

ANALYSIS OF DIFFUSION FLAMES WITH FUEL DROPLETS IN THE REACTION ZONE

Luciano Hennemann, hennemann@lcp.inpe.br

Antonio Seridonio, seridonio@lcp.inpe.br

Fernando F. Fachini, fachini@lcp.inpe.br

Laboratório de Combustão e Propulsão - LCP
Instituto Nacional de Pesquisas Espaciais - INPE
12630-000, Cachoeira Paulista, SP, Brazil

***Abstract.** This work analyses the external structure of diffusion flames established in counterflow configuration assuming fuel droplets inside the flame structure together with fuel in the gas phase. The model with reactants in the gas phase is called flamelet and this model will be called spraylet. The conservation equations were used adding extra source terms corresponding to the fuel in the liquid phase. In the energy conservation equation, the extra term is a sink which has a strength proportional to the product of the droplet vaporization rate and the latent heat. On the other hand, in the fuel species conservation equation, the extra term is a source which has a strength proportional to the droplets vaporization rate. The results point out the stability of the flame established in spray combustion.*

***Keywords:** spraylet, droplet, flamelet, diffusion flame.*

1. INTRODUCTION

Spray combustion is present in many devices, from rocket motor to house heating. The atomization of the liquid fuel in a combustion chamber is obtained when a jet or sheet of liquid is broken in droplets by aerodynamic forces, or an external mechanical energy applied through rotating or vibrating devices. The atomization process has a random behavior, so the resulting spray can be characterized by a large spectrum of different droplet sizes. Sprays are more dense in the first layers after the injection and more rarefied near the flame. The main target of the atomization is to increase the surface area between the liquid and gas phases to achieve high rates of evaporation. In diffusion flames, reducing the droplet diameter will provide high rates of volumetric heat release (Couto, 2000).

Studies with a dense cloud spray were made by Hallett (2000), where commercial petroleum is simulated with a large number of components. A quasi-steady droplet evaporation model was based on a technique of continuous thermodynamics. Williams (1985) described the importance of the spray dilution. The ratio of the volume occupied by the condensed phase to the volume occupied by the gas must be small avoiding the excess of particles collisions. With small and volatile droplets, in deflagration terms, the vaporization occurs completely and the fuel from vaporization of droplets mixes with the oxidizer in the convective and diffusive deflagration zone. This process must be done before reaching the diffusive-reactive zone and this zone will remain unchanged. But with large particles and nonvolatile fuels, the deflagration represents the combustion in premixed systems with a nonpremixed sub-structure. Kim and Sung (2003) investigated a spray of n-heptane using a model of evaporation with high pressure considering equilibrium between the liquid and gas phases. Considering source terms, Eulerian and Lagrangian descriptions were used for gas and droplet phases respectively. Two evaporation models were used for low and high pressures based on the Spalding theory (Spalding, 1953). The model shows that the lifetime of the droplets in a spray is longer at high pressures with low ambient temperature and it is shorter at a high ambient temperature.

Watanabe *et al.* (2007) studied flamelets within two-phase combustion, exploring the properties of spray fuel n-decane in a laminar counterflow using two-dimensional numerical simulation. The effects of strain rate, equivalent ratio and droplets size in terms of mixture fraction and scalar rate were examined. The motion of the droplet was calculated using a Lagrangian method. Large differences in the trends were found among the spray flame and the gaseous diffusion flame in respect of mass fractions of chemical species, gas temperature and scalar dissipation rate. The temperature of the spray flames becomes much higher than gaseous diffusion flame due to the lower scalar dissipation rate and also when premixed and diffusion combustion occurs simultaneously in the spray flame. Li (1997) discussed spray combustion in laminar stagnation flows in sprays structures such counterflowing diffusion flames. He analyzed droplet and spray

characteristics and details in the structure of the flame. Experiments with spray counterflowing burners were made in laboratory and the geometry of the flame was analyzed. Li (1997) observed that the axial velocity and all state variables (species concentrations, temperature, etc) depend on the axial coordinate and so, the conservations equations can be reduced from partial to ordinary differential equations, simplifying the theoretical and numerical analysis. For small droplets in counterflowing streams, the vaporization plane and the flame sheet decrease the distance of separation when the strain rate increases. The flame structure is determined by the ratio of heat of vaporization to heat of combustion and thus, the spray flames are distinguished from gaseous-fuel flames. Liñán (1974) studied the structure of steady state diffusion flames. A counterflow diffusion flame model was used, intending to make an asymptotic analysis on structures of diffusion flame for large activation energies. He also investigated the analytical expressions for ignition and extinction conditions, analyzing the behavior of the temperature and the *Damköhler* number for the regimes: nearly frozen, partial burning, premixed flame and near-equilibrium diffusion flame.

