Effects of Soot Formation on Shape of a Nonpremixed Laminar Flame Established in a Shear Boundary Layer in Microgravity

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Abstract. A numerical study was performed to give a quantitative description of a heavily sooting, nonpremixed laminar flame established in a shear boundary layer in microgravity. Controlling mechanisms of three dimensional flow, combustion, soot and radiation are coupled. Soot volume fraction were predicted by using three approaches, referred respectively to as the fuel, acetylene and PAH inception models. It is found that the PAH inception model, which is based on the formation of two and three-ringed aromatic species, reproduces correctly the experimental data from a laminar ethylene diffusion flame. The PAH inception model serves later to better understand flame quenching, flame stand-off distance and soot formation as a function of the dimensionless volume coefficient, defined as $C_q = V_F/V_{ox}$ where $V_F$ is the fuel injection velocity, and $V_{ox}$ air stream velocity.

The present experiments showed that a blue unstable flame, negligible radiative feedback, may change to a yellow stable flame, significant radiative loss with an increase of $C_q$; this experimental trend was numerically reproduced. The flame quenching occurs at the trailing edge due to radiative heat loss which is significantly amplified by increasing $V_F$ or decreasing $V_{ox}$, favouring soot formation. Along a semi-infinite fuel zone, the ratio, $d_f/d_b$, where $d_f$ is the flame standoff distance, and $d_b$ the boundary layer thickness, converges towards a constant value of 1.2, while soot resides always within the boundary layer far away from the flame sheet.

1. Introduction

The most likely scenario of a flame incidentally initiated and spread on board of a spacecraft is a wall of combustible material adjacent to a low Reynolds number gas flow (forced by the venting system) and exposed to a critical ignition source. As a major portion of heat released from the igniting stage of combustion is transported by forced convection in the flow direction, the superior mode of spread is of co-current (forward) type. Under conditions of reduced gravity in spacecraft where the effects of buoyancy are small, due to the absence of natural convection, radiation becomes the...
predominant mode of heat transfer even for a small forward diffusion flame [1]. A proper evaluation of material flammability requires a detailed understanding of the effect of oxidizer flow velocity on local soot concentrations, to which the structure of the flow field in the vicinity of the flame connects. Konsur et al. [2] have attempted to describe the sooting behaviour of non-buoyant jet diffusion flame by using the Smoke-Point concept proposed originally by Markstein et al. [3]. Co-current flame spread over a solid plate could then be linked to a critical soot concentration [4] controlling the trailing edge quenching. Despite the practical utility of this approach, the local soot concentrations have not been comprehensively described. Several experimental investigations [5, 6] have demonstrated how changes in blowing affect soot formation and thus, flame structure in the absence of natural convection. Numerical simulations have been performed [7] to determine two regimes (attached and detached flows) of a low Reynolds number flow in the absence of natural convection, function of blowing and thermal expansion, but without radiation due to lack of adequate soot formation model.

Up to now, the exact elementary reactions and species, and chemical processes of soot formation are not fully understood. Currently, for predicting local soot concentration, extensive efforts are devoted in 3D CFD codes to the semi-empirical soot models [8-11], involving the inception, coagulation, surface growth and oxidation processes. Non-buoyant ethylene laminar jet diffusion flames have been modelled by assuming the nucleation and growth of soot are first-order functions of acetylene concentrations [8, 9]. Recent research suggests that the growth of aromatics is the rate limiting step rather than the formation of the first ring [10]. Vovelle et al. [11] showed that in decane flames, aromatic hydrocarbons are formed from acetylene. Anderson et al. [12] has shown that even a small quantity of aromatic hydrocarbons in the fuel can significantly increase soot emissions. Hall et al. [13] in their study of laminar methane flame, developed a soot inception rate based on the formation of two and three-ringed aromatic species from single ring aromatic species using a simplified reaction mechanism. While no guarantees are given that validation of the soot models [8-13] applies to a co-current, boundary type laminar flame under microgravity. Thus this paper tends to evaluate three approaches for soot formation, referred respectively to as the fuel, acetylene and PAH inception models, in such flame. For this, a detailed kinetic reaction mechanism [14], including 736 reversible

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2. Theoretical model

In order to conform as much as possible to the experimental configuration [5, 6], the starting point of the analysis is the set of three-dimensional elliptic, reacting flow equations that governs the phenomena of interest here. This set consists of the conservation equations of mass, momentum, energy and species. In a heavily sooting flame such as fire, as the radiation spectrum of soot is continuous, it is possible to assume that the gas behaves as a gray medium, and the radiative transfer equation without scattering is solved by using a discrete expression adapted to a Finite Volume Method. The calculation of the gray absorption coefficients, $\kappa$, of a sooting diffusion flame (mixture of soot, CO$_2$ and H$_2$O ) is based on the work of Grosshandler (RadCal) [15]. The simulations were performed using the Fire Dynamics Simulator (FDS) software [16]. The precise formulation of the differential equations describing the model and the numerical technique can be found elsewhere [16], and will not be repeated here. For such low Reynolds number reacting flow, comparison between the numerical results and experimental standoff distances to validate the accuracy of FDS code has been presented in detail by Rouvreau et al. [7]. In this study, for investigating quenching of a laminar flame due to radiation losses, soot models were implemented within the FDS code by the authors.

