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SPRAY-FLAMELET APPROACH BY MEANS OF A MONOTONIC CUMULATIVE MIXTURE FRACTION VARIABLE

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Abstract. *The external structure of the spray-flamelet can be described using the Schvab-Zel'dovich-Liñan formulation. The mixture-fraction variable Z normally employed for the description of gaseous diffusion flames leads to non-monotonicity behavior for spray flames due to extra fuel supplied by vaporization of droplets distributed into the flow. Therefore, spray flames depend not only on Z and the scalar dissipation rate, but also on the spray source term. Since the mixture fraction is locally normal to the surface of stoichiometric mixture, its cumulative value, $Z_C = \int_{-\infty}^{z} Z(t)dt/Z_C^T$, can also be considered as a coordinate variable that guarantees monotonicity. This new quantity includes spatial information about the whole mixture fraction due to gaseous phase and droplet vaporization. For pure gaseous flow, the well-established description in terms of Z is recovered. The spray-flamelet structure and the new equations of temperature and mass fractions in terms of Z_C are derived. The proposed formulation is applied in a counterflow configuration. The numerical results are obtained for ethanol spray and presented for the temperature and mass fractions in terms of Z_C. The accuracy of the results confirms the validity of the proposed formulation.*

Keywords: *counterflow diffusion flame, spray-flamelet, cumulative mixture fraction, monotonic variable*

Nomenclature

$\bar{l}_c$	characteristic length
$\dot{\bar{m}}_k$	vaporization rate
$\dot{\omega}_k$	dimensionless specific chemical reaction rate
ν_k	stoichiometric mass coefficient
ρ	dimensionless gas density
Θ	dimensionless temperature
c_p	specific heat
D	diffusion coefficient
K	conductivity
k	index of the species ($k = 1, \cdots, n$)
l_k	dimensionless latent heat
Le_k	fuel Lewis number
Le_O	oxygen Lewis number

$N_{k_{spray}}$ total number of droplets in the spray

Pe Peclet number

q_k dimensionless heat of combustion

S_k dimensionless source of mass due to the presence of droplets in the flow field

u_i dimensionless gas velocity in i direction

$V_{k_{spray}}$ spray volume

(Θ_B) T_B (dimensionless) boiling temperature

(a_k) $\bar{a}_k$ (dimensionless) droplet radius

(Y_O) $\bar{Y}_O$ (dimensionless) oxidant mass fraction

(Y_{Fk}) $\bar{Y}_{Fk}$ (dimensionless) fuel mass fraction of species k

1. INTRODUCTION

The flame structure of laminar gaseous diffusion flames is tipically studied in terms of the gaseous mixture fraction (Peters, 1984). Besides enabling a computationally more efficient solution in composition space compared to the solution in physical-space, the mixture fraction concept is also used in turbulent combustion models. By simply extending this formulation to spray flames, though it enables the analysis tools developed for gaseous flames to be further applied, the classical gaseous mixture-fraction becomes non-monotonic due to vaporization sources (Luo *et al.*, 2013; Sanchez *et al.*, 2015; Franzelli *et al.*, 2015; Olguin and Gutheil, 2014). The constraint of monotonicity is required to guarantee the existence of the derivative and of a single valued solution. In addition to the gaseous mixture fraction, other composition spaces have been proposed such as the total mixture fraction (Smith *et al.*, 2000; Vié *et al.*, 2013; Urzay *et al.*, 2014) and the conserved mixture fraction (Franzelli *et al.*, 2015). The above definitions are not monotonicity preserving due to differential diffusion between liquid and gaseous phases and the presence of a slip velocity between the phases. An effective composition variable combining the gaseous mixture fraction and the liquid-to-gas mass ratio was applied to the analysis of counterflow spray flames (Franzelli *et al.*, 2015). This variable was employed for the derivation of a spray-flamelet formulation that were solved together with closure models for the scalar dissipation and the velocity field. The flame structure response to variations of droplet diameter and strain rate were correctly reproduced by this formulation. The focus of this work is to propose an alternative monotonic variable that enables the description of spray flames. This new variable, called cumulative mixture fraction Z_C, consists of the integration of the usual gaseous mixture fraction Z over physical space. This formulation leads to an initially increasing function that reaches a plateau at later times thereby guaranteing its monotonicity. In the present manuscript, the spray-flamelet equations in Z_C-space are derived and preliminary simulation results are presented, in both, physical and composition space.

