# FLAME STRUCTURE OF DIESEL SURROGATE COMBUSTION IN A COUNTERFLOW DIFFUSION FLAME

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***Abstract:*** *In 2014, Mario Molina Center performed a study concerning air pollutants in Asunción. The results showed that population of Asunción is exposed to high levels of air pollution particles (ranging between 2.5 and 10 microns) and nitrogen dioxide that threatens their health. In addition, the study showed that transport has an important role in this problem, due to the fact that emission of particles is one of the main problems of Diesel engines (about 80 % of the total fleet in Paraguay). Most of experimental studies of Diesel fuel combustion are performed using internal combustion engines, in order to characterize the emission and performance of the engine. From the numerical point of view, many studies are performed using homogeneous reactors. However, mainly due to the complexity of its chemical composition, there are only few studies on kinetic modeling of such fuel in a 1D configuration. This paper presents numerical studies of Diesel surrogate combustion in laminar counterflow diffusion flame configuration. The key objective of the study is to understand the flame structure of Diesel fuel and validate the kinetic models used in the simulations. The kinetic modelling for Diesel oxidation in the counterflow diffusion flame was performed using the COUNTERFLOW code within the REGATH package developed at EM2C laboratory (Centrale Supelec, France), that takes into account the detailed kinetic and transport phenomena (heat and mass transfer) through a numerical predictive 1D code. A kinetic model was chosen to carry the simulations. This model consists of 150 species and 759 reactions. A surrogate Diesel fuel composed of n-heptane and toluene was chosen to represent Diesel chemistry. Different equivalence ratios and strain rates of Diesel counterflow diffusion flames were studied. The flames structures were analysed and presented.*

***Keywords:*** *Diesel, Counterflow flames, Freely propagating flames*

## 1. INTRODUCTION

In 2014, Mario Molina Center performed a study concerning air pollutants in Asunción. The results showed that population of Asunción is exposed to high levels of air pollution particles (ranging between 2.5 and 10 microns) and nitrogen dioxide that threatens their health. In addition, the study showed that transport has an important role in this problem, due to the fact that emission of particles is one of the main problems of Diesel engines (about 80 % of the total fleet in Paraguay).

Diesel is a complex real fuel, which is derived from conventional petroleum sources, and is composed of hundreds of compounds. Although the composition of petroleum-based diesel fuel is highly variable, there are some trends (Farrell *et al* 2007): The carbon numbers of the components range from approximately $C_{10} - C_{22}$. An average carbon number is 14 or 15. These characteristics indicate the difficulty of using diesel 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. Development of models that represent all these components is prohibitive because the model would be too large for current computational resources.

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.

Most of experimental studies of Diesel fuel combustion are performed using internal combustion engines, in order to characterize the emission and performance of the engine. From the numerical point of view, many studies are performed using homogeneous reactors. However, mainly due to the complexity of its chemical composition, there are only few studies on kinetic modeling of such fuel in a 1D configuration.

This paper presents numerical studies of Diesel surrogate combustion in laminar counterflow diffusion flame configuration. The key objective of the study is to understand the flame structure of Diesel fuel and validate the kinetic models used in the simulations.

The kinetic modelling for diesel oxidation in a 1D freely propagating gaseous premixed flame and 1D gaseous diffusion counterflow flame was performed using the REGATH package developed at EM2C laboratory (N. Darabiha *et al* 1993, Candel *et al* 2011 and Franzelli *et al* 2013), that takes into account the detailed kinetic and transport phenomena (heat and mass transfer) through a numerical predictive 1D code.

The kinetic model of Andrae et al (2011) was chosen to carry the simulations. This model consists of 150 species and 759 reactions. A surrogate Diesel fuel composed of n-heptane and toluene was chosen to represent Diesel chemistry. Different equivalence ratios and strain rates of Diesel counterflow diffusion flames were studied. The flames structures were analysed and presented.

