Dimensional

 $=r*/r_s^*$ 

 $W_{i}$ 

 $=c_{n,\infty}^*\tilde{T}^*/Q^*$ 

 $= W_i^*/W_\infty^*$ 

 $B^*$ 

# **Droplet Ignition with Variable Properties** and Distinct Binary Diffusion Coefficients

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The ignitibility of a fuel droplet in an oxidizing environment has been analyzed by a matched asymptotic analysis of large activation energy. Overall one-step irreversible chemical kinetics with arbitrary fuel and oxidizer reaction orders are considered. The variable thermophysical properties are taken to depend on temperature and composition with distinct binary diffusion coefficients. The analysis shows that the appropriate definition of the mixture Lewis number relevant to the ignition phenomena is  $\Sigma_j Le_{Fj,\infty} X_j,\infty$ , the Lewis number for each binary system weighted by the molar concentration of each species. The major effects of the variable thermophysical properties on ignition are partly through the droplet mass evaporation rate and partly through the thermal driving force  $\beta$ . The former affects the reduced Damköhler number, and an increase in the latter increases the ignition Damköhler number. If proper care is taken of the mixture Lewis number, the frozen evaporation rate of the droplet, and the thermal driving force, the results of previous analyses involving constant properties with equal binary diffusion coefficients can be used.

# Nomenclature

= pre-exponential factor in the Arrhenius law

```
c_p^*
c_{p,\circ}^*
D_{ij}^*
        = specific heat of fuel vapor at constant pressure
        = specific heat of fuel vapor evaluated at T_{\infty}^*
        = mass diffusion coefficient of species pair i and j
E^*
        = activation energy
H^*
        = effective latent heat of evaporation
h*
        = specific enthalpy
        = pressure
        = heat of combustion per unit mass of fuel consumed
        = universal gas constant
        = radial coordinate
        = instantaneous radius of the droplet
        = temperature
T_a^*
V^*
        = activation temperature, E^*/R^{\circ *}
        = diffusion velocity
v*
        = velocity
W^*
        = molecular weight
\bar{W}^*
        = average molecular weight of the mixture
λ*
        = thermal conductivity
        = density
Nondimensional
        =c_p^*/c_{p,\infty}^*
Ď
        = Damköhler number
D_{ij}
        =D_{ij}^*/D_{ij,\infty}^*
H
        =H^*/Q
h
Le_{ij,\infty} = (\lambda_{\infty}^*/c_{p,\infty}^*)/(\rho_{\infty}^*D_{ij,\infty}^*)
        = mass evaporation rate, (\rho^* v^* r^{*2})/(r_s^* \lambda_{\infty}^* / c_{n,\infty}^*)
        = overall reaction order with respect to species i
n
        = \Sigma_i n_i
```

```
X
        = mole fraction
β
        = thermal driving force for droplet evaporation,
          \sum_{i} \gamma_{i,f} h_i(T_{\infty}) - \sum_{i} \gamma_{i,f} h_i(T_s) + H
        = mass flux fraction
_{\Gamma}^{\gamma}
        = perturbation in mass flux fraction
\delta_{ij}
        =\delta_{ij}=1 if i=j; \delta_{ij}=0 if i\neq j
        = reduced Damköhler number
Δ
        = small perturbation parameter, T_{\infty}^2/T_a
\epsilon
        = inner stretching variable
        = perturbation in temperature
        = \lambda^*/\lambda^*_{\alpha}
λ
        = stoichiometric molar coefficient
        = perturbation in molar concentration
χ
Subscripts
\boldsymbol{F}
        = fuel
        = frozen state
        = ignition
        = i = 1 fuel, i = 2 oxidizer, i > 2 inert gases
i
        = oxidizer
0
P
        = products
        = droplet surface
S
        = ambience
```

