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NUMERICAL STUDY OF GASOLINE-ETHANOL BLENDS IN A COUNTERFLOW PREMIXED FLAME

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Abstract. *Gasoline is a complex real fuel, with a wide variation in composition between commercial gasolines. These characteristics indicate the difficulty of using this fuel for numerical studies. In order to avoid these difficulties, simplified synthetic fuels, called "surrogate fuels" are used. On the other hand, ethanol is a renewable, biodegradable, non-toxic fuel that can be produced from plants such as corn, sugar cane, beets, etc. In many countries, gasoline is normally blended with ethanol. In order to acquire a better understanding of combustion fundamental phenomena, it is preferable to study flames configurations with flows relatively simple that are easy to control. The counterflow laminar flames meet these criteria: the flow is well known, it can be modeled from theoretical and numerical points of view and experimentally it can be controlled in a relatively easy manner. This paper presents numerical studies of gasoline-ethanol blends combustion in laminar counterflow gaseous premixed flames configuration. The key objective of the study is to analyze the flame structure of different gasoline-ethanol blends. A gasoline model (containing ethanol), a semi-detailed mechanism with 150 species and 759 reactions, was chosen to carry the simulations. Laminar flame velocities were estimated as a function of equivalence ratio for different gasoline-ethanol blends. And laminar gasoline-ethanol counterflow premixed flames structures were presented and analyzed, also for different blends.*

Keywords: *Gasoline, Ethanol, Kinetic modeling, Counterflow, Premixed flame*

1. INTRODUCTION

Gasoline is a complex real fuel, with a wide variation in composition between commercial gasolines. In this sense, gasoline composition depends on origin and as a result of this there is no fixed combustion properties that could be applied worldwide.

These characteristics indicate the difficulty of using gasoline for experimental studies associated with numerical simulations. In effect, due to its complex and varying composition, the number of possible reaction pathways in a chemical reaction mechanism increases drastically. Such mechanisms development is challenging, and its simulations extremely time-consuming as it requires enormous computing resources, even for homogeneous reactors systems.

In order to avoid these difficulties, simplified synthetic fuels, called "surrogate fuels", with shorter chain lengths and known physical chemical properties are chosen to carry combustion studies. The term surrogate refers to a simpler representation of a real complex fuel.

The purpose of using surrogates is to simplify the combustion mechanism by using a single fuel molecule or a blend of relatively small molecules to represent the real fuel. Numerically, the use of surrogate fuels reduces significantly the number of possible chemical reactions in the kinetic scheme, while still representing the main properties of the real fuel.

On the other hand, ethanol is a renewable, biodegradable, non-toxic fuel that can be produced from plants such as corn, sugar cane, beets, etc. In many countries, gasoline is normally blended with ethanol. For example, in Paraguay and Brazil E24 (24% ethanol) can be found in most gas stations.

Chemical kinetic mechanisms for hydrocarbon fuels have been the focus of intense research for several decades.

However, there is surprisingly little information on the combution properties and pathways of common liquid fuels. This is due in part to the difficulty in representing real fuels containing hundreds of components with a wide variation in composition by surrogate fuels for the purpose of chemical kinetic modelling. Nevertheless, due to the increasing number of researchers working in the development of either kinetic modelling or experimental database of this fuel, this field has experienced a significant amount of recent developments.

In this sense, the most common gasoline surrogate chosen over the last decades are iso-octane or binary mixtures of iso-octane and n-heptane, the primary reference fuels (PRF) for determining octane ratings for spark ignition engine fuels (Bradley *et al* 1998).

More recently, Pitz *et al* 2007 came to a consensus that iso-octane, n-heptane and toluene should be included in any gasoline surrogate. N-heptane and iso-octane were chosen since they are the primary reference fuel components and toluene was chosen because it is the most abundant aromatic in gasoline.

Following these authors a gasoline model fuel (a n-heptane/iso-octane/toluene mixture) have been chosen in this study, since this ternary mixture was shown to be a very good surrogate of the commercial gasoline in terms of laminar burning velocity representation.

Since ethanol is an alternative fuel to gasoline, the purpose of this study is to characterize the influence of the addition of ethanol on the combustion properties of a commercial gasoline.

