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Radiation, thermal diffusion and kinetic effects in evaporation and combustion of large and moderate size fuel droplets

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Abstract—This paper analyzes quasi-steady combustion and evaporation of large and moderate size single fuel droplets in a quiescent atmosphere taking into account the kinetic effects, variable thermo-physical properties, thermal diffusion and radiation. An analytical solution is obtained for the heat and mass fluxes in the neighbourhood of the large burning droplets in the case of high reaction rates. The analytical formulae are derived for temperature and concentration distributions and heat and mass fluxes in the vicinity of the burning or evaporating droplet. The contribution of the various effects to the heat and mass fluxes is analyzed. It is shown that the effect of thermal diffusion is essential in the case of evaporation or combustion of fuel droplets with internal heat sources (i.e. when temperature at the surface of fuel droplet is higher than an ambient temperature) in a binary gas mixture with significant differences in molecular weights or diameters. Also it is shown that the effect of radiation is significant in case of evaporation and combustion of large droplets. The theoretical results are compared with the available experimental data.

1. INTRODUCTION

The theory of evaporation and combustion of fuel droplets has been developed intensively during the past few decades. Detailed discussion of this subject may be found in reviews by Law [1] and Sirignano [2]. The classical droplet vaporization and combustion model is described in many textbooks on combustion (see e.g. Lefebvre [3] and Williams [4]). However, this model employs many oversimplified assumptions:

(1) average values of the thermophysical properties;

(2) Lewis number in the gas phase in the neighbourhood of the droplet is equal to 1;

(3) the effect of Stefan's flow on heat and mass transfer in the neighbourhood of the droplet is neglected;

(4) the vaporization rate of the droplet in stagnant environment is multiplied by an empirical factor $0.5Nu_0$, where Nu_0 is the Nusselt number for a solid sphere;

(5) the droplet surface is assumed to be at the normal boiling temperature;

(6) fuel leaves the surface of the droplet by diffusion only (in this case relative concentration in the neighbourhood of the droplet $C_1 \ll 1$).

In case of combustion of fuel droplets, high temperature differences occur in the neighbourhood of burning droplets and using the mean coefficients of heat and mass transfer causes significant errors.

In reality, the Lewis number varies in the range from 1 to 4 during the vaporization period [5]. Many factors, e.g. the variable thermophysical properties, Knudsen layer, evaporation, radiation, affect the value of the Nusselt number [6, 7]. However in spite of the fact that the assumptions of the classical model are violated in many cases, it is widely used in the most advanced computations of evaporation and combustion of sprays [8, 9]. Many of the latter approaches are based on the assumption that the spray evaporation rate is the same as that for an isolated drop in a stagnant ambient fuel vapor atmosphere.

In case when vapor leaves the surface by diffusion only, Saiton and Nagano [10] analyzed large droplet evaporation in a hot stagnant gaseous atmosphere taking into account variable thermophysical properties. Significant discrepancies between constant and variable thermophysical properties solutions were obtained.

In the case of combustion of fuels with high flame front temperature (i.e. T_f is in range 1800–2500 K), the fuel leaves the surface of the droplet mostly by convection. In this case the assumption that fuel leaves the surface by diffusion only (i.e. $C_1 \ll 1$), adopted in the previous studies, is not valid.

In numerical investigations of vaporization and combustion of fuel droplets and their applications to the modeling of spray-fueled combustors, droplet evaporation rate calculations are based on the d^2 law:

$$\frac{\mathrm{d}(d^2)}{\mathrm{d}t} = K = \text{const.} \tag{1}$$

In the case of evaporation or combustion of moderate size droplets, $0.01 \leqslant Kn \leqslant 0.3$ (Kn is a Knudsen

NOMENCLATURE

A	molecules of gas components
C_v	$= n/\Sigma_i n_i$ dimensionless concentration
d	droplet diameter
$D_{j,N}$	binary diffusion coefficient
$\mathbf{j}$	flux density
j	flux density in radial direction
h	specific enthalpy
k	coefficient of thermal conductivity
$K_T^{(T)}, K_n^{(n)}$	temperature and concentration jumps
$K_T^{(n)}, K_n^{(T)}$	cross coefficients
K_T	thermodiffusion ratio
L	latent heat of evaporation
m	mass of a molecule
$\dot{m}$	evaporation rate
n	concentration
q	heat of combustion
Q_T	heat flux
Q_1, Q_2	mass flux
r	radial coordinate
R	radius of droplet
R^*	universal gas constant
T	temperature
t	time
$\mathbf{v}$	mass velocity of the gas
x_f	distance between droplet surface and flame front.

Greek symbols

ν, ε	stoichiometric coefficients
ρ	gas density
τ_s	$= T^{(s)}/T_f$
τ_f	$= T_f/T_\infty$.

Subscripts

e	external value
f	value at the flame front
i, j	species i or j
$1, 2, \ldots, N$	number of species
s	value at the droplet surface
∞	value at infinity.

Superscripts

(1), (2)	number of zone
(s)	value at the droplet surface.

number), the d^2 law is not valid since K in expression (1) is not constant because it includes kinetic corrections depending upon the Knudsen number [11].

In order to abandon some approximations of the classical droplet evaporation and combustion model, it is necessary to undertake thorough investigation of droplet evaporation kinetics.

The present investigation attempts to develop the gaseous phase quasi-steady model of evaporation and combustion of large size and moderate size fuel droplets in a more general case, when relative differences of concentration in the neighborhood of a droplet are small, i.e.

$$\frac{|C_1 - C_{1\infty}|}{C_{2\infty}} \ll 1 \tag{2}$$

taking into account the influence of variable thermophysical properties and internal heat sources and thermal diffusion. The developed model does not employ the assumption about small temperature differences in the neighborhood of the burning droplet.

In the next section the important evaporation characteristics of fuel droplets with internal heat sources are discussed. The quasi-steady model of combustion in the case when fuel leaves the surface by diffusion and relative differences of concentration in the neighborhood of a droplet are small is presented in the second section.

2. VAPORIZATION OF LARGE SIZE AND MODERATE SIZE FUEL DROPLETS IN A STAGNANT AMBIENT ATMOSPHERE

Consider a spherical droplet of pure fuel immersed into a stagnant binary gas mixture at high temperature T_∞, with the concentration of volatile species $C_{1\infty}$. It is assumed also that the internal sources within the droplet heat the droplet's surface uniformly. The influence of gravitational convection on the process of evaporation is neglected. Since the characteristic times of heat and diffusive relaxation are small we can consider steady-state evaporation.