2. MODEL DESCRIPTION

A planar counterflow configuration is considered, consisting of a mono-disperse fuel spray injected from the left and air from the right side of the stagnation plane, as shown in Fig. 1. The governing equations are formulated in an Eulerian frame of reference assuming steady-state, constant gas density and the low-Mach number approximation. An infinite reaction rate of the Burke-Schumann kinetic mechanism is considered, enabling the diffusion flame to be described in terms of the extended Shvab-Zel'dovich model. The set of droplets composing the spray are assumed to be monodisperse, mono-temperature and monokinetic. The spray is considered dilute and there is no interaction between droplets or secondary break-up. This simple model avoids physical and chemical aspects previously addressed by Continillo and Sirignano (1990); Fachini (1999); Fachini *et al.* (1999). No leakage of fuel and oxidant through the flame is considered. There is no droplet-gas relative motion. The droplets are injected close to the flame region at their boiling temperature and are assumed to vaporize completely (Maionchi and Fachini, 2013; Maionchi, 2017).

A single global reaction step is used to represent the combustion processes according to

$$F + \nu_k O_2 \rightarrow (1 + \nu_k) P + q_k.$$

The flow field is described by linear functions of the axial and transverse spatial components of the velocity given respectively by $(u, v) = (-Az, Ax)$. This consideration means that the flow field is not modified by mass addition due to droplet vaporization or by volume change of the gaseous phase caused by temperature variation (Maionchi and Fachini, 2013). The model for the vaporization of isolated droplets was developed in a previous work (Maionchi and Fachini, 2013). The solution of the problem is obtained by solving the differential equations for the mixture fraction Z and the excess of enthalpy H in Z_C-space which can be readily converted to physical space using appropriate transformations. The temperature and mass fraction profiles can be computed from from Z and H.

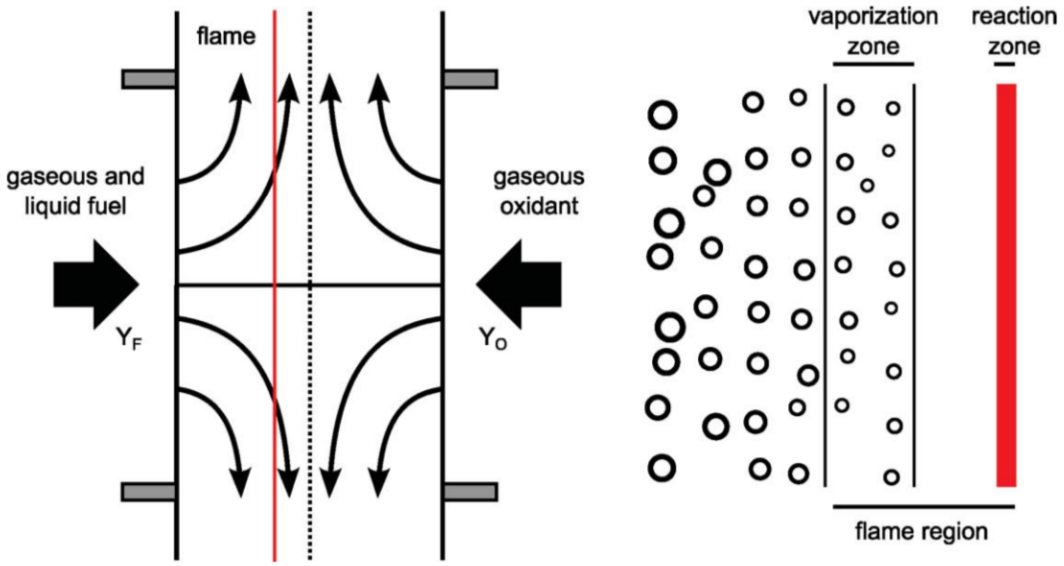


Figure 1. Spray-flamelet model with multi-component fuel injected from the left and air from the right side. The droplets are shown in the flame region.

2.1 The Gaseous Phase

The gaseous phase can be described by the following dimensionless conservation equations of mass, chemical species mass fractions and energy (Maionchi and Fachini, 2013; Maionchi, 2017),

$$\frac{\partial}{\partial x_i}\left[\rho u_i \begin{pmatrix} 1 \\ Le_O Y_O \\ Le_{F_k} Y_{F_k} \\ \Theta \end{pmatrix}\right] = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial}{\partial x_i}\begin{bmatrix} 0 \\ Y_O \\ Y_{F_k} \\ \Theta \end{bmatrix}\right) + \begin{bmatrix} 0 \\ \sum\limits_k \dot{\omega}_k \\ \dot{\omega}_k \\ -\sum\limits_k q_k \dot{\omega}_k \end{bmatrix} + \begin{bmatrix} S_m \\ 0 \\ \delta_{lk} S_k \\ S_e \end{bmatrix}, \tag{1}$$

The sources of mass and energy are given by $S_m = \sum\limits_k \delta_{lk} S_k$ and $S_e = -\sum\limits_k \delta_{lk} l_k S_k$ on the fuel side, and equal to zero on the oxidant side.