# Superscript

\* = dimensional quantity

### I. Introduction

It is often assumed in many theoretical analyses of combustion problems that gas-phase mass and heat transport coefficients are constants, and the Lewis number is unity. This invariably results in the Shvab-Zeldovich formulation, which considerably simplifies an otherwise usually formidable mathematical analysis. However, deviation of the Lewis number from unity exists, which is sometimes responsible for new phenomena in combustion, such as the diffusive-thermal instability of premixed flames. For heavy hydrocarbon liquid fuels, heat and mass transport coefficients differ, under normal operating conditions, by a factor of more than two or three. Further, these coefficients are concentration and temperature dependent. Although it is simplifying in mathematical manipulations and elucidating in physical phenomena to suppress such dependence of these coefficients, it is, in reality, inade-

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quate in producing reliable quantitative estimates, especially for situations of practical interest where large variations in temperature and species concentrations occur. Another frequently invoked assumption is the equality of the binary diffusion coefficients for all pairs of species present in the system under study. This assumption is physically unrealistic for a gas mixture comprised of species with widely different molecular structures and weights, as in the case of a hydrocarbon droplet auto-igniting in air.

Because of its relevance to the performance of liquid-fueled combustors, one of the important parameters in the analysis of spray combustion is the ignition of fuel droplets. As compared to the pure vaporization case, the initiation of vigorous chemical reaction results in sharper concentration and temperature variations in the gas phase, with corresponding spatial and temporal variations in the thermophysical properties. Hence, there exists a need to establish an improved ignition criterion that includes the variable property effects.

In most ignition analysis of a fuel droplet, it is usually assumed that the fuel droplet is situated in a hot oxidizing environment of infinite expanse. Heat from the hot ambience is transported radially inward, while the fuel vapor generated at the droplet surface is transported radially outward, without undergoing appreciable chemical reactions, to reach and mix with the hot oxidizer, where the temperature is the highest and the chemical reaction is most likely to occur due to the strong temperature dependence of the Arrhenius reaction rate. The ignition event is significantly affected by concentration and temperature variations, due to their strong influence on the rates at which heat and mass are transported.

Based on a quasisteady theory, Law<sup>2</sup> derived an ignition criterion that is valid for unity reaction orders and unity Lewis numbers for fuel and oxidizer. Later, Law and Chung<sup>3</sup> gave a modified criterion to account for fuel vapor in the ambience, which is typical in a spray environment. However, the assumption of unity reaction order and Lewis number was still retained. Recently, Mawid and Aggarwal4 extended Law's analysis to include the effect of arbitrary reaction orders with respect to the fuel and oxidizer, but the unity Lewis number for both fuel and oxidizer was again employed in their analysis. In summary, the constant thermophysical properties and equal binary diffusion coefficients have been assumed in all of the preceding analyses. Hence, the success of their results, to a certain degree, depends on the judicious selection of the types of species, their relative concentrations, and the reference temperature at which all the assumed constant properties are evaluated.

For droplet combustion, the diffusion flame-sheet model of the constant thermophysical properties due to Godsave<sup>5</sup> has been considerably extended to account for the effects of variable thermophysical properties and general nonunity Lewis numbers.<sup>6-12</sup> A summary with discussion in this aspect has been given by Williams.<sup>1</sup> It is beyond the scope of the present paper to review the theory of droplet combustion. However, the variable transport property formulation of droplet combustion due to Law and Law<sup>10,11</sup> and that of droplet vaporization due to Law<sup>13</sup> will be incorporated into the present analysis of droplet ignition.

In the present paper, the work of Law<sup>2</sup> and Mawid and Aggarwal<sup>4</sup> is extended to include variable thermophysical properties with concentration and temperature dependence, arbitrary Lewis numbers, and arbitrary reaction orders with respect to the fuel and oxidizer. Since the purpose of the present work is to examine the effects of variable thermophysical properties on the ignition criterion, the emphasis will be placed on the derivation of the reduced and ignition (critical) Damköhler numbers.