In order to acquire a better understanding of combustion fundamental phenomena, it is preferable to study flames configurations with flows relatively simple that are easy to control. The counterflow laminar flames meet these criteria: the flow is well known, it can be modeled from a theoretical point of view and experimentally it can be controlled in a relatively easy manner. The interest of these stretched flames also lies in the fact that they act as the main element to describe some turbulent combustion models.

This paper presents numerical studies of gasoline-ethanol blends combustion in laminar counterflow gaseous premixed flames configuration. The key objective of the study is to analyze the flame structure of different gasoline-ethanol blends.

The kinetic modelling for gasoline-ethanol blend oxidation in the counterflow premixed flame was performed using the COUNTERFLOW code within the REGATH package developed at EM2C laboratory, that takes into account the detailed kinetic and transport phenomena (heat and mass transfer) through a numerical predictive 1D code. The gasoline model (containing ethanol) of Andrae *et al* 2011, a semi-detailed mechanism with 150 species and 759 reactions, was chosen to carry the simulations. It consists of a detailed description of toluene oxidation and skeletal mechanisms of iso-octane and n-heptane.

Laminar flame velocities were obtained as a function of equivalence ratio for different gasoline-ethanol blends. And laminar gasoline-ethanol counterflow premixed flames structures were presented and analyzed, also for different blends.

2. GASOLINE AND ETHANOL CHEMICAL STRUCTURE

Gasoline is a refined product of petroleum consisting of a mixture of hydrocarbons, additives, and blending agents. The composition of gasolines varies widely, depending on the crude oils used, the refinery processes available, the overall balance of product demand, and the product specifications. The typical composition of gasoline hydrocarbons (% volume) is as follows: 4-8% alkanes; 2-5% alkenes; 25-40% isoalkanes; 3-7% cycloalkanes; 1-4% cycloalkenes; and 20-50% total aromatics (0.5-2.5% benzene) (IARC 1989).

As explained in Section 1, a n-heptane (C_7H_{16})/ iso-octane (C_8H_{18})/ toluene ($C_6H_5CH_3$) mixture have been chosen as a surrogate of the commercial gasoline. Chemical structures of these surrogates are presented in Figure 1. The percentages used in this study were suggested by Dryer *et al* 2011 and were as follows (% volume): 48.73 % n-heptane, 27.76 % iso-octane and 23.51% toluene.

Unlike gasoline, ethanol is composed of a single molecule: C_2H_5OH. Chemical structure of ethanol is presented in Figure 2. This fuel has been used for several decades in internal combustion engines, especially blended with gasoline. More than any other major country, Brazil relies on ethanol as an engine fuel.

3. LAMINAR FLAME VELOCITY

The laminar burning velocity is a physicochemical property dependent on the temperature, pressure, and mixture composition (fuel type, equivalence ratio, and amount of diluents). As a result, the laminar burning velocity provides invaluable information on the combustion properties and the underlying oxidation chemistry of the given fuel. It is also an important parameter in the design of engines, burners and other equipment where combustion is involved. Several experimental setups can be used to measure the laminar burning velocity of fuels: flat flame burners, combustion chambers, counterflow burners, etc. (Ranzi *et al* 1998)

It is found that a detailed knowledge of laminar premixed flames will provide insights into such properties as heat release rate, flammability limits, propagation rates, quenching and emissions characteristics. It is also common to use measured burning velocities to validate chemical kinetic schemes. Although the majority of fuel is probably burnt in turbulent combustion, data on laminar burning velocities are still needed as input to many turbulent combustion models.

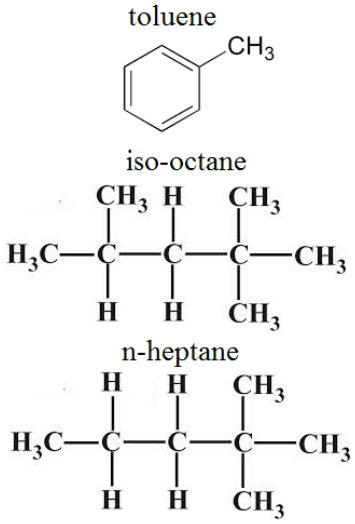

Figure 1. Gasoline surrogates chemical structures

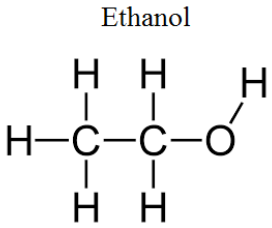

Figure 2. Ethanol chemical structure

Also, in internal combustion engines the initial combustion is laminar, so again there is a need for the laminar burning velocity (Takashi *et al*).