The elimination of the chemical reaction rate can be achieved by the Schvab-Zel'dovich-Liñan formulation (Liñan, 1991; Liñan and Williams, 1993; Liñan, 2001; Maionchi, 2017), which leads to the following equations

$$\frac{\partial}{\partial x_i}\left(\rho u_i \int_0^Z L(Z) dZ\right) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Z}{\partial x_i}\right) + \frac{S_Z}{1+\sum\limits_k \Phi_k}, \tag{2a}$$

$$\frac{\partial}{\partial x_i}\left(\rho u_i H_N\right) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial H}{\partial x_i}\right) + \frac{S_H}{1+\sum\limits_k \Phi_k}. \tag{2b}$$

in which $H_N = H + \int_0^Z N(Z) dZ$. The distributed source terms $S_Z(Z)$ and $S_H(Z)$ and the functions $L(Z)$ and $N(Z)$ are given by

$$S_Z(Z) = \begin{cases} 0, & Z < Z_f, \\ S_m + \frac{\partial}{\partial x_i}\left[\rho u_i \sum_{k=2}^n (Le_1 - Le_k) Y_{F_k}\right], & Z > Z_f, \end{cases} \tag{3a}$$

$$S_H(Z) = \begin{cases} 0, & Z < Z_f, \\ S_e - S_m + \sum\limits_k \delta_{lk} q_k S_k + \frac{\partial}{\partial x_i}\left\{\rho u_i \sum_{k=2}^n [(Le_1 - 1)(q_1 - 1) - (Le_k - 1)(q_k - 1)] Y_{F_k}\right\}, & Z > Z_f, \end{cases} \tag{3b}$$

$$L(Z) = \begin{cases} Le_0, & Z < Z_f, \\ Le_1, & Z > Z_f, \end{cases} \tag{3c}$$

$$N(Z) = \begin{cases} 1 - Le_0, & Z < Z_f, \\ (1 - Le_1)(1 - q_1), & Z > Z_f. \end{cases} \tag{3d}$$

The mixture fraction and the excess of enthalpy are defined as

$$Z \equiv \frac{1+\sum_k Y_{F_k} - Y_O}{1+\sum_k \Phi_k}, \qquad H = \frac{\Theta + \sum_k (q_k - 1) Y_{F_k} + Y_O}{1+\sum_k \Phi_k}, \tag{4}$$

in which $\Phi_k = \nu_k Le_O \bar{Y}_{F_{k-\infty}} / (Le_{F_k} \bar{Y}_{O_{+\infty}})$ is the mixture strength representing a modified equivalence ratio for diffusion flames. Note at the flame position $Y_O = Y_{F_k} = 0$, leading to $Z_f = (1+\sum_k \Phi_k)^{-1}$ and $H_f = \Theta_f (1+\sum_k \Phi_k)^{-1}$.

Besides Eqs. (2) and (3), $n-1$ conservation equations of the following type must be integrated for $k = 2, \cdots, n$ to solve the problem,

$$Le_{F_k} \frac{\partial (\rho u_i Y_{F_k})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_{F_k}}{\partial x_i} \right) + \delta_{lk} S_k, \tag{5}$$

which assumes that there is no escape of reactants at the flame. Note that the Lewis number Le_1 and the heat release rate q_1 in Eq. (3) are related to the only fuel whose conservation equation (5) does not need to be integrated. In the counterflow configuration, the boundary conditions are given by

$$\begin{aligned} &Z \equiv 1, \quad H = [\Theta_{-\infty} + \sum_k (q_k - 1)\Phi_k]/(1+\sum_k \Phi_k), \quad \text{for} \quad x_i \to -\infty, \\ &Z = 0, \quad H = (\Theta_{+\infty} + 1)/(1+\sum_k \Phi_k), \qquad\qquad\quad \text{for} \quad x_i \to +\infty. \end{aligned} \tag{6}$$

The source term is given by $S_k = M_k \lambda_k$, which is obtained from non-dimensionalization of the governing conservation equations (Maionchi and Fachini, 2013). Part of this term describing the vaporization process in Eqs. (2) is zero for i) $z < z_0$ (i.e. $M_k = 0$), and ii) $z > z_a$, in which droplets are totally vaporized (i.e. $\lambda_k = 0$). The model assumes that all droplets have to vaporize before the flame position z_f, which means that $z_a < z_f$.