Under the above assumptions the system of mass and energy conservation equations is [12]

$$\operatorname{div} \mathbf{j}_i = 0 \tag{3}$$

$$\operatorname{div} \mathbf{j}_T = 0 \tag{4}$$

where mass and thermal energy fluxes are determined taking into account the Stefan's flow:

$$\mathbf{j}_i = n_i \mathbf{v} - \frac{m_j n^2}{\rho} D\left(\nabla C_i + (-1)^{i+1} \frac{K_T}{T_e} \nabla T_e\right) \tag{5}$$

$$\mathbf{j}_T = \sum_i h_i m_i \mathbf{j}_i - k_e \nabla T_e \tag{6}$$

$$(i, j = 1, 2, i \neq j).$$

Note that in a binary gas mixture the thermodiffusion ratio (the ratio of thermal diffusion coefficient to diffusion coefficient) $K_T > 0$ when $m_1 > m_2$, and $K_T < 0$ when $m_1 < m_2$.

The boundary conditions for equations (5)–(6) allow the existence of temperature and concentration jumps at the surface of a droplet [11]:

$$(T_e - T_i)|_{r=R} = K_T^{(T)} \frac{\partial T_e}{\partial r}\bigg|_{r=R} + K_T^{(n)} T_\infty \frac{\partial C_1}{\partial r}\bigg|_{r=R} \tag{7}$$

$$(C_1 - C_1^{(s)}(T_i))|_{r=R} = K_n^{(n)} \frac{\partial C_1}{\partial r}\bigg|_{r=R} + \frac{K_n^{(T)}}{T_\infty} \frac{\partial T_e}{\partial r}\bigg|_{r=R}. \tag{8}$$

These boundary conditions must be supplemented with the condition of continuity of energy flux at the droplet surface:

$$\frac{W_T}{4\pi R^2} = ((L_1 - h_1) m_1 \mathbf{j}_1 + \mathbf{j}_T + \mathbf{j}_R)|_{r=R}. \tag{9}$$

Conditions at infinity are

$$T_e|_{r\to\infty} = T_\infty \quad C_1|_{r\to\infty} = C_{1\infty} \tag{10}$$

where $C_v = n_v/\Sigma_i n_i$ is a relative concentration, $K_T^{(T)}, K_n^{(n)}$ are coefficients of temperature and concentration jumps [11, 16], $K_T^{(n)}, K_n^{(T)}$ are cross coefficients [11], $\mathbf{j}_i$ is density of a mass flux, $\mathbf{j}_T$ is density of a heat flux, $\mathbf{j}_R$ is density of a radiative flux, m_i is mass of the molecule species i, D is diffusion coefficient, W_T is total power density of internal heat sources, L is latent heat of evaporation, h_i is enthalpy. Since the molecules of species 2 are not absorbed at the droplet surface the integral flux $Q_2 = 4\pi r^2 j_2 = 0$ (i.e. $\mathbf{j}_2 = 0$). Taking into account that $C_2 = 1 - C_1$ we arrive at the following expression for mass velocity of the gas:

$$v_r = -\frac{m_1 n}{C_2 \rho} D \left(\frac{dC_1}{dr} + \frac{K_T}{T_e}\frac{dT_e}{dr}\right). \tag{11}$$

Substituting equation (11) into the expression (7) for j_1 yields

$$j_1 = -\frac{Dn}{C_2}\left(\frac{dC_1}{dr} + \frac{K_T}{T_e}\frac{dT_e}{dr}\right). \tag{12}$$

Using equations (11), (12) the conservation equations (3)–(6) can be represented as follows:

$$\frac{d}{dr}\left[r^2\left(\frac{Dn}{C_2}\left(\frac{dC_1}{dr} + \frac{K_T}{T_e}\frac{dT_e}{dr}\right)\right)\right] = 0 \tag{13}$$

$$\frac{d}{dr}\left[r^2\left(h_1 m_1 j_1 - k_e \frac{dT_e}{dr}\right)\right] = 0. \tag{14}$$

In the general case the coefficients of heat conductivity and diffusion depend upon the temperature and concentration. However, in case when a condition (2) is satisfied, the dependence of thermal conductivity coefficient on relative concentration C_1 can be neglected. Thus we can consider k_e as a function of T_e only:

$$k_e = k_e(T_e, C_{1\infty}). \tag{15}$$

Expanding the thermodiffusion ratio into the Taylor's series and neglecting higher order terms we obtain

$$K_T = K_T^{(0)} + K_T^{(1)}(C_1 - C_{1\infty}) \tag{16}$$

where

$$K_T^{(0)} = K_T(T_e, C_{1\infty}), \quad K_T^{(1)} = \frac{\partial K_T(T_e, C_{1\infty})}{\partial C_1}\bigg|_{C_1 = C_{1\infty}}.$$

If condition (2) is satisfied, we can assume that $C_2 = C_{2\infty}$. Then equation (14) can be easily integrated to yield

$$h_1 m_1 j_1 - k_e \frac{dT_e}{dr} = \frac{A}{r^2} \tag{17}$$

where $A = Q_T/4\pi$ and Q_T is a constant integral heat flux.

After integrating equations (17) and (13) we obtain

$$\int_{T_\infty}^{T_e} \frac{k_e}{(Q_T - h_1 m_1 Q_1)} dT_e = \frac{1}{4\pi r} \tag{18}$$

$$\frac{Dn}{C_{2\infty}}\left(\frac{dC_1}{dr} + (K_T^{(0)} + K_T^{(1)}(C_1 - C_{1\infty}))\frac{1}{T_e}\frac{dT_e}{dr}\right) = \frac{G}{r^2} \tag{19}$$

where $G = Q_1/4\pi$ and Q_1 is a constant integral mass flux.

