DROPLET COMBUSTION

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Abstract. *This work presents a new strategy combining the Shvab-Zel'dovich and flamelet formulations to solve the droplet combustion problem, in which thermodynamic and transport properties are considered dependent on composition and temperature. By following Shvab-Zel'dovich procedure, combinations among the conservation equations are used to eliminate the chemical reaction term. Four independent functions (three mixture fraction functions and excess enthalpy) are found and they are conservative in the whole domain. The first mixture fraction function combines the fuel and oxidant species conservation equations, the second one combines fuel and* H_2O *species conservation equations and the last one, fuel and* CO_2 *species conservation equations. The excess enthalpy function is formed by a combination among fuel and oxidant species and energy conservation equations. By following the flamelet description, the excess of enthalpy and the fuel and* H_2O *and fuel and* CO_2 *mixture fractions are written in terms of fuel and oxidant mixture fraction. The integration of the equations for these three functions can be done by any very well known methods. The dependence of these three functions on spatial coordinate is found by the integration of the fuel and oxidant mixture fraction equation. This new strategy accelerates the integration of the system of equations because the two eigenvalues of the problem, i.e. the droplet surface temperature and vaporisation constant, are determined separately. The first one is found by the excess enthalpy equation written in the mixture fraction space and the second one is found by the mixture fraction conservation equation.*

Keywords: *Droplet Combustion, Diffusion Flame, Shvab-Zel'dovich Formulation...*

1. INTRODUCTION

Spray combustion (reacting multi-phase flow), as well as non reacting and reacting mono-phase flows, present processes in different spatial and temporal scales. With the now-a-days computational capability, a simulation of this kind of problem is not feasible economically in certain cases and not possible in other cases. To avoid the integration of all processes in all scales, the simulation grid is chosen to cover the processes in the largest spatial scales and the processes in the other scales are included in the simulation via parameters, which are determined by separated analysis. If the sub-grid processes can be described analytically, those parameters are determined by expressions, with practically no cost to the largest scales problem simulation. In most of time, those parameters are not determined by an analytical expression, but by a numerical solution. In these cases, the cost to obtain the numerical solution of the sub-grid processes is counted on the whole problem simulation time. Thereby, beyond representing well the physics, the sub-grid processes modelling must be computationally economic. The combustion of individual droplet problem is the sub-grid information necessary to perform the spray combustion simulation. Therefore, the model for the droplet combustion must be simple, fast integrated and represent well the experimental results. In this sense, the present work proposes a procedure to describe the droplet combustion by making use of an extended Shvab-Zel'dovich and flamelet formulations considering the thermodynamical properties dependent on composition and temperature.

It is not the aim of this paper to explore the all aspects of the droplet combustion, but to present this new procedure. Thereby, even with a extensive literature on droplet combustion, only those papers linked closely to the development of the procedure will be mentioned.

The description of the droplet combustion is relatively simple for normal pressure, because the gas phase close to the droplet behaves quasi-steadily when analized by the droplet lifetime. The problem of droplet combustion presents a analytical solution for the case of thermodynamic and the transport coefficients constant (Spalding, 1953; Godsave, 1953). To avoid the integration of the conservation equations with the chemical reaction term, it was imposed the condition of infinitely thin flame, which permitted to divide the domain in two zones (fuel zone and oxygen zone) and to perform the integration of the conservation equations. At the flame, it was imposed continuity and flux conservation. An improvement on the model occurred by imposing a linear variation of the thermodynamic and transport coefficients on the temperature (Goldsmith and Penner, 1954). Instead of integrating the equations avoiding to cross the flame, it was used the Shvab-Zel'dovich procedure to eliminate the chemical reaction term, which permitted to integrate continuously from one boundary to another. The next step in the improvement of the droplet combustion model was done by incorporating the dependence of the transport coefficients on a power of the temperature (Kassoy and Williams, 1968). The complete dependence on the composition and temperature of the transport coefficients was considered, but the process of integration of the equations avoided to cross the flame (Raghunandan and Mukunda, 1977). Another strategy was adopted, using the previous model but incorporating the Shvab-Zel'dovich formulation to eliminate the chemical reaction term (Williams, 1985).