The aim of this work is to use the model proposed by Liñán (1974) considering part of the fuel in the liquid phase. This term will simulate droplets in the gaseous fuel stream. An analysis will be demonstrated for the outer zone and we will analyse the behavior of the flame position and flame temperature changing the fuel mass fraction. This work is organized as follows. The first section contain all the formulation adopted. The second section presents the solution obtained to the model. The third section shows the main results and the last presents our conclusions.

2. FORMULATION

The flow geometry is composed by two opposite flows. The gaseous fuel comes through the left stream and the gaseous oxidant comes from the right stream. The flame stabilizes near the plane that contains the stagnation point. We will admit in this work fuel partially in liquid phase to simulate the spray combustion. The injection of the liquid fuel occurs near the flame, in order to find fuel in liquid phase inside the flame (see Figure 1).

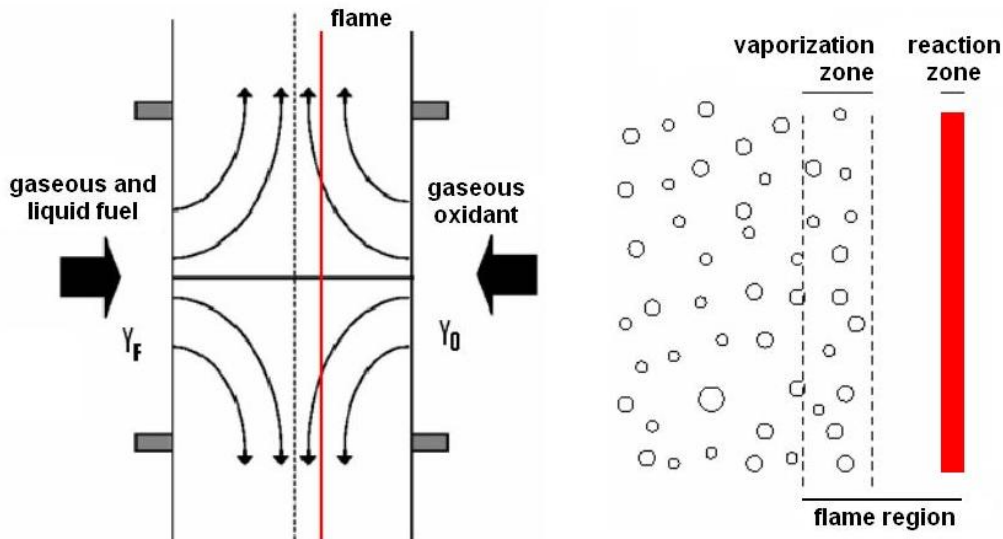


Figure 1. Spraylet model adopted and droplets in the flame region.

Because of the presence of the liquid in this problem, the conservation equations will have source terms. For the fuel species conservation equation, the source term is determined by the distribution of the number of droplets per volume multiplied by the mass vaporization rate. For the energy conservation equation, the sink term is determined by the distribution of the number of droplets per volume multiplied by the mass vaporization rate and the latent heat. The following set of equations describe the fuel and oxidant mass fractions and the temperature of the flow,

$$\bar{\rho}\bar{u}\frac{\partial}{\partial\bar{z}}\begin{Bmatrix}\bar{Y}_O \\ \bar{Y}_F \\ \bar{h}\end{Bmatrix}=\frac{\partial}{\partial\bar{z}}\left(\begin{Bmatrix}\bar{\rho}\bar{D}_O \\ \bar{\rho}\bar{D}_F \\ \bar{K}\end{Bmatrix}\frac{\partial}{\partial\bar{z}}\begin{Bmatrix}\bar{Y}_O \\ \bar{Y}_F \\ \bar{T}\end{Bmatrix}\right)+\begin{Bmatrix}-\bar{\nu} \\ -1 \\ \bar{Q}\end{Bmatrix}\bar{W}+\begin{Bmatrix}0 \\ \bar{N}\bar{\dot{m}} \\ -\bar{N}\bar{\dot{m}}\bar{l}\end{Bmatrix}. \quad (1)$$