2.1. Combustion and soot formation

In gaseous combustion, the chemical compositions are found by using an appropriate reaction mechanism. For providing the local concentration of soot precursory species, such as acetylene (C$_2$H$_2$), benzene (C$_6$H$_6$) and phenyl (C$_6$H$_5$), a detailed kinetic reaction [14], including 736 reversible
reactions and 99 species has to be used to model the combustion for ethylene/air. This reaction mechanism consists of a set of elementary reactions with corresponding rate parameters. The rate coefficient for reaction is calculated from an Arrhenius expression. These rate parameters, together with the elementary reactions and their stoichiometric coefficients, constitute the reaction mechanism. The rate laws for the species can be calculated by using a time consuming stiff ODE solvers. However, any attempt to use Arrhenius expression for a detailed kinetic [14] coupled with a three dimensional elliptic, reacting flow is discouraged due to a problem of computational cost. In this study, the reaction mechanism of NO\textsubscript{x} included in the detailed kinetic [14], is not taken into account. This treatment does not affect the soot precursory species (C\textsubscript{2}H\textsubscript{2}, C\textsubscript{6}H\textsubscript{6}, C\textsubscript{6}H\textsubscript{5}, etc) due to lack of the interaction between the NO\textsubscript{x} formation and the reaction of other species.

In combustion, the mixture fraction is a conserved quantity traditionally defined as the (mass) fraction of the gas mixture that originates in the fuel stream. The mixture fraction is a function of space and time, commonly denoted Z(x,t). Therefore, many combustion models employ a detailed, cost effective kinetic reaction by tabulating the kinetics in terms of mixture fraction and only the mixture fraction is tracked in the calculation [17]. This implies that all species of interest of combustion products can be described in terms of the mixture fraction alone. The correspondence between the mass fraction of an individual species and the mixture fraction is called its “state relation”. This state relation can be obtained by using the OPPDIF (Opposed Diffusion Flames) computer code [18] which is performed by using subroutines from the chemical program library Chemkin.

![Figure 1. State relation between chemical species and mixture fraction](image)

For obtaining such state relation for combustion of fuel/air, OPPDIF [18] requires the chemical and physical input parameters, such as the fuel type, the initial temperature value of fuel and oxygen, the initial value of fuel and oxygen mass fraction, pressure and strain rate. While this state relation is independent of reactant and oxidizer flow rates. As an illustration, dependence of the main chemical species on mixture fraction is presented in Figure 1. These chemical compositions profiles for combustion of ethylene /air as a function of the mixture fraction (cf. Fig.1) correspond to the temperature (T\textsubscript{f}=T\textsubscript{ox}=300 K), pressure (P=1 atm) and composition (X\textsubscript{O\textsubscript{2}}= 0.35) found in the experiment [6]. A small value of the strain rate (<0.0003) which is much lower than the critical extinction value, is assigned, corresponding to the chemical equilibrium conditions. By looking at the relative locations of the chemical species as a function of the mixture fraction, high amounts of the phenyl (C\textsubscript{6}H\textsubscript{5}), acetylene (C\textsubscript{2}H\textsubscript{2}) and hydrogen (H\textsubscript{2}) take place in fuel-rich region around a mixture fraction value of 0.2. It is found that an abundant benzene is formed around a mixture fraction of 0.9, and maximum of the benzene mass fraction attains up to 0.6. At the start of a simulation, the detailed
chemical species involved are tabulated as a function of mixture fraction. During the simulation, the local value of all the species is found by table-lookup according to the local mixture fraction value [16].

The two time-dependent conservation equations for soot particles number, \( N \) (particles/m³) and soot mass density, \( M \) (kg/m³) are incorporated in FDS [16].

\[
\frac{\partial pN}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho \left( \frac{u_j + u_i^{th}}{\partial x_j} \right) \frac{\partial N}{\partial x_j} \right) = \dot{\omega}_{N,inc} + \dot{\omega}_{N,coa}
\]

(1)

\[
\frac{\partial pM}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho \left( \frac{u_j + u_i^{th}}{\partial x_j} \right) \frac{\partial M}{\partial x_j} \right) = \dot{\omega}_{M,inc} + \dot{\omega}_{M,gro} + \dot{\omega}_{M,oxi}
\]

(2)

where \( u_i^{th} \) is the thermophoretic velocity components:

\[
u_i^{th} = -0.54 \frac{\mu}{\rho} \frac{\partial \ln T}{\partial x_i}
\]

(3)

The first term in Eq.(1) represents the rate of soot particle inception and the second the soot coagulation. The second term in Eq.(2) represents the surface growth of soot, and the last the soot oxidation rate. Three approaches, referred respectively to as the fuel, acetylene and PAH inception models, are tested.