More recently, extensions for the droplet combustion were presented. The problem, in which the transport coefficients were considered dependent on a power of the temperature and constant specific heat, was solved analytically (Fachini, 1999). This model was able to treat the Lewis number for the fuel and oxygen constant but different from unity. To avoid the integration of the chemical reaction term, the Shvab-Zel'dovich's formulation was employed, but even with that the integration was only possible with the partition of the domain in fuel zone and oxygen zone. The continuous integration in whole domain is possible only in a numerical way (Lima et al., 2006). This numerical procedure was used to analyse the influence of soot in the droplet combustion (Fachini, 2006). This strategy of analysis, an extension for the droplet model is proposed with thermodynamic coefficients dependent on the composition and temperature and the transport coefficients dependent on a temperature power.

The dependent variables from the Shvab-Zel'dovich's formulation are conserved, i.e. the equations for the mixture fraction functions and excess enthalpy do not present source term. However, they are not passive because the flow field influentiates their behaviour. The flow field acts on the droplet problem by two mechanisms: fluxes of the excess enthalpy and the mixture fraction functions at the droplet surface and the differences among the molecular diffusive velocities. The first source is eliminated combining the mixture fraction functions and the excess enthalpy in a such way that the fluxes of the new variables are zero at the droplet. However, to eliminate the second source is necessary to impose Lewis number equal to one (Sirignano, 2002). This imposition limits the application of the passive, conservative variables (super-scalar variables) formulation to fuels with molecular weight close to that of the ambient oxidant gas.

2. MATHEMATICAL FORMULATION

Formulation of quasi-steady droplet combustion is presented elsewhere (Fachini, 1999). Thus, because of that only the essential parts of it will be explicitly presented.

Considering the ambient conditions to be characterised by the temperature T_∞, density ρ_∞, oxygen mass fraction $Y_{O\infty}$. Without loosing any important feature of the problem, the transport coefficients (thermal conductivity and diffusion coefficient) are supposed to depend on a power of temperature, according to $k/k_\infty = D_i/D_{i\,\infty} = (T/T_\infty)^n = \theta^n$. The pressure specific heat for the gases mixture is determined by $\sum_i Y_i\, c_{pi}$. The non-dimensional quasi-steady conservation equations, describing the gas phase around the droplet with radius $\bar{a}$ at time t ($\bar{a}_0$ at the time $t = 0$), are expressed by

$$x^2 \varrho v = \lambda(\tau) \tag{1}$$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left\{\begin{array}{c} Le_F y_F \\ Le_O y_O \\ Le_H y_H \\ Le_C y_C \\ h \end{array}\right\} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \theta^n \frac{\partial}{\partial x}\left\{\begin{array}{c} y_F \\ y_O \\ y_H \\ y_C \\ \theta \end{array}\right\}\right) = \dot{\omega}_F Le_F \left\{\begin{array}{c} -1 \\ -S \\ S_H \\ S_C \\ Q \end{array}\right\} \tag{2}$$

The definition of the non-dimensional independent variables are as following: the time $\tau \equiv t/t_c$, where t_c is the vaporisation time $t_c \equiv \varepsilon(\bar{a}_0^2/\alpha_\infty)$ and the radial coordinate $x \equiv r/\bar{a}_0$; $\varepsilon \equiv \rho_\infty/\rho_l$ is the ratio of the gas density to the liquid density and $\alpha_\infty \equiv k_\infty/(\rho_\infty c_{p\infty})$ is the thermal diffusivity. The definition of the non-dimensional dependent variables (temperature, density, oxygen mass fraction, fuel mass fraction and velocity, respectively) are as following: $\theta \equiv T/T_\infty$, $\varrho \equiv \rho/\rho_\infty$, $y_O \equiv Y_O/Y_{O\infty}$, $y_F \equiv Y_F$ and $v \equiv V\bar{a}_0/\alpha_\infty$. The parameters in Eqs. (2) are defined as: Lewis number $Le_i \equiv \alpha_\infty/D_{i\,\infty}$ ($i = F, O \equiv O_2, N \equiv N_2, H \equiv H_2O, C \equiv CO_2$), $S_H \equiv Le_H\nu_H/Le_F$, $S_C \equiv Le_C\nu_C/Le_F$, $S \equiv Le_O\nu_O/[Y_O(\infty)Le_F]$, $\nu_{O_2}/Y_O(\infty)$ is mass of air to burn stoichiometrically a unit of mass of fuel according to the reaction $F + \nu_O O_2 \rightarrow \nu_H H_2O + \nu_C CO_2$. Heat of combustion Q is defined as $Q \equiv q/(Le_F c_{p\infty} T_\infty)$. The function h represents the enthalpy, defined as

$$h \equiv \frac{1}{c_{p\infty}T_\infty}\int_{T_{ref}}^{T}\sum_i Y_i c_{pi} dT$$

in which $i = F,\ O,\ N,\ H,\ C$ and $c_{p\infty} = Y_O(\infty)c_{pO}(T_\infty) + Y_N(\infty)c_{pN}(T_\infty)$.