The vaporization rate is given by $\lambda_k = c_p \dot{\bar{m}}_k / 4\pi \bar{a}_{k_0} \bar{K}_{+\infty}$ in which the index 0 denotes the initial droplet radius. It can be obtained from the model for the vaporization of isolated droplets (Maionchi and Fachini, 2013). The spray combustion parameter, which combines properties of mass transfer Le_O, heat transfer Pe, chemical reaction $(\nu_k / \bar{Y}_{O_{+\infty}})$, flow field $(\bar{l}_c / \bar{a}_{k_0})$, and spray $(\bar{a}_{k_0}^3 N_{k_{spray}} / V_{k_{spray}})$, is given by

$$M_k = 4\pi \left(\frac{Le_O}{Pe} \right) \left(\frac{\nu_k}{\bar{Y}_{O_{+\infty}}} \right) \left(\frac{\bar{l}_c}{\bar{a}_{k_0}} \right)^2 \left(\frac{\bar{a}_{k_0}^3 N_{k_{spray}}}{V_{k_{spray}}} \right). \tag{7}$$

The combustion process can be conveniently studied by analyzing this parameter only and not the individual influence of each of the properties just described.

2.2 The Spray-Flamelet Strucuture

The laminar spray-flamelet equations follow the formulation derived in (Peters, 1984; Franzelli *et al.*, 2015), accounting for the vaporization source term due to the presence of droplets. It is assumed that the physical coordinate along the direction normal to the surface of stoichiometric mixture fraction can be expressed in terms of the generic variable ξ according to the transformation $(x_1, x_2, x_3) \to (\xi(x_i), \xi_2, \xi_3)$. The spatial derivatives yield

$$\frac{\partial}{\partial x_1} = \frac{\partial \xi}{\partial x_1} \frac{\partial}{\partial \xi}, \qquad \frac{\partial}{\partial x_i} = \frac{\partial}{\partial \xi_i} + \frac{\partial \xi}{\partial x_i} \frac{\partial}{\partial \xi}, \quad for \quad i = 2, 3. \tag{8}$$

The high-order contributions are neglected because the derivatives along the ξ-direction are much larger in comparison to the ξ_2 and ξ_3 directions.

The transformation from the physical space to the new system of coordinates leads to the following expressions for

the gas phase:

$$\sqrt{\frac{\chi_\xi}{2D}}\frac{\partial(\rho u_i)}{\partial\xi} = S_m, \tag{9a}$$

$$\Sigma^\dagger_{\xi,Le_O}\frac{\partial Y_O}{\partial\xi} = \frac{\rho\chi_\xi}{2}\frac{\partial^2 Y_O}{\partial\xi^2} + \sum_k \dot{\omega}_k, \tag{9b}$$

$$\Sigma^\dagger_{\xi,Le_{F_k}}\frac{\partial Y_{F_k}}{\partial\xi} = \frac{\rho\chi_\xi}{2}\frac{\partial^2 Y_{F_k}}{\partial\xi^2} + \dot{\omega}_k + \delta_{kF}S_k - Le_{F_k}Y_{F_k}S_m, \tag{9c}$$

$$\Sigma^\dagger_{\xi,1}\frac{\partial\Theta}{\partial\xi} = \frac{\rho\chi_\xi}{2}\frac{\partial^2\Theta}{\partial\xi^2} - \sum_k q_k\dot{\omega}_k + S_e - \Theta S_m, \tag{9d}$$

$$\Sigma^\dagger_{\xi,1}\frac{\partial}{\partial\xi}\left(\int_0^Z L(Z)dZ\right) = \frac{\rho\chi_\xi}{2}\frac{\partial^2 Z}{\partial\xi^2} + \frac{S_Z}{1+\sum\limits_k \Phi_k} - S_m\int_0^Z L(Z)dZ, \tag{9e}$$

$$\Sigma^\dagger_{\xi,1}\frac{\partial H}{\partial\xi} + \Sigma_\xi\frac{\partial}{\partial\xi}\left(\int_0^Z N(Z)dZ\right) = \frac{\rho\chi_\xi}{2}\frac{\partial^2 H}{\partial\xi^2} + \frac{S_H}{1+\sum\limits_k \Phi_k} - S_m H_N, \tag{9f}$$

in which

$$\Sigma_\xi = \rho u_i\frac{\partial\xi}{\partial x_i}, \qquad \Sigma^\dagger_{\xi,\epsilon} = \left[\epsilon\Sigma_\xi - \frac{\chi_\xi}{2D}\frac{\partial(\rho D)}{\partial\xi} - \frac{\rho D}{2}\frac{\partial}{\partial\xi}\left(\frac{\chi_\xi}{2D}\right)\right], \qquad \chi_\xi = 2D\left(\frac{\partial\xi}{\partial x_i}\right)^2, \tag{10}$$

and the last term is defined as scalar dissipation rate.

