Int. J. Heat Mass Transfer. Vol. 30, No. 9, pp. 1949–1961, 1987
Printed in Great Britain

0017-9310/87 $3.00+0.00

Modeling of a dilute vaporizing multicomponent fuel spray

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(*Received* 15 *September* 1986 *and in final form* 23 *February* 1987)

Abstract—A simplified spray environment is used to represent the multicomponent nature of liquid fuels and to examine the sensitivity of their vaporization behavior to the various liquid- and gas-phase models. Liquid-phase models are the diffusion limit, the infinite diffusion, and the vortex. Gas-phase models are the Ranz–Marshall correlation and the axisymmetric model. Three subsets of equations are solved by a hybrid Eulerian–Lagrangian, explicit–implicit scheme. Results demonstrate that the fuel vapor distributions are extremely sensitive to the models considered, that the internal circulation is less important for the multicomponent case as compared to the single component, that the multicomponent results are in complete contrast to those for the single component, and that an acceptable spray model should realistically consider the diffusive–convective processes inside and outside the droplet. For most spray situations, the diffusion-limit model is recommended.

1. INTRODUCTION

ONE ASPECT of spray combustion research which remains mostly unexplored is the representation of the multicomponent nature of fuel. Most of the liquid fuels utilized in practical systems are mixtures of many compounds with wide variation in properties. The single-component vaporization models cannot be used for these fuels since the vaporization/combustion characteristics of multicomponent fuel sprays are distinctly different from those of the single-component sprays due to several reasons. First of all, the behavior of an isolated droplet changes significantly if the droplet contains more than one fuel. The effect of transient heat transport inside the droplet is probably not important in predicting the droplet behavior for the single-component case. For the multicomponent case, however, the transient thermal and specially the liquid mass transport may be the rate-controlling process and must be included in the modeling. Thus, the single-component droplet models which neglect the liquid transport effects [1] and still yield reasonable predictions of droplet vaporization rate, cannot be employed for the multicomponent case. Another difference between the two cases is due to the phenomenon of microexplosion. For the multicomponent case, the volatile component is trapped inside the droplet due to high mass diffusional resistance where it may be heated beyond its boiling point. This can start the homogeneous nucleation leading to microexplosion. Obviously, this phenomenon, which may also be used to improve the combustion characteristics of heavy fuels [2], cannot be explained by the single-component theory. The spray-combustion characteristics of multicomponent fuels may also be profoundly different from those of the single-component fuel due to droplet dynamics. Certain regions of the combustor may be relatively rich in the volatile fuel while others may have a high concentration of less volatile fuel. The non-uniform fuel distributions may significantly influence not only the phenomena of ignition, flame stability and pollutant formation, but also the dominant burning mechanism itself.

The objective of this paper is to study the representation of the multicomponent nature of fuel in spray modeling. The combustion aspects are not studied in the first analysis. Only the vaporization aspects are examined. The dynamics and vaporization of the spray in a laminar, hot gas stream flowing in a tube are analyzed. In particular, the local as well as global effects of different liquid- and gas-phase models on the spray vaporization characteristics are examined. The liquid-phase models considered are the infinite-diffusion, the diffusion-limit, and the vortex models. The gas-phase models which account for the convective motion between droplet and gas, are the Ranz–Marshall correlation and a model based on the simplified analysis of gas flow over a droplet.

The vaporization/combustion behavior of an isolated single-component fuel droplet is fairly well understood and comprehensive models for its prediction have been generated [2]. Only the simplest of these models have been used in spray modeling, however, due to the many complexities involved. Recently, more detailed droplet models have been studied by Aggarwal *et al.* [3] where the effects of several liquid- and gas-phase models were investigated for the single-component fuel sprays. The major conclusion was that the transient heat transport in the liquid may not effect the global behavior of an isolated droplet much, but can influence the spray vaporization significantly. In the present study, the vapo-

NOMENCLATURE

B_k	given in Appendix
C_D	drag coefficient
C_k	ratio of gas and liquid-thermal conductivities
D	gas diffusivity
D'_c	initial gas diffusivity [$\text{cm}^2\,\text{s}^{-1}$]
K	$\rho'_c D'_c/\alpha'_l \rho'_k$
L_i	heat of vaporization for fuel i
Le	Lewis number for the liquid fuel
L_r	ratio of gas-phase length scale and initial droplet radius, L'_c/r'_{k0}
L'_c	gas-phase length scale [cm]
M	non-dimensional vaporization rate given in equations (25) and (26)
n_k	non-dimensional droplet number per unit area or number of droplets in a group
Re	Reynolds number based on droplet diameter and interphase velocity
r'	radial distance inside the droplet [cm]
r_k	droplet radius
r'_{k0}	initial droplet radius [cm]
t	time variable
t_r	ratio of convective time scale to diffusive time scale in the gas phase, $(t'_c L'_c)/D'_c$
T	gas temperature
T_B	non-dimensional boiling temperature of volatile fuel
T_l	liquid temperature inside the droplet
T'_{bn}	normal boiling temperature of volatile component [K]
T'_0	initial liquid temperature [K]
T_k	droplet surface temperature
V	gas velocity
V_k	droplet velocity
W_i	molecular weight of species i
x	spatial coordinate for the gas properties
Δx	grid size for the gas-phase calculations
X_k	position of a droplet group
X_{lis}	liquid mole fraction of fuel species i at the droplet surface
X_{is}	vapor mole fraction of species i at the droplet surface
Y_{fi}	fuel vapor mass fractions for the gas-phase equations, also the value at infinity for the liquid-phase equations
Y_{is}	fuel vapor mass fractions at the droplet surface
Y_{fs}	total fuel vapor mass fraction at the droplet surface
Y_{li}	liquid mass fraction of fuel i inside the droplet.

Greek symbols

α'_l	liquid thermal diffusivity [$\text{cm}^2\,\text{s}^{-1}$]
ε_i	fractional mass vaporization rate of fuel i
μ	gas viscosity
ρ	gas density
ρ'_k	liquid density [$\text{g}\,\text{cm}^{-3}$]
ρ_r	ratio of initial gas density to liquid density
ρ'_c	initial gas density [$\text{g}\,\text{cm}^{-3}$].

Subscripts

1	volatile fuel
2	non-volatile fuel
k	droplet group; one group enters the tube after every predetermined time interval
∞	gas-phase property for the liquid-phase equations.

rization characteristics of the multicomponent fuel sprays are studied. By considering several liquid- and gas-phase models, it is shown that the transient processes of thermal and mass transport in the liquid not only have a strong influence on the droplet behavior but a much stronger influence on the spray behavior. This paper may be considered an extension of an earlier paper [3] where the different models have been examined for the single-component fuel sprays.