## 2. DIESEL CHEMICAL STRUCTURE

Diesel is a complex combination of hydrocarbons produced by the distilation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of $C_{10} - C_{20}$. The composition 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 diesel shows approximately, by volume, 66% of saturated hydrocarbons, 30% aromatics (benzene derivatives) and 4% olefins (unsaturated hydrocarbons).

Due to the complex chemical structure of diesel, simplified synthetic fuels, called surrogate fuels, with shorter chain lengths are chosen to carry numerical combustion studies.

There has been much recent progress in the area of surrogate fuels for diesel. In the last few years, experiments and modeling have been performed on higher molecular weight components of relevance to diesel fuel. Chemical kinetic models have been developed for all the n-alkanes up to 16 carbon atoms. Also, there has been experimental and modeling work on lower molecular weight surrogate components such as n-decane and n-dodecane that are most relevant to jet fuel surrogates, but are also relevant to diesel surrogates where simulation of the full boiling point range is desired (W. Pitz *et al* 2011).

According to a recent paper (Hernandez *et al* 2014), a mixture of toluene and n-heptane was the best diesel surrogate in comparison to other species surrogates. Chemical structures of these surrogates are presented in Figure 1.

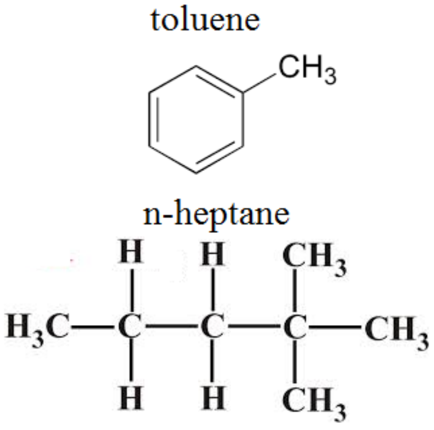

Figura 1: Diesel surrogates chemical structures

We have studied 4 mixtures of toluene and n-heptane to represent Diesel chemistry, suggested by different authors. These mixtures (in volume) are presented below:

- Mixture A: 48% n-heptane/52% toluene (Hernández *et al* 2008)
- Mixture B: 62.15% n-heptane/37.85% toluene (Hernández *et al* 2014)
- Mixture C: 80% n-heptane/20% toluene (Luo *et al* 2012)
- Mixture D: 70% n-heptane/30% toluene (Corcione *et al* 2004)

In this study, we have estimated flame velocities as a function of equivalence ratio for Mixtures A to D, and the one closer to Commercial Diesel experimental flame velocity was chosen.

## 3. NUMERICAL APPROACH

### 3.1 Freely propagating premixed flames governing equations

We consider a steady, isobaric, quasi-one-dimensional flame propagation configuration. A diesel/air mixture is injected from one side, and a premixed flame propagates freely towards fresh gases with the corresponding laminar flame velocity. In order to get a stabilized flame (instead of a propagating flame) one must inject fresh gases with a velocity equal to the laminar flame velocity.

Gaseous phase are described by the following balance equations (mass, energy and species, respectively). It must be noted that there is one species conservation equation for each species present in the numerical model $(N_{sp})$.

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

$$\rho_g v_g c_{p_g} \frac{\partial T_g}{\partial z} = \frac{\partial}{\partial z}\left(\lambda_g \frac{\partial T_g}{\partial z}\right) - \sum_{k=1}^{K} h_k W_k \Omega_k - \left(\sum_{k=1}^{K} \rho_g Y_k V_{kz} c_{p_{gk}}\right) \frac{\partial T_g}{\partial z}, \tag{2}$$

$$\rho_g v_g \frac{\partial Y_k}{\partial z} = -\frac{\partial}{\partial z}\left(\rho_g Y_k V_{kz}\right) + W_k \Omega_k, \qquad k = 1, ....N_{sp} \tag{3}$$

The above system of equations is completed by the ideal gas equation.

