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# Numerical simulations of microgravity ethylene/air laminar boundary layer diffusion flames

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ABSTRACT

Microgravity ethylene/air laminar boundary layer diffusion flames were studied numerically. Two oxidizer velocities of 250 and 300 mm/s and three fuel injection velocities of 3, 4, and 5 mm/s were considered. A detailed gas-phase reaction mechanism, which includes aromatic chemistry up to four rings, was used. Soot kinetics was modeled by using a pyrene-based model including the mechanisms of nucleation, heterogeneous surface growth and oxidation following the hydrogen-abstraction acetylene-addition (HACA) mechanism, polycyclic aromatic hydrocarbon (PAH) surface condensation and soot particle coagulation. Radiative heat transfer from CO, $CO_2$, $H_2O$ and soot was calculated using the discrete ordinate method (DOM) coupled to a wide-band correlated-k model. Model predictions are in quantitative agreement with the available experimental data. Model results show that H and OH radicals, responsible for the dehydrogenation of sites in the HACA process, and pyrene, responsible for soot nucleation and PAH condensation, are located in a thin region that follows the stand-off distance. Soot is produced in this region and, then, is transported inside the boundary layer by convection and thermophoresis. The combustion efficiency is significantly lower than 1 and is reduced as the flow residence time increasing, confirming that these sooting micro-gravity diffusion flames are characterized by radiative quenching at the flame trailing edge. In particular, this quenching phenomenon explains the increase in flame length with the oxidizer velocity observed in previous experimental studies. The effects of using approximate radiative-property models, namely the optically-thin approximation and gray approximations for soot and combustion gases, were assessed. It was found that the re-absorption and the spectral dependence of combustion gases and soot must be taken into account to predict accurately temperature, soot volume fraction, flame geometry and flame quenching.



## 1. Introduction

Nowadays microgravity combustion studies have been largely encouraged by the successful landing of Mars mission and the idea of conduct the first manned mission to this planet for 2030. In this sense, the fire safety plays an important role in order to maintain protected, during the mission, the crew and the spacecraft. The materials employed and ambient conditions should be therefore an important research subject. In fact, at the very early stages of space flight development, oxygen concentration in spacecraft was almost 100%, and combustible materials present in the spacecraft were flammable under such oxygen concentration, which resulted in high risk of fire. At present, the oxygen concentration in spacecraft is currently less, such as 21% normally established in the International Space Station (ISS) [1]. Flame behavior under microgravity conditions is quite different from that on the Earth due to the absence of buoyancy forces [2] and thus, understanding microgravity combustion to manage possible hazards associated with unwanted fires is crucial to minimize risks of future missions.

A canonical scenario for the fire safety purpose in microgravity is the Laminar Boundary Layer Diffusion Flame (LBLDF) where a flame sets over a fuel plate supported by a low oxidizer flow blowing parallel to this surface. This situation can be analyzed theoretically by using the Emmons theory [3]. It is associated with flame spread over solid and liquid fuel flat-surfaces with opposed flow [4–9] and co-current flow [10–12], fabric materials [13,14] and electrical wires [15–18]. Also, it is of great importance to obtain insights on flame spread and extinction in materials used in the spacecraft infrastructure, payloads, crew member clothes and wires of electrical circuits. This configuration using a LBLDF at microgravity has been extensively studied by the group of researchers around Torero [19–25]. In some of these studies, the con-

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**Nomenclature**

| | |
|---|---|
| $f_s$ | Soot volume fraction (ppm) |
| $g$ | Cumulative $k$-distribution function (–) |
| $g_k$ | $k$th quadrature points (–) |
| $I_{b\eta}$ | Spectral blackbody intensity (W sr$^{-1}$m$^{-1}$) |
| $I_\eta$ | Spectral intensity (W sr$^{-1}$m$^{-1}$) |
| $k$ | Absorption coefficient variable (m$^{-1}$) |
| $L_b$ | Porous burner length (m) |
| $L_f$ | Flame length (m) |
| $p$ | Pressure (Pa) |
| $\dot{Q}_R$ | Heat loss per unit volume by radiation (W m$^{-3}$) |
| $t_{\text{res}}$ | Residence time (s) |
| $T$ | Temperature (K) |
| $u$ | Velocity in the $x$-direction (m s$^{-1}$) |
| $U_{ox}$ | Oxidizer injection velocity (m s$^{-1}$) |
| $v$ | Velocity in the $z$-direction (m s$^{-1}$) |
| $V_F$ | Fuel injection velocity (m s$^{-1}$) |
| $w_k$ | $k$th quadrature weight (–) |
| $x$ | Coordinate along the plate (m) |
| $x_i$ | Molar concentrations of the $i$th gaseous species (–) |
| $Y$ | Mass fraction (–) |
| $z$ | Coordinate in the vertical direction (m) |