In this study, laminar flame velocities as a function of the equivalence ratio have been obtained in the case of ethanol, gasoline, and different blends of these two fuels using the 1D-PREMIXED code within the REGATH package.

4. COUNTERFLOW CONFIGURATION

4.1 Governing equations

We consider an axisymmetric counterflow configuration shown in Figure 3. A gasoline-ethanol/air mixture is injected from both the right and left sides. We model our system using similarity approach by searching for similar solutions of gaseous flow equations in the vicinity of the central axis (N. Darabiha *et al* 1993, Franzelli *et al* 2013 and D. Alviso *et al* 2015). These similar solutions have the form: gas density $\rho_g = \rho_g(z)$, gas radial velocity $u_g = r\,U_g(z)$, gas axial velocity $v_g = v_g(z)$, gas temperature $T_g = T_g(z)$ and species mass fractions $Y_k = Y_k(z)$, $k = 1, ...N_{sp}$ (N_{sp} is the number of species).

By assuming a pressure gradient in the radial direction so that $-\frac{1}{r}\frac{\partial p}{\partial r} = J$ is constant along the z axis, the gaseous phase are described by the following balance equations (mass, momentum, energy and species, respectively). It must be noted that there is one species conservation equation for each species present in the numerical model (N_{sp}).

$$2\rho_g U_g + \frac{\partial \rho_g v_g}{\partial z} = 0, \tag{1}$$

$$\rho_g U_g^2 + \rho_g v_g \frac{\partial U_g}{\partial z} = \frac{\partial}{\partial z}\left(\mu_g \frac{\partial U_g}{\partial z}\right) + J, \tag{2}$$

$$\rho_g v_g c_{p_g} \frac{\partial T_g}{\partial z} = \frac{\partial}{\partial z}\left(\lambda_g \frac{\partial T_g}{\partial z}\right) - \sum_{k=1}^{K} h_k W_k \Omega_k - \left(\sum_{k=1}^{K} \rho_g Y_k V_{kz} c_{p_{gk}}\right) \frac{\partial T_g}{\partial z}, \tag{3}$$

$$\rho_g v_g \frac{\partial Y_k}{\partial z} = -\frac{\partial}{\partial z}\left(\rho_g Y_k V_{kz}\right) + W_k \Omega_k, \qquad k = 1, ...N_{sp} \tag{4}$$

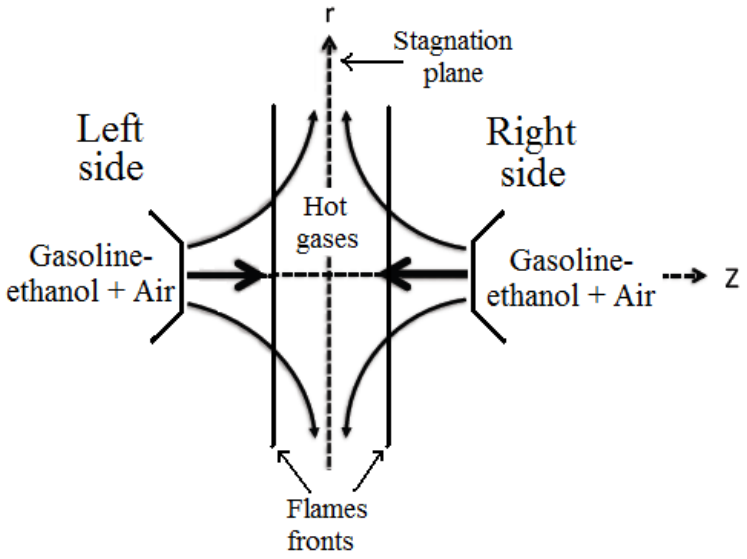

Figure 3. Counterflow premixed flames configuration

In these equations μ_g is the gaseous mixture viscosity. $c_{p_{gk}}$ and c_{p_g} are the heat capacity at local constant pressure of species k and of the mixture respectively. h_k, W_k, Ω_k are the specific enthalpy, the molar weight and the molar chemical production rate of the k^{th} species respectively, and V_{kz} is the diffusion velocity of the k^{th} species in the axial direction.