Here we have four terms that mean; the first one a convective term, the second term is a diffusive term, the third term is the chemical reaction and the last one is a source term that was included. The variables that have an overwriten bar will be transformed on nondimensional units using these boundary conditions

$$\begin{cases}\bar{z}=-\infty, \bar{Y}_F=Y_{F-\infty}, \bar{T}=\bar{T}_{-\infty}, \bar{Y}_O=0, \bar{\rho}=\bar{\rho}_{-\infty} \\ \bar{z}=\infty, \bar{Y}_O=Y_{O+\infty}, \bar{T}=\bar{T}_{+\infty}, \bar{Y}_F=0, \bar{\rho}=\bar{\rho}_{+\infty}.\end{cases} \quad (2)$$

Since the flame is close to the stagnation point A , the flow velocity is approximated by $\bar{u} = -A\bar{z}$. So, we shall use this following nondimensional variables: the mixing layer $z \equiv \bar{z}/\bar{l}_c$, the oxidant mass fraction $y_O \equiv \bar{Y}_O/\bar{\nu}Y_{F-\infty}$, where $\bar{\nu}$ is stoichiometric mass ratio, fuel mass fraction $y_F \equiv \bar{Y}_F/Y_{F-\infty}$, the temperature $T \equiv c_p\bar{T}/\bar{Q}Y_{F-\infty}$ with specific heat c_p and heat release \bar{Q} , the density $\rho = \bar{\rho}/\bar{\rho}_c$, where $\bar{\rho}_c = \rho_{+\infty}$, the velocity $u = \bar{u}/\bar{u}_c$, where $\bar{u}_c = A\bar{l}_c$. Note that the characteristic length \bar{l}_c is determined by $\bar{K}/\bar{\rho}_c c_p A \bar{l}_c^2 = 1$, where \bar{K} is thermal conductivity. The source term is composed by \bar{N} , that is the number os droplets of fuel, the property \bar{l} is the latent heat needed to evaporate the mass of droplet and \bar{m} is the rate of mass vaporized and depends on the latent heat supplied. The properties are

$$W \equiv \frac{\bar{W}\bar{l}_c}{Y_{F-\infty}\bar{u}_c\bar{\rho}_c}; \quad Q \equiv \frac{\bar{Q}}{\bar{Q}Y_{F-\infty}}; \quad N\bar{m} \equiv \frac{\bar{N}\bar{m}}{Y_{F-\infty}\bar{u}_c\bar{\rho}_c}; \quad l \equiv \frac{\bar{l}}{\bar{Q}}; \quad (3)$$

$$\bar{l}_c \equiv \sqrt{\frac{D_{OF}}{A}}; \quad D_F = D_O = \frac{\bar{K}}{\bar{\rho}_c c_p}; \quad \frac{\bar{K}}{\bar{\rho}_c c_p A \bar{l}_c^2} \equiv 1; \quad \bar{u} = -A\bar{z}; \quad L_{eF} = L_{eO} = 1. \quad (4)$$

Here D_O and D_F are the diffusion coefficients for oxidant and fuel and W is the molecular weight. Remember that in the problem, the normalized oxidant mass fraction leads to $\alpha^{-1} = \nu Y_{F-\infty}/Y_{O+\infty}$, which is called equivalence ratio.

In this analysis we assume for simplicity that the thermodynamic and transport coefficients are constant. The energy and species conservation equations in the nondimensional form are (Liñán, 1974):

$$\frac{d^2 T}{dz^2} + z \frac{dT}{dz} = -D y_O y_F e^{-T_a/T} + N \bar{m} l \quad (5)$$

$$\frac{d^2 y_F}{dz^2} + z \frac{dy_F}{dz} = D y_O y_F e^{-T_a/T} - N \bar{m} \quad (6)$$

$$\frac{d^2 y_O}{dz^2} + z \frac{dy_O}{dz} = D y_O y_F e^{-T_a/T}, \quad (7)$$

which satisfies the boundary conditions

$$\begin{cases} z \rightarrow -\infty, & y_O = 0, & y_F = 1, & T = T_{-\infty} \\ z \rightarrow +\infty, & y_O = \alpha, & y_F = 0, & T = T_{+\infty}. \end{cases} \quad (8)$$