Since temperature T_e depends on coordinate r only, we can choose T_e as an independent variable in equation (19):

$$\left(\left[\frac{dC_1}{dT_e} + (K_T^{(0)} + K_T^{(1)}(C_1 - C_{1\infty}))\frac{1}{T_e}\right]\frac{dT_e}{dr}\right) = \frac{Q_1}{4\pi r^2}. \tag{20}$$

Substitution of equation (17) into equation (20) yields

$$\frac{dC_1}{dT_e} + (K_T^{(0)} + K_T^{(1)}(C_1 - C_{1\infty}))\frac{1}{T_e} = \frac{C_{2\infty} Q_1}{(Q_T - h_1 m_1 Q_1)}\frac{k_e}{Dn}. \tag{21}$$

Denoting $\Phi = C_1 - C_{1\infty}$, equation (21) can be rewritten as

$$\frac{d\Phi}{dT_e} = -\eta_1(T_e)\Phi + \eta_2(T_e) + \eta_3(T_e) \tag{22}$$

where

$$\eta_1(T_e) = \frac{K_T^{(1)}}{T_e}, \quad \eta_2(T_e) = -\frac{K_T^{(0)}}{T_e},$$

$$\eta_3(T_e) = \frac{C_{2\infty} Q_1}{(Q_T - h_1 m_1 Q_1)}\frac{k_e}{Dn}.$$

Solution of this equation yields the explicit expression for concentration distribution C_1:

$$C_1 = C_{1\infty} + \exp\left(-\int_{T_\infty}^{T_e} \eta_1(T)\,\mathrm{d}T\right) \times \left[\int_{T_\infty}^{T_e} \eta_2(T) \exp\left(\int_{T_\infty}^{T} \eta_1(\xi)\,\mathrm{d}\xi\right)\mathrm{d}T + \int_{T_\infty}^{T_e} \eta_3(T) \exp\left(\int_{T_\infty}^{T} \eta_1(\xi)\,\mathrm{d}\xi\right)\mathrm{d}T\right]. \quad (23)$$

Substituting C_1 and T_e in the boundary conditions (7), (8) we obtain the system of algebraic equations to determine $T_e^{(s)}$, $T_i^{(s)}$, Q_T and Q_1:

$$T_e^{(s)} - T_i^{(s)} = \frac{1}{4\pi R^2 k_s}\left((Q_T - h_1 m_1 Q_1) \times \left([K_{T_s}^{(0)} + K_{T_s}^{(1)}(C_1^{(s)} - C_{1\infty})]\frac{T_\infty}{T_e^{(s)}} K_T^{(n)} - K_T^{(T)}\right) + Q_1 C_{2\infty} T_\infty \frac{k_s}{n_s D_s} K_T^{(n)}\right) \quad (24)$$

$$C_1^{(s)} - C_1(T_i^{(s)}) = \frac{1}{4\pi R^2 k_s}\left(\frac{(Q_T - h_1 m_1 Q_1)}{T_\infty} \times \left([K_{T_s}^{(0)} + K_{T_s}^{(1)}(C_1^{(s)} - C_{1\infty})]\frac{T_\infty}{T_e^{(s)}} K_T^{(n)} - K_T^{(T)}\right) + Q_1 C_{2\infty} \frac{k_s}{n_s D_s} K_T^{(n)}\right) \quad (25)$$

$$W_T = Q_T + (L - h_1) m_1 Q_1 + 4\pi R^2 j_R \quad (26)$$

$$\int_{T_\infty}^{T_e^{(s)}} \frac{k_e}{(Q_T - h_1 m_1 Q_1)}\,\mathrm{d}T_e = \frac{1}{4\pi R} \quad (27)$$

where

$$k_s = k_e|_{r=R}, \quad n_s = n|_{r=R}, \quad D_s = D|_{r=R},$$

$$T_i^{(s)} = T_i|_{r=R}, \quad T_e^{(s)} = T_e|_{r=R}, \quad C_1^{(s)} = C_1|_{r=R}.$$

In cases when effects of temperature and concentration jumps on the process of evaporation can be neglected equations (24)–(25) reduce to

$$T_e|_{r=R} = T_i|_{r=R} = T_s; \quad C_1|_{r=R} = C_1^{(s)}(T_i). \quad (28)$$

From the system of equations (24)–(27) it is seen that, in the case when effects of temperature and concentration jumps and radiation are negligible, the temperature at the droplet surface does not depend upon r. If effects of the Stefan's flow and radiation on the process of heat and mass transfer are negligible, the expressions for the temperature and concentration distributions may be simplified. In this case we can obtain the concentration and temperature distributions C_1, T_e and thermal and mass fluxes Q_T and Q_1 from the expressions

$$C_1 = C_{1\infty} + \exp\left(-\int_{T_\infty}^{T_e} \frac{K_T^{(1)}}{T}\,\mathrm{d}T\right) \times \left[\int_{T_\infty}^{T_e} \frac{K_T^{(0)}}{T} \exp\left(-\int_{T_\infty}^{T} \frac{K_T^{(1)}}{\xi}\,\mathrm{d}\xi\right)\mathrm{d}T + \frac{C_{2\infty} Q_1}{Q_T}\int_{T_\infty}^{T_e} \frac{k_e}{nD} \exp\left(-\int_{T_\infty}^{T} \frac{K_T^{(1)}}{\xi}\,\mathrm{d}\xi\right)\mathrm{d}T\right] \quad (29)$$

$$\int_{T_\infty}^{T_e^{(s)}} k_e\,\mathrm{d}T = \frac{R}{r}\int_{T_\infty}^{T_e} k_e\,\mathrm{d}T \quad (30)$$

where

$$Q_T = 4\pi R \int_{T_\infty}^{T_e^{(s)}} k_e\,\mathrm{d}T \quad (31)$$

$$Q_1 = Q_T \frac{C_1^{(s)} - C_{1\infty} + \exp\left(-\int_{T_\infty}^{T_e} \frac{K_T^{(1)}}{T}\right) \times \int_{T_\infty}^{T_e} \frac{K_T^{(0)}}{T} \exp\left(-\int_{T_\infty}^{T_e} \frac{K_T^{(1)}}{\xi}\,\mathrm{d}\xi\right)\mathrm{d}T}{C_{2\infty}\int_{T_\infty}^{T_e} \frac{k_e}{nD} \exp\left(-\int_{T_\infty}^{T} \frac{K_T^{(1)}}{\xi}\,\mathrm{d}\xi\right)\mathrm{d}T}. \quad (32)$$