The solutions have the form: gas density $\rho_g = \rho_g(z)$, 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).
In these equations $c_{p_{gk}}$ and $c_{p_g}$ are the heat capacity at local constant pressure of species $k$ and of the mixture respectively. $h_k$, $W_k$, $\Omega_k$ 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.

### 3.1.1 Numerical conditions

The kinetic modeling for diesel oxidation in the 1D freely propagating flame was performed using the 1D-PREMIXED code within the REGATH package (N. Darabiha *et al* 1993, Candel *et al* 2011 and Franzelli *et al* 2013) with detailed thermochemical 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.

Diesel/air freely propagating premixed flames operating condition have been chosen, considering the equivalence ratio ($\phi$): from $\phi = 0.6$ to $\phi = 1.4$. The mixture stream is kept at an initial temperature of 470 K. The pressure is equal to one atmosphere.

## 3.2 Counterflow diffusion flames governing equations

We consider an axisymmetric counterflow configuration shown in Figure 2. Air is injected from the left side whereas a mixture of diesel and nitrogen is injected from the right side. 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 and D. Alviso *et al* 2015). These similar solutions have the form: gas density $\rho = \rho(z)$, gas radial velocity $u = r\,U(z)$, gas axial velocity $v = v(z)$, gas temperature $T = T(z)$ and species mass fractions $Y_k = Y_k(z)$, $k = 1, ...N_{sp}$ ($N_{sp}$ is the number of species).

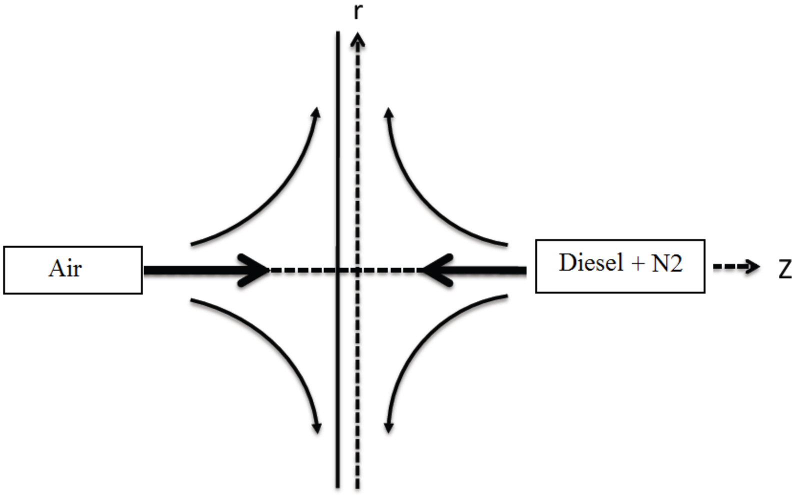

Figura 2: Counterflow diffusion flame configuration

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 (Franzelli *et al* 2013):

$$2\rho U + \frac{\partial \rho v}{\partial z} = 0, \tag{4}$$

$$\rho U^2 + \rho v \frac{\partial U}{\partial z} = \frac{\partial}{\partial z}\left(\mu \frac{\partial U}{\partial z}\right) + J, \tag{5}$$

$$\rho v c_p \frac{\partial T}{\partial z} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial T}{\partial z}\right) - \sum_{k=1}^{K} h_k W_k \Omega_k - \left(\sum_{k=1}^{K} \rho Y_k V_{kz} c_{p_k}\right)\frac{\partial T}{\partial z}, \tag{6}$$

$$\rho v \frac{\partial Y_k}{\partial z} = -\frac{\partial}{\partial z}\left(\rho Y_k V_{kz}\right) + W_k \Omega_k, \qquad k = 1, ....N_{sp} \tag{7}$$

In these equations $\mu$ is the gaseous mixture viscosity. $c_{p_k}$ and $c_p$ are the heat capacity at local constant pressure of species $k$ and of the mixture respectively. $h_k$, $W_k$, $\Omega_k$ 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 $\frac{\partial J}{\partial z} = 0$.