2.1.1. Fuel inception model.

The first approach is developed by Moss et al. [19], which incorporates the essential physical process of soot inception, coagulation and surface growth in terms of the local temperature, \( T \), and the mole fraction of fuel (ethylene) gas, \( X_F \).

\[
\dot{\omega}_{N,inc} = C_\alpha N_A \rho^2 T^{1/2} X_F e^{-T_u/T} \]

(4)

\[
\dot{\omega}_{N,coa} = \frac{C_\beta}{N_A} T^{1/2} N^2
\]

(5)

\[
\dot{\omega}_{M,inc} = \frac{C_\delta}{N_A} \dot{\omega}_{N,inc}
\]

(6)

\[
\dot{\omega}_{M,gro} = C_\gamma \rho T^{1/2} X_F e^{-T_f/T} N^{1/3} M^{2/3}
\]

(7)

2.1.2. Acetylene inception model

In the second approach, a conventional soot inception model, for which acetylene (\( \text{C}_2\text{H}_2 \)) is assumed the only soot precursor, is proposed by Leung et al. [9] via a simple two-step soot chemistry scheme.

\[
\text{C}_2\text{H}_2 \rightarrow 2\text{C}_s + \text{H}_2
\]

(8)

\[
\text{C}_2\text{H}_2 + n\text{C}_s \rightarrow (n + 2)\text{C}_s + \text{H}_2
\]

(9)

The soot inception rate is expressed as,

\[
\dot{\omega}_{N,inc} = c_1 N_A \left[ \frac{Y_{\text{C}_2\text{H}_2}}{W_{\text{C}_2\text{H}_2}} \right] e^{-\frac{21100}{T}}
\]

(10)
where \( c_1 \) is a scaling factor, given as \( c_1=54 \text{ s}^{-1} \), and \( T \) the gas temperature. The soot coagulation rate is determined by Lindstedt [20] based on the collision frequency defined by Puri et al.[21].

\[
\dot{\omega}_{N,\text{coa}} = \left( \frac{24R}{\rho_{\text{soot}} N_A} \right)^{1/2} \left( \frac{6}{\pi \rho_{\text{soot}}} \right)^{1/6} T^{1/2} M^{1/6} N^{11/6} \tag{11}
\]

\[
\dot{\omega}_{M,\text{inc}} = \frac{M_p}{N_A} \dot{\omega}_{N,\text{inc}} \tag{12}
\]

The surface growth of soot is proposed by Frenklach et al. [22].

\[
\dot{\omega}_{M,\text{gro}} = c_4 \left( \rho \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right) e^{\frac{12100}{T}} \left( \frac{6M}{\rho_{\text{soot}}} \right)^{2/3} \tag{13}
\]

where \( c_4 \) is a scaling factor, given as \( c_4=9000.6 \text{ kg.m.kmol}^{-1}.\text{s}^{-1} \), \( M_p \) (=12011 kg/kmol) molar mass of a soot nucleus, \( \rho_{\text{soot}} \) density of a soot particle, \( R \) the universal gas constant and \( W_i \) molecular weight of species, \( i \).

### 2.1.3. PAH inception model
Several theoretical and experimental works [10,11,13], highlight the importance of poly-aromatics species (PAH) as result of intermediary reactions in soot inception processes. Hall et al. [13] developed a soot inception model, which is based on the formation rates of two and three ringed aromatics (\( C_{10}H_7 \) and \( C_{14}H_{10} \)) from acetylene (\( C_2H_2 \)), benzene (\( C_6H_6 \)) and the phenyl radical (\( C_4H_5 \)). The growth mechanism of PAH is composed of consecutive repeated reactions that can be classified in two steps mechanism, called HACA (H-Abstraction-C\(_2\)H\(_2\)-Addition). The first one is an abstraction mechanism of hydrogen.

\[
2C_2H_2 + C_6H_5 \rightarrow C_{10}H_7 + H_2 \tag{14}
\]

The second one is the addition reaction of acetylene.

\[
C_2H_2 + C_4H_6 + C_6H_5 \rightarrow C_{14}H_{10} + H_2 + H \tag{15}
\]

Based on the laminar flame data, the resulting inception rate is expressed as,

\[
\dot{\omega}_{\text{inc}} = \frac{8N_A}{M_p} \left[ c_2 \left( \rho \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right)^2 \frac{Y_{C_6H_5} W_{H_2}}{W_{C_4H_6} Y_{H_2}} \right]^{-\frac{4378}{T}} + c_3 \left[ \rho \frac{Y_{C_2H_2} Y_{C_4H_6} Y_{C_6H_5} W_{H_2}}{W_{C_2H_2} W_{C_4H_6} W_{C_6H_5} Y_{H_2}} \right]^{-\frac{6390}{T}} \tag{16}
\]

where \( c_2 = 127 \times 10^{8.88} \) and \( c_3 = 178 \times 10^{9.50} \). The rates for coagulation and surface growth are identical to these in the acetylene inception model (section 2.1.2).