Since the fuel oxidation kinetic mechanism is supposed to be one-step and the reaction rate follows Arrhenius type,

$$\dot{\omega}_F = \frac{Ba_0^2}{\alpha_\infty}\frac{\rho_\infty^{n_1+n_2-1}}{W_O^{n_1}W_F^{n_2}} y_O^{n_1} y_F^{n_2} exp(-\theta_a/\theta) \tag{3}$$

where W_i is the molecular weight of species i and the non-dimensional activation energy is defined by $\theta_a \equiv E/RT_\infty$;

The non-dimensional vaporisation rate is $\lambda = \dot{m}/(4\pi\bar{a}_0 k_\infty/c_p)$ and the non-dimensional droplet radius, $a = \bar{a}/\bar{a}_0$. According to d^2 law, the ratio λ/a, known as vaporisation constant and defined as β, depends on the heat flux to the droplet imposed by the flame and is a constant value.

Equations (2) are integrated from the droplet surface $x = a$ to the ambient atmosphere $x \to \infty$, the flame is at a position between these two boundaries. The conditions for these two boundaries are: at $x = a \equiv \bar{a}/\bar{a}_0$:

$$\frac{x^2\theta^n}{Le_H}\frac{\partial y_H}{\partial x} = \lambda y_H, \quad \frac{x^2\theta^n}{Le_C}\frac{\partial y_C}{\partial x} = \lambda y_C,$$

$$-\frac{x^2\theta^n}{Le_F}\frac{\partial y_F}{\partial x} = \lambda(1 - y_{Fs}), \quad x^2\theta^n\frac{\partial \theta}{\partial x} = \lambda l + q^- = \lambda l',$$

$$\theta = \theta_s, \quad y_F = y_{Fs} = exp[\gamma(1 - \theta_b/\theta_s)] \tag{4}$$

and for $x \to \infty$:

$$\theta - 1 = y_O - 1 = y_F = y_H = y_C = 0 \tag{5}$$

The subscript s represents the droplet surface condition. The non-dimensional latent heat l is expressed by $L/(c_pT_\infty)$, q^- is the heat to inside the droplet. The modified non-dimensional latent heat γ is defined as $\gamma = L/RT_b$.

In this work, it is admitted uniform temperature profile inside the droplet and close to the boiling value, $\theta = \theta_s < \theta_b$. Thereby, the mass conservation equation for the liquid phase leads to

$$\frac{da^2}{d\tau} = -2\frac{\lambda}{a} \tag{6}$$

The closure for the system of equations is provided by the dimensionless equation of state of the gas, $\varrho\theta = 1$.

According to the type of the problem, at the flame $x = x_p$, the properties are

$$\theta - \theta_p = y_F - y_{Fp} = y_0 - y_{Op} = 0 \tag{7}$$

Equation (7) expresses the droplet problem in a general form, either fuel and oxygen leak by the flame. Under reactants leakage condition, the flow field analysis does not provide a closed solution. The flame properties (position and temperature of the flame) and the droplet properties (droplet temperature and vaporisation rate) are determined as a function of the fuel leakage quantity. For these conditions, the Shvab-Zel'dovich formulation with the excess enthalpy $H \equiv (S + 1)\theta/Q + y_F + y_O$ and the fuel and oxygen mixture fraction $Z \equiv Sy_F - y_O + 1$ (Fachini, 1999),

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\left(x^2\theta^n\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\left\{\begin{array}{l}[(Le_F - 1)/S]\,\partial Sy_F/\partial x + \\ \\ (1 - Le_O)\partial(-y_O)/\partial x - [(S+1)/Q]\partial(\theta - h)/\partial x\end{array}\right\} = 0 \tag{8}$$

$$\frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \frac{1}{x^2}\left(x^2\theta^n\frac{\partial Z}{\partial x}\right) + \frac{\lambda}{x^2}\left\{\begin{array}{l}(Le_F - 1)\partial Sy_F/\partial x + \\ \\ (Le_O - 1)\partial(-y_O)/\partial x\end{array}\right\} = 0 \tag{9}$$

is not able to solve the problem in a closed form. To determine the solution is necessary to integrate the species conservation equations together with Eqs. (8) and (9).