### 3.2.1 Numerical conditions

The boundary conditions of the system are given in Table 1. The distance between the two injections was kept constant to 20 mm.

| | $left\,(z = -10\ mm)$ | $right\,(z = 10\ mm)$ |
|---|---|---|
| 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 | $u_g = 0$ | $u_g = 0$ |

Tabela 1: Boundary conditions

The set of equations 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 (see (N. Darabiha *et al* 1993 and Giovangigli *et al* 1998). The grid is adapted to first and second order derivatives of all variables and the smallest grid size is 5 $\mu m$.

The kinetic modeling for diesel oxidation in the counterflow flame was performed using the REGATH-1D- COUNTERFLOW code of the REGATH package with detailed thermochemical and transport properties developed at EM2C laboratory.

We have performed numerical studies of five different combinations (I-V) of equivalence ratio ($\phi$) and velocity injection ($V$) gathered in Table 2. Injection velocities are the same at both left and right sides.

| Diesel flames References | | | |
|---|---|---|---|
| $\phi \backslash V$ | 30 | 40 | 50 |
| 3.3 | I | - | - |
| 4.3 | II | IV | V |
| 5.3 | III | - | - |

Tabela 2: Diesel flames conditions, velocities ($V$) are in $cm\ s^{-1}$

## 4. RESULTS AND DISCUSSION

### 4.1 Freely propagating flames

As the laminar burning velocity provides invaluable information on the combustion properties, we have first used the kinetic scheme proposed by Andrae *et al* 2011 to simulate 1-D freely propagating diesel premixed flames.

Flame velocities as a function of equivalence ratio are presented in Figure 3, for commercial diesel (Chong *et al* 2011, experimental results in continous black line), and for Mixtures A to D (see Section 2. in continous colour lines) using Andrae chemical scheme. In this figure one can see that the maximum flame velocity for commercial diesel is obtained for an equivalence ratio of 1.2, whereas those of mixtures A to D are obtained for an equivalence ratio of 1.1

As one can see for equivalence ratios lower than 1 (lean flames) the mixtures A to D give consistents results and follow the trend, the closest to commercial diesel been mixture D (red line). However, for equivalence ratios higher than 1 (rich flames), mixtures A to D do not reproduce very well (do not follow the trend) commercial diesel flame velocity.

Considering standard deviation for equivalence ratios from 0.6 to 1.4 the mixture D (red line, 70% n-heptane/30% toluene (Corcione *et al* 2014) is the one closer to commercial Diesel flame velocity. Therefore, this was the mixture chosen to represent diesel chemistry and analyse the flame structure in the next section.

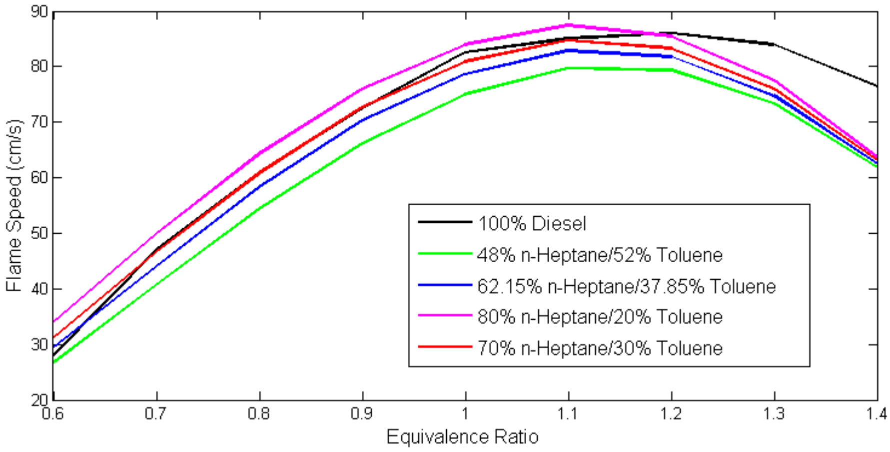

Figura 3: Diesel flame velocity as a function of equivalence ratio. 100 % Diesel corresponds to Commercial Diesel experimental flame velocity (black line)

## 4.2 Counterflow diffusion flames

### 4.2.1 Typical flame structure

Figures 4 to 5 present a typical counterflow diffusion diesel flame structure. The boundary conditions correspond to Flame IV (see Table 2). As it can be seen the distance between the left and right sides is 20 mm.