2.3 The Liquid Phase

The model for the vaporization of isolated droplets was developed in a previous work (Maionchi and Fachini, 2013). Since the droplets follow the flow, the time dependence of the droplet radius and the vaporization rate can be written in terms of the generic variable ξ and its velocity in the spray-flamelet. The solution of the mass conservation equation is given by the following expression

$${a_k}^2 = 1 - 2\int_{\xi_0}^{\xi}\frac{\beta_k(\xi)}{u}d\xi, \quad \beta_k(\xi) = \ln\left(1 + \bar{Y}_{O+\infty}\frac{\Theta(\xi)-\Theta_B}{\nu_k l_k}\right), \tag{11}$$

in which the vaporization function is defined in terms of the vaporization rate, $\beta_k(\xi) = \lambda_k(\xi)/a_k(\xi)$ and is obtained from the classical model for droplet vaporization. The conversion from the droplet scale to the spray scale is performed considering that the ambient temperature far from the droplet corresponds to the local temperature in the spray.

2.4 The Cumulative Mixture Fraction as the Generic Variable ξ

The definition of Z_C consists in the cumulative of function Z in the one-dimensional physical space ($x_i = z$ and $u_i = u$) normalized by its value considering the entire domain, that is,

$$Z_C(z) = \frac{1}{Z_C^T}\int_{-\infty}^{z} Z(t)dt, \qquad Z_C^T = \int_{-\infty}^{\infty} Z(t)dt \tag{12}$$

Assuming the generic variable to be a strictly monotonic function, i.e. $\xi = Z_C$ for counterflow spray flames, the following simplifications are obtained

$$\frac{dZ_C}{dz} = \frac{Z}{Z_C^T}, \qquad z = z_i + Z_C^T\int_{Z_{c0}}^{Z_c}\frac{dZ_C}{Z}, \qquad \Sigma_{Z_C} = \rho u_i\frac{Z}{Z_C^T}, \qquad \chi_{Z_C} = \frac{2D}{(Z_C^T)^2}Z^2. \tag{13}$$

In this description, the complete spray-flamelet equations are reduced to

$$\frac{Z}{Z_C^T}\frac{d(\rho u)}{dZ_C} = S_m, \tag{14a}$$

$$\frac{Z}{Z_C^T}\frac{d}{dZ_C}\left[\rho D\frac{Z}{Z_C^T}\frac{dY_O}{dZ_C} - Le_O\rho u Y_O\right] = -\sum_k \dot{\omega}_k, \tag{14b}$$

$$\frac{Z}{Z_C^T}\frac{d}{dZ_C}\left[\rho D\frac{Z}{Z_C^T}\frac{dY_{F_k}}{dZ_C} - Le_{F_k}\rho u Y_{F_k}\right] = -\delta_{kF}S_k - \dot{\omega}_k, \tag{14c}$$

$$\frac{Z}{Z_C^T}\frac{d}{dZ_C}\left[\rho D\frac{Z}{Z_C^T}\frac{d\Theta}{dZ_C} - \rho u\Theta\right] = -S_e + \sum_k q_k\dot{\omega}_k, \tag{14d}$$

$$\frac{Z}{Z_C^T}\frac{d}{dZ_C}\left[\rho D\frac{Z}{Z_C^T}\frac{dZ}{dZ_C} - \rho u\int_0^Z L(Z)dZ\right] = -\frac{S_Z}{1+\sum_k \Phi_k} \tag{14e}$$

$$\frac{Z}{Z_C^T}\frac{d}{dZ_C}\left[\rho D\frac{Z}{Z_C^T}\frac{dH}{dZc} - \rho u\left(H + \int_0^Z N(Z)dZ\right)\right] = -\frac{S_H}{1+\sum_k \Phi_k} \tag{14f}$$

Note that the distributed source terms $S_Z(Z)$ and $S_H(Z)$ are still given by Eqs. (3a) and (3b) by taking $\partial/\partial x_i == (Z/Z_C^T)\partial/\partial Z_C$. For simplicity, the model considers constant thermo-diffusive properties, $\rho = 1$ and potential flow in the z direction, i.e. $u = -z$. The spatial variable z in these equations can be obtained from its definition in Eq. (13). The solution of the problem can be obtained by solving Eqs. (14e) and (14f) for Z and H together with Eq. (14c) without the chemical reaction term for $k = 1, \cdots n-1$. The temperature and mass fraction profiles can be extracted from Z and H using their definitions from Eq. (4).

2.5 Results and Discussion

Ethanol and *n*-heptane were considered as the spray fuels for the simulations ($k = 1$). Small amounts of hydrogen or methane were injected as secondary gaseous fuels ($k = 2$). The following parameters are considered in the simulations: $z_0 = -1.5$, $\bar{T}_{-\infty} = 700K$, $\bar{T}_{+\infty} = 300K$, $\bar{Y}_{O+\infty} = 0.21$, $c_p(\text{medium}) = 1.0kJ/kgK$ (average c_p of the multi-component mixture) and $M_1 = 32$, in order to agree with the values adopted previously in Maionchi and Fachini (2013); Maionchi (2017). The transport, thermodynamic and chemical parameters for each fuel participating in the reactions are given in Table 1.

Table 1. Chemical parameters.