The equations for H and Z satisfy the boundary conditions at the droplet surface $x = a$, which are determined from Eq. (3),

$$H_s \equiv \frac{(S+1)}{Q}\theta_s + y_{Fs}, \quad F_H \equiv \frac{x^2\theta^n}{\lambda}\left.\frac{\partial H}{\partial x}\right|_a = \frac{(S+1)}{Q}l' - Le_F(1 - y_{Fs}), \tag{10}$$

$$Z_s \equiv Sy_{Fs} + 1, \qquad F_Z \equiv \frac{x^2\theta^n}{\lambda}\left.\frac{\partial Z}{\partial x}\right|_{x=a} = -SLe_F(1 - y_{Fs}) \tag{11}$$

at the flame $x = x_p$, the boundary conditions are given from Eq. (7),

$$H(x_p) = (S + 1)\theta_p/Q + y_{Fp} + y_{Op}, \qquad Z(x_p) = Sy_{Fp} - y_{Op} + 1, \tag{12}$$

and for the ambient atmosphere $x \to \infty$

$$H(\infty) = (S + 1)/Q + 1, \qquad Z(\infty) = 0, \tag{13}$$

3. BURKE-SCHUMANN KINETIC

Burke-Schumann kinetic mechanism considers the reactions infinitely fast, thereby by the flame there is no leakage of reactants. The following condition is satisfied $y_F.y_O = 0$, or $y_{Fp} = y_{Op} = 0$ at the flame. Under this condition, the flame takes place where the fuel flux meets the oxidant flux in stoichiometric proportion and the position is defined as $x = x_p = x_f$. Thereby, by imposing no leakage condition, Eqs. (8) and (9) simplify to (Fachini, 1999; Fachini et al., 1999),

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left(H + \int_{Z_s}^{Z} N(Z)dZ\right) - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\theta^n\frac{\partial H}{\partial x}\right) = \frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[\frac{(S+1)}{Q}(\theta - h)\right] \tag{14}$$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} L(Z)dZ - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\theta^n\frac{\partial Z}{\partial x}\right) = 0 \tag{15}$$

in which

$$N(Z) = \begin{cases} (Le_F - 1)/S, & Z > 1 \\ (1 - Le_O), & Z < 1 \end{cases}, \qquad L(Z) = \begin{cases} Le_F, & Z > 1 \\ Le_O, & Z < 1 \end{cases}$$

From the definition of the functions H and Z, the original variables are defined as following:

$$\theta = \begin{cases} [H - (Z-1)/S]Q/(S+1), & Z > 1 \\ [H + (Z-1)]\,Q/(S+1), & Z < 1 \end{cases}, \qquad \begin{matrix} y_F = (Z-1)/S, & Z > 1 \\ y_O = (1 - Z), & Z < 1 \end{matrix}$$

The fuel and H_2O and fuel and CO_2 mixture fractions are found in the same way as the previous conservative functions,

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left(Le_H\, y_H + S_H\, Le_F\, y_F\right) - \frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2\theta^n\frac{\partial}{\partial x}(y_H + S_H\, y_F)\right] = 0 \tag{16}$$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left(Le_C\, y_C + S_C\, Le_F\, y_F\right) - \frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2\theta^n\frac{\partial}{\partial x}(y_C + S_C\, y_F)\right] = 0 \tag{17}$$