The above system of equations is completed by the ideal gas equation and by specifying the equation $\frac{\partial J}{\partial z} = 0$.

4.2 Numerical conditions

The boundary conditions of the system are given in Table 1. The distance between the left side and the right side is 40 mm, which is the typical distance found in a counterflow premixed configuration.

Table 1. Boundary conditions

	$left\,(z = -20\ mm)$	$right\,(z = 20\ mm)$
Gas temperature	$T_g = T_g^{left}$	$T_g = T_g^{right}$
Species mass fractions	$Y_k = Y_k^{left}$	$Y_k = Y_k^{right}$
Gas axial velocity	$v_g = v_g^{left}$	$v_g = v_g^{right}$
Gas radial velocity	$u_g = 0$	$u_g = 0$

The set of equations for the gaseous phase is then replaced by a fully coupled set of discrete relations. The solution of this system is then based on a global adaptive nonlinear method using Newton iterations (N. Darabiha *et al* 1993). The grid is adapted to first and second order derivatives of all variables and the smallest grid size is 5 μm.

The kinetic modeling for gasoline-ethanol blends oxidation in the counterflow flame was performed using the REGATH-1D-COUNTERFLOW code of the REGATH package (N. Darabiha *et al* 1993, Candel *et al* 2011) with detailed thermo-chemical and transport properties developed at EM2C laboratory. The inputs to each simulation include a chemical kinetic reaction mechanism, a dataset of thermochemical properties and a dataset of transport properties.

To carry gasoline-ethanol blends flame simulations, the mechanism due to Andrae *et al* 2011 (including ethanol) consisting of 150 species and 759 reactions was chosen. This model consists of a semi-detailed description of toluene oxidation and skeletal mechanisms of iso-octane and n-heptane.

A double gasoline-ethanol/air counterflow premixed flames operating condition have been chosen, considering the equivalence ratio (ϕ) and the injection velocity (V): $\phi = 0.7$ and $V = 43.3\ cms^{-1}$ at the left side, and $\phi = 0.7$ and $V = 56.2\ cms^{-1}$ at the right side. Both the left and right streams are kept at an initial temperature of 300 K. The pressure is equal to one atmosphere.

5. RESULTS AND DISCUSSION

5.1 Freely propagating flames

As the laminar burning velocity provides invaluable information on the combustion properties (see Section 3.), we have first used the kinetic scheme proposed by Andrae *et al* 2011 to simulate 1-D freely propagating gasoline-ethanol/air premixed flames using 1D-PREMIXED code within the REGATH package.

Gasoline-ethanol blends studied in this work were as follows: pure gasoline ($E0:0\%$ ethanol), pure ethanol ($E100:100\%$ ethanol), $E30:30\%$ (volume) ethanol and $E50:50\%$ (volume) ethanol.