# II. Formulation

The problem under consideration is the quasisteady, isobaric, and spherically symmetric process of a single component fuel droplet vaporizing in an infinite, quiescent, and hot

environment, which consists of known concentrations of an oxidizer and noncondensable inert gases. Effects due to gravity and thermal radiation are neglected, and the heat of combustion is taken to be constant. Species diffusion arising only from concentration gradients is assumed with negligible thermal diffusion (Soret effect). The thermophysical properties are functions of temperature and species concentrations, and the species binary diffusion coefficients are all distinct. Further assumed is that the overall chemical reaction between the fuel and oxidizer is one step, irreversible, and with arbitrary reaction orders with respect to each of the reactant concentrations. Hence, the reaction can be represented by

$$\nu_F F + \nu_O O + \text{inerts} \xrightarrow{K} \nu_P P + \text{inerts} - \nu_F W_F^* Q^*$$

where the term  $\nu_F W_F^* Q^*$  represents the heat of combustion, and  $\kappa$  is described by the Arrhenius law of reaction rate with constant pre-exponential frequency factor  $B^*$ . The overall reaction orders with respect to the fuel and oxidizer are denoted by  $n_F$  and  $n_o$ , respectively, which are not necessarily the same as the stoichiometric coefficients  $\nu_F$  and  $\nu_o$ .

With the preceding assumptions, it can be shown<sup>1</sup> that gasphase conservation equations for oxidizer O, fuel F, and energy can be expressed as follows:

$$\frac{\dot{m}}{r^2} \frac{\mathrm{d}\gamma_i}{\mathrm{d}r} = -\frac{\nu_i W_i}{\nu_E W_E} \dot{\omega} \tag{1}$$

$$\frac{\dot{m}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} \left( \sum_{i} \gamma_i h_i \right) - \frac{1}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} \left( r^2 \lambda \frac{\mathrm{d}T}{\mathrm{d}r} \right) = \dot{\omega}$$
 (2)

$$\frac{\mathrm{d}X_i}{\mathrm{d}r^*} = \sum_j \frac{X_i X_j}{D_{ii}^{*}} (V_j^* - V_i^*) \qquad (i = 1, 2, \dots, N)$$
 (3)

where  $\gamma_i$  is the mass-flux fraction of chemical species i, and  $\gamma_i$  does not necessarily lie between the values of 0 and 1.<sup>1</sup> However,  $\Sigma_i \gamma_i \equiv 1$  holds. The summation sign is to be performed over all of the species present in the system, unless otherwise stated.

The chemical reaction term  $\dot{\omega}$  is given by

$$\dot{\omega} = \mathfrak{D}\left(\frac{1}{T}\right)^n X_F^{n_F} X_o^{n_O} \exp\left(-\frac{T_a}{T}\right) \tag{4}$$

where

$$\mathfrak{D} = \frac{c_{p,\infty}^*}{\lambda_{\infty}^*} \nu_F W_F^* B^* \left( \frac{p^* c_{p,\infty}^*}{R^{\circ *} O^*} \right)^n r_s^{*2}$$
 (5)

is the system Damköhler number.

The boundary conditions for Eqs. (1-3) are given below: As  $r \to \infty$ :

$$X_i = X_{i,\infty}(1 - \delta_{iF}) \tag{6}$$

$$T = T_{\infty} \tag{7}$$

At r = 1:

$$\gamma_i = \delta_{iF} \tag{8}$$

$$\lambda_s \frac{\mathrm{d}T}{\mathrm{d}r} = mH \tag{9}$$

$$T = T_s = \text{const}$$
 (10)

where  $\delta_{iF} = 0$  for  $i \neq_F$ , and  $\delta_{iF} = 1$  for i = F. Hence, it is understood that  $X_F = 0$  as  $r \to \infty$ .

Note that Eq. (3) is the one-dimensional form of the Stefan-Maxwell equation, hence the diffusion coefficients  $D_{ij}^*$  are the mass diffusivity of the species pair i-j in a binary mixture consisting of only the species i and j. According to the kinetic theory of gases, <sup>14</sup> the  $D_{ij}^*$  are symmetric in i and j and virtually

independent of species mole fractions. But they are inversely proportional to the pressure, and increase with increasing temperature. Therefore, they may be expressed in the following form<sup>11</sup>:

$$D_{ij}^* = \left(\frac{d_{ij}^* T^*}{p^*}\right) f_D^*(T^*) \tag{11}$$

where  $d_{ij}^*$  are constants and  $f_{ij}^*(T^*)$  acknowledges the nonlinear temperature dependence.