The present study is important because none of the works reported so far have considered the multicomponent nature of the fuel in the spray modeling, though the isolated droplet containing a multicomponent fuel has been investigated [4–12]. This study is different from these investigations in that we are considering a spray situation here whereas the referred works considered an isolated droplet. The results, presented later, indicate that the spray characteristics are much more sensitive to the various liquid- and gas-phase models than a single droplet study would indicate.

The physical situation considered, the equations governing the variation of gas- and liquid-phase properties, and the various models are described in the next section. Then, the results are discussed and, finally, the conclusions are presented.

2. THE PHYSICAL MODEL

The physical situation considered is that of a bicomponent fuel spray flowing in a one-dimensional tube. The spray consists of a continuous laminar flow of hot air and an intermittent injection of droplets. A simplified spray statistics is considered in the sense that a deterministic model is employed, and that a monodisperse spray is assumed. Further, the continuous liquid injection is simulated by an intermittent one where one group of droplets is injected in each time interval. The effect of relaxing these assumptions will be examined in a subsequent study. The injection time interval or the frequency depends upon the overall fuel–air ratio, the mass flow rate of air, the droplet spacing, the droplet velocity at the injection point, and the droplet size. The droplet size and the slip velocity are adjusted to provide a Reynolds number, based on these parameters, of about 100 initially. After injection, as a droplet group moves in the hot gas stream, it accelerates. At the same time, the droplets in this group are heated and the vaporization is initiated. These processes influence the state of the gas, i.e. the gas stream is retarded, cooled and enriched with vapors of component fuels. The changes in the gas-phase properties in turn influence the dynamics and vaporization of droplets which are subsequently injected. All these gas-phase and liquid-phase processes are modeled by a system of unsteady, one-dimensional equations. The subsystem of the gas-phase equation is written in Eulerian coordinates whereas the liquid phase is represented in Lagrangian coordinates. The two subsystems are coupled through the exchange rate terms which represent the rates of mass, momentum and energy transfer between the phases. The two subsystems of equations are given below.

2.1. *Gas phase equations*

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(\rho V)=S_\rho \tag{1}$$

$$\frac{\partial Y_i}{\partial t}+V\frac{\partial Y_i}{\partial x}-Dt_r\frac{\partial^2 Y_i}{\partial x^2}=S_i. \tag{2}$$

The equations are in non-dimensional form. The terms on the right-hand side are the source/sink terms and provide the coupling between the gas and liquid phases. These are given in the Appendix. Equation (1) is the standard continuity equation in one-dimensional unsteady form with the source term representing the rate of production of fuel vapors. Equation (2) governs the variations of species concentrations and temperature in the gas phase. Thus Y_i can be represented by a row matrix given by

$$Y=Y_{f1},Y_{f2},Y_O,T. \tag{3}$$

The equation for the oxygen mass fraction (Y_O) is not required for the present case but will be relevant when spray combustion is considered. The values at the tube entrance are used for non-dimensionalizing the respective variables. In addition, the tube length and gas velocity at the entrance are used as the length and velocity scales, respectively. The assumptions used in writing these equations are quite standard and are discussed in an earlier work [3]. The set of equations for the gas phase is completed by the equation of state and the relation for the dependence of gas diffusivity on temperature. These relations in non-dimensional form are

$$\rho=1/T \tag{4}$$

$$D=T. \tag{5}$$

Equation (4) is based on the constant pressure assumption and equation (5) assumes that the product ρD is constant. It is noteworthy, however, that ρD is considered to be temperature dependent in the gas film surrounding individual droplets and is evaluated by using the one-third rule [13].

2.2. *Liquid-phase equations*

$$\frac{\mathrm{d}X_k}{\mathrm{d}t}=V_k \tag{6}$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}t}=\rho_r L_r^2 t_r\left\{\frac{3}{16}\frac{C_D\mu Re_k(V-V_k)}{r_k^2}\right\} \tag{7}$$

$$\frac{\mathrm{d}r_k^2}{\mathrm{d}t}=-2\rho_r L_r^2 t_r M_k \tag{8}$$

where

$$C_D=\frac{24}{Re_k}\left(1+\frac{Re_k^{2/3}}{6}\right) \tag{9}$$

$$Re_k=\frac{2}{t_r L_r}\frac{r_k\rho}{\mu}|V-V_k|. \tag{10}$$

Equations (6)–(8) govern the variation of position, velocity, and size, respectively, for the droplet group represented by subscript k. M_k represents the non-dimensional vaporization rate and is described in the next subsection. Note that the non-dimensionalization gives rise to three dimensionless groups t_r, L_r and ρ_r.

The basic premise of this paper is the following. The accurate prediction of the spray vaporization as well as combustion behavior may critically depend on the realistic representation of the coupling terms between the phases. These terms would depend on:

(a) how accurately the transient processes in the droplet are represented;

(b) how accurately the phenomena in the gas-film surrounding a droplet or a group of droplets are accounted for;

(c) and how accurately the spray statistics is modeled.

The present study focuses on the first two aspects in the sense that various liquid- and gas-phase models for the processes inside and outside the droplets are examined for the multicomponent-fuel sprays. A dilute spray is considered. Thus, there is no direct effect of the droplet interaction on the spray calculations. The effect of non-diluteness will be considered in a subsequent study. Of course, there is still indirect droplet interaction since the droplets influence the gas phase which in turn effects the droplets.

The coupling terms, as given in the Appendix, contain basically three unknowns, namely the fractional vaporization of each component fuel (ε_i), the vapor mass fraction of each fuel species at the surface, and the droplet surface temperature. A relationship between the last two is obtained by using the assumptions of ideal liquid mixture and phase equilibrium. In addition, the gas-phase process in the film surrounding the droplets is considered quasi-steady, which is valid for ρ_r much smaller than unity and the pressures much lower than the critical values. Raoult's law for ideal mixtures and the Clasius–Clapeyron relation for phase equilibrium [5] are then used. This leaves ε_i and T_k as the two unknowns. The various models, which differ in the determination of these two, are discussed next.

2.3. *The description of the liquid- and gas-phase models*

The liquid-phase models are the diffusion-limit, the infinite-diffusion, and the vortex models. To account for the convective motion between droplet and gas, the Ranz–Marshall correlation and an axisymmetric model, based on the simplified analysis of gas flow over a droplet are considered. The details of these models can be found in refs. [4–8, 10, 11]. Only the essential features are given here.