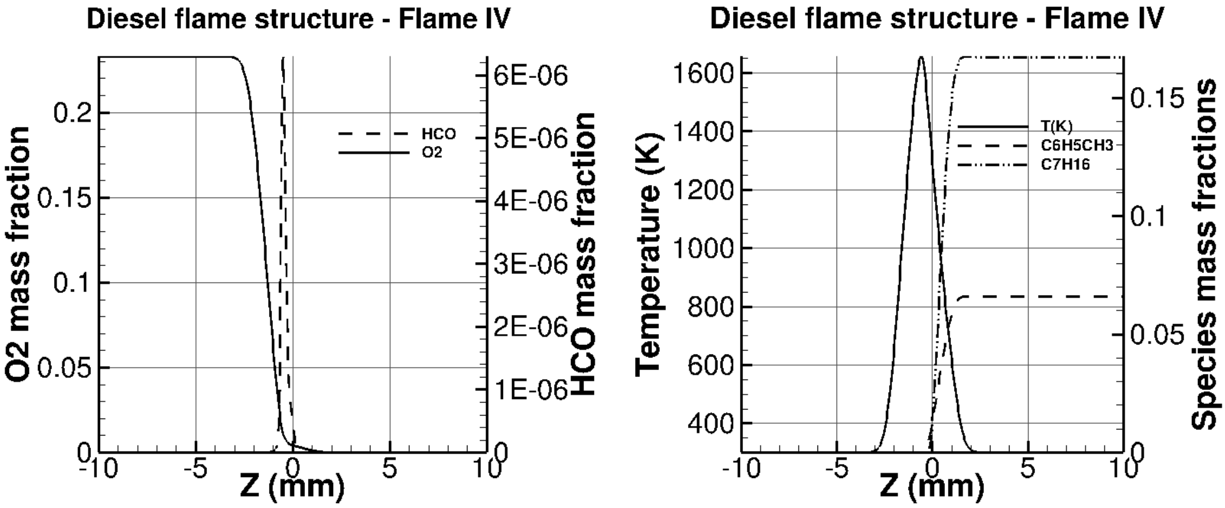

Figura 4: Counterflow diffusion Diesel flame structure - Flame IV

Figure 4 (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 diesel/air flame front is located at about $z = -0.5\ mm$. The $HCO$ mass fraction profile at this point has a local maximum of $6.2E-06$. At the left side $O_2$ mass fraction remains constant until $z = -3\ mm$ and then decreases very rapidly.

Figure 4 (right) presents the gas temperature and fuel species profiles. As explained, Diesel is represented by 2 surrogates: n-heptane ($C_7H_{16}$) and toluene ($C_6H_5CH_3$). These surrogates are injected at the right side with an equivalence ratio of 4.3. Fuel species react with the oxidizer $O_2$, therefore $C_7H_{16}$ and $C_6H_5CH_3$ mass fractions remains constant until $z = 2\ mm$ and then decreases very rapidly.. In the same figure, gas temperature increases very rapidly from 300 K to 1620 K near the flame front.

Figure 5 (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. This Figure also presents the axial velocity profile between the two sides, where one can verify that there is first an acceleration and then a deceleration of the gas when approaching from both sides to the flame zone. The stagnation point (axial velocity $V = 0$) is located at $z = 0\ mm$.