From Eq. (11), the definition of mass-flux fraction  $\gamma_i$ , and the relation between mole and mass fraction, Eq. (3) can be expressed as follows<sup>11</sup>:

$$r^{2} \frac{\mathrm{d}X_{i}}{\mathrm{d}r} = \sum_{j} Le_{ij,\infty} \left( \frac{\gamma_{j}}{W_{j}} X_{i} - \frac{\gamma_{i}}{W_{i}} X_{j} \right) \frac{\dot{m}}{f_{D}(T)} \quad (i = 1, 2, \dots, N)$$
(12)

where

$$Le_{ij,\infty} = \lambda_{\infty}^* / (\rho_{\infty}^* c_{p,\infty}^* D_{ij,\infty}^*)$$
 (13)

is the Lewis number, and  $f_D(T) = f_D^*(T^*)/f_D^*(T_\infty^*)$ .

#### III. Frozen Solution

In this regime, all the chemical reactions are frozen due to the large value of the activation energy (that is,  $T_a \rightarrow \infty$ ). Hence, Eq. (1) reduces to

$$\frac{\mathrm{d}\gamma_{i,f}}{\mathrm{d}r} = 0\tag{14}$$

which, together with the boundary condition, Eq. (8), yields

$$\gamma_{i,f} = \delta_{iF} \tag{15}$$

The species concentration, Eq. (12), can be expressed as

$$\frac{\mathrm{d}X_{i,f}}{\mathrm{d}\zeta} = -\sum_{j} Le_{ij,\infty} \left( \frac{\gamma_{j,f}}{W_{j}} X_{i,f} - \frac{\gamma_{i,f}}{W_{i}} X_{j,f} \right)$$

$$(i = 1, 2, \dots, N) \qquad (16)$$

where

$$\zeta = \int_{r}^{\infty} \frac{\dot{m}_f}{r'^2 f_D \{ T_f(r') \}} \, \mathrm{d}r' \tag{17}$$

is a new independent variable. Then the concentration distribution can be obtained<sup>11</sup> as

$$X_{i,f}(\zeta) = \sum_{k} K_{i,k} \exp(\Lambda_k \zeta) \quad (i = 1, 2, \dots, N)$$
 (18)

where  $\Lambda_k$  are the eigenvalues of the coefficient matrix in Eq. (16). Substituting Eq. (18) into the left side of Eq. (16) and evaluating at  $\zeta = 0$   $(r \to \infty)$  with the boundary condition [Eq. (6)] yields

$$\sum_{k} K_{i,k} \Lambda_{k} = -\sum_{j} Le_{ij,\infty} \left( \frac{\gamma_{j,f}}{W_{j}} X_{i,\infty} - \frac{\gamma_{i,f}}{W_{i}} X_{j,\infty} \right)$$

$$(i = 1, 2, \dots, N) \qquad (19)$$

Hence the integration constants  $K_{i,k}$  are determined.

With the boundary conditions in Eqs. (7), (9), and (10), Eq. (2) can be reduced, in terms of  $\zeta$ , as follows

$$\sum_{i} \gamma_{i,f} h_i(T_f) + \frac{\lambda}{f_D(T_f)} \frac{\mathrm{d}T_f}{\mathrm{d}\zeta} = h_\infty - \beta \tag{20}$$

where  $\beta$  is defined as

$$\beta = h_{\infty} - h_s + H \tag{21}$$

with  $h_{\infty} = \sum_i \gamma_{i,f} h_i(T_{\infty})$  and  $h_s = \sum_i \gamma_{i,f} h_i(T_s)$ . For frozen flow, only fuel vapor moves (see Eq. 15); hence,  $\beta$  becomes

$$\beta = H + \int_{T_c}^{T_{\infty}} c_p(T_f) \, \mathrm{d}T_f \tag{22}$$

where H is an effective latent heat of evaporation, which includes the enthalpy of evaporation, and the amount of energy spent on heating the droplet interior per unit mass of fuel evaporated. To evaluate the parameter  $\beta$  and the droplet evaporation rate later on, the parameters H and  $T_s$  need to he known. These can be determined from a droplet heating analysis, as it is done by Law,  $^{2,15}$  Law and Chung,  $^3$  and Mawid and Aggarwal.  $^4$ 