In the above expression the temperature at the droplet surface $T_e^{(s)}$ can be obtained from the expressions (24)–(25) neglecting the convective terms:

$$T_e^{(s)} - T_i^{(s)} = \frac{1}{4\pi R^2 k_s}\left(\left([K_{T_s}^{(0)} + K_{T_s}^{(1)}(C_1^{(s)} - C_{1\infty})]\frac{T_\infty}{T_e^{(s)}} K_T^{(n)} - K_T^{(T)}\right) Q_T + Q_1 C_{2\infty} T_\infty \frac{k_s}{n_s D_s} K_T^{(n)}\right) \quad (33)$$

$$C_1^{(s)} - C_1(T_i^{(s)}) = \frac{1}{4\pi R^2 k_s}\left(\left([K_{T_s}^{(0)} + K_{T_s}^{(1)}(C_1^{(s)} - C_{1\infty})]\frac{T_\infty}{T_e^{(s)}} K_T^{(n)} - K_T^{(T)}\right)\frac{Q_T}{T_\infty} + Q_1 C_{2\infty} \frac{k_s}{n_s D_s} K_T^{(n)}\right). \quad (34)$$

It is easy to show that in case when $K_T^{(T)} = K_n^{(n)} = K_T^{(n)} = K_n^{(T)} = 0$ (when droplets are large) the equations (33), (34) can be rewritten as

$$T_e^{(s)} = T_i^{(s)} \quad C_1^{(s)} = C_1(T_i^{(s)}). \quad (35)$$

Using the above results allows one to estimate temperature and concentration distributions in the neighborhood of a droplet and heat and mass fluxes, taking into account thermal diffusion and variable thermophysical properties.

Finally, the radius of evaporating droplet can be found from the equation

$$R^2 \frac{\mathrm{d}R}{\mathrm{d}t} = -\frac{m_1}{4\pi\rho_d} Q_1 \quad (36)$$

where ρ_d is droplet density, t is time, R is radius of the droplet. Since generally Q_1 (in case of nonzero temperature and concentration jumps) depends upon the radius R, the equation (38) can be only integrated numerically. However for large size droplets (when $K_T^{(T)} = K_n^{(n)} = K_T^{(n)} = K_n^{(T)} = 0$) and when effects of radiation are neglected, temperature $T_e^{(s)} = T_i^{(s)}$, and mass flux Q_1 do not depend upon radius. If $C_{1\infty} = 0$ (in this case $K_T^{(0)} = 0, K_T^{(1)} = \text{const.}$) and effect of the temperature and concentration jumps on the process of heat and mass transfer of the droplet is neglected, the expression for the mass flux from the droplet reads

$$Q_1 = 4\pi R \frac{C_{1s}\tau_s^{K_T^{(1)}}}{\int_{T_\infty}^{T_e^{(s)}} \frac{k_e}{nD}(1+K_T^{(1)})\,\mathrm{d}T} \int_{T_\infty}^{T_e^{(s)}} k_e\,\mathrm{d}T \quad (37)$$

where

$$\tau_s = \frac{T_e^{(s)}}{T_\infty}.$$

Given the power dependence of coefficients k_e and D on temperature,

$$k_e = k_\infty \left(\frac{T_e}{T_\infty}\right)^\alpha \quad D = D_\infty \left(\frac{T_e}{T_\infty}\right)^{1+\beta} \quad (38)$$

the expression for the mass flux Q_1 reads

$$Q_1 = 4\pi R n_\infty D_\infty \frac{(1+K_T^{(1)}+\alpha-\beta)(\tau_s^{\alpha+1}-1)}{(\alpha+1)(\tau_s^{1+K_T^{(1)}+\alpha-\beta}-1)} C_{1s}\tau_s^{K_T^{(1)}}. \quad (39)$$

The ratio of the values of mass flux determined, neglecting the effect of thermal diffusion Q_1^*, to that when thermal diffusion is accounted for is

$$\frac{Q_1^*}{Q_1} = \frac{(1+\alpha-\beta)(\tau_s^{1+K_T^{(1)}+\alpha-\beta}-1)}{(1+K_T^{(1)}+\alpha-\beta)(\tau_s^{1+\alpha-\beta}-1)} \tau_s^{-K_T^{(1)}} \quad (40)$$

where

$$Q_1^* = Q_1|_{K_T=0}.$$

3. COMBUSTION OF LARGE SIZE AND MODERATE SIZE FUEL DROPLET IN A STAGNANT AMBIENT ATMOSPHERE

In the combustion of large and moderate size fuel droplets two regions with large temperature differences in the neighborhood of a burning droplet are formed. The heat and mass transfer between a fuel vapor and combustion products that are formed in the vicinity of a flame front occurs in the region between a droplet surface and a flame front. In the external region the oxidizer flows to the flame front and heat flux and combustion products flow into a stagnant gaseous atmosphere. Assume that the combustion products do not affect the process of combustion and that the rate of mixing is high and the relative concentration differences of oxidizer in the neighborhood of a droplet are small. In this case the influence of the Stefan's flow on heat and mass transfer is negligible.

The equation of chemical reaction will be assumed as follows:

$$v_j^{(k)} A_j + v_{j,i}^{(k)} A_i = \sum_{l=1}^{N-1} \varepsilon_{j,l}^{(k)} A_l \quad (41)$$

where A_j, A_i, A_l denote molecules of gas component, droplet substance and combustion products, correspondingly, $v_j^{(k)}, v_{j,i}^{(k)}, \varepsilon_{j,l}^{(k)}$ are stoichiometric coefficients and index $j = 1, 2$ denotes gas component or droplet substance (first or second species, correspondingly).

Thus a gas mixture in the neighborhood of a burning droplet is composed of the molecules of gas of surrounding media. The external zone consists of a mixture of oxidizer, products of reaction and the gases of surrounding media.

Under the above assumptions the problem of gaseous phase quasi-steady combustion must be formulated in two domains. The first region is $R \leqslant r \leqslant R+x_f$, where R = radius of a droplet, and x_f is distance between a droplet surface and a flame front. The corresponding system of conservation equations similar to equations (3)–(6) for $R \leqslant r \leqslant R+x_f$ reads [12]

$$\operatorname{div}\mathbf{j}_i = 0$$

$$\operatorname{div}\mathbf{j}_T^{(1)} = 0 \quad (42)$$

$$\mathbf{j}_i = n_i\mathbf{v} - \frac{m_j n^2}{\rho} D_{ij}^{(1)}\left(\nabla C_i + (-1)^{i+1}\frac{K_T}{T_e^{(1)}}\nabla T_e^{(1)}\right)$$

$$\mathbf{j}_T^{(1)} = \sum_i h_i m_i \mathbf{j}_i - k_e^{(1)}\nabla T_e^{(1)} \quad (i, j = 1, 3, i \neq j) \quad (43)$$

where superscript 1 denotes the values in the first zone.