By expressing the fuel mass fraction in terms of mixture fraction Z in Eqs. (16) and (17) and integrating Eqs. (14) and (17) from the droplet surface up to a position x, the following system of equations are found

$$\frac{\partial H}{\partial(\lambda/x)} = -\frac{1}{\theta^n}\left\{H - H_s + F_H + \int_{Z_s}^{Z} N(Z)dZ - \frac{(S+1)}{Q}\left[(\theta - h) - (\theta_s - h_s)\right]\right\} \tag{18}$$

$$\frac{\partial Z}{\partial(\lambda/x)} = -\frac{1}{\theta^n}\left\{\int_{Z_s}^{Z} L(Z)dZ + F_Z\right\} \tag{19}$$

$$\frac{\partial y_H}{\partial(\lambda/x)} = -\frac{1}{\theta^n}\left\{Le_H\, y_H + S_H\, Le_F\left[\left.\frac{(Z-1)}{S}\right|_{Z>1} - 1\right] - \frac{S_H}{S}\left.\frac{\partial(Z-1)}{\partial(\lambda/x)}\right|_{Z>1}\right\} \tag{20}$$

$$\frac{\partial y_C}{\partial(\lambda/x)} = -\frac{1}{\theta^n}\left\{Le_C\, y_C + S_C\, Le_F\left[\left.\frac{(Z-1)}{S}\right|_{Z>1} - 1\right] - \frac{S_C}{S}\left.\frac{\partial(Z-1)}{\partial(\lambda/x)}\right|_{Z>1}\right\} \tag{21}$$

The value of F_H and F_Z are given by Eqs. (10) and (11).

The system of equations (18) to (21) has two eigenvalues: the droplet surface temperature θ_s and the vaporisation constant $\beta \equiv \lambda/a$. As the equations are written, the determination of these eigenvalues occurs simultaneously and together with the solution.

3.1 Simplification for the condition $\theta_s < \theta_b$

For the condition $\theta_s < \theta_b$, the fuel mass fraction at the droplet surface never reaches the value one. Thus, the fuel mass fraction flux at that position is different from zero, according Eq. (4), and the Z flux is different from zero. As a consequence, the right side of Eq. (19) is also different from zero at $x = a$, $\int_{Z_s}^{Z} +F_Z \neq 0$. Under this condition, the excess enthalpy H and the fuel and H_2O and fuel and CO_2 mixture fractions equations, Eqs. (18), (20) and (21), to can be expressed as a function of the mixture fraction Z as following (Fachini, 1999; Lima et al., 2006; Fachini, 2006)

$$\frac{dH}{dZ} = \frac{H - H_s + F_H + \int_{Z_s}^{Z} N(Z)dZ - [(S+1)/Q]\,[(\theta - h) - (\theta_s - h_s)]}{\int_{Z_s}^{Z} L(Z)dZ + F_Z} \tag{22}$$

$$\frac{dy_H}{dZ} = \frac{Le_H\; y_H}{\int_{Z_s}^{Z} L(Z)dZ + F_Z} + \frac{1}{\int_{Z_s}^{Z} L(Z)dZ + F_Z} \left\{ \begin{array}{r} S_H\; Le_F\; [(Z-1)/S - 1]|_{Z>1} \\ -S_H\; Le_F|_{Z<1} \end{array} \right\} - \left\{ \begin{array}{r} S_H/S|_{Z>1} \\ 0|_{Z<1} \end{array} \right\} \tag{23}$$

$$\frac{dy_C}{dZ} = \frac{Le_C\; y_C}{\int_{Z_s}^{Z} L(Z)dZ + F_Z} + \frac{1}{\int_{Z_s}^{Z} L(Z)dZ + F_Z} \left\{ \begin{array}{r} S_C\; Le_F\; [(Z-1)/S - 1]|_{Z>1} \\ -S_C\; Le_F|_{Z<1} \end{array} \right\} - \left\{ \begin{array}{r} S_C/S|_{Z>1} \\ 0|_{Z<1} \end{array} \right\} \tag{24}$$

$$\frac{\partial Z}{\partial(\lambda/x)} = -\left[\frac{\theta^n}{\int_{Z_s}^{Z} L(Z)dZ + F_Z}\right]^{-1} \tag{25}$$

From Eq. (25), the mixture fraction Z is a function of the position, $Z = Z(x)$. From Eqs. (10), (11) and (13), the behaviour of Z can be studied. Since $Z_s > Z(\infty)$ and $\partial Z/\partial x|_a < 0$, then Z decreases monotonically and $x = x(Z)$ is found.

The advantage of this formulation over that represented by Eqs. (18) to (21) is the decouple of the eigenvalues. As can be seen, the system of equations represented by (22), (23) and (24) can be integrated independently from (25). Therefore, the eigenvalue θ_s is determined independently from the other one, β. Once knowing θ_s and the temperature profile $\theta(Z)$, the value for Z_s is specified and problem characterised by Eq. (19) is solved and β and $Z = Z(x)$ are determined with the imposition of two boundary conditions: $Z(x = a) = Z_s$ and $Z(x \to \infty) = 0$, according to Eqs. (11) and (13).