Accurate expressions for mixture thermal conductivity like the Tondon-Saxena formula<sup>16</sup> depend inseparably on the temperature and species concentrations; this renders the analytical solution to Eq. (20) almost impossible, except for a binary system.<sup>13</sup> Following Law and Law<sup>10,11</sup> in droplet combustion, and Law<sup>13</sup> in droplet evaporation, the simple linear molar mixing rule, originally suggested by Kennard,<sup>17</sup> is adopted here. Hence, the mixture thermal conductivity, in dimensionless form, is

$$\lambda = \sum_{i} \alpha_{i} X_{i} f_{\lambda}(T) \tag{23}$$

Substituting Eq. (23) into Eq. (20) and integrating from  $\infty$  leads to

$$\int_{T_{\infty}}^{T_f} \frac{f_{\lambda}(T_f')}{f_D(T_f')} \frac{\mathrm{d}T_f'}{\Sigma_i \gamma_{i,f} h_i(T_f') - h_{\infty} + \beta} = -\int_0^{\zeta} \frac{\mathrm{d}\zeta'}{\Sigma_i \alpha_i X_{i,f}(\zeta')} \tag{24}$$

where  $X_{i,f}(\zeta)$  is given in Eq. (18). The temperature distribution can be obtained from Eq. (24) if the dependence of the specific enthalpy for the pure gas  $h_i$  on the temperature, as well as  $f_{\lambda}(T)$  and  $f_D(T)$ , is specified. However, the nice feature for the present analysis of droplet ignition is that these specific functional forms are not required.

Evaluating at the droplet surface, Eq. (24) becomes

$$\int_{T_s}^{T_{\infty}} \frac{f_{\lambda}(T_f')}{f_D(T_f')} \frac{\mathrm{d}T_f'}{\Sigma_i \gamma_{i,f} h_i(T_f') - h_{\infty} + \beta} = \int_0^{\xi_s} \frac{\mathrm{d}\zeta'}{\Sigma_i \alpha_i X_{i,f}(\zeta')}$$
(25)

which gives the relation  $\zeta_s = \zeta_s (T_s, T_{\infty})$ , whereas  $\zeta_s$  is proportional to the droplet evaporation rate  $m_f$  according to

$$\zeta_s = \int_1^\infty \frac{\dot{m}f}{r'^2 f_D \left[ T_f(r') \right]} \, \mathrm{d}r' \tag{26}$$

Therefore, the droplet evaporation rate can be determined from Eqs. (25) and (26). By comparing with the constant property results of Law,<sup>2</sup> Law and Chung,<sup>3</sup> and Mawid and Aggarwal,<sup>4</sup> it is clear that  $\dot{m}_f$  is affected by the specific dependence of the thermophysical properties on the concentration and temperature distributions.

# IV. Ignition Analysis

For ignition analysis, which follows that of Law,<sup>2</sup> Law and Chung,<sup>3</sup> and Mawid and Aggarwal,<sup>4</sup> the flowfield is divided into two regions: an outer, convective-diffusive region that is free from the chemical reactions, and an inner diffusive-reactive region where all the chemical reactions occurring in the system are concentrated.

In the outer, convective-diffusive region, all the chemical reactions are frozen due to the strong temperature dependence of Arrhenius kinetics, but the mass flux fraction, species concentration, and temperature distributions differ from their

frozen solution by a small amount of order  $\epsilon=T_{\infty}^2/T_a$ . The lengthy presentation of the perturbation terms is avoided here since they are not prerequisite for the following analysis. The detailed process is very similar to those in Refs. 2–4. The mass evaporation rate is also expanded in the powers of  $\epsilon$ 

$$\dot{m} = \dot{m}_f + \epsilon \dot{m}_1 + O(\epsilon^2) \tag{27}$$

where  $\dot{m}_1$  is the first-order perturbation to the droplet vaporization rate.