Note that T_a is the nondimensional activation energy of the Arrhenius term. The *Schvab-Zeldovich* procedure is applied to reduce the number of equations. The resulting equations describe the functions $H \equiv (T + l y_F)/(1 - l) + y_O$ and $Z \equiv y_F - y_O$, which are known in the literature as excess of enthalpy and mixture fraction respectively

$$\frac{d^2 H}{dz^2} + z \frac{dH}{dz} = 0 \quad (9)$$

$$\frac{d^2 Z}{dz^2} + z \frac{dZ}{dz} = -N \bar{m}. \quad (10)$$

3. SOLUTION

Physically, the liquid fuel in droplet form arrives from one side of the flame and the oxidant arrives from the other side, and so, these flows are opposed in the viscous layer without reactant leakage from the flame. The droplets are released at a certain distance and the gaseous fuel stream pushes them to the flame. The conservation equations are defined from $z \rightarrow -\infty$ to $z \rightarrow +\infty$ but they are described in a more convenient way from 0 to 1, using

$$x = \frac{1}{2} \operatorname{erfc}\left(\frac{z}{\sqrt{2}}\right), \quad (11)$$

which is the solution of the homogeneous part of Eq. (10). By performing the transformation z to x on Eq. (9) and (10) one finds

$$\frac{d^2 H}{dx^2} = 0, \quad (12)$$

$$\frac{d^2 Z}{dx^2} = -2\pi e^{z^2} N \bar{m}, \quad (13)$$

recalling that $H \equiv (T + l y_F)/(1 - l) + y_O$ and $Z \equiv y_F - y_O$ and satisfy

$$\begin{cases} x = 0, & H = (T_{-\infty} + l)/(1 - l); & Z = 1 \\ x = 1, & H = T_{+\infty}/(1 - l) + \alpha; & Z = -\alpha. \end{cases} \quad (14)$$

The solution of Eq. (12) with the boundary conditions from Eq. (14) is

$$\frac{1}{1-l}(T + ly_F) + y_O = \frac{1}{1-l}(T_{-\infty} + l) + \left[\frac{1}{1-l}(\beta - l) + \alpha \right] x, \quad (15)$$

where $\beta \equiv T_{+\infty} - T_{-\infty}$ (Liñán, 1974). By applying the condition on the flame, $y_F = y_O = 0$, $T = T_e$ at $x = x_e$, the flame temperature is found from Eq. (15)

$$T_e = T_{-\infty} + l + [\beta - l + \alpha(1-l)]x_e. \quad (16)$$

By observing Eq. (16), the flame temperature T_e is a function of the flame position x_e . Thus an extra expression relating T_e and x_e is necessary to solve the problem.

In the fuel side of the flame, the source term $N\dot{m}$ determines the fuel entering in the gas phase domain by the vaporization of the cloud of droplets. The present work admits that the vaporization rate distribution is similar to a *Gaussian Distribution*, $N\dot{m} \equiv (\bar{M}/2\pi)e^{-(z^2-z_i^2)}$. For the distribution, Eq. (13) with the boundary condition Eq. (14) presents an analytical solution,

$$Z = y_F = -Mx^2 + \left(\frac{Mx_e^2 - 1}{x_e} \right) x + 1, \quad (17)$$

and the boundary conditions that are satisfies $Z = 1$ at $x = 0$ and $Z = 0$ at $x = x_e$. Note that $M \equiv (\bar{M}/2)e^{z_i^2}$. In the oxidant side of the flame the source term is null, the solution of Eq. (13) with the boundary condition Eq. (14) and $Z = 0$ at the flame $x = x_e$ is

$$Z = -y_O = -(x - x_e) \frac{\alpha}{1 - x_e}. \quad (18)$$

The next step is to define the position of the flame x_e , which is still unknown. As the flame is small, in many cases, the chemical reaction term can be represented by the *Delta of Dirac* function. So, Eq. (13) will be written inserting a *Delta of Dirac*, where $w_F = m\delta(x - x_e)$

$$\frac{d^2 y_F}{dx^2} = 2\pi e^{z^2} \left[m\delta(x - x_e) + \frac{\bar{M}}{2\pi} e^{-(z^2 - z_i^2)} \right] \quad (19)$$

$$\frac{d^2 y_O}{dx^2} = 2\pi e^{z^2} m\delta(x - x_e). \quad (20)$$

For this distribution, the solution of Eq. (13) use the boundary conditions Eq. (14) and $Z = 0$ at the flame $x = x_e$. By integrating these equations around the flame

$$\frac{dy_F}{dx} \Big|_{x_e^-} = -m \int_{x_e^-}^{x_e^+} 2\pi e^{z^2} \delta(x - x_e) dx + \int_{x_e^-}^{x_e^+} \frac{\bar{M}}{2\pi} e^{-(z^2 - z_i^2)} dx \quad (21)$$