The boundary conditions for equations (42)–(43) are

$$(T_e^{(1)} - T_i)|_{r=R} = K_T^{(T)} \left.\frac{\partial T_e^{(1)}}{\partial r}\right|_{r=R} + K_T^{(n)} T_f \left.\frac{\partial C_1}{\partial r}\right|_{r=R} \quad (44)$$

$$(C_1 - C_1^{(s)}(T_i))|_{r=R} = K_n^{(n)} \left.\frac{\partial C_1}{\partial r}\right|_{r=R} + \frac{K_n^{(T)}}{T_f} \left.\frac{\partial T_e^{(1)}}{\partial r}\right|_{r=R} \quad (45)$$

$$h_1 m_1 \mathbf{j}_1|_{r=R} = (L_1 m_1 \mathbf{j}_1 + \mathbf{j}_T^{(1)} + \mathbf{j}_R^{(1)})|_{r=R}. \quad (46)$$

Assume that the chemical reaction rate is large and that all molecules of the fuel react with oxidizer. Then energy and mass conservation equations in the domain $R+x_f \leqslant r < \infty$ can be represented as follows:

$$\operatorname{div}(k_e^{(2)}\nabla T_e^{(2)}) = 0$$

$$\operatorname{div}(nD_{j,N}^{(2)}\nabla C_2) = 0 \quad (47)$$

with the regular boundary conditions of temperature and energy flux continuity at the flame front:

$$T_e^{(1)}|_{r=R+x_f} = T_e^{(2)}|_{r=R+x_f} = T_f \quad (48)$$

$$\left(qm_2Q_2+k_{\mathrm{e}}^{(2)}\frac{\partial T_{\mathrm{e}}^{(2)}}{\partial r}\right)\Bigg|_{r=R+x_{\mathrm{f}}} = \left(\mathbf{j}_T^{(1)}+\gamma\sigma\left(T_{\mathrm{e}}^{(1)^4}-T_\infty^4\right)\right)\Bigg|_{r=R+x_{\mathrm{f}}}. \quad (49)$$

The flux of oxidizer at the flame front Q_2 is determined by a stoichiometric relation [17],

$$\nu_1Q_2 = \nu_2Q_1. \quad (50)$$

The flame thickness is assumed to be infinitely small, i.e.

$$C_1^{(\mathrm{s})}|_{r=R+x_{\mathrm{f}}} = 0 \quad (51)$$

where Q_2 is an oxidizer flux to the flame front.

Conditions at infinity are

$$T_{\mathrm{e}}^{(2)}|_{r\to\infty} = T_\infty \quad C_1|_{r\to\infty} = C_{1,\infty}. \quad (52)$$

Since there are no restrictions on the temperature differences in the neighborhood of a droplet, the diffusion coefficient and heat conductivity are considered to be functions of temperature and pressure,

$$k_{\mathrm{e}}^{(1)} = k_{\mathrm{e}}^{(1)}\left(T_{\mathrm{e}}^{(1)},p\right) \quad k_{\mathrm{e}}^{(2)} = k_{\mathrm{e}}^{(2)}\left(T_{\mathrm{e}}^{(2)},p\right)$$

$$D_{j,N} = D_{j,N}(T,p).$$

Therefore the solution of the problem of combustion reduces to solving the above conservation equations in the domain $R \leqslant r \leqslant R+x_{\mathrm{f}}$ (it was done in the previous section) and solving the conservation equations in the domain $R+x_{\mathrm{f}} \leqslant r < \infty$. Thus the values $T_{\mathrm{e}}^{(\mathrm{s})}, T_i^{(\mathrm{s})}, Q_T^{(1)}, Q_1$ can be found from a system of equations similar to (24)–(27):

$$T_{\mathrm{e}}^{(\mathrm{s})}-T_i^{(\mathrm{s})} = \frac{1}{4\pi R^2k_{\mathrm{s}}^{(1)}}\left((Q_T-h_1m_1Q_1)\left([K_{T_{\mathrm{s}}}^{(0)} + K_{T_{\mathrm{s}}}^{(1)}(C_1^{(\mathrm{s})}-C_{1\infty})]\frac{T_{\mathrm{f}}}{T_{\mathrm{e}}^{(\mathrm{s})}}K_T^{(n)}-K_T^{(T)}\right) + Q_1C_{2\infty}T_{\mathrm{f}}\frac{k_{\mathrm{s}}^{(1)}}{n_{\mathrm{s}}D_{\mathrm{s}}^{(1)}}K_T^{(n)}\right) \quad (53)$$

$$C_1^{(\mathrm{s})}-C_1\,(T_i^{(\mathrm{s})}) = \frac{1}{4\pi R^2k_{\mathrm{s}}^{(1)}}\left(\frac{(Q_T-h_1m_1Q_1)}{T_{\mathrm{f}}}\left([K_{T_{\mathrm{s}}}^{(0)} + K_{T_{\mathrm{s}}}^{(1)}\,(C_1^{(\mathrm{s})}-C_{1\infty})]\frac{T_{\mathrm{f}}}{T_{\mathrm{e}}^{(\mathrm{s})}}K_T^{(n)}-K_T^{(T)}\right) + Q_1C_{2\infty}\frac{k_{\mathrm{s}}^{(1)}}{n_{\mathrm{s}}D_{\mathrm{s}}^{(1)}}K_T^{(n)}\right) \quad (54)$$

$$W_T = Q_T^{(1)}+(L-h_1)\,m_1Q_1+4\pi R^2\gamma\sigma\,(T_{\mathrm{e}}^{(\mathrm{s})^4}-T_{\mathrm{f}}^4) \quad (55)$$

$$\int_{T_{\mathrm{f}}}^{T_{\mathrm{e}}^{(\mathrm{s})}}\frac{k_{\mathrm{e}}^{(1)}}{(Q_T^{(1)}-h_1m_1Q_1)}\mathrm{d}T_{\mathrm{e}} = \frac{1}{4\pi R}. \quad (56)$$

Equations (53)–(56) include the unknown values of temperature and location of flame front T_{f}, x_{f}, which can be found by combining the analytical solutions of conservation equations (47) and stoichiometric relation (50):

$$qm_2\frac{\nu_2}{\nu_1}Q_1 = Q_T^{(1)}-4\pi\,(R+x_{\mathrm{f}})\int_{T_\infty}^{T_{\mathrm{f}}}k_{\mathrm{e}}^{(2)}\,\mathrm{d}T_{\mathrm{e}} \quad (57)$$

$$qm_2Q_1 = -4\pi(R+x_{\mathrm{f}})\frac{\nu_1}{\nu_2}C_{2\infty}\frac{\displaystyle\int_{T_\infty}^{T_{\mathrm{f}}}k_{\mathrm{e}}^{(2)}\,\mathrm{d}T_{\mathrm{e}}}{\displaystyle\int_{T_\infty}^{T_{\mathrm{f}}}\frac{k_{\mathrm{e}}^{(2)}}{nD^{(2)}}\mathrm{d}T_{\mathrm{e}}}. \quad (58)$$