For the inner, diffusive-reactive region, the species concentrations and temperature are also perturbed from their frozen solutions by a small amount of the order of  $\epsilon$ , such that

$$T_{in} = T_{\infty} + \epsilon \left[ \theta(\eta) - \beta \eta \right] + O(\epsilon^2)$$
 (28)

$$\gamma_{i,in} = \gamma_{i,f} + \Gamma_i(\eta) + O(\epsilon)$$
 (29)

$$X_{i,in} = X_{i,\infty} + \epsilon \left[ \sum_{k} K_{i,k} \Lambda_k \eta + \chi_i(\eta) \right] + O(\epsilon^2)$$
 (30)

where  $\eta$  is the inner stretching variable, defined as

$$\eta = \frac{\dot{m}_f}{r} \frac{1}{\epsilon} \tag{31}$$

Note that although the chemical reactions have small effects on the temperature and concentrations as assumed in Eqs. (28) and (30), they exert significant influences on the mass flux fraction as shown in Eq. (29) and as confirmed later on.

As  $r \to \infty$  ( $\epsilon \to 0$ ), Eq. (17) becomes, to the leading-order term,  $\zeta = \eta \epsilon$ . By the inner expansion given in Eqs. (28) and (30), it can be seen that  $f_D(T) = 1 + O(\epsilon)$ , and Eq. (23) becomes  $\lambda = 1 + O(\epsilon)$ . Therefore, in terms of the inner stretching variable, and with the help of Eq. (19), the energy equation, Eq. (2), becomes, to the leading order term

$$\eta^4 \frac{\mathrm{d}^2 \theta}{\mathrm{d}\eta^2} = -\Delta \left( \eta + \frac{\chi_F}{\Sigma_j Le_{Fj,\infty} X_{j,\infty} / W_F} \right)^{n_F} \exp(\theta - \beta \eta) \qquad (32)$$

where

$$\Delta = \dot{m}_f^2 (\mathfrak{D} \epsilon^{n_F - 3}) \left(\frac{1}{T_{\infty}}\right)^n \left(\frac{1}{W_F}\right)^{n_F} X_{o, \infty}^{n_o}$$

$$\times \exp\left(-\frac{T_a}{T_{\infty}}\right) \left(\sum_{j} L e_{Fj, \infty} X_{j, \infty}\right)^{n_F}$$
(33)

is the reduced Damköhler number, and is regarded as  $\Delta = O(1)$ .

Similarly, Eq. (1) can be shown to take the following form

$$\eta^{4} \frac{\mathrm{d}\Gamma_{i}}{\mathrm{d}\eta} = \frac{\nu_{i}W_{i}}{\nu_{F}W_{F}} \Delta \left( \eta + \frac{\chi_{F}}{\Sigma_{j}Le_{Fj,\infty}/W_{F}} \right)^{n_{F}} \times \exp(\theta - \beta\eta) \qquad (i = 1, 2, \dots, N) \quad (34)$$

which confirms that the inner expansion of the mass flux fraction as assumed in Eq. (29) is correct in order of the magnitude in terms of  $\epsilon$ .

For the species concentrations, the left side of Eq. (12) is expressed in terms of the inner variable  $\eta$ ; then the derivative of the both sides of the equation is taken with respect to  $\eta$ . Taking account of Eq. (34) while keeping in mind that  $\Delta = O(1)$ , the species molar concentrations in the inner region are derived as

$$\eta^{4} \frac{\mathrm{d}^{2}\chi_{i}}{\mathrm{d}\eta^{2}} = -\sum_{j} Le_{ij,\infty}(\nu_{j}X_{i,\infty} - \nu_{i}X_{j,\infty}) \frac{1}{\nu_{F}W_{F}} \Delta$$