$$\frac{dy_O}{dx} \Big|_{x_e^+} = m \int_{x_e^-}^{x_e^+} 2\pi e^{z^2} \delta(x - x_e) dx, \quad (22)$$

since that the second term of Eq. (21) is much smaller than 1, therefore

$$\frac{dy_F}{dx} \Big|_{x_e^-} = -\frac{dy_O}{dx} \Big|_{x_e^+}. \quad (23)$$

By imposing the condition of Eq. (23) on Eq. (17) and (18), we determine the flame position x_e

$$x_e^3 - x_e^2 + \frac{(1 + \alpha)}{M} x_e - \frac{1}{M} = 0. \quad (24)$$

The *Cardano-Tartaglia* method is applied in order to find the solutions for Eq. (24). This procedure shows that there are two imaginary roots and one real.

4. RESULTS

In this work, ethanol (C_2H_6OH) is the simulated fuel and oxygen is the oxidant. The considered properties are: the heat combustion $Q = 27899 \text{ kJ/kg}$ (Avallone and Baumeister, 1987), the latent heat $l = 846 \text{ kJ/kg}$ (Turns, 2000), the specific heat $c_p(\text{medium}) = 1.947 \text{ kJ/kgK}$ (Turns, 2000) and the ambient temperature is $T_{+\infty} = T_{-\infty} = 300 \text{ K}$, consequently $\beta = 0$. The stoichiometric mass coefficient is $\nu = 2.0869$ based on one-step chemical kinetics



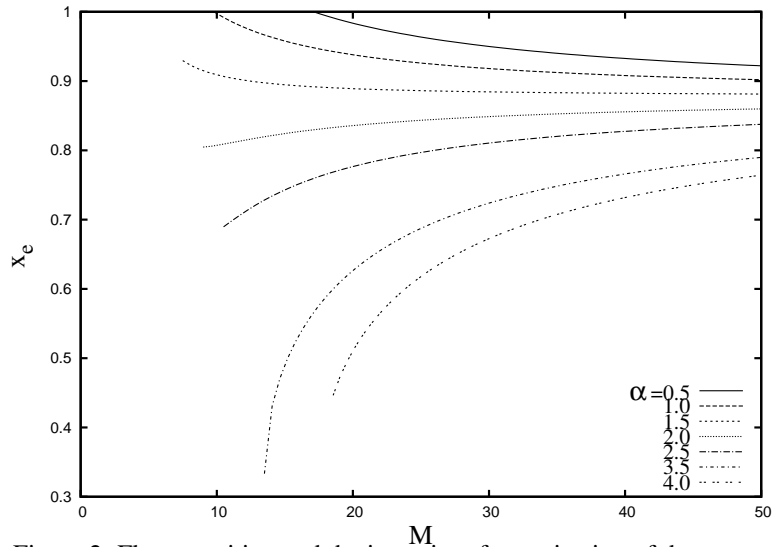


Figure 2. Flame position and the intensity of vaporization of the source.

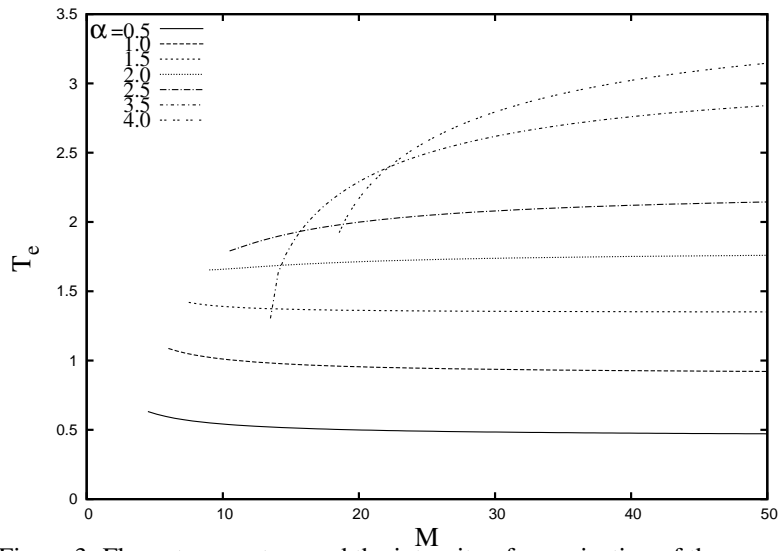


Figure 3. Flame temperature and the intensity of vaporization of the source.