4. COMMENTS

The problem integration can follow by two ways: explicit or implicit. The explicit method is as following. The solution of Eq. (22) permits to determine the temperature at the droplet surface θ_s, the eigenvalue of the excess enthalpy equation and, at same time, the limit of the mixture fraction Z space Z_s ($0 \leq Z \leq Z_s$) via Eq. (4). As part of the solution of Eq. (22), the flame temperature θ_f ($Z = 1$) is obtained. Note that the limit of the boundary $Z = Z_s$ in the mixture fraction Z space depends on H_2O and CO_2 mass fractions, which are initially a guess. The equations for y_H and y_C [Eqs. (23) and (24)] can be integrated to have a better approximation for those species profiles. The procedure is repeated up to converging the solutions. After that, the integration of the equation for mixture fraction Z is proceeded to determine the dependence of the dependent variables on the physical space x. The position of the flame x_f is determined by imposing the condition $Z = 1$. The implicit method consists of integrating simultaneously Eqs. (22) to (25).

The problem presents another eigenvalue besides the droplet surface temperature θ_s, the vaporisation constant $\beta \equiv \lambda/a$. As expressed by the mixture fraction equation, this eigenvalue is the boundary of the problem in the physical space, $\lambda/x = \lambda/a$, at $Z = Z_s$. All parameters in the problem influentiate the vaporisation constant β, $\beta = \beta(n, Le_F, Le_O)$.

The difference between the specific heat constant model and the specific heat variable model is expressed explicitly by the source term in the excess enthalpy equation (18),

$$[(S+1)/Q][(\theta - h) - (\theta_s - h_s)]$$

Note that, the source term becomes zero for specific heat constant.

According to the equation for function H, the model for droplet combustion with specific heat constant is overestimated in parts of the domain where the condition $(\theta - h) - (\theta_s - h_s) < 0$ is found and is underestimated where $(\theta - h) - (\theta_s - h_s) > 0$. The effect of considering specific heat constant is already known, but the present work reveals directly this feature in the model.

It is worth to mention that transport coefficients as well as thermodynamic coefficients have influence on the droplet properties, i.e. vaporisation rate β and the droplet temperature θ_s, and on the flame properties, i.e. flame position x_f flame temperature θ_f. Explicitly on the excess enthalpy equation via enthalpy, thermodynamic coefficients influentiate the temperature profile, as seen in Figure 1, and implicitly on the reactants profiles via temperature dependence of transport coefficients on temperature (see Figure 2).

The considered hypotheses are infinitely thin flame (or infinitely fast reaction) and the transport coefficients are proportional. From this analysis, it is seen that the second hypotheses can be partially modified. The proportionality among the transport coefficients is still necessary, but it can be different depending on which flame side (fuel zone or oxygen zone) is being considered.