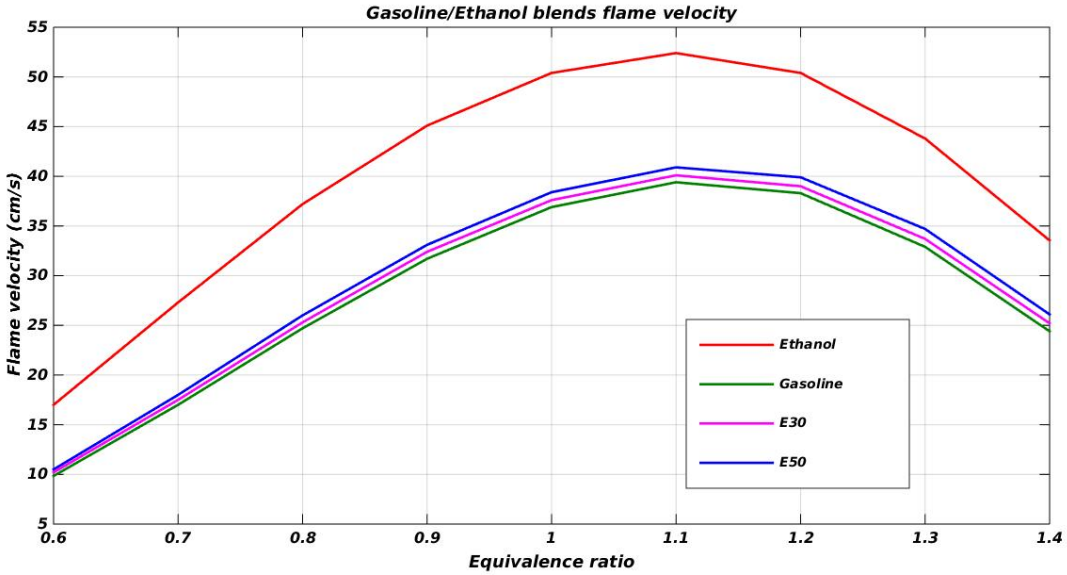

Figure 4. Gasoline-ethanol blends flame velocity as a function of equivalence ratio

Gasoline-ethanol blends flame velocities estimated as a function of equivalence ratio are presented in Figure 4, where one can see that the maximum flame velocities for pure ethanol (red curve) and gasoline (green curve) are obtained for an equivalence ratio of 1.1.

In Figure 5 one can also see that the influence of adding ethanol is almost negligible up to $E50$ (blue curve), concerning the blend flame velocity. This can be due to the fact that as the blend is made in volume, and ethanol molecular weight is small compared to that of gasoline (46 to be compared to about 105), the percentage of ethanol in mass in the blend is relatively small (31.08%), therefore the blend flame velocity is very close to that of pure gasoline, at least up to $E50$.

5.2 Counterflow premixed flames

Figures 5 and 6 present a typical pure gasoline flame structure. The boundary conditions correspond to those presented in Section 4.2 ($\phi = 0.7$ and $V = 43.3\ cms^{-1}$ at the left side ($z = -20\ mm$), and $\phi = 0.7$ and $V = 56.2\ cms^{-1}$ at the right side ($z = 20\ mm$)).

Figure 5 (left) presents the profiles of two important species: O_2 and HCO. Species O_2 is the oxidizer, and HCO is a species that indicates the flame front position: this species is present only in the reaction zone. From this Figure one can see that two premixed gasoline/air flame fronts are located at about $z = -8\ mm$ and $z = 4\ mm$. The HCO mass fraction profile at these points have a local maximum of $9.0E-06$ and $6.5E-06$, respectively. These flames are not symmetric due to the different injection velocities. At the left side O_2 mass fraction remains constant until $z = -9\ mm$ and then decreases very rapidly, whereas at the right side it remains constant until $z = 5\ mm$ and then also decreases very rapidly.

Figure 5 (right) presents the gas temperature and fuel species profiles. Gasoline is represented by 3 surrogates: n-heptane (C_7H_{16}), iso-octane (C_8H_{18}) and toluene ($C_6H_5CH_3$). These surrogates are injected at both left and right sides with an equivalence ratio of 0.7. Fuel species react with the oxidizer O_2, therefore C_7H_{16}, C_8H_{18} and $C_6H_5CH_3$ profiles are very similar to O_2 profile. In the same figure, gas temperature increases very rapidly from 300 K to 1850 K within 1 mm near the flame fronts.

Figure 6 (left) presents H_2O species and axial velocity profiles. Water vapor (H_2O) is one of the main products in any combustion process, and from this Figure one can see the profile is very similar to that of temperature. In a counterflow

premixed flame configuration, flames are stabilized at a position where the flame velocity matches the flow velocity. Therefore, this Figure presents the axial velocity profile between the two sides, where one can verify (Figure 4) the value of gasoline flame velocity for an equivalence ratio of 0.7 (about 17 cms^{-1}). The stagnation point (axial velocity $V = 0$) is located at $z = -2\ mm$.

Figure 6 (right) presents the fuel heat release (kg/m^3) profile along with O_2 species profile, where it can be seen that HCO species (Figure 5 (left)) is a good indicator of the flame front position.