The simulations are presented in two figures for a representative range of the parameters α . For all cases, the oxygen mass fraction is $Y_{O+\infty} = 1$ and the changes on α correspond to the fuel concentration changes. By analyzing Fig. (2) it is possible to observe the behavior of the flame position x_e as a function of M and Fig. (3), the flame temperature T_e as a function of M . Recalling that M represents the vaporization rate of the droplets. A detailed analysis of Eq. (24) reveals that the flame position x_e has physical meaning only if the condition $M > 3(1 + \alpha)$ is satisfied.

For $\alpha = 0.5$ the gaseous fuel mass fraction is very close to unit. In this condition unphysical solutions are found as shown in Fig. (2) and (3): the flame establishes out of the boundary $x_e > 1$ for $4.5 < M < 17.6$. Despite of physical solution observed for $M > 17.6$, because the flame position is inside the boundary ($x_e > 0.9$), the flame temperature indicates an unphysical condition $T_e \sim 0.5$. For the case $\alpha = 1.0$, which corresponds to $Y_{F-\infty} \sim 0.5$, there is an unphysical solution for $6 < M < 9.84$. Contrary to the case $\alpha = 0.5$, the solutions for $M > 9.84$ have physical meaning ($x_e < 1$) and ($T_e \sim 1$).

Under the condition that $\alpha = 4.0$ ($Y_{F-\infty} = 0.12$), the unphysical solutions are also observed for $15 < M < 18.55$. It is not complete clear, but in that range the flame temperature should be very low. Note that in the range $18.55 < M < 22$, the flame temperature is below the case $\alpha = 3.5$. For $M > 22$, the system with $\alpha = 4.0$ is more efficient than with $\alpha = 3.5$. For all cases, the flame position and the flame temperature does not present any significant variation for $M > 30$.

5. CONCLUSION

This work presents an analysis of the external flame structure obtained with two opposite jets (the fuel and oxidant are not premixed) and considering fuel droplets mixed with gaseous fuel. This spraylet model uses a sink term in the energy conservation equation, which is the product of the droplet vaporization rate and the latent heat. A source term is included in the fuel species conservation equation, determining the droplets vaporization rate. The flame position and the flame temperature are considered as function of the vaporization rate of droplets with different fuel concentrations in the gaseous stream. The best result obtained is $\alpha = 4.0$ ($Y_{F-\infty} = 0.12$) because Te has the greatest variation in temperature. Observing the intersection of the curves $\alpha = 4.0$ and $\alpha = 3.5$ in Figure (3), the highest temperature is obtained when $M > 22$. The same analysis can be done for $\alpha = 3.5$ ($Y_{F-\infty} = 0.14$) the highest temperature is in the limit $16 < M < 22$. The behavior of the temperature in these curves are in accordance with the flame positions, as shown in Fig. (2). Small α means high concentration of fuel in gas phase and so, the flame position is pushed to the infinite and the problem does not have solution.

6. REFERENCES

- Avallone, E.A. and Baumeister, T., 1987. *Mark's Standart Handbook for Mechanical Engineers*. McGraw-Hill, New York, USA.
- Couto, H.S., 2000. "Atomização e sprays". In *Proceedings of the II Escola de Combustão*. São José dos Campos, SP, Brazil.
- Hallett, W.L.H., 2000. "A simple model for the vaporization of droplets with large numbers of components". *Combustion and Flame*, Vol. 121, pp. 334–344.
- Kim, H. and Sung, N., 2003. "The effect of ambient pressure on the evaporation of a single droplet and a spray". *Combustion and Flame*, Vol. 135, pp. 261–270.
- Li, S.C., 1997. "Spray stagnation flames". *Progress in Energy and Combustion Science*, Vol. 23, pp. 303–347.
- Liñán, A., 1974. "The asymptotic structure of counterflow diffusion flames for large activation energies". *Acta Astronautica*, Vol. 1, pp. 1007–1039.
- Spalding, D.B., 1953. "The combustion of liquid fuels". In *Fourth Symposium (International) on Combustion*. The Combustion Institute, Pittsburgh, p. 847.
- Turns, S.R., 2000. *An Introduction to Combustion-Concepts and Applications*. McGraw-Hill, Pennsylvania, USA.
- Watanabe, H., Kurose, R., Hwang, S.M. and Akamatsu, W., 2007. "Characteristics of flamelets in spray flames formed in a laminar counterflow". *Combustion and Flame*, Vol. 148, pp. 234–248.
- Williams, F.A., 1985. *Combustion Theory*. The Benjamin/Cummings Publishing Company Inc, Menlo Park, California, USA.

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.