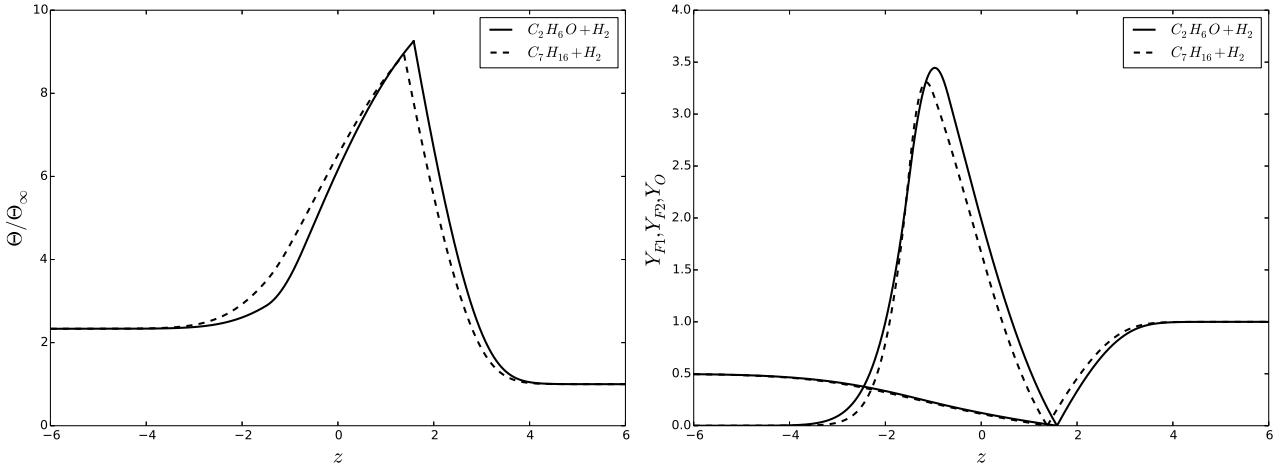
Fuel	Le	ν	$\bar{q}(kJ/g)$	$\bar{l}(kJ/g)$	$T_B(K)$
C_2H_6O	1.3	2.087	29.7	0.846	351
C_7H_{16}	1.9	3.52	48.5	0.320	371
CH_4	0.8	4.0	55.5	-	-
H_2	0.3	8.0	141.0	-	-

The simulation of biphasic and multicomponent fuels was evaluated directly in the physical space in a previous work (Maionchi, 2017). One of the results is showed in Fig. 2 for the profiles of $\Theta(z)$ and $Y_{F_k}(z)$. In this case ethanol and *n*-heptane were considered as the sprays and a small amount of hydrogen was injected, showing a quasi-universal behaviour. The flame position is characterized by $Y_O = Y_{F_1} = Y_{F_2} = 0$ in Fig. 2b which, as expected, coincides with the place where de temperature is maximum, as can be seen in Fig. 2a. The peak observed in the mass fractions appears due to the vaporization of the droplets that works as a source of heat and mass.

Note that for each position z there is only one corresponding value of Θ and Y_{F_k}, showing that these variables are uniquely defined in the physical space. In order to describe the spray-flamelet, this characteristic must be maintained in the general ξ-space. Figures 3, 4 and 5 show results for two ξ-spaces: Z and Z_C. It is evident that $Z(z)$ is a non-monotonic function and that Z_C is an optimal space for spray-flamelet description.

In Figure 3, the dependence of the temperature Θ and the mass fractions Y_{F_k} on the mixture fraction Z is presented. These simulations were performed for ethanol sprays with a small injection of light/heavy secondary fuels (methane or hydrogen), showing that these variables present a quasi-universal behaviour in the spray flamelet description (Maionchi, 2017). From these results it is possible to identify the flame position, where $Z = (1+0.5)^{-1} = 0.667$ ($Y_O = Y_{F_1} = Y_{F_2} = 0$) where the temperature reaches its maximum value.

For $Z < 1$, $\Theta(Z)$ and $Y_{F_k}(Z)$ are single-valued. However, in the range $1 < Z < Z_{max}$, there are two possible values of these variables for a given Z. Consequently, $\Theta(Z)$ and $Y_{F_k}(Z)$ are not uniquely defined in the whole Z-space. It