*Greek letters*

| | |
|---|---|
| $\chi$ | Combustion efficiency (–) |
| $\chi_R$ | Radiant fraction (–) |
| $\varepsilon$ | Emissivity (–) |
| $\phi$ | Scalar variable (–) |
| $\eta$ | Wavenumber (m$^{-1}$) |
| $\kappa$ | Absorption coefficient (m$^{-1}$) |
| $\rho$ | Density (kg m$^3$) |

*Subscripts*

| | |
|---|---|
| $F$ | Flame |
| $max$ | Maximum |
| $ox$ | Oxidizer |
| $R$ | Radiative |
| ref | Reference |
| $s$ | Soot |
| $\infty$ | Oxidizer |
| $\eta$ | Wavenumber |

*Abbreviations*

| | |
|---|---|
| DOM | Discrete ordinate method |
| FVM | Finite volume method |
| OI | Oxygen concentration in the oxidizer flow |
| SOD | Stand-off distance (m) |
| WBCK | Wide-band correlated-k |
| WB | Wide band |
| NB | Narrow band |

densed fuel was replaced by a porous gas burner which was justified by obtaining large experimental times, no fuel surface regression and because in this configuration the flame is easier to ignite and to control [23–26].

The absence of buoyancy normally enhances the residence time favoring the production of soot and increasing the radiative heat transfer to the detriment of convection. Consequently, the competing processes between soot formation and soot oxidation, and the resulting flame radiation, controls the flame length ($L_f$) and the heat flux toward the solid surface. In particular, it was found that flame length increases mainly with the oxidizer velocity ($U_{ox}$) [23–25,27]. This behavior is opposite to that expected when complete combustion occurs, suggesting that extinction takes place at the flame trailing edge [27], as expected from Ref. [28].

Two mechanisms can lead to flame quenching. The first mechanism [29,30] (the kinetic extinction) occurs when the mixing time (or residence time) becomes significantly lower than the characteristic time for the chemical reactions (low Damkhöler number, $Da$). The other mode of quenching, opposite to the kinetic mode, is the radiative quenching. It exists only in the presence of radiative heat loss, and occurs at long residence times (large $Da$). The energy loss through radiation causes a decrease in flame temperature, leading to a reduction of the reaction rates. Quenching takes place when excess heat loss significantly lowers the reaction rate such that the flame can no longer sustain itself [31]. The radiative quenching has been less studied than the kinetic quenching because it is more difficult to observe on earth as the intrusion of buoyant force accelerates the flow and reduces the residence times. The microgravity environment offers unique conditions to investigate radiative flame quenching due to the large residence times encountered. Also, this phenomenon is expected to be enhanced by larger quantities of soot produced and reinforced radiation for this type of laminar diffusion flames.

The main objective of the present study is to provide a better description of the structure for an ethylene LBLDFs generated in microgravity conditions and to demonstrate numerically the existence of flame quenching at the trailing edge of the flame providing also a better comprehension of this phenomenon. This work is carried out by using a numerical model involving detailed chemistry and advanced soot production and radiation models. Finally, different radiative property models are tested to evaluate the influence in the prediction of flame structure, soot production and quenching induced by the radiation heat loss mechanism.

## 2. Numerical model

The overall continuity equation, the Navier–Stokes equations in the low Mach number formulation, and transport equations for gas-phase species mass fraction including the soot mass fraction, the soot number density per unit mass of mixture, and energy were solved in a 2D rectangular coordinates system ($x$, $z$) using a finite volume method (FVM) on a staggered grid. The gravitational term was set to zero to simulate the gravity reduced environment. Correction diffusion velocities in both $x$- and $z$-directions were used to ensure that the mass fractions of gaseous species and soot sum to unity. The thermophoretic velocities of soot in both the $x$- and $z$-directions were accounted for, as were the interactions between the gas-phase chemistry and the soot chemistry. The source term in the energy equation due to radiation heat transfer was calculated using the discrete ordinates method (DOM) with the absorption coefficients calculated from a wide-band correlated-k (WBCK) model as described below. The kinetic mechanism developed by Slavinskaya and Frank [32] to predict the formation of polycyclic aromatic hydrocarbons (PAH) and their growth up to four aromatic rings was used in present work. It consists of 94 species and 723 reactions. Transport properties are calculated from the CHEMKIN database [33].

### 2.1. Soot model

The soot model is, on the whole, the same as used by Guo et al. [34] and was based on the work of Apple et al. [35]. However, two major differences have been introduced. The steric factor for the H-abstraction-$C_2H_2$-addition (HACA) process is a constant set equal to 0.1 to be consistent to the works of Slavinskaya and coworkers [32,36,37]. In addition, the contribution of surface growth due to PAH-surface condensation has been added.

The soot model assumes that soot particles are spherical and locally monodisperse, leading to a formulation involving two transport equations: one for the mass concentration of soot particles