Assuming power law dependence of the thermal conductivity and diffusivity on temperature,

$$k_{\mathrm{e}}^{(m)}\,(T_{\mathrm{e}}^{(m)}) = k_0^{(m)}\left(\frac{T_{\mathrm{e}}^{(m)}}{T_0}\right)^{\alpha}$$

$$D^{(m)}\,(T_{\mathrm{e}}^{(m)}) = D_0^{(m)}\left(\frac{T_{\mathrm{e}}^{(m)}}{T_0}\right)^{1+\beta}, \quad (59)$$

the expression of the mass flux from the fuel droplet reads

$$Q_1 = 4\pi Rn_{\mathrm{f}}D_{\mathrm{f}}\frac{(R+x_{\mathrm{f}})}{x_{\mathrm{f}}} \times\frac{(1+\alpha_1-\beta_1)(\Theta_{\mathrm{s}}^{1+\alpha_1}-1)}{(1+\alpha_1)(\Theta_{\mathrm{s}}^{1+\alpha_1-\beta_1}-1)}(C_{1\mathrm{s}}-C_{1\mathrm{f}}) \quad (60)$$

where $\Theta_{\mathrm{s}} = T_{\mathrm{e}}^{(\mathrm{s})}/T_{\mathrm{f}}$ and $m = 1, 2$ is a zone number.

The expression (60) can be obtained similarly to the expression (39). The evolution of the radius R of the burning droplet can be found from equation (36).

4. RESULTS AND CONCLUSIONS

The above model of vaporization of droplets in a hot and radiant environment was applied to study the process of evaporation and combustion of fuel droplets in a binary gas mixture. Analysis of expressions for the mass fluxes of evaporating or burning droplets [equations (32), (60)] shows that the effect of thermal diffusion is essential in cases of evaporation or combustion of fuel droplets in a binary gas mixture with thermal diffusion ratio of the order of 0.1–0.5 or higher. It is known that the coefficients of thermal diffusion are large for gas mixtures with significant differences in molecular weights or diameters. The results of numerical calculations of dependence of Q_1/Q_1^* vs τ_{s} in the case of a droplet with internal heat sources (i.e. $\tau_{\mathrm{s}} > 1$, where $\tau_{\mathrm{s}} = T_{\mathrm{s}}/T_\infty$), which are performed according to expression (40), are presented in Fig. 1. Note that the existence of internal heat sources can be taken into account by setting the ratio $\tau_{\mathrm{s}} > 1$. The results presented in this figure show that the difference between the fluxes of volatile component calculated, taking into account the thermal diffusion Q_1 and neglecting the effects of thermal diffusion Q_1^*,

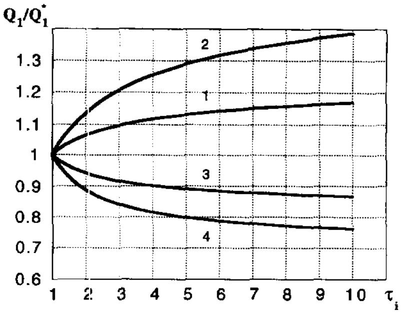

Fig. 1. Effect of thermal diffusion on droplet evaporation (combustion) with internal heat sources. (1) $\alpha = \beta$, $K_T = 0.2$. (2) $\alpha = \beta$, $K_T = 0.4$. (3) $\alpha = \beta$, $K_T = -0.2$. (4) $\alpha = \beta$, $K_T = -0.4$.

can be of the order of 20% when the relative temperature difference is high.

The analysis of the expression for the mass flux of combusting droplets [equation (60)] shows that the ratio of the mass fluxes calculated with and without thermal diffusion for the combusting droplets is identical to expression (40). The results of numerical calculation in the case of combusting droplets (i.e. without internal heat sources $\tau_i = T_f/T_s < 1$) are presented in Fig. 2.

It can be seen from this plot that effects of thermal diffusion on the process of combustion are significant in cases when temperature differences in the neighborhood of the droplets are large. In reality, the temperature differences in the neighborhood of the combusting fuel droplets when the fuel leaves the surface by diffusion vary in the range τ_i from 0.1 to 0.7. However, even in these cases, the effect of thermal diffusion on the process of combustion is significant.

The d^2–t diagram for *n*-heptane droplet evaporating in nitrogen, obtained from the present model, is shown in Fig. 3. Line 1 is plotted for an ambient temperature $T_\infty = 100°C$ and line 2 for an ambient temperature $T_\infty = 300°C$. As seen from these plots, the theoretical results are in fairly good agreement with experimental data [18].

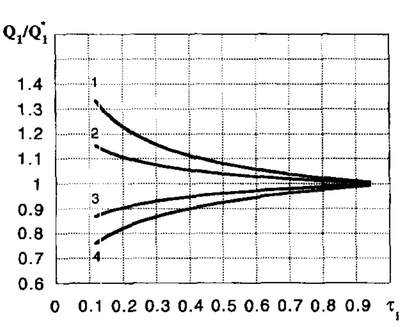

Fig. 2. Effect of thermal diffusion on droplet evaporation (combustion) without internal heat sources. (1) $\alpha = \beta$; $K_T = -0.2$. (2) $\alpha = \beta$; $K_T = -0.1$. (3) $\alpha = \beta$; $K_T = 0.1$. (4) $\alpha = \beta$; $K_T = 0.2$.

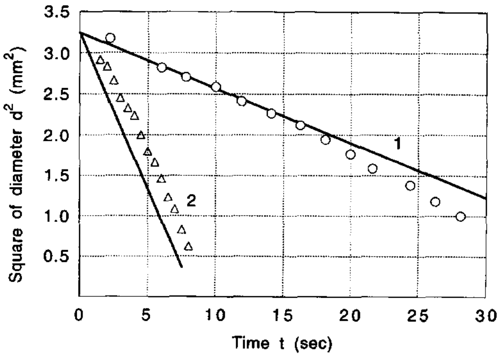

Fig. 3. Variation of square of diameter vs time (*n*-heptane droplet evaporating in nitrogen). (1) $T_\infty = 100°C$. (2) $T_\infty = 300°C$. (○) Experimental data [18] for $T_\infty = 100°C$. (△) Experimental data [18] for $T_\infty = 300°C$.