2.3.1. *The diffusion-limit model.* This model is most relevant when the Reynolds number (*Re*) is relatively small, say, of the order of unity. The transient heat and mass transport in the liquid are assumed to be governed by the unsteady heat and mass diffusion equations. A transformation is used to cast the moving boundary problem into a fixed one. The final form of the equations to be solved are:

$$\frac{\partial T_1}{\partial t_b} = \frac{\partial^2 T_1}{\partial \bar{r}^2} + \frac{\partial T_1}{\partial \bar{r}}\left(\frac{2}{\bar{r}} - \bar{r}MK\right) \tag{11}$$

$$\frac{\partial Y_{1i}}{\partial t_b} = \frac{1}{Le}\frac{\partial^2 Y_{1i}}{\partial \bar{r}^2} + \frac{\partial Y_1}{\partial \bar{r}}\left(\frac{1}{Le}\frac{2}{\bar{r}} - \bar{r}MK\right) \tag{12}$$

with the initial and boundary conditions as

$$T_1(\bar{r}, 0) = 0 \tag{13}$$

$$\begin{aligned} \frac{\partial T_1}{\partial \bar{r}} &= \frac{C_k M(H-L)}{T_B - T_0} \\ \frac{\partial Y_{1i}}{\partial \bar{r}} &= Le\, MK(Y_{1is} - \varepsilon_i). \end{aligned} \tag{14}$$

The non-dimensional radial distance, time, and liquid temperature are defined, respectively, as

$$\bar{r} = r'/r'_k$$

$$t_b = \alpha'_1 \int_0^{t'} \frac{dt'}{r'^2_k} \tag{15}$$

$$T_1 = \frac{T'_1 - T'_0}{T'_{bn} - T'_0}.$$

The governing equations are stiff due to the large Lewis number. A Crank–Nicolson implicit scheme [14] with a variable size grid is employed to solve them.

2.3.2. *The infinite-diffusion model.* This model, which has also been referred to as the batch-distillation or the complete-mixing model [6, 8], assumes that the liquid temperature and composition remain uniform as the droplet vaporizes. The model may be relevant when the droplet lifetime is small as compared to the liquid-mass-diffusion time. The temporal variations of droplet composition and temperature are determined from the overall mass and energy conservation

$$\frac{dm_i}{dt_b} = 3\varepsilon_i MKr_k^3 \tag{16}$$

$$\frac{dT_k}{dt_b} = 3C_k M(H-L). \tag{17}$$

The equations are similar to the other liquid-phase equations and are solved by a second-order Runge–Kutta procedure.

2.3.3. *The vortex model.* The conditions of complete mixing, as assumed in the infinite-diffusion model, is never realized in most combustor situations [8]. As discussed by Sirignano [8, 9], even with large internal circulation, the liquid temperature and composition become uniform along the liquid streamlines, but not across them. Sirignano and co-workers [8, 9, 15, 16] have conducted a detailed study of a multicomponent vaporizing droplet in a highly convective environment. Their model, referred to as the vortex model, considers a steady-state gas-phase consisting of inviscid and boundary-layer regions. Inside the droplet, a liquid-phase boundary layer surrounding an inviscid liquid-flow region is considered. The inviscid liquid motion is assumed to be given by Hill's vortex. It is further agreed that the liquid motion may be assumed quasi-steady although heat and mass transport are unsteady. This model, still too complicated for a comprehensive spray analysis, has been further simplified by neglecting the liquid-phase boundary layer [10, 11]. Then the equations are

$$\frac{1}{b_1}\frac{\partial T_1}{\partial \bar{t}} = \phi\frac{\partial^2 T_1}{\partial \phi^2} + [1 + C(\bar{t})\phi]\frac{\partial T_1}{\partial \phi} \tag{18}$$

$$\frac{1}{b_1}\frac{\partial Y_{1i}}{\partial \bar{t}} = \frac{\phi}{Le}\frac{\partial^2 Y_{1i}}{\partial \phi^2} + \left[\frac{1}{Le} + C(\bar{t})\phi\right]\frac{\partial Y_{1i}}{\partial \phi} \tag{19}$$

where

$$d\bar{t} = \frac{b_1}{b_0}\frac{\alpha'_1}{r'^2_k}dt' \tag{20}$$

and

$$C(\bar{t}) = \frac{2}{b_1}\left(\frac{1}{r_k}\right)^{3/2}\frac{d}{d\bar{t}}(r_k^{3/2}) = -A_1 MK \tag{21}$$

and ϕ is the dimensionless stream function [11]. The initial conditions are

$$\begin{aligned} T_1(\phi, 0) &= 0 \\ Y_{1i}(\phi, 0) &= Y_{1i0} \end{aligned} \tag{22}$$

and the boundary conditions are

at $\phi = 0$

$$\frac{\partial T_l}{\partial \phi} = \frac{1}{b_1}\frac{\partial T_l}{\partial \bar{t}}$$

and (23)

$$\frac{\partial Y_{li}}{\partial \phi} = \frac{Le}{b_1}\frac{\partial Y_{li}}{\partial \bar{t}}$$

at $\phi = 1$

$$\frac{\partial T_l}{\partial \phi} = \frac{A_2 C_k M(H-L)}{T_B - T_0}$$

$$\frac{\partial Y_{li}}{\partial \phi} = Le\, A_2 C_k M(Y_{lis} - \varepsilon_i). \tag{24}$$

Here, A_1, A_2 are constants with their values being 3/17 and 3/16, respectively [11]. The value of b_1 is 17.

2.3.4. *Gas-phase models.* To account for the gas-phase convection, the traditional approach has been to modify the spherically-symmetric results by an empirical correction

$$M_k = (1+0.3Re_k^{1/2})\ln(1+B_k) \tag{25}$$

where the term multiplying the logarithmic term represents the correction. Sirignano [8] has analyzed the quasi-steady axisymmetric gas-phase boundary layer outside the droplet. By assuming further that the solution can be represented by a weighted average of the stagnation point region and the shoulder (flat plate) region [11], the following expression has been obtained:

$$M_k = A_1\, Re_k^{1/2} f(B_k) \tag{26}$$

where the constant A_1 is evaluated by comparison with the more exact analyses. The constant was found to be $4/\sqrt{\pi}$. f is the Blassius function [8].

2.4. *The numerical procedure*

There are three subsets of equations to be solved, namely, the gas-phase equations (1)–(5), the liquid-phase equations (6)–(8), and the droplet equations (11)–(26). A hybrid numerical scheme is employed to solve them. The gas-phase equations are solved by an explicit finite-difference scheme. The liquid-phase equations for the position, velocity, and size of each droplet group are integrated by a second-order Runge–Kutta procedure. The details of the hybrid scheme are discussed in refs. [3, 14, 17]. The droplet equations, which govern the variations of temperature and composition in each droplet or group of droplets, are solved by the Crank–Nicolson scheme for the diffusion-limit and vortex models, and by the Runge–Kutta method for the infinite-diffusion model. The results are presented in the next section.