### 2.1.4. Soot Particles Oxidation
The soot oxidation in Eq.(2) is assumed to proceed through two reaction steps,

\[
\frac{1}{2}O_2 + C_s \rightarrow CO \tag{17}
\]
\begin{align}
\text{C}_2 + \text{OH} & \rightarrow \text{CO} + \text{H} \quad (18) \\
\text{Lee et al.} \ [23] \text{ measured and modelled the } \text{O}_2 \text{ and OH dependence of the soot oxidation in a laminar diffusion flame. By assuming that the kinetics of surface reactions are the limiting mechanism, the specific rate of soot oxidation is expressed by,} \\
\dot{\omega}_{\text{M,oxi}} &= -c_5 \tau p \frac{\text{Y}_{\text{OH}}}{\text{W}_{\text{OH}}} \text{T}^{1/2} \left( \pi N \right)^{1/3} \left( \frac{6\text{M}}{\rho_{\text{soot}}} \right)^{2/3} - c_6 \rho \frac{\text{Y}_{\text{O}_2}}{\text{W}_{\text{O}_2}} \text{T}^{1/2} \left( \pi N \right)^{1/3} \left( \frac{6\text{M}}{\rho_{\text{soot}}} \right)^{2/3} e^{-\frac{19778}{T}} \quad (19) \\
\text{where } c_5 &= 105.81 \text{kg.m.kmol}^{-1}.\text{K}^{-1/2}.\text{s}^{-1}, \quad c_6 = 18903.51 \text{kg.m.kmol}^{-1}.\text{K}^{-1/2}.\text{s}^{-1} \text{ and a value of 0.13 is assigned to the collision efficiency, } \tau .
\end{align}

2.2 Numerical technique

Low speed solvers used in FDS [16] explicitly eliminate compressibility effects that give rise to acoustic (sound) waves for low-Mach number flows (<0.3). The Boussinesq approximation invoked – the fluid is still considered thermally-expandable. Due to the use of the low Mach number approximation, the divergence of the flow plays a very important role in the overall solution scheme. The temperature is extracted from the density via the equation of state. The fidelity of the numerical solution of the entire system of equations is tied to the pressure/velocity coupling thanks to a direct Poisson solver [16]. All spatial derivatives are approximated by second-order finite differences and the flow variables are updated in time using an explicit second-order predictor-corrector scheme. The convective terms are written as upwind-biased differences in the predictor step and downwind-biased differences in the corrector step. The thermal and material diffusion terms are pure central differences in both the predictor and corrector steps [16]. In this study, the fuel temperature of 300 K and the atmospheric pressure (P=1 atm) are imposed at the porous burner boundaries, conforming to the experimental conditions [5, 6]. At the free boundaries, zero gradient conditions are used for the farfield boundary values of the mass fractions.

3. Results and discussions

The sketch of the experimental setup [5, 6] with the relevant burner dimensions is displayed in Fig.2(a,b). In the experiment, microgravity conditions are attained by means of parabolic flights that provide a gravity level of 10^(-3)g during 22 seconds. The experimental set-up corresponds to a square porous burner (L_p=W_p=5 cm, cf. Fig.2b) which is embedded in the plane at z=0, centred in the y direction and at 5 cm from the inlet of a large enclosed combustion chamber. Porous burners have been used regularly in an attempt to simplify experiments by avoiding the coupling between heat feedback from the flame and fuel supply so that longer experimentation time can be achieved. The pyrolysis products of a condensed fuel are simulated by injecting ethylene with a constant velocity, V_F, through a porous burner. The dimensions of the computational domain, as shown in Fig.2(a,b), are 8L_p in the windward direction, and 4L_p in both the lateral and normal directions so that boundary conditions can be set to conform as much as possible to the experimental configuration. The grid system contains 240 x 80 x 60 cells, and cells of 1 mm are concentrated around the reacting zone. The resolution tests indicated that the computations are grid independent when the cell dimensions are lower than 2 mm. Thus this grid system is considered as the best trade-off between accuracy and cost for a three-dimensional reacting flow simulation. A further reduction in the grid size results in a significant reduction in the time step ( \Delta t < 0.0005 s) for satisfying the CFL stability condition.