Constant of evaporation K determined by expression (1) is an important characteristic of the process of evaporation. In the case when the burning rate is limited by the rate of evaporation, K is equal to the constant of combustion. The classical evaporation model yields the following expression for the evaporation constant:

$$K = \frac{8k_e \ln(1+B)}{\rho_l c_p} \tag{61}$$

where B is the transfer number for steady-state evaporation, ρ_l is density of liquid and c_p is specific heat. The transfer number B is determined at the steady-state condition $B = B_T = B_M$ (where

$$B_T = c_p \frac{(T_\infty - T_s)}{L} \qquad B_M = \frac{Y_{F_s}}{1 - Y_{F_s}}$$

and T_s = steady-state value of surface temperature). The various modifications and refinements of the above expression (61) are employed in many investigations dealing with evaporation and combustion of single droplets and sprays (see e.g. refs. [1, 5, 9]). Comparison of values of the evaporation constant and the droplet temperature obtained with the present model and from formula (61) for an alcohol droplet with the radius 0.15 mm, evaporating in air in the range of ambient temperature 100–350°C, is shown in Fig. 4. The estimations of the value of radiation flux

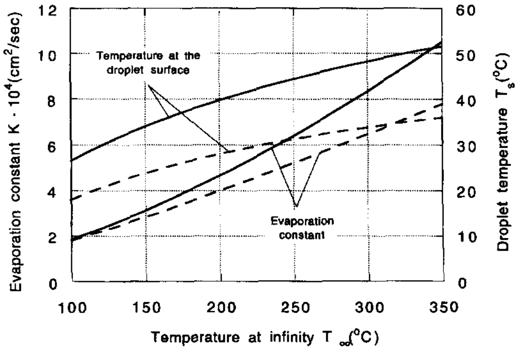

Fig. 4. Variation of temperature at the droplet surface and evaporation constant vs ambient temperature for alcohol droplets. (——) Present model. (----) Classical model [formula (61)].

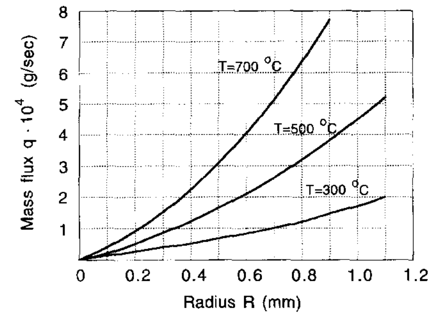

Fig. 5. Variation of the mass flux vs radius for the alcohol droplets.

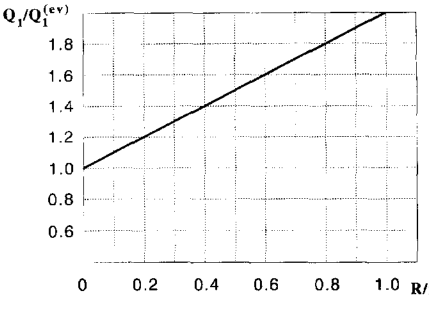

Fig. 7. Effect of the distance from a droplet surface to a flame front upon the ratio of a mass flux from a burning droplet to a mass flux of evaporating droplet, with the temperature at infinity equal to a flame front temperature.

show that, in this case, the contribution of radiation flux to the mass flux is less than 5% and the d^2 law is valid. The results presented in Fig. 4 demonstrate the significant discrepancy between the results obtained with the classical model and our model. For ambient temperature 350°C, the classical model underestimates the evaporation constant K by 25%. As seen from Fig. 4, the discrepancy between the temperature at the droplet surface obtained by the present method and steady-state droplet temperature used for calculation of evaporation constant according to the classical model is more significant. The latter is one of the main reasons for underestimation of evaporation constant in the classical model.

In case when the temperature differences in the neighborhood of the droplet are large, the effect of radiation must be taken into account. Results of numerical calculation of the dependence of mass flux q $(q = m_1 Q_1)$ on the radius for the evaporating alcohol droplets are presented in the Fig. 5. These results were obtained taking into account the effects of radiation. It is seen from these plots that the dependence of mass flux on radius for the evaporating droplet is nonlinear in a case when radiation is taken into account. In the opposite case (i.e. when radiation effects are neglected), as shown in Fig. 6 (curves 2 and 4), the dependence is linear. It is readily seen from these plots that, in the case when droplets are large, the effect of radiation is significant. The difference between the results obtained when radiation is taken into account (curves 1 and 3) and those neglecting radiation effects (curves 2 and 4), is of order 100% for the large droplets.

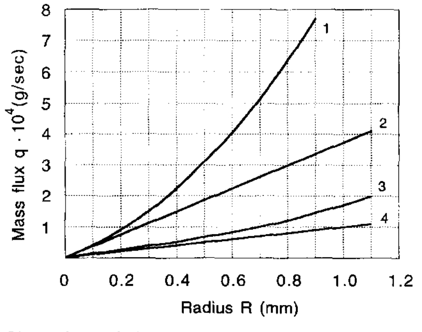

Fig. 6. Variation of the mass flux vs radius for the alcohol droplets. (1) $T_\infty = 700°C$, radiation is taken into account. (2) $T_\infty = 700°C$, radiation is not taken into account. (3) $T_\infty = 300°C$, radiation is taken into account. (4) $T_\infty = 300°C$, radiation is not taken into account.

When mixing and chemical reaction rates are large, the combustion is limited by evaporation rate. This allows consideration of the combustion process as evaporation at adiabatic flame front temperature [19, 20]. In this case expression of fuel mass flux can be obtained from expression (41), setting $K_T^{(1)} = 0$:

$$Q_1^{(\mathrm{ev})} = 4\pi R n_\mathrm{f} D_\mathrm{f} \frac{(1+\alpha_1-\beta_1)(\Theta_\mathrm{s}^{1+\alpha_1}-1)}{(1+\alpha_1)(\Theta_\mathrm{s}^{1+\alpha_1-\beta_1}-1)}(C_{1\mathrm{s}}-C_{1\mathrm{f}}). \tag{62}$$

The dependence of $Q_1/Q_1^{(\mathrm{ev})}$, on R/x_f [where Q_1 is mass flux calculated from equation (60) and $Q_1^{(\mathrm{ev})}$ is mass flux calculated from equation (62)] is shown in Fig. 7. The comparison between the exact results obtained from expression (60) with the approximate formula (62) shows that the adiabatic flame temperature approximation underestimates the mass flux. In a typical case of combustion of fuel droplets with $R/x_\mathrm{f} \simeq 0.3$, the effect of this underestimation amounts to 30%. As can be seen from Fig. 7, expression (62) can be used only when $R/x_\mathrm{f} \ll 1$. In the opposite case when $R/x_\mathrm{f} \simeq 1$ one must use the exact relation (60).

