)\right] \tag{A9}$$

In the above relations, S_{Yf} and S_{Yo} are the source and sink terms for the fuel vapor and oxidizer mass fractions, x_{fs} the mole fraction at the droplet surface, M'_a the molecular weight of the gas phase (excluding fuel vapor), T'_{bn} the liquid fuel boiling temperature at the normal pressure p'_n, p the prevailing pressure, and k represents the summation over all droplet groups which happen to be in a given gas-phase mesh, of size Δx. A phase equilibrium assumption has been made at the droplet surface and the Clausius-Clapeyron relation [Eq. (A9)] has been used. The different methods of computing the droplet surface temperature T_k distinguish the various liquid-phase models examined in the present spray problem. These have been discussed in Sec. II.

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