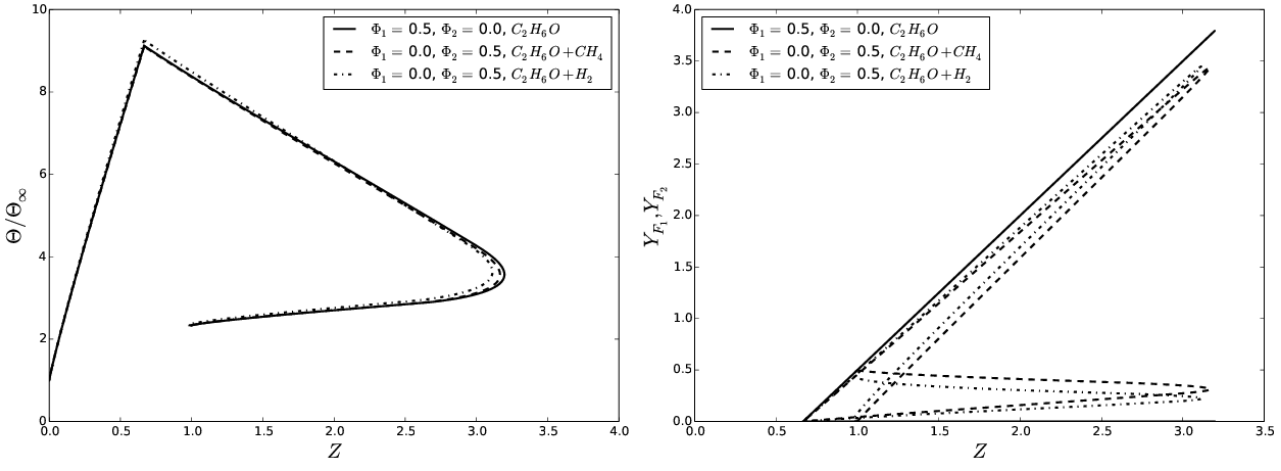
(a) (b)

Figure 2. (a) Temperature and (b) mass fractions profiles in physical space z for ethanol and *n*-heptane sprays with injection of hydrogen. Both variables are uniquely defined in the z-space.

means that a description of the spray-flamelet in Z-space is not properly defined, since it would be impossible to convert this solution back to the physical space z.

The mixture fraction Z is a monotonic function of z when the reactants are only in the gaseous phase (Peters, 1984). However, as can be seen in Fig. 4a, a given value of Z in the peak region corresponds to different positions in the physical space. Comparing to the classical results, the addition of the liquid phase is responsible for this peak.

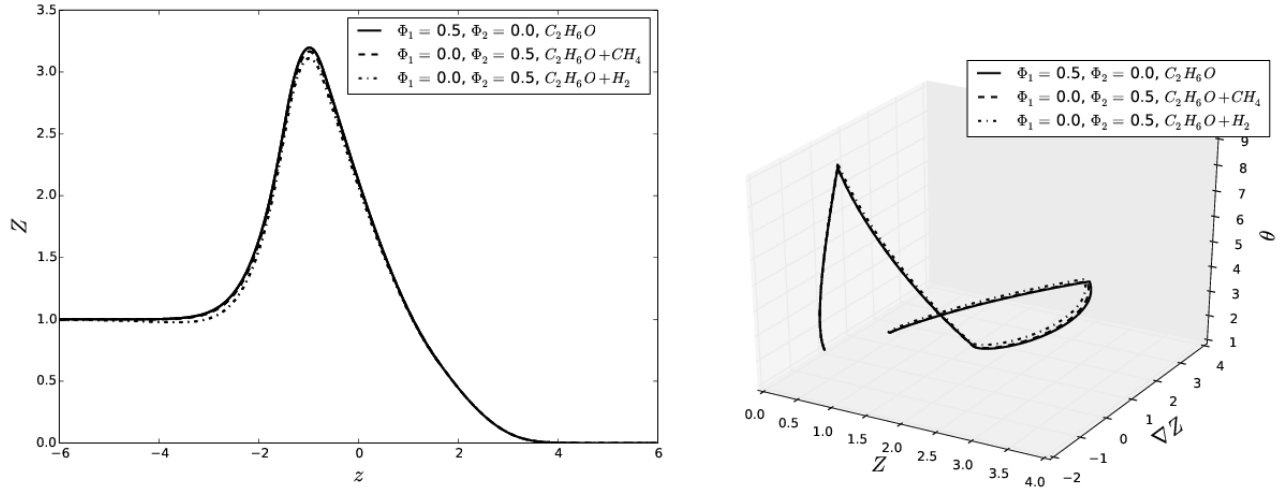
A non-monotonic behaviour is not desirable for spray-flamelet descriptions, which is the case if it is evaluated in the Z-space. A possible solution for this problem would be to describe the temperature and the mass fraction not only in terms of Z but also of another variable. In Fig. 4(b), for example, the temperature is presented as a function of Z and its gradient ∇Z (the same can be done for Y_{F_k}). It shows that for a pair of values $(Z, \nabla Z)$ just one value of temperature (or Y_{F_k}) can be found. Note that the results presented in Fig. 3 are projections of $\Theta(Z, \nabla Z)$ and $Y_{F_k}(Z, \nabla Z)$ onto the Z-space. Although this procedure could solve the problem of the non-monotonicity, it brings complications related to the mathematical description by treating it in two instead of one dimension as in the former case.