As the experiment, a uniform oxidizer flow at the inlet with a composition of 35% oxygen and 65% nitrogen flows parallel to the surface with a constant velocity, V_{ox}. This type flame can be described by the ratio between buoyant forces and inertia, defined as follows, \( \xi = \frac{\text{Gr}_x}{\text{Re}_x^{5/2}} \), where Re_x is the Reynolds number and Gr_x the Grashof number [24]. The experimental work [24] shows that if the
magnitude of the forced flow is small, an almost vertical plume is formed (cf. Fig.3a), indicating a predominant natural convection ($\xi > 1$). While microgravity reduces buoyancy enough to enable a much lower ratio ($\xi \leq 1$) even for a low Reynolds number flow ($Re < 100$), inducing a boundary layer diffusion flame (cf. Fig.3b). From Fig.4 for the velocity vectors in microgravity, it appears that energy release from an exothermic chemical reaction enhances the flow perturbations at the leading edge enough to enable an establishment of a parabolic nature boundary layer behind of that region. A low Reynolds number flow ($Re < 100$) is maintained all along the flame and parallel to the surface. The velocity overshoots in the line where fuel and oxidizer are delivered in stoichiometric proportions as a consequence of thermal expansion and interaction of the fuel and oxidizer flows.

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Figure 2. Computational domain and the coordinate system

![Side view](image1)

![Top view](image2)

(a) calculated iso-contours of the temperature (side view)  
(b) disposition of the fuel zone (top view)

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Figure 3. Structure of non premixed reacting flow from experiment

![Normal gravity](image3)

![Micro-gravity](image4)

(a) normal gravity  
(b) micro-gravity
Figure 4. Predicted velocity vectors of a boundary layer type laminar diffusion flame in microgravity

The sooting behaviour of such laminar diffusion flame is characterized by using the laser induced incandescence technique (LII). The basic principle of LII relies on the detection of the thermal radiation from the soot particles that have been heated up to vaporization temperature by means of high energy laser pulse. Given in Fig.5(a-d) is the comparison between the predicted and measured soot volume fractions across the height, z, at various axial locations \(x/L_p\) = 0.5, 1, 1.5 and 2 for \(V_\alpha = 0.25\) m/s and \(V_f = 0.005\) m/s. Based on the Moss model [19], both the soot inception and surface growth rates are determined solely from the mole fraction of fuel (ethylene) gas. This simplification gives a relatively good agreement with the measurement only in the fuel injection zone (\(x/L_p \leq 1\)) where the fuel concentration is important. However, far away from the fuel injection zone (\(x/L_p > 1.5\)), the Moss model [19] underpredicts by a factor of 5-6 times the measured value. Based on the same soot surface growth model (Eq.13), the predicted soot by using the PAH inception model is an order of magnitude larger than that by using the acetylene inception model. It seems that the PAH inception model reproduces correctly both the general shape and the peak value (about 5 ppm) of experimentally-determined soot volume fraction. By looking at their locations, the measured peak is placed just above the plate surface at \(z = 3\) mm, while the calculated one by using the PAH inception model occurs at \(z = 5\) mm, meaning an over-prediction of the vertical stratification of the soot layer.
Soot volume fraction is integrated over the soot layer in the z direction, as follows:

\[ F_{\text{soot}}(x) = \int_{z=0}^{Z_{\text{max}}(x)} f_{\text{soot}}(x,z) \, dz \],

where \( Z_{\text{max}}(x) \) is the height so that \( f_{\text{soot}}(x,z)=0 \) for \( z>Z_{\text{max}}(x) \) at a given \( x \). A global description of the integrated soot production, \( F_{\text{soot}} \), along x-axis as a function of both \( V_{\text{ox}} \) and \( V_{\text{F}} \) is presented in Figs.6(a,b). It seems that the PAH inception model reproduces the aforementioned sensitivity of the experimental soot formation to both \( V_{\text{ox}} \) and \( V_{\text{F}} \). A decreasing of \( F_{\text{soot}} \) from 60 to 30 (ppm)mm (cf. Fig.6a) is induced with an increase of the oxidizer flow velocity, \( V_{\text{ox}} \), from 0.06 to 0.25 m/s at a fuel injection velocity of 0.005 m/s. An inverse dependence of soot formation on the mainstream flow is predicted, and these tendencies are consistent with the experimental observation of Konsur et al.[2] based on the global residence time, defined as the ratio of the characteristic flame length, \( L_{f} \), to the oxidizer velocity. While an enhancement of \( F_{\text{soot}} \) (cf. Fig.6b) from 20 to 38 (ppm)mm occurs with an increase of the fuel injection velocity, \( V_{\text{F}} \), from 0.003 to 0.005 m/s at an oxidizer velocity of 0.25 m/s. The peak values of the integrated soot volume fraction are located far away from the trailing edge (\( x/L_{f}>1 \)). It is found that the extent of the measured soot is always within the zone of \( x/L_{f}<3 \). It should be noted that the measured soot volume fraction distribution is converted from LII intensity image, and its accuracy depends on the accuracy of the proportionality constant required for correction due to attenuations of both the laser beam and the collected signal. Besides, for the low fuel injection velocity of \( V_{\text{F}}=0.003 \) m/s, the flames considered have the particularity of being mostly two-dimensional. While for high \( V_{\text{F}} \), the flames considered develop strongly three-dimensional features far away from the trailing edge, affecting the collected signal for LII. This analyse is supported by the fact that the predicted soot profile follows closely the experimental trend for the low fuel injection velocity of 0.003 m/s, because the soot formation occurs within the extent of the collected signal for LII. While for the fuel injection velocity beyond 0.004 m/s, general shape of the predicted soot profiles has qualitative agreement with the experimental data. The error in numerical simulation may be linked to the constants used in the semi-empirical soot model, and accuracy of this type soot model seems to be strongly linked to the configuration studied. Generally, only a qualitative agreement with the measured soot volume fraction is achieved by using these standard constants [10]. It is felt that the difference is due to a combination of experimental uncertainties and the error in the numerical simulation.