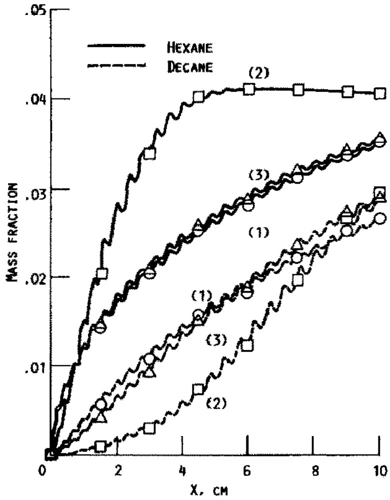


FIG. 1. Profiles of hexane (volatile) and decane (non-volatile) vapor mass fractions in the tube as predicted by the three liquid-phase models: (1) diffusion limit; (2) infinite diffusion; (3) vortex.

3. THE DISCUSSION OF RESULTS

The results are now presented for a spray consisting of hot air and bicomponent fuel droplets flowing in an open tube. The tube length is 10 cm. The fuels are n-hexane and n-decane. Their boiling temperatures differ by about 100 K. The initial air temperature is 1000 K, the velocity is 10 m s^{-1}, and the pressure is 10 atm. The overall fuel–air ratio is stoichiometric. The initial droplet diameter is 100 μm. The initial Reynolds number based on this size and slip velocity is 114. The liquid Lewis number is assumed to be 10. The effects of different liquid- and gas-phase models on the spray vaporization behavior are discussed in the following subsections.

3.1. *The effects of liquid-phase models*

Three liquid-phase models and their influence on the spray behavior are investigated by comparing the gas- and liquid-phase properties as predicted by the models. It is appropriate to present the comparison in terms of the fuel vapor distributions, owing to their high sensitivity to the models. The first set of results is given in Figs. 1–5. Initial liquid mass fractions of hexane and decane are uniform with each equal to 0.5. The injection interval is 0.49 ms, i.e. one group of droplets is injected every 0.49 ms. Each group contains 400 droplets and the initial spacing between two successive groups is 0.5 mm. The effect of varying these parameters is discussed later. The tube length is 10 cm. About 80% of the mass is vaporized by the time the droplets reach the tube exit. Figure 1 gives the distribution of vapor mass fraction of hexane and decane in the tube at t = 15 ms. By this time, the first group of droplets reaches the tube exit. The important observations are given below.

(1) As compared to the diffusion-limit and vortex models, the infinite-diffusion model grossly over-

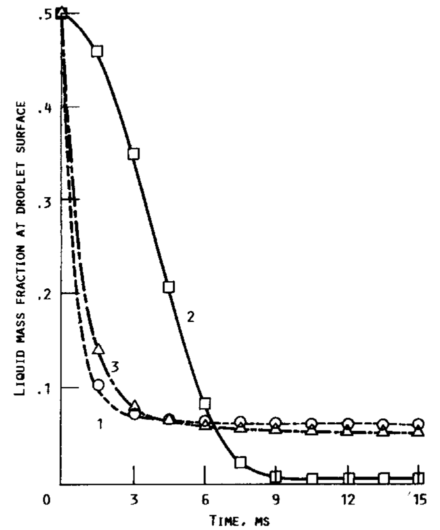


FIG. 2. Liquid mass fraction of hexane at the droplet surface vs time for the first droplet group: (1) diffusion limit; (2) infinite diffusion; (3) vortex.

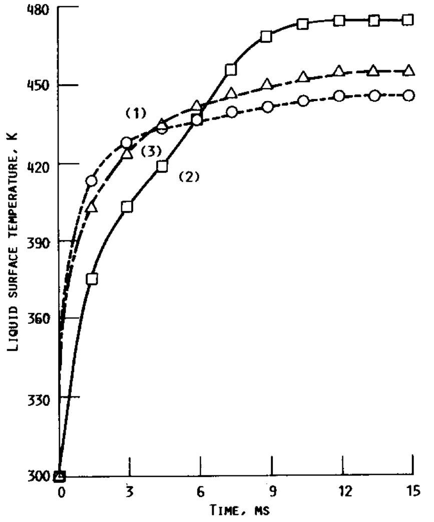
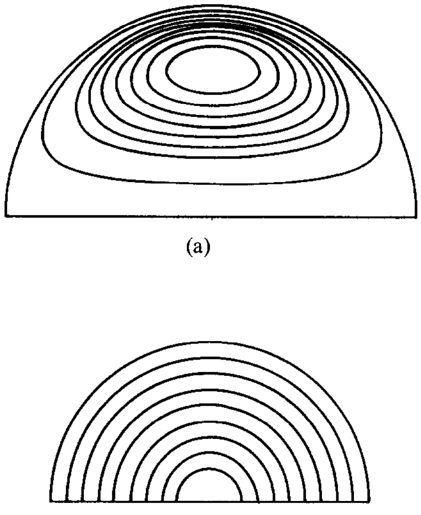


FIG. 3. Droplet surface temperature vs time for the first droplet group: (1) diffusion limit; (2) infinite diffusion; (3) vortex.

predicts and underpredicts the vapor mass fraction of the volatile and non-volatile components, respectively. The differences which are as much as 50% for hexane and 100% for decane, are directly attributable to the interphase processes. As indicated in Fig. 2, the infinite-diffusion model overpredicts the liquid mass fraction of hexane during the first half of droplet lifetime. The liquid hexane which is depleted at the surface due to vaporization is instantaneously replenished because of the infinite-diffusion assumption. For the other two models, the rate of supply of liquid hexane is slow due to the high liquid-phase Lewis number.

(2) The above result is in contrast to that for the single-component fuel spray [3]. For the latter, the infinite-diffusion model underpredicts the fuel vapor



(a)

(b)

FIG. 4. Lines of constant liquid temperature and of constant hexane mass fraction: (a) vortex model; (b) diffusion-limit model.

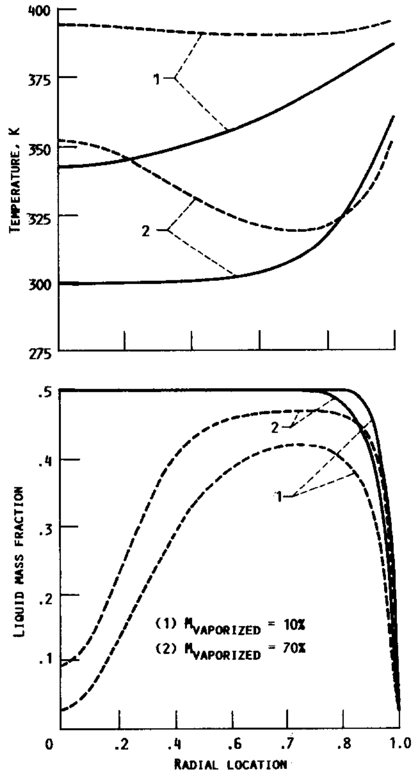


FIG. 5. Comparison of internal liquid-temperature and hexane-mass-fraction profiles at two different times for the two models: ———, diffusion-limit model; – – – –, vortex model.

distribution (in the first half of the tube) as compared to the other two models. This is due to the fact that the infinite-diffusion model predicts a lower surface temperature which amounts to a lower vapor mass fraction at the droplet surface and thus lower vaporization rate. The surface temperature effect is also present in the multicomponent case, as seen in Fig. 3 and also in Fig. 1 near the tube entrance, but is overshadowed by the large liquid-hexane concentration at the droplet surface, as seen in Fig. 2.