The effects of the kinetic jumps on evaporation rate is shown in Fig. 8 for alcohol droplets of two sizes. The values of coefficients of temperature and concentration jumps were adopted from ref. [16]. As can be seen from these plots, the kinetic effects are significant ($\simeq 12\%$) at the final stages of droplet combustion. Note that the kinetic effects slow down the combustion process.

The effect of kinetic jumps on integral mass flow is shown in Fig. 9. The results presented in this figure demonstrate that the integral mass flow is less when kinetic effects are taken into account. The difference between the integral mass fluxes calculated with and without kinetic jumps can be of order $\simeq$ 12% for 5 μ droplets.

In the case of combustion of hydrocarbon fuels, the

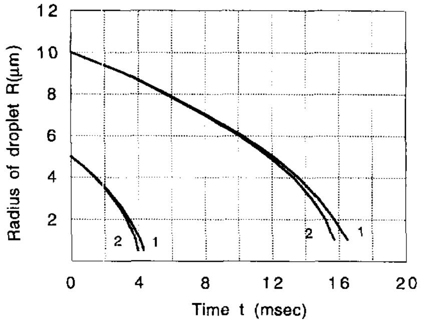

Fig. 8. Effect of temperature and concentration jumps on evaporation rate ($T_\infty = 100°C$). (1) Temperature and concentration jumps are taken into account. (2) Temperature and concentration jumps are not taken into account.

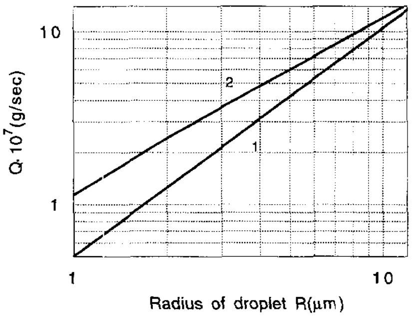

Fig. 9. Effect of temperature and concentration jumps on total mass flux ($T_\infty = 300°C$). (1) Temperature and concentration jumps are taken into account. (2) Temperature and concentration jumps are not taken into account.

diffusion model, which neglects the dependence of the transport coefficients (i.e. diffusivity and heat conductivity) upon concentration, is not valid. The reason is that, in the latter case, the concentration differences in the vicinity of the droplet surface are quite significant and condition (2) is violated. Therefore, the consistent solution of the problem must take into account that heat conductivity and diffusion coefficients are functions of temperature and concentration of gaseous mixture components, i.e. $k = k(T, C_i)$, $D = D(T, C_i)$.

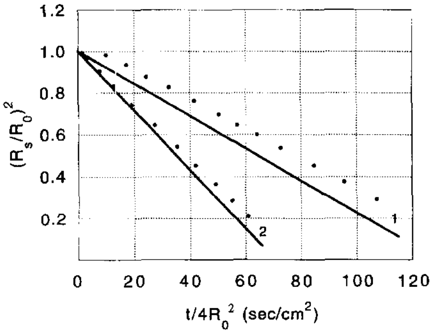

Fig. 10. Variation of radius of burning droplet vs time. (1) O_2/N_2: 21/79; 0.15 atm environment, $R_0 = 0.51$ mm. (2) O_2/N_2: 75/25; 0.1 atm environment, $R_0 = 0.57$ mm. (——) Theory. (●) Experimental data [21].

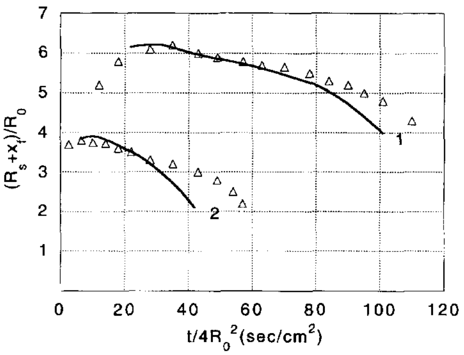

Fig. 11. Variation of flame front location vs time. (1) O_2/N_2: 21/79; 0.15 atm environment, $R_0 = 0.51$ mm. (2) O_2/N_2: 75/25; 0.1 atm environment, $R_0 = 0.57$ mm. (——) Theory. (△) Experimental data [21].

Such an approach was employed in calculations of combustion of *n*-octane droplets. The comparison of the prediction of the theoretical model with experimental results [21] is presented in Figs. 10 and 11.

In these calculations the convective terms in equations (5)–(6) were preserved. The agreement of theoretical and experimental results is fairly good. In the calculations we adopted the lumped values of the coefficients of diffusivity and heat conductivity from ref. [19]. The dependence of these coefficients upon temperature and concentration was accounted for when solving the system of nonlinear algebraic equations (53)–(56). In the solution we adopted the concentration dependence of k_0 in expression (59), as recommended in ref. [19], and the dependence of diffusion coefficient upon concentration was neglected.

5. SUMMARY

The quasi-steady model of combustion and evaporation of large and moderate size single fuel droplets in a quiescent atmosphere, taking into account the kinetic effects, variable thermophysical properties, thermal diffusion and radiation, was developed. The comparison of the theoretical results, obtained with the aid of this model, with experimental data demonstrated the validity of the developed model.

An analytical solution is obtained for heat and mass fluxes in the neighborhood of the large burning droplets in the case of high reaction rates. The analytical formulae are derived for temperature and concentration distributions and heat and mass fluxes in the vicinity of the burning (evaporating) droplet.

The analysis of the contribution of the radiation, thermal diffusion and kinetic jump effects on the heat and mass fluxes showed that the relative contribution of these effects is quite significant in the range of parameters encountered in many combustion systems. It is shown that the effect of thermal diffusion is essential in the case of evaporation or combustion of fuel droplets with internal heat sources (i.e. when temperature at the surface of fuel droplet is higher than an ambient temperature) in a binary gas mixture with significant differences in molecular weights or diameters.

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