Figure 5. Comparison between computation and experiment for the soot volume fraction at different axial locations.
Effect of the soot inception model on the geometric characteristics of a co-current flame is evidenced in Fig. 7(a-d). As compared to the experiment (cf. Fig. 7d), the disagreement with or without (cf. Fig. 7a) radiation is carried through the entire flame, becoming most evident in the quenching or extinction region behind the trailing edge. Absence of radiation induces a large flame stand-off distance (cf. Fig. 7a), implying the lack of oxygen inside the boundary layer so that excessive fuel is burned into an area of freestream where oxygen is available. Particularly for the flame considered here, presence of soot particles in the combustion gas mixture greatly enhances radiation from the flame. Although, a zero gravity numerical simulation is performed, the fluid and combustion are strongly coupled through the contributions of the heat release rate and the thermal radiation associated with soot formation, inducing a major influence on the flame structure through radiation loss. Therefore, in the previous work [7], 40% of energy had to be subtracted numerically from the heat release rate for providing a correct flame structure due to neglecting thermal radiation. Besides, if the soot is underpredicted (cf. Fig. 7b) by using the acetylene inception model, the flame significantly exceeds the measured flame zone at the trailing edge. The experimental flame shape is correctly hold with the PAH inception model (cf. Fig. 7c), and thus it is used in the following study.
Most of the work [26, 27, 28] in reactive boundary layer with blowing concentrated on the description of flame standoff over a semi-infinite fuel surface ($L_p \rightarrow \infty$). This case is also selected in this demonstration to clearly illustrate the effect of radiation on the flame characteristics over a large fuel size. For describing the effect of injection in boundary layer with blowing, a dimensionless volume coefficient, $C_q = V_f/V_{ox}$, defined by Schlichting [29], is currently employed. The work of Rouvreau et al. [7] clearly indicated that for the low values of $C_q \leq 0.08$ considered here, the low Reynolds number flow remains attached. Therefore, the different assumptions used within the boundary layer formulation should be validated for conditions in which there is no separation. Given in Figure 8 is the ratio, $d_f/d_b$, between the flame standoff distance, $d_f$, and the boundary layer thickness, $d_b$. The boundary layer thickness, $d_b$, is defined as the distance above the surface where the parallel component of velocity reaches 99% of the main flow velocity. The flame stand-off distance, $d_f$, is the distance between the plate and the flame sheet where oxygen and fuel is delivered in stoichiometric proportions corresponding to the maximum HRR. Near the leading edge, the flame is positioned very close to the porous plate edge, and the flame establishes inside the viscous boundary layer, denoting the importance of diffusion there. As $x$ increases along an infinite fuel zone (cf. Fig.8), both $d_f$ and $d_b$ move away from the plate into an area of higher velocity, and the ratio, $d_f/d_b$, converges to one single
curve and toward a constant value of 1.2, implying that the flame sheet crosses the momentum boundary layer. While an asymptotical solution without the consideration of radiative loss from the reactive boundary layer model [26] suggests that the flame resides always within the boundary layer, and seems still incapable of predicting this type flame. Moreover, the flame stand-off distance, $d_f$, is an order of magnitude larger than that predicted by a Shvab-Zeldovich analysis, as described by Emmons [27] for a reacting boundary layer flow with blowing. The works of Andreussi [28] concluded that the Shvab-Zeldovich analysis is only adequate for freestream velocities higher than 1.2 m/s. Consequently, the natural constraints imposed by buoyancy in the absence of radiation heat transfer prevent complete validation of this model.