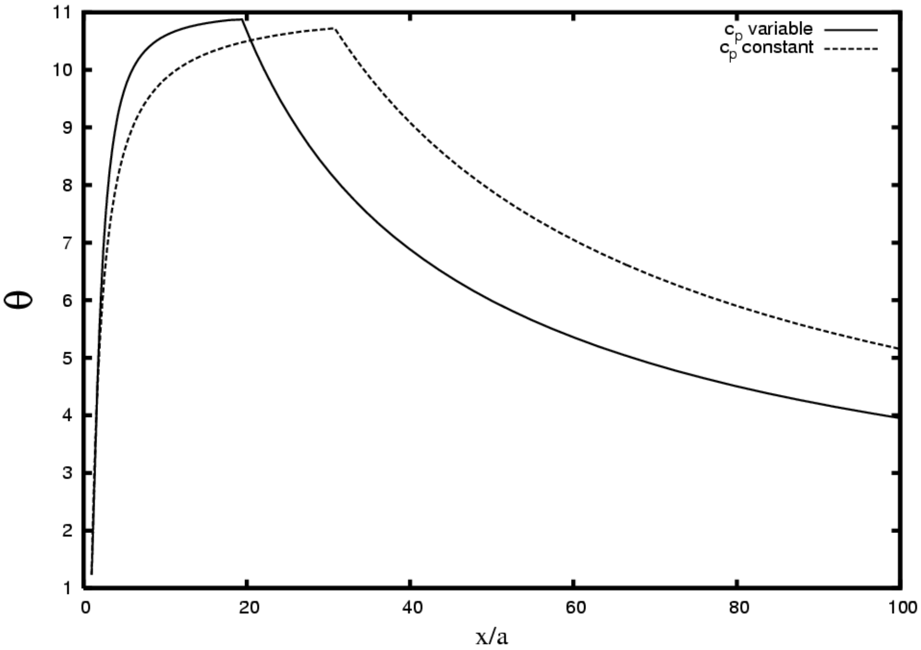

Figure 1. Non-dimensional temperature $\theta \equiv T/T_\infty$ as a function of non-dimensional radius x/a

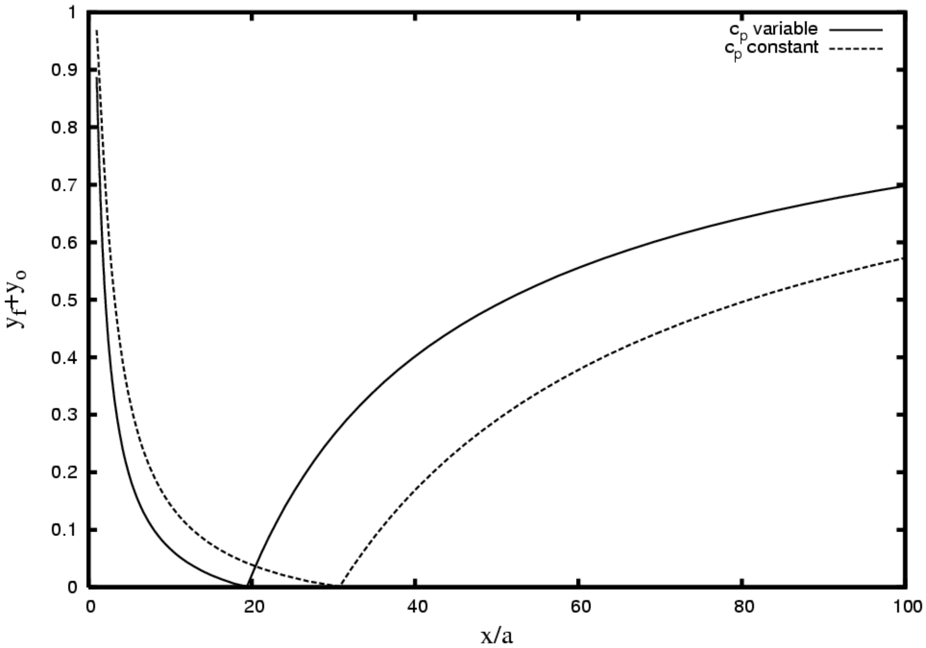

Figure 2. Reactants mass fractions $y_f + y_o$ as a function of non-dimensional radius x/a

The figures 1 and 2 show the temperature and reactants profiles around a droplet of radius a. The maximum value of θ in figure 1 and the minimum value for the $y_f + y_o$ function determine the value of the flame position x_f. These figures show that the flame position comes closer to the experimental value when the variation of the thermodynamics coefficients on the temperature and composition is considered. This value decreases from 30.75 to 19.41. The value $x_f = 19.41$ is still far from the experimental one, that is about 7 and the causes for the discrepancies among the experimental results and theoretical results are due to the soot formation and radiative energy loss (Jackson and Avedisian, 1994; Mikami et al., 1994; Jackson and Avedisian, 1996; Nayagan et al., 1998; Manzello et al., 2000). Thereby, the inclusion in the model of these two processes will bring the experimental results close to the theoretical results (Kumar et al., 2002; Fachini, 2006).

5. CONCLUSION

In order to include a droplet combustion model in a spray combustion simulation, the model must represents well the physics and be very computationally economic. Based on that, it is presented a droplet combustion model in which is considered the thermodynamic and transport coefficients variable with temperature and composition. The Shvab-Zel'dovich formulation is employed to avoid the chemical reaction term and to reduce the system of equations and the flamelet formulation is employed to avoid the calculation of the two eigenvalues simultaneously. Due to the characteristic of the problem, the system of equations could be simplified to a first order ordinary differential equation system. This system of equations permits to be integrated explicitly or implicitly.

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