(3) The predictions of diffusion-limit and vortex models are remarkably similar, both in terms of the gas-phase and the liquid-phase properties. The result is not all that surprising. What it means is that the internal circulation, which is accounted for in the vortex model, does not effect the transport rates inside the droplet in any significant way. The presence of internal circulation causes uniformity of temperature and composition only along the streamlines. Across the streamlines, which are indicated in Fig. 4 (the lines of constant liquid temperature and composition for the diffusion-limit case are also shown), the mass diffusion process is still slow and rate limiting. Another evidence of the similarity between these to models is provided in Fig. 5. The distribution of liquid temperature and hexane mass fraction inside a droplet are shown in the early and later part of its lifetime. Note that, for comparison purposes, the two-dimensional axisymmetric distribution (being a function of radius and azimuthal angle) of the vortex model has been transformed into the one-dimensional distribution by averaging over spherical surfaces. The internal circulation is quite efficient for making the liquid temperature uniform but not the composition, owing to the large Lewis number. That explains why the predictions of the vortex and diffusion-limit models are so similar for the multicomponent case. Another interesting consequence of the above result is that the internal circulation is less effective for the multicomponent case as compared to the single-component case. This is further illustrated in later results. The remarkable similarity also gives credence to the concept that the effect of liquid motion can be incorporated in the diffusion-limit model by using an effective diffusivity, which may be a function of the Reynolds number and the initial composition.

(4) Undulations in the gas-phase properties (Fig. 1) are due to the well-defined period of injection for the droplets. For example, the peaks in the mass fraction profiles represent the instantaneous locations of droplet groups, and the distance between successive peaks corresponds to the droplet spacing. These undulations are expected to be present even when the injection is more random; only that they will not be so well defined. It is further noteworthy that the undulations are also related to the fact that a hybrid Eulerian–Lagrangian approach has been used and that the gas-phase properties have been resolved over a scale of droplet spacing. The Eulerian–Eulerian approach will effectively average the liquid-phase effects and thus not reveal the undulations. The effect is further examined by changing the droplet spacing at the same overall equivalence ratio and droplet size. The results are shown in Fig. 6, where the droplet spacing is one-half of that in Fig. 1. The magnitude of undulations is smaller because the number of droplets with each droplet group is now reduced by a factor of two.

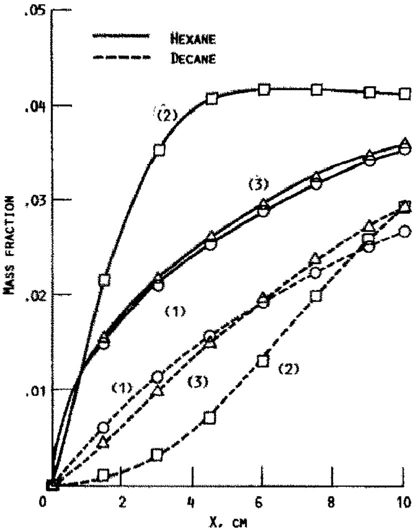


FIG. 6. Profiles of hexane- and decane-vapor mass fractions in the tube as predicted by the three liquid-phase models: (1) diffusion limit; (2) infinite diffusion; (3) vortex.

(5) It is also relevant to examine the effect of spray statistics on the spray vaporization behavior. The comparison of Figs. 1 and 6 indicates that the effect is insignificant, except for the undulations as discussed above.

The major observation so far is that the liquid-phase models strongly influence the vaporization behavior of multicomponent fuel sprays, especially the local values of the fuel vapor concentrations. This is a significant result since such large differences in the fuel vapor distribution would have a strong effect on the subsequent spray combustion behavior. Let us also examine the effects of liquid-phase models on a more global basis. For this purpose, we compare the total vapor mass in the tube for the different models. Figure 7 gives the total mass of hexane vapor as a function of time for the multicomponent as well as the single-component fuel sprays. The vapor mass increases with time as more droplet groups enter the tube and vaporize. A steady state is eventually reached (at about 13 ms), where the rate of fuel vapor produced equals the rate of fuel vapor leaving the tube. The most important observation here is that the global vaporization characteristics are also quite sensitive to the liquid-phase models for the multicomponent case. For the single-component case, however, the liquid models do not have much effect on the total fuel vapor mass. This is another indication of the fact that the isolated droplet behavior is not very sensitive to the liquid models for the single-component case, but is quite sensitive for the multicomponent case.

3.2. *Effect of initial liquid composition on spray vaporization*

Results are now presented to examine the influence of initial liquid composition on the local as well as

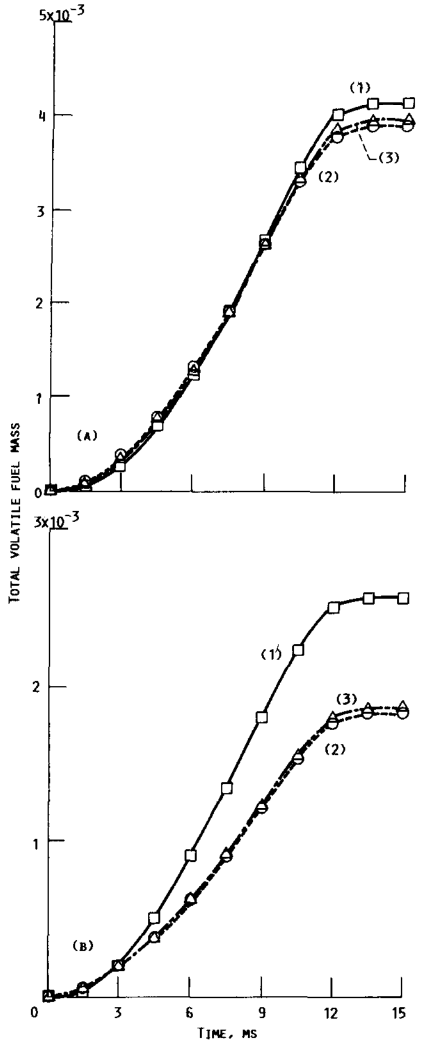


FIG. 7. Variation of total hexane vapor mass in the tube with time for (1) diffusion-limit, (2) infinite-diffusion and (3) vortex models: (a) single-component case; (b) multi-component case.

global spray characteristics. This study is important for two reasons. One is that we want to assess the sensitivity of the spray vaporization process to the liquid-phase models for different initial compositions in the droplet. Secondly, it is relevant to examine the effect of fuel impurities on the spray vaporization behavior. Results are shown in Figs. 8–10. The major observations are given below.