Contrary to the flame standoff distance along a semi-infinite fuel zone (cf. Fig.8), the maximum soot formation occurs always inside the boundary layer ($d_{soot}/d_b<1$) far away from the stoichiometric line, as shown in Figure 9. Fujita et al. [30] observed that soot particles trajectories inside a laminar boundary layer diffusion flame in microgravity do not follow exactly the gas movement due to thermophoretical effects. This is evidenced by a significant deviation of soot particles from the stoichiometric line due to the dominant thermal expansion which prevents soot particles approaching the flame. The peak soot production is placed just over the plate surface in the fuel rich zone (cf. Fig.5), and its location does not follow the response of flame standoff to changes in mainstream parameters.

Flame standoff is of great importance on the heat flux over a material surface. After a threshold pyrolysis temperature is attained, all heat flux to the material surface is used entirely for pyrolysis. Given in Fig.10 is the normalized total heat flux over a semi-infinite fuel surface, where $q_{pyro}$ is the heat release rate per unit area (kW/m$^2$) from a flame. Microgravity flames are typically smooth (cf. Fig.3b) with a large heat feedback close to the leading edge where the fraction of the total energy released by the flame to the surface may be higher than 10%. Because heat flux is proportional to the flame temperature level and its location (view factor), with an increase of the flame standoff distance downstream (cf. Fig.8), the maximum temperature moves away from the surface, implying a reduction in the view factor from flame to the wall. This leads to a decrease of the fraction of the total energy to the surface, approaching an asymptotic solution of about 2% for $C_q$ below 0.02.
Diffusion flame quenching is of both fundamental and practical interest to applications such as fire spread over a condensed fuel surface. Gas phase quenching or extinction phenomena are often described using the Damköhler number, $\overline{D_s} = \frac{\tau_{re}}{\tau_{ch}}$, which is the ratio of a characteristic residence time, $\tau_{re}$, over a characteristic chemical time, $\tau_{ch}$, defined respectively as follows:

$$\tau_{re} = \left( \frac{V_{in}}{\alpha_{\infty}} \right)^{-1}$$

$$\tau_{ch} = \left[ \rho_{\infty} A T_f \exp(-E/R T_f) \right]^{-1}$$

(20)

Where $\alpha_{\infty}$ is the free-stream thermal diffusivity, $A$ the pre-exponential factor, and $E$ the activation energy. From equation (20), flame extinction can be characterized as either kinetic (i.e. diffusion) or radiative loss. Kinetic extinction is unlikely in the absence of natural convection where buoyancy is not available to accelerate (strain) the flow field and consequently, to reduce residence times, $\tau_{re}$, by enhancing mixing. Whereas radiative extinction is expected at long residence times, and thus occurs at very low strain rates. Microgravity experiments [5, 6] allowed the first observation of flame quenching, this being for boundary layer diffusion flame. The effect of soot formation on the flame temperature, $T_f$, which is the dominant factor for the characteristic chemical time $\tau_{ch}$, along a semi-infinite fuel zone ($L_p \to \infty$) is presented in Fig.11. The horizontal flame length, $L_c$, is defined as the distance of the 600°C contour from the leading edge (cf. Fig.2a), and this definition appears to be very close to the experimental visible flame [5, 6]. As given in Figure 12 is the flame length and its stand-off distance along a semi-infinite fuel zone as a function of $C_q$. It can be seen that the lack of adequate radiative heat transfer dominated by soot formation, leads to a flame temperature of 2000 °C downstream the leading edge, and to an infinite flame length (cf. Fig.12a). In fact, because of radiative heat loss from this heavily sooting flame, the flame temperature does not surpass 1300°C and decreases along the x-axis. This implies longer chemical times and thus, lower Damköhler numbers,
up to a flame quenching due to radiative heat loss around a soot concentration of $F_{\text{soot}} \approx 50$ (ppm)mm, consistent to the Smoke-Point concept [2, 4]. It is found that a decrease of $C_q$ results in an increase in the flame length (cf. Fig.12b) due to reduction in soot formation (cf. Fig.6a).

4. Conclusions

This numerical study highlights the importance of soot formation on the quenching of a microgravity diffusion flame established in a shear boundary layer. The acetylene or fuel inception model underestimates the soot amount behind the trailing edge, and thus entails an overestimation of flame length. The behaviour of the soot production is reasonably well predicted by using PAH inception model despite the fact that a qualitative agreement with the measured soot volume fraction is achieved for a high value of $C_q$. It is felt that the difference between prediction and experiment is due to a combination of experimental uncertainties and the error in the numerical simulation linked to the semi-empirical soot model. Both prediction and experiment suggest that soot production is enhanced with decreasing the oxidizer flow velocity or increasing the fuel injection rate, further emphasizing the role of radiation on the geometric characteristics of a co-current, boundary layer laminar flame under microgravity. It can be concluded that a large $C_q$ favours soot formation, and consequently, flame quenching due to a significant radiative heat loss. For a low Reynolds number reacting flow in microgravity, the flame establishes outside the viscous boundary layer, while the soot resides within the boundary layer far away from the stoichiometric line, implying the less importance of diffusion as compared to expansion and convection. A microgravity diffusion flame seems “open-tip” because quenching occurs before the fuel is fully consumed, so that fuel accumulates at the stoichiometric line. As a consequence, the flames significantly exceed at the trailing edge for $C_q$ below 0.02. A maximum in the flame length for oxidizer velocities below those encountered in natural convection, represents a greater hazard for fire safety in spacecraft. These results are valid only for gaseous fuel and oxidizer, and should not be directly extrapolated to condensed fuel burning. Therefore, ongoing work is accounting for the PAH inception model for predicting flame spread over a condensed fuel surface in microgravity.