(a) (b)

Figure 3. (a) Temperature and (b) mass fractions profiles as functions of the mixture fraction Z. Comparison between different secondary fuels (methane and hydrogen) for ethanol spray. For $Z > 1$, which corresponds to the peak of the vaporization zone, both Θ and Y_{F_k} are not uniquely defined.

Finally, the profiles of temperature and fuel/oxidant mass fraction in the Z_C-space are shown in Fig. 5. These simulations were performed for light/heavy main fuels sprays (ethanol or *n*-heptane) with a small injection of hydrogen, also confirming that the temperature and the mass fractions variables present a quasi-universal behaviour in the spray flamelet description. In this space, one can still identify the flame position where $Y_F = Y_O = 0$ and the temperature reaches its

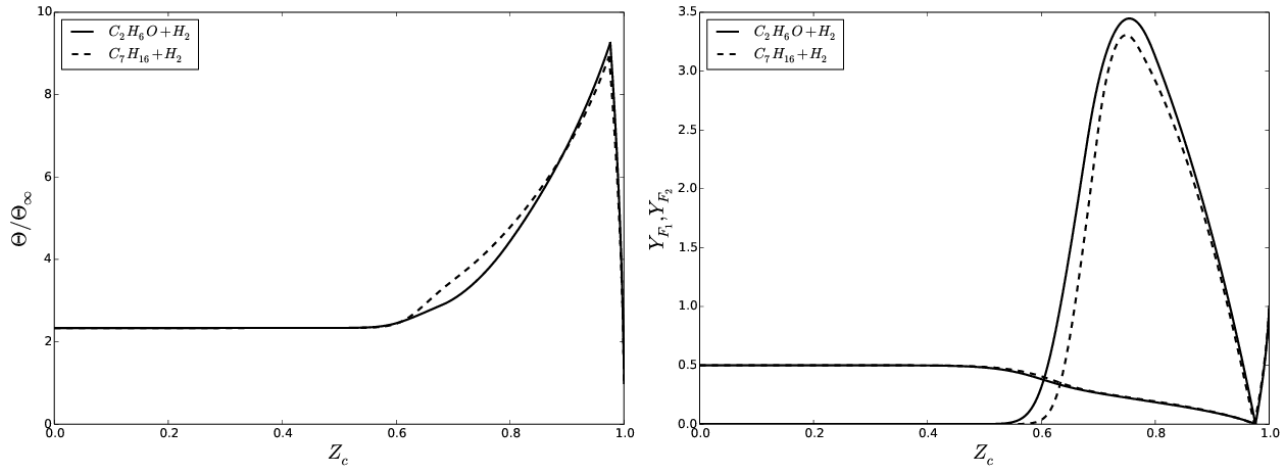


(a) (b)

Figure 4. (a) The non-monotonic mixture fraction Z in physical space z. The peak responsible for this behaviour is due to the vaporization source not present in the classical flamelet description. (b) The temperature (as well as the mass fractions) in $(Z, \nabla Z)$-space, since is uniquely defined can be used as an alternative to describe spray-flamelets.

maximum value.

Comparing these results with those presented in Fig. 2, it can be seen that the non-uniqueness problem pointed out earlier for $\Theta(Z)$ and $Y_{F_k}(Z)$ was solved using Z_C-space. By choosing the monotonic function $Z_C(z)$, the spray-flamelet description in the Z_C-space guarantees that both $\Theta(Z_C)$ and $Y_{F_k}(Z_C)$ are uniquely defined as in physical space. Moreover, an advantage over the description in the $(Z, \nabla Z)$-space is that the description remains one-dimensional.



(a) (b)

Figure 5. (a) Temperature and (b) mass fractions profiles as functions of the cumulative mixture fraction Z_C. Comparison between ethanol and *n*-heptane sprays with injection of hydrogen. Both temperature and mass fractions are uniquely defined in the Z_C-space, providing a potential solution to the problem presented in Fig. 3 for Θ and Y_{F_k} in the Z-space.

3. Conclusions

The monotonic cumulative mixture fraction variable Z_C was proposed for the description of the spray-flamelet structures. The flamelet formulation was derived and the feasibility of directly evaluating the resulting spray-flamelet equations in Z_C-space. On the contrary of the classicaly used $Z(z)$ for flamelet description, $Z_C(z)$ is a monotonic function, allowing temperature $\Theta(Z_C)$ and mass fractions $Y_{F_k}(Z_C)$ to be uniquely described in this space. In future, the model will be extended by considering relative velocities between droplets and gaseous phases as well as droplets injected at temperatures different than their boiling temperature. This work is also a first step towards the development of spray- flamelet based turbulent models, which will require development of subgrid scale models for the composition-space variable Z_C

as well as evaporation source terms.

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