$$\times \left(\eta + \frac{\chi_{F}}{\Sigma_{j}Le_{Fj,\infty}X_{j,\infty}/W_{F}}\right)^{n_{F}} \exp(\theta - \beta\eta)$$

$$(i = 1, 2, \dots, N) \qquad (35)$$

Application of the local Shvab-Zeldovich formulation to Eqs. (32) and (35) would result in explicit expressions for the species concentrations. Particularly, for i = F, we have

$$\theta + \frac{\chi_F}{\Sigma_j L e_{Fj,\infty} X_{j,\infty} / W_F} = 0$$
 (36)

when considering the finiteness of  $\theta$  and  $\chi_i$  as  $\eta \to \infty$ , and the boundary conditions at  $\eta = 0$ . Substituting Eq. (36) into Eq. (32) yields

$$\eta^4 \frac{\mathrm{d}^2 \theta}{\mathrm{d}\eta^2} = -\Delta (\eta - \theta)^{n_F} \exp(\theta - \beta \eta) \tag{37}$$

and the appropriate boundary conditions are

$$\theta = 0 \quad \text{at } \eta = 0$$

$$\frac{d\theta}{d\eta} = 0 \quad \text{as } \eta \to \infty$$
(38)

It is clear that Eq. (37) is the only equation that needs to be solved for the present problem. After the temperature is obtained, the species concentrations can be determined from Eq. (36), and the first-order perturbation term to the droplet evaporation rate can be found from  $\dot{m}_1 = \theta(\infty)/\beta$ .

# V. Results and Discussion

By comparing Eq. (37) with the results of Mawid and Aggarwal, it is apparent that whether the thermophysical properties are variable or just constant, the ignition phenomena are governed by the same type of equations. And further, the ignition Damköhler numbers  $\Delta_I$  for these cases are equal provided that the value of  $\beta$  is the same. Also the definition of  $\beta$  as shown in Eq. (22) suggests that the appropriate specific heat  $c_p$  should be that of the fuel vapor rather than that of the inert gases as frequently used.

The previous analyses of Law<sup>2,15</sup> and Mawid and Aggarwal<sup>4</sup> are special cases of the present analysis, and their results can be readily obtained from the present by invoking simplifying assumptions concerning the reaction orders and thermophysical properties. Conversely, their numerical results can be readily used to obtain the ignition Damköhler number for the present case. For example, from the results of Law<sup>15</sup> it can be shown that for  $\beta < 0.35$  and  $n_F = 1$ 

$$\Delta_I(\beta) = 1.05 \exp(6.40\beta) \tag{39}$$

whereas Mawid and Aggarwal's results<sup>4</sup> yield for  $\beta \le 0.3$  and  $n_F = 0.25$ 

$$\Delta_I(\beta) = 1.40 \exp(6.463\beta)$$
 (40)

For large values of  $\beta$ , there is no simple analytical relation between  $\Delta_I$  and  $\beta$ , and a numerical solution is required to generate the value of  $\Delta_I$  for given  $\beta$  and  $n_F$ . However, as shown by Law, <sup>15</sup> the interesting range of  $\beta$  relevant to the ignition phenomena is  $0 < \beta < 1$ . In fact, for many practical combustion systems involving hydrocarbon fuels,  $\beta$  is usually of the order of 0.1 or less.

The analysis indicates that, for the leading order term, the specific dependence of the thermal conductivity and binary diffusion coefficients on temperature and composition does not affect the ignition Damköhler number. However, their effects do show up if the analysis is performed to the next (second) order. Therefore, they only have a minor contribution to  $\Delta_I$ . The main influences of variable thermophysical properties on the ignition phenomena are through the droplet evaporation rate  $m_f$ , which appears in the reduced Damköhler number  $\Delta$  as the square factor. As is obvious from Eqs. (25) and (26), any variations in temperature and concentration fields, on which the thermophysical properties depend, con-

tribute to variations in  $\dot{m}_f$ . In reality, the nature of the variable thermophysical property effects on  $\dot{m}_f$  is very complicated, and Eqs. (25) and (26) have to be solved by numerical methods.