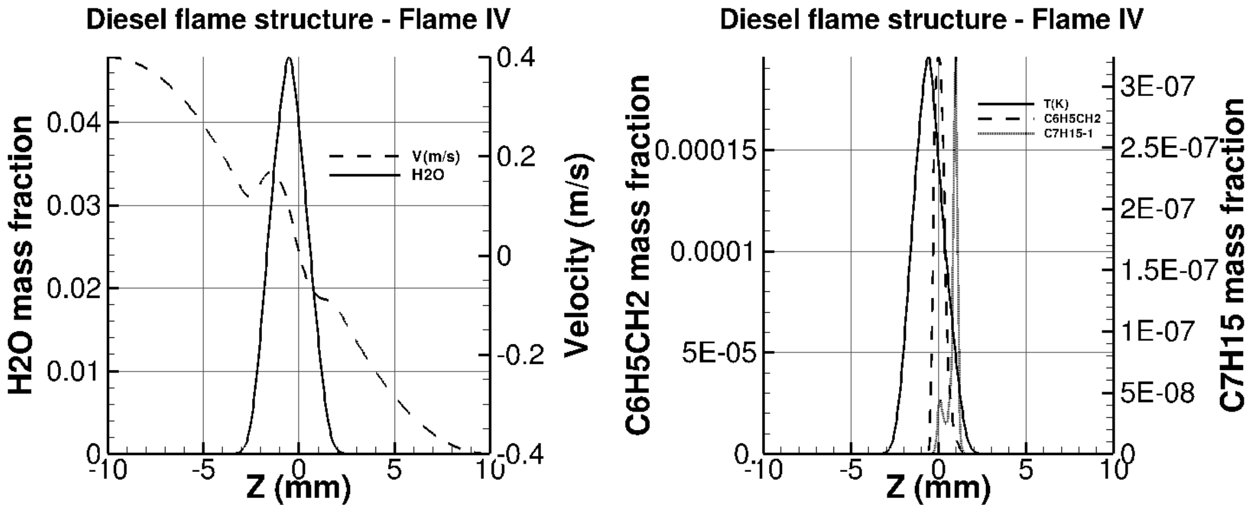

Figura 5: Counterflow diffusion Diesel flame structure - Flame IV

Figure 5 (right) presents the gas temperature profile along with $C_7H_{15}$ and $C_6H_5CH_2$ species profiles. In hydrocarbon flames, ignition usually begins with an H atom abstraction. Consequently, as n-heptane and toluene start to decrease, $C_7H_{15}$ and $C_6H_5CH_2$ species start to increase. These species in turn decomposes into other radicals, explaining its presence in a thin region.

### 4.2.2 Influence of equivalence ratio

Figure 6 presents $O_2$ and $HCO$ species profiles for Flames I (left) and III (right). These flames have different equivalence ratios and same injection velocities (see Table 2).

It is noted that oxygen is consumed more rapidly in Flame III than in Flame I (different equivalence ratios). In addition, although there is a slight difference between $HCO$ mass fractions maximum, what really matters is the flame position. In diffusion flames, the position is defined by the stoichiometry, thus, as the amount of fuel increases (higher equivalence ratio) the flame position slightly shifts toward the oxygen (in order to find stoichiometry).