(1) Fuel vapor mass fractions are quite sensitive to the liquid-phase models (see Fig. 8). The sensitivity is specially strong when the initial liquid mass fraction of either fuel constituent is more than 0.1. When this mass fraction is less than 0.1, the multicomponent spray behaves more like a single-component spray.

(2) The differences between the diffusion-limit model and the vortex model are much smaller than those between the infinite-diffusion model and these two. As a matter of fact, the differences between these

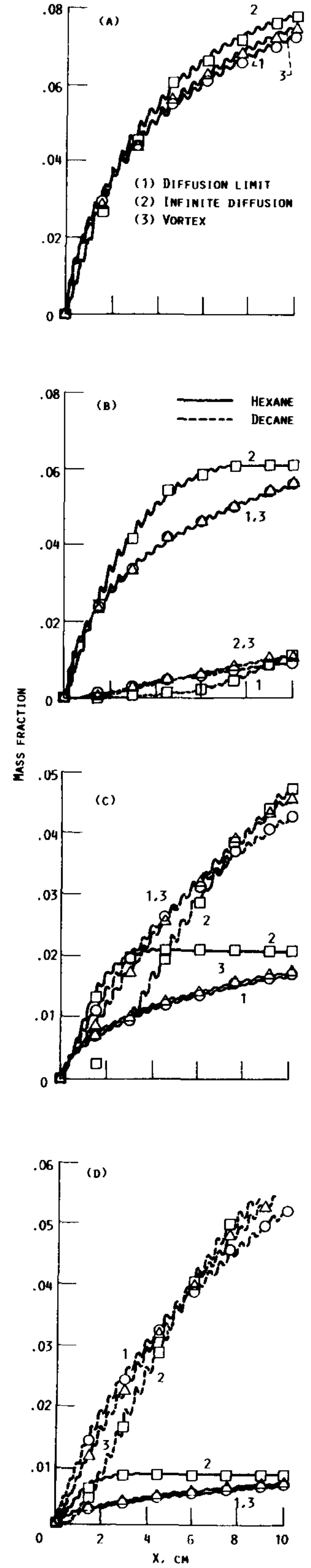


FIG. 8. Comparison of the hexane- and decane-vapor mass fractions in the tube for the three liquid-phase models: (a) initial mass fraction of liquid hexane, $Y_L = 1.0$; (b) $Y_L = 0.75$; (c) $Y_L = 0.25$; (d) $Y_L = 0.1$.

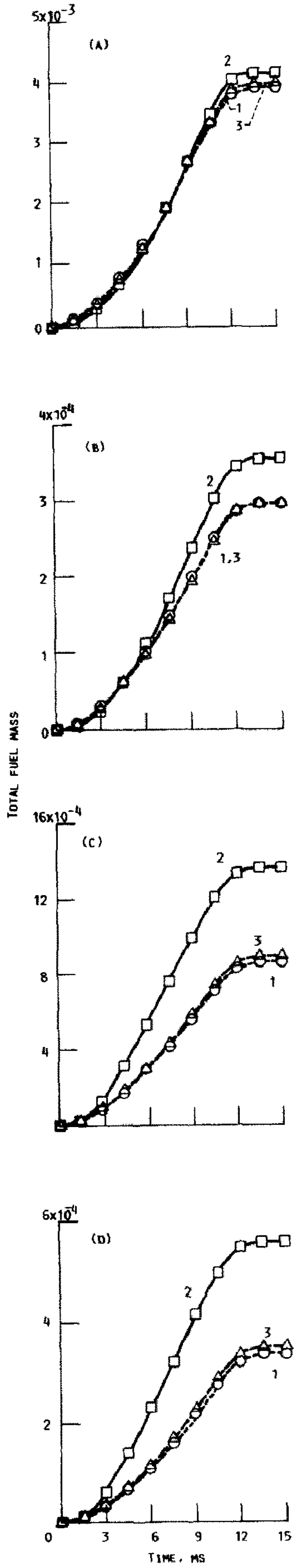


FIG. 9. Comparison of the total hexane-vapor mass vs time for the three liquid-phase models. Four different cases as indicated in Fig. 8.

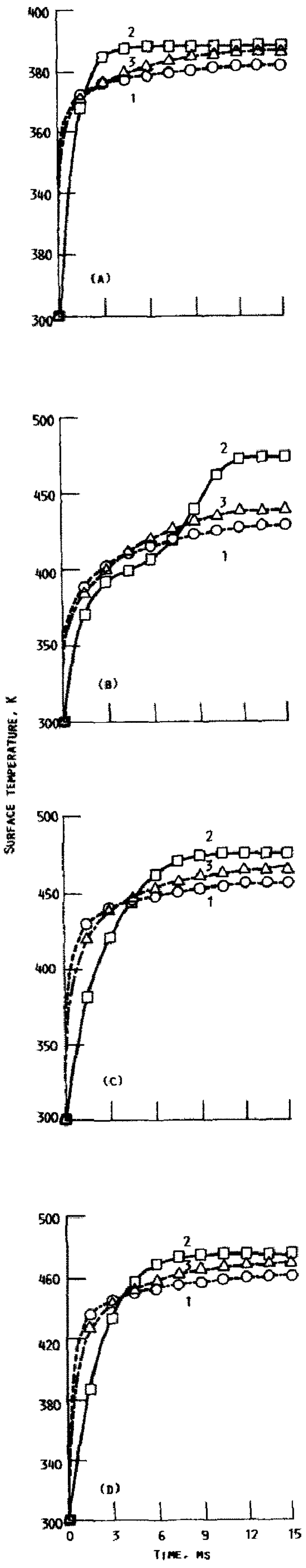


FIG. 10. Comparison of the droplet surface temperature for the first droplet group vs time for the three liquid-phase models. Four different cases as indicated in Fig. 8.

two models are relatively large for the single-component case as compared to the multicomponent case. This again confirms the earlier observation that the internal circulation has a relatively weak effect, owing to the large Lewis number, for the multicomponent case.

(3) The total fuel–vapor mass of volatile component, given in Fig. 9, indicates that the effect of liquid-phase models is more significant when the initial liquid mass fraction of either fuel constituent is 0.1 or greater. The plots for the non-volatile component (not shown) indicate a similar behavior.

(4) The surface temperature vs time plots for the first group of droplets are shown in Fig. 10. The first and last graphs represent the typical single-component behavior (see ref. [3]). An interesting result is seen in Figs. 10(b) and 3. The droplet vaporization process as predicted by the infinite-diffusion model is more like batch distillation when the initial concentrations of the volatile components are relatively large. This result is not significant, however, for the spray vaporization behavior.