References

[1] Olson, S.L., T’ien, J.S., 2000, Combustion and Flame, 121(3), p.439.
[2] Konsur, B., Megaridis, C.M., Griffin, D.W., 1999, Combustion and Flame 118 (4), p.509.
[3] Markstein, G.H., De Ris, J., 1985, 20th Symposium (international) on Combustion (Pittsburgh: The Combustion Institute), p.1637.
[4] T’ien, J.S., 1990, Combustion and Flame, 80, p.335.
[5] Legros, G., Joulin, P., Vantelon, J.P., Fuentes, A., Torero, J.L., 2006, Combustion Science and Technology, p.178.
[6] Fuentes, A., Legros, G., Claverie, A., Joulin, P., Vantelon, J.P., Torero, J.L., 2007, 31th Symposium (international) on Combustion (Pittsburgh: The Combustion Institute), p.2685.
[7] Rouvreau, S., Torero, J.L., Joulin, P., 2005, Combustion Theory and Modelling, 9 (2), p.137.
[8] Lui, F., Guo, H.S., Gregory, J., Smallwood, J., Ömer, L., 2002, Journal of Quantitative Spectroscopy & Radiative Transfer, 73, p.409.
[9] Leung, K.M., Lindstedt, R.P., Jones, W.P., 1991, Combustion and Flame, p.289.
[10] Wen, Z., Yun, S., Thomson, M.J., Lighthorne, M.F., 2003, Combustion and Flame, 135, p.323.
[11] Vovelle, C., Delfan, J.L., Reuillon, M., 1994, Springer-Verlag, Berlin, p.50.
[12] Anderson, H., McNally, C.S., Pfeifferle, L.D., 2000, 28th Symposium (international) on Combustion (Pittsburgh: The Combustion Institute), p.2577.
[13] Hall, R.J., Smooke, M.D., Colket, M.D., 1997, Gordon & Breach, p.189.
[14] Dagaut, P., Nicolle, A., 2005, Combustion and Flame, 140, p.161.
[15] W. Grosshandler, 1993, NIST technical Note TN 1402, National Institute of Standards and Technology, Maryland.
[16] Mcgrattan, K.B., Glenn, P.F., Jason, E.F., 2008, Fire Dynamics Simulator.
[17] Poinsot T. and Veynante, D., 2005, Second Edition, ISBN:1-930217-10-2, R.T. Edwards, Inc., P.O. Box 27388, Philadelphia, PA, 19118 USA.
[18] Lutz, A.E., Kee, R.J., Grcar, J.F., Rupley, F.M., 1997, Sandia National Laboratories Technical Rep. SAND96-8243.
[19] Moss, J.B., Stewart, C.D., Young, K.J., 1995, Combustion and Flame, 101, p. 491.
[20] Lindstedt, P.R., 1994, Springer-Verlag, p.417.
[21] Puri, R., Richardson, T.F., Santoro, R.J., 1993, Combustion and Flame, 92 (3), p.320.
[22] Frenklach, M., Clary, D.W., Gardier, J., Stein, S.E., 1984, 20th Symposium (international) on Combustion (Pittsburgh: The Combustion Institute), p.887.
[23] Lee, K.B., Thring, M.W., Beer, J.M., 1962, Combustion and Flame, 6, p.137.
[24] Torero, J.L., Bonneau, L., Most, J.M., Joulain, P., 1994, 25th Symposium (international) on Combustion (Pittsburgh: The Combustion Institute), p.1701.
[25] Brahmi, L., Vietoris, T., Rouvreau, S., Joulain, P., David, L., Torero, J.L., 2005, AIAA Journal, Vol.43, No.8, p.1725.
[26] Liu, S., Catalin, G., Fotache, 2008, Combustion and Flame, 154, p.378.
[27] Emmons, H., 1956, Z. Angew. Math. Mech., 36, p.60.
[28] Andreussi, P., 1982, Combustion and Flame, 45, p.1.
[29] Schlichting, H., 1979, Seventh Edition, McGraw-Hill.
[30] Fujita, O., Ito, K., Ito, H., Takeshita, Y., 1997, 4th NASA International Microgravity Combustion Workshop, p.217.