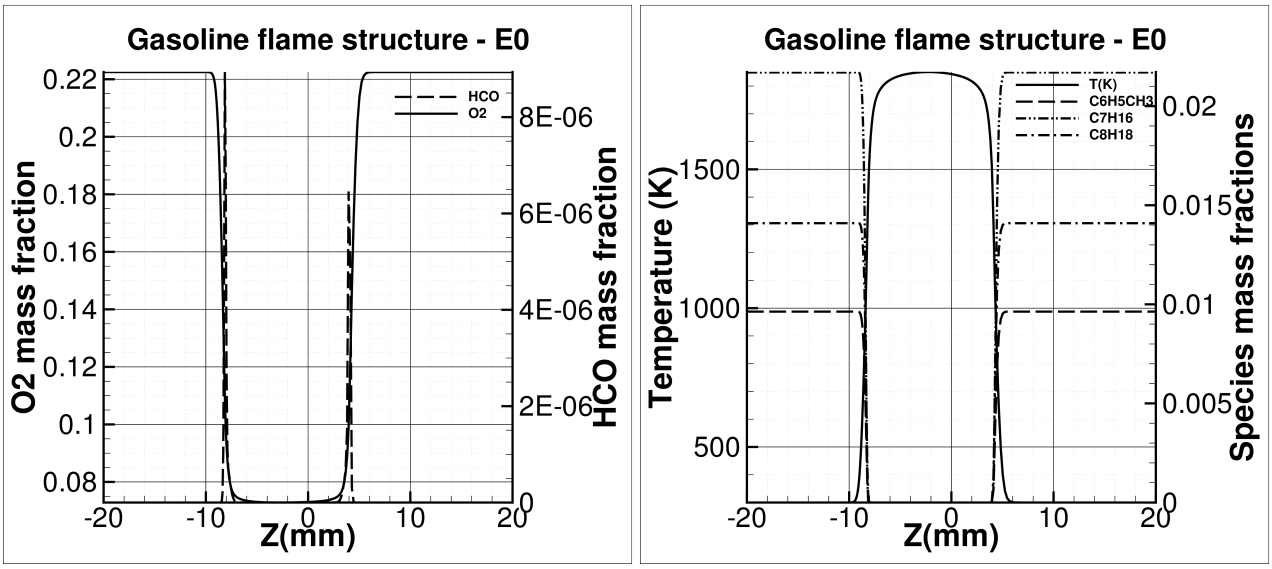

Figure 5. Gasoline ($E0$) counterflow premixed flame structure

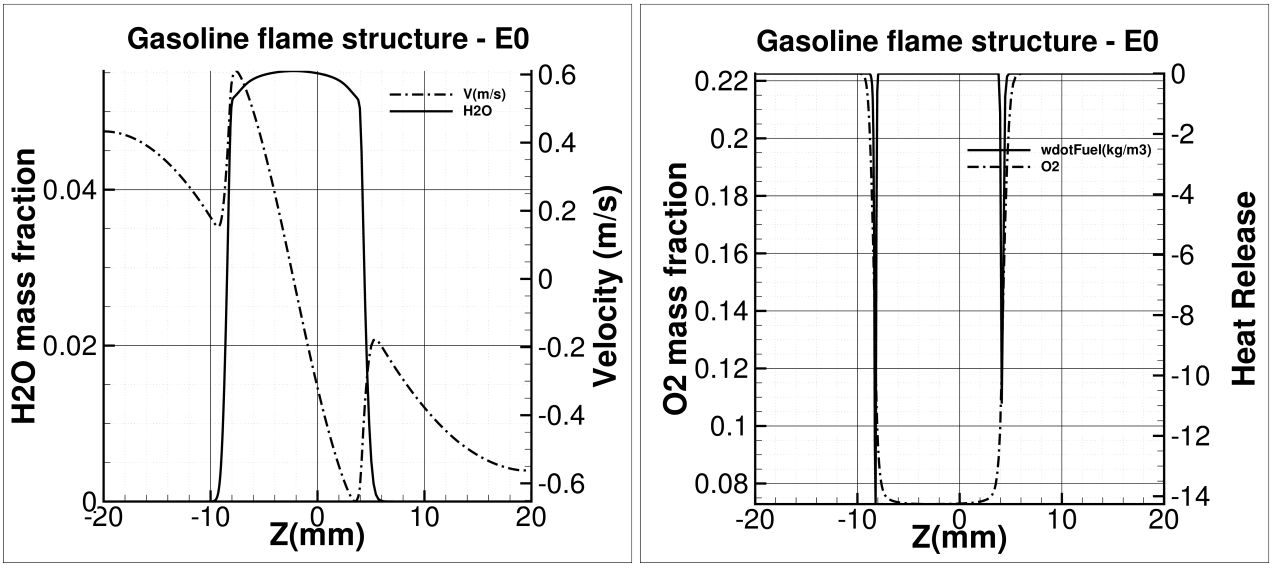

Figure 6. Gasoline ($E0$) counterflow premixed flame structure

Figures 7 and 8 present a $E30$ (30% ethanol and 70% gasoline in volume) gasoline-ethanol blend flame structure.

Figure 7 (left) presents O_2 and HCO profiles. From this Figure one can see that for $E30$ the flame fronts are located at about $z = -8.5\ mm$ and $z = 4.2\ mm$. Therefore, the addition of ethanol (up to $E30$) has a almost negligible effect on the flame positions.

In Figure 7 (right) gas temperature and fuel species profiles are shown. Gasoline is represented by its 3 surrogates: C_7H_{16}, C_8H_{18} and $C_6H_5CH_3$. Ethanol is represented by C_2H_5OH. Fuel species profiles: C_7H_{16}, C_8H_{18}, $C_6H_5CH_3$ and C_2H_5OH, are very similar to those presented for $E0$. The difference is the mass fraction of these species, due to the addition of ethanol. In the same figure, gas temperature increases very rapidly from 300 K to 1853 K, to be compared to that of $E0$ (1850 K). Therefore, the influence of the addition of ethanol is also almost negligible concerning the maximum gas temperature for these operating conditions.

Figure 8 (left) presents H_2O species and axial velocity profiles, which are also very similar to those presented for $E0$. Finally, Figure 8 (right) presents the fuel heat release (kg/m^3) and O_2 species profiles, where once again it can be seen that HCO species is a good indicator of the flame front position.