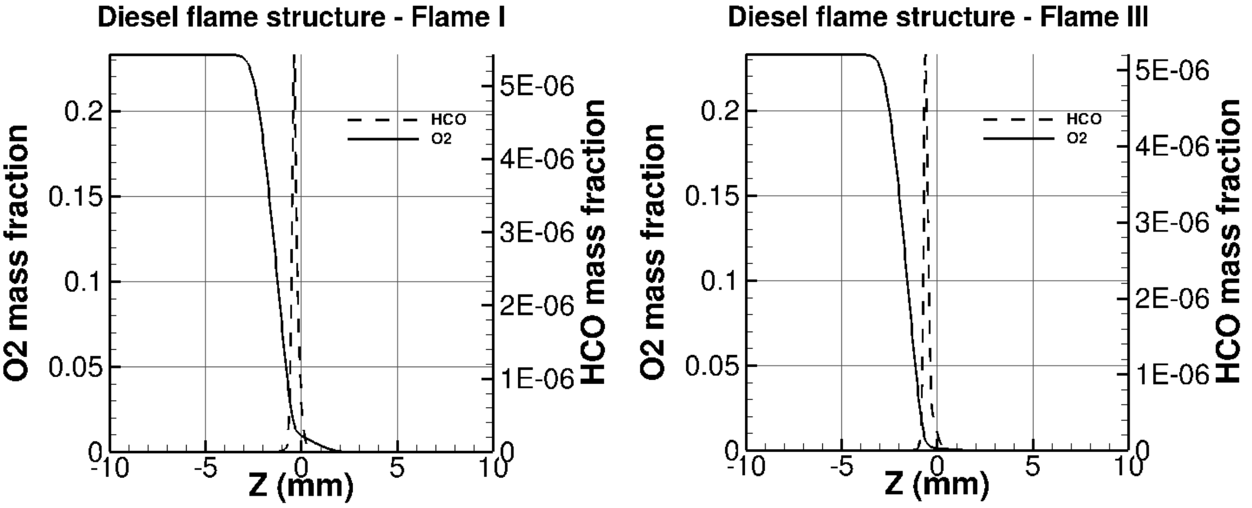

Figura 6: Counterflow diffusion Diesel flame structure - Flame I (left), Flame III (right)

Figure 7 presents the gas temperature and fuel species profiles for Flames I (left) and III (right). It is noted that the maximum temperature is higher in Flame III (higher equivalence ratio) as expected.

### 4.2.3 Influence of injection velocity

Figure 8 presents $O_2$ and $HCO$ species profiles for Flames II (left) and V (right). These flames have different injection velocities and same equivalence ratio (see Table 2).

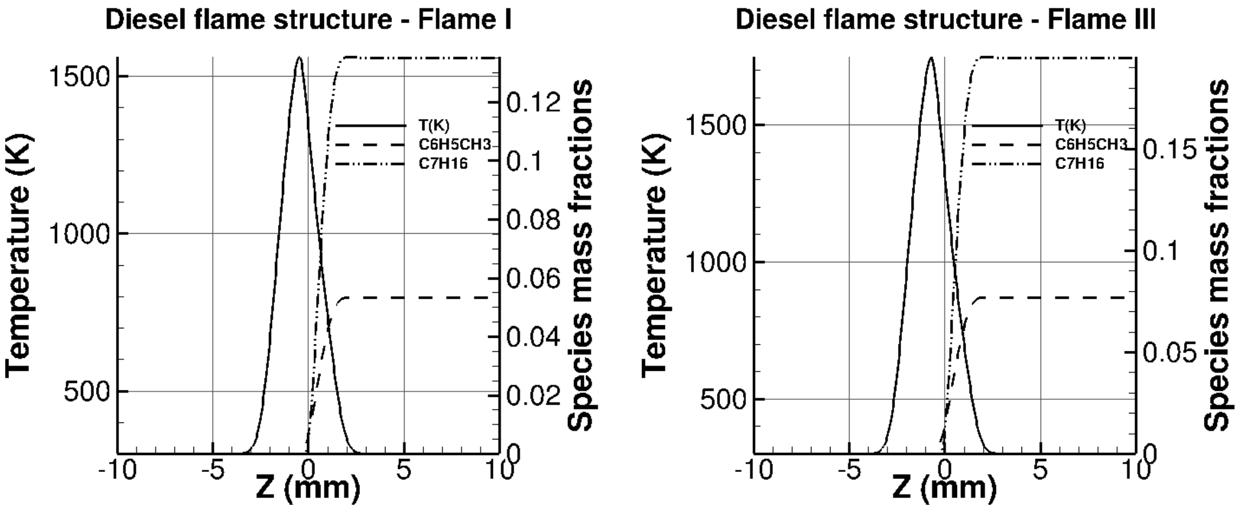

Figura 7: Counterflow diffusion Diesel flame structure - Flame I (left), Flame III (right)

According to the HCO species profile, it can be seen that there is almost no difference between the flame front positions, as the increase of the gas flow is the same at both left and right sides. In addition, there is a decrease in flame thickness for Flame V, due to the higher injection velocity at both left and right sides: the flame front is more stretched.