The nonlinear nature of the specific heat of the fuel vapor  $c_p$  on the temperature would exert a significant effect on the ignition Damköhler number, since as Eqs. (39) and (40) indicate, the ignition Damköhler number  $\Delta_I$  is very sensitive to the value of  $\beta$ . It is clear from the definition of  $\beta$  that a stronger temperature dependence of  $h_F$  (or  $c_p$ ) would increase the value of  $\beta$ , which increases the value of  $\Delta_I$  exponentially. This means that an increase in  $\beta$  would be prohibitive to ignition. It can also be seen that for droplets with liquid-phase transient heating and for heavy hydrocarbon fuels, the ignition Damköhler number will be higher, and thus ignition becomes more difficult.

The fuel reaction order  $n_F$  affects both reduced and ignition Damköhler numbers, whereas the oxidizer reaction order  $n_o$  has only weak influence on the ignition Damköhler number. This is expected from the fact that the ignition event occurs in the neighborhood of the oxidizer-rich ambience, where the temperature is the highest. Hence the oxidizer concentration in the inner reaction zone is much in excess of what would be required stoichiometrically by the amount of the fuel consumed there. However, should the concentration of the oxidizer be limited in the inner reaction zone (such that  $X_{o,\infty}$  is of order  $\epsilon$ ), then the ignition Damköhler number  $\Delta_I$  will also depend on  $n_o$ , in addition to  $n_F$  and  $\beta$ .

If the present results are compared with those corresponding to the case of equal binary diffusion coefficients, it is observed that the reduced Damköhler numbers for both cases are identical, provided that

$$Le_{\infty} = \sum_{j} Le_{Fj,\infty} X_{j,\infty}$$
 (41)

This relation indicates that the frequently invoked assumption of the equal binary diffusion coefficients is acceptable provided that the Lewis number is evaluated according to Eq. (41).

As for the nonunity Lewis number effect, the factor  $\Sigma_i$  $Le_{F_{i,\infty}}X_{i,\infty}$  in  $\Delta$  indicates that any individual  $Le_{F_{i,\infty}}$  change has to be felt in the value of the sum to make any contribution to the ignition phenomenon. An increase in the value of this sum will increase the Damköhler number  $\Delta$ , which is beneficial to the occurrence of an ignition. This would be expected since a larger value in the sum implies that overall, heat transport is faster than the mass transport and that heat transport is the controlling factor whereas mass diffusion is self-adjusting. However, change in Lewis numbers  $Le_{Fj,\infty}$  usually accompanies changes in the other thermophysical properties. Therefore, the overall effects on  $\Delta$  have to be determined for specific cases. It should also be mentioned that if the droplet surface temperature is not a constant but has a perturbation in the amount of, say,  $\epsilon T_{s1}$ , then it can be shown that the results of the present ignition analysis are unaffected, but the value of  $\theta(\infty)$  is now increased by a constant amount proportional to  $T_{s1}$ .

### VI. Conclusions

The effects of variable thermophysical properties on the ignitibility of a single component fuel droplet in a hot oxidizing environment have been analyzed by means of large activation energy asymptotics. The system and reduced Damköhler numbers and their corresponding ignition counterparts have been derived. A comparison with the results of the case of constant or variable thermophysical properties but with equal binary diffusion coefficients reveals that the

specific heat should be that of the fuel rather than that of the inert gases, and the mixture Lewis number should be defined as  $\Sigma_j Le_{F_{i,\infty}} X_{j,\infty}$ .

The effects of the variable thermophysical properties on ignition are partly through the mass evaporation rate  $m_f$  and partly through  $\beta$ , which directly influences the ignition Damköhler number. The ignition Damköhler number increases both with increasing  $\beta$  and decreasing fuel reaction order  $n_F$  and is weakly dependent on the oxidizer reaction order  $n_o$ , unless the oxidizer concentration at the ambience is limited. Since  $n_F$  also appears in the reduced Damköhler number, the overall effects of  $n_F$  on ignition have to be judged for specific cases.

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