The major conclusion from Figs. 8–10 is that the multicomponent nature of fuel spray is significant when the initial liquid concentration of either constituent fuel is more than 10%. Then an accurate representation of the heat and mass transport inside the droplet is extremely important.

3.3. *Comparison of gas-phase models*

The comparison of two gas-phase models, which account for the effect of slip on the interphase heat and mass transfer, is illustrated in Fig. 11. The vortex model is used for the liquid phase in both the cases. Thus, the differences are entirely due to the gas-phase models. It is seen that the Ranz–Marshall correlation overpredicts the vapor mass fractions of both hexane and decane. That means the correlation predicts a relatively larger influence of gas-phase convection. This is also manifested in a larger value of the droplet surface temperature due to a higher rate of heat transfer for the Ranz–Marshall correlation. As a consequence, the mass fraction of liquid hexane at the surface is lower for this model, as illustrated in Fig. 12. The results, shown in Fig. 11, are consistent with those for an isolated droplet as well as for single-component spray as discussed in ref. [3]. Since the axisymmetric model is valid only when the Reynolds number (*Re*) is significant (see equation (9)), it has been suggested that we should switch from this model to the Ranz–Marshall correlation when *Re* drops below a certain value. This is investigated by using the axisymmetric model for *Re* greater than 10 and the Ranz–Marshall model for smaller *Re*. The results are almost the same as those for the axisymmetric model, given in Figs. 11 and 12. This suggests that the Reynolds number remains significant, at least greater than 10, during most of the droplet lifetime and notable differences exist between the predictions of the two gas-phase models. Obviously, more work is needed, by way of experimental results and more sophisticated models, before drawing any definite conclusions regarding the gas-phase models.

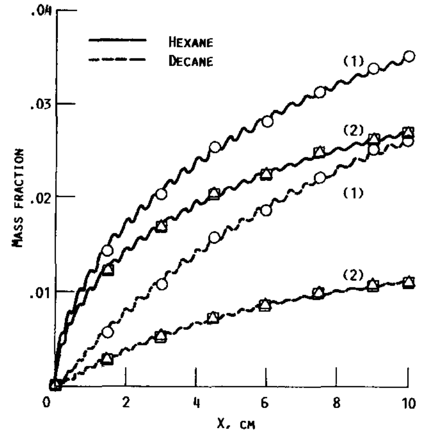


Fig. 11. Profiles of hexane (volatile) and decane (non-volatile) vapor mass fractions in the tube as predicted by the two gas-phase models: (1) Ranz–Marshall correlation; (2) simplified axisymmetric model.

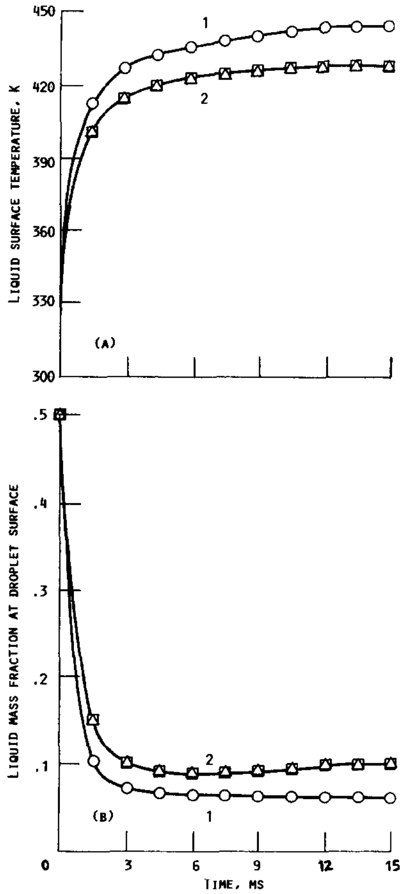


Fig. 12. Comparison of surface temperature and hexane-vapor mass fraction vs time for the two gas-phase models: (1) Ranz–Marshall correlation; (2) simplified axisymmetric model.

4. GENERAL CONCLUSIONS

A simplified spray environment has been used to represent the multicomponent nature of liquid fuels and to examine the sensitivity of their vaporization behavior to the various liquid- and gas-phase models. The liquid-phase models studied are the diffusion limit, the infinite diffusion, and the vortex, with the last two accounting for the effect of internal circulation. The effect of slip between the phases is considered by comparing the Ranz–Marshall correlation and a simplified axisymmetric model. In addition, the effect of initial spray statistics and of initial liquid composition are examined. The conclusions are given below.

(1) The predictions of the infinite-diffusion model, in terms of the fuel vapor distributions, are markedly different from those of the other two models. The vapor mass fractions of the volatile and non-volatile components are grossly overpredicted and underpredicted, respectively, by the infinite-diffusion model. The differences are attributable to the large concentration gradients inside the droplet which are ignored by this model.

(2) The results are in complete contrast to those for the single-component fuel spray. First, the fuel vapor distribution of the volatile component is grossly overpredicted by the infinite-diffusion model for the multicomponent case, whereas it is generally underpredicted for the single-component case. Second, the differences between the infinite-diffusion and the other two models are much more severe for the multicomponent case. The comparison of the models at different initial liquid compositions reveal that the differences are maximum when the constituent fuels are present in equal proportions.

(3) The predictions of the diffusion-limit and vortex models are remarkably similar. In fact, the differences between these models are smaller for the multicomponent case as compared to the single-component case. This behavior can be explained by the temperature and concentration profiles inside the droplet. This also suggests that the internal circulation is less important for the multicomponent case.

(4) The differences between the predictions of the two gas-phase models are quite significant. The Ranz–Marshall correlation overpredicts the fuel vapor mass fractions of both volatile and non-volatile components, as compared to the axisymmetric model. The behavior is similar for the single-component fuel sprays.

(5) The effect of the presence of other fuels on the vaporization behavior of pure fuel sprays is also examined. The results indicate that the effect is important when the initial concentration of the less volatile fuel is more than 10%.

5. CONCLUDING REMARKS

The numerical results for simplified multicomponent fuel sprays clearly demonstrate that the spray vaporization behavior is extremely sensitive to the liquid- and gas-phase models. Since the fuel vapor distributions are remarkably different, the expectation is that the ignition and combustion characteristics of the multicomponent fuel sprays will also be sensitive to the liquid- and gas-phase models. This is presently under investigation.