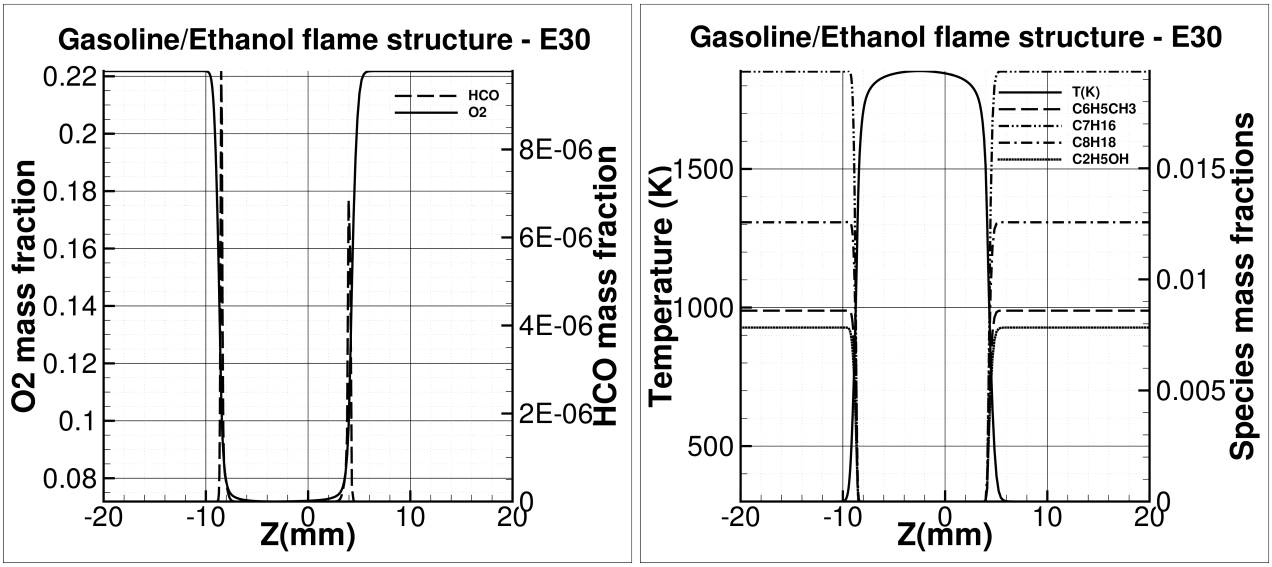

Figure 7. Gasoline-ethanol blend ($E30$) counterflow premixed flame structure

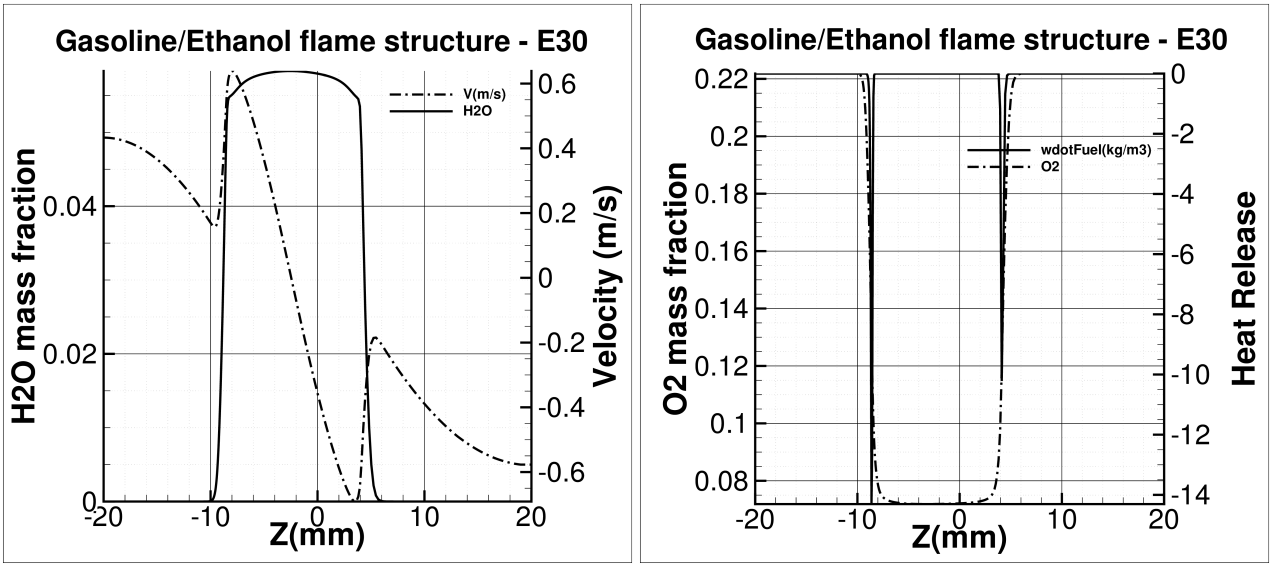

Figure 8. Gasoline-ethanol blend ($E30$) counterflow premixed flame structure

6. CONCLUSIONS

This paper has presented numerical studies of gasoline-ethanol blends combustion in laminar counterflow gaseous premixed flames configuration. The key objective of the study was to analyze the flame structure of different gasoline-ethanol blends. A gasoline model (containing ethanol), a semi-detailed mechanism with 150 species and 759 reactions, was chosen to carry the simulations.

Laminar flame velocities were estimated as a function of equivalence ratio for different gasoline-ethanol blends. The maximum flame velocities for pure ethanol and gasoline are obtained for an equivalence ratio of 1.1. Also, it was shown that the influence of adding ethanol is almost negligible up to $E50$ (50% ethanol), concerning the blend flame velocity. This can be due to the fact that as the blend is made in volume, and ethanol molecular weight is small compared to that of gasoline (46 to be compared to about 105), the percentage of ethanol in mass in the blend is also small, therefore the blend flame velocity is very close to that of pure gasoline, at least up to $E50$.

Laminar gasoline-ethanol counterflow premixed flames structures were presented and analyzed. Gas temperature, fuel heat release, axial velocity, oxidizer, fuel surrogates and other species profiles were presented for two gasoline-ethanol blends ($E0$ and $E30$). Concerning the two premixed flame fronts, the addition of ethanol has a almost negligible effect on the flame positions. And concerning the maximum gas temperature, $E0$ reaches a value of 1850 K, whereas for $E30$ is 1853 K, which shows also that the effect of the addition of ethanol on the maximum gas temperature is not very important, at least for blends up to $E30$.

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