The physical situation considered here is that of a dilute spray in a convective hot environment, typical of the gas-turbine combustors. For this situation, where the vaporization rate is much faster than the liquid mass diffusion rate, the infinite-diffusion model should be avoided in spray combustion calculations, especially for the multicomponent fuels. The diffusion-limit model is recommended for these calculations because it is easier to use than the vortex model and also because the internal circulation does not seem to have any significant effect for the multicomponent case. It should be added, however, that the infinite-diffusion model cannot be ruled out for other situations, where the vaporization is rate-controlling; for example low temperature environments and dense sprays. Further validation of the gas- and liquid-phase models is, of course, needed. This includes the comparison of the models in more realistic spray situations, for example recirculating flows, as well as the comparison with experimental data. The author is pursuing efforts in these areas. Regarding the comparison with experimental data, it would be most useful to construct a simple experiment which can create the physical situation considered here. Measurements of fuel vapor profiles and of droplet size distributions in a vaporizing spray would then greatly facilitate the suggested comparison.

Acknowledgment—The study was initiated under a Summer Faculty Fellowship from the NASA Lewis Research Center. The diligent typing of this manuscript by Miss Denise Burt is appreciated.

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APPENDIX A

The source/sink terms for the gas-phase equations

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

$$S_{fi} = \frac{S_\rho}{\rho}(\varepsilon_i - Y_{fi}), \quad i = 1, 2 \tag{A2}$$

$$S_0 = -\frac{S_\rho}{\rho} Y_0 \tag{A3}$$

$$S_T = -\frac{S_\rho}{\rho}\{H + T - T_k\} \tag{A4}$$

$$H = H_1 + \Sigma\varepsilon_i L_i = \frac{(1 - Y_{fs})(T_\infty - T_k)}{Y_{fs} - Y_{f\infty}} \tag{A5}$$

$$B_k = \frac{T_\infty - T_k}{H} = \frac{Y_{fs} - Y_{f\infty}}{1 - Y_{fs}} \tag{A6}$$

$$m_k = 4\pi\rho D r_k M_k \tag{A7}$$

$$Y_{fs} = \Sigma Y_{is} \tag{A8}$$

$$Y_{f\infty} = \Sigma Y_{fi} \tag{A9}$$

$$\varepsilon_i = \mathrm{Y}_{is} + (1 - Y_{fs})\frac{Y_{is} - Y_{fi}}{Y_{fs} - Y_{f\infty}} \tag{A10}$$

$$L = \Sigma\varepsilon_i L_i \tag{A11}$$

$$\dot{m}_i = \varepsilon_i \dot{m} \tag{A12}$$

$$X_{lis} = \frac{Y_{lis}/W_i}{\Sigma_j Y_{ljs}/W_j} \tag{A13}$$

$$X_{is} = \frac{1}{p_\infty} X_{lis} p^0_{is} \tag{A14}$$

$$p^0_{is} = \exp\left[\frac{L_i W_i}{R}\left\{\frac{1}{T'_{bn}} - \frac{1}{T'_k}\right\}\right] \tag{A15}$$

$$Y_{is} = \frac{X_{is} W'_i}{W'_a(1 - \Sigma_j X_{js}) + \Sigma_j W_j X_{js}}. \tag{A16}$$

MODELISATION D'UN COMBUSTIBLE DILUE, PULVERISE QUI SE VAPORISE

Résumé—On utilise un environnement simple d'aérosol pour représenter la nature des combustibles multicomposants liquides et pour examiner la sensibilité de la vaporisation à différents modèles de phases liquides et gaz. Les modèles à phase liquide sont la limite de diffusion, la diffusion infinie et le vortex. Les modèles à phase gazeuse sont la formule de Ranz–Marshall et le modèle axisymétrique. Trois sous-systèmes d'équations sont résolus par un schéma explicite–implicite, hybride Eulerien–Lagrangien. Les résultats démontrent que les distributions de combustible vaporisé sont extrêmement sensibles aux modèles considérés, que la circulation interne est moins importante pour le cas multicomposant en comparaison du cas à un seul composant, que les résultats pour multicomposants sont en complète opposition avec ceux relatifs au monocomposant et qu'un modèle acceptable d'aérosol peut considérer les mécanismes diffusifs–convectifs à l'intérieur. et à l'extérieur de la gouttelette. Pour la plupart des situations d'aérosol, on recommande le modèle de limite de diffusion.

MODELLHAFTE BESCHREIBUNG EINER VERDÜNNTEN VERDAMPFENDEN WOLKE AUS ZERSTÄUBTEM VIEL-KOMPONENTEN-BRENNSTOFF

Zusammenfassung—Mit einer vereinfachten Sprühströmung wird die Viel-Komponenten-Natur flüssiger Brennstoffe dargestellt und die Empfindlichkeit ihres Verdampfungsverhaltens im Hinblick auf die verschiedenen Flüssig- und Gasphasen-Modelle untersucht. Als Flüssigphasen-Modelle werden solche mit begrenzter Diffusion, mit unbegrenzter Diffusion und mit Wirbel verwendet. Gas-Phasen-Modelle sind die Ranz–Marshall-Korrelation und das achsensymmetrische Modell. Drei Gleichungsuntersysteme werden mit einer hybriden Euler/Lagrange-Explizit/Implizit-Methode gelöst. Ergebnisse zeigen, daß die Verteilung der Brennstoffdämpfe besonders empfindlich bezüglich der verwendeten Modelle sind, daß die innere Zirkulation für Viel-Komponenten-Systeme weniger bedeutend ist als für Einzelstoffe, daß sich die Ergebnisse für Viel-Komponenten-Systeme vollkommen von denen für Einzelstoffe unterscheiden, und daß ein akzeptables Zerstäubungsmodell die diffusions-konvektionsgesteuerten Vorgänge innerhalb und außerhalb eines Tröpfchens berücksichtigen muß. Für die meisten Zerstäubungsvorgänge wird das Modell mit begrenzter Diffusion empfohlen.

МОДЕЛИРОВАНИЕ ИСПАРЕНИЯ МНОГОКОМПОНЕНТНОГО ЖИДКО-ТОПЛИВНОГО ФАКЕЛА

Аннотация—Упрощенная модель факела использована для иллюстрации многокомпонентной природы жидких топлив и исследования характера их испарения на основании различных жидко-и газофазных моделей. Использовались жидкофазные модели трех типов: контролируемая диффузия, диффузия с бесконечной скоростью и вихревые модели. Для описания газовой фазы использовалась корреляция Рэнца–Маршалла и осесимметричная модель. С помощью гибридной явно-неявной схемы Эйлера–Лагранжа решались три подсистемы уравнений. Результаты исследования показывают, что профили паров топлива чрезвычайно чувствительны к рассматриваемым моделям; внутренняя циркуляция менее важна для случая многокомпонентных жидких топлив, чем для однокомпонентных; и данные, полученные для многокомпонентной системы находятся в полном противоречии с результатами для однокомпонентного случая. Кроме того, показано, что приемлемая модель факела должна учитывать реальные диффузионно–конвективные процессы внутри капли и за ее пределами. Для большинства случаев рекомендуется применять модель контролируемой диффузии.