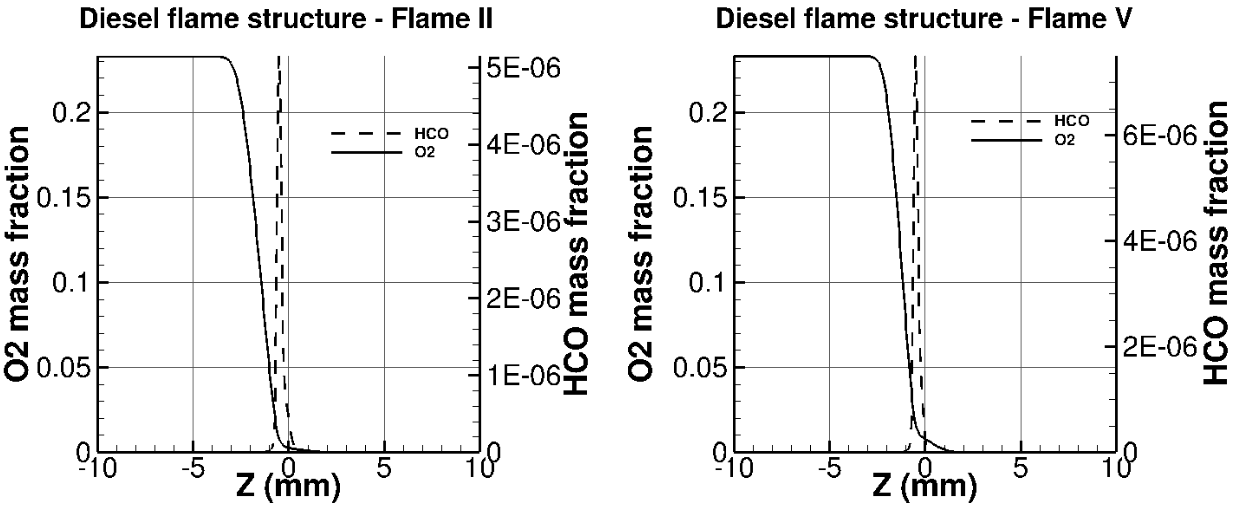

Figura 8: Counterflow diffusion Diesel flame structure - Flame II (left), Flame V (right)

Figure 9 presents the gas temperature and fuel species profiles for Flames II (left) and V (right). It is observed that the fuel mass fractions remain constant (same equivalence ratio). Furthermore, an increase of about 80 K in the maximum temperature of Flame II it can be seen compared to that of Flame V, this is because a flame tends to cool as the flows velocities increase.

## 5. CONCLUSIONS

This paper has presented numerical studies of diesel combustion in a 1D freely propagating gaseous premixed flame configuration and 1D gaseous counterflow diffusion flame configuration. The key objective of the study was to understand the flame structure of Diesel fuel and validate the kinetic models used in the simulations.

The kinetic modelling for diesel oxidation in a 1D freely propagating gaseous premixed flame and 1D gaseous diffusion counterflow flame was performed using the REGATH package developed at EM2C laboratory (N. Darabiha *et al* 1993, Candel *et al* 2011 and Franzelli *et al* 2013).

The kinetic model of Andrae et al (2011) was chosen to carry the simulations. This model consists of 150 species and 759 reactions. A surrogate Diesel fuel composed of n-heptane and toluene was chosen to represent Diesel chemistry.

In this study, we have estimated flame velocities as a function of equivalence ratio for 4 different mixtures of n-heptane and toluene, and the one closer to Commercial Diesel experimental flame velocity was chosen (70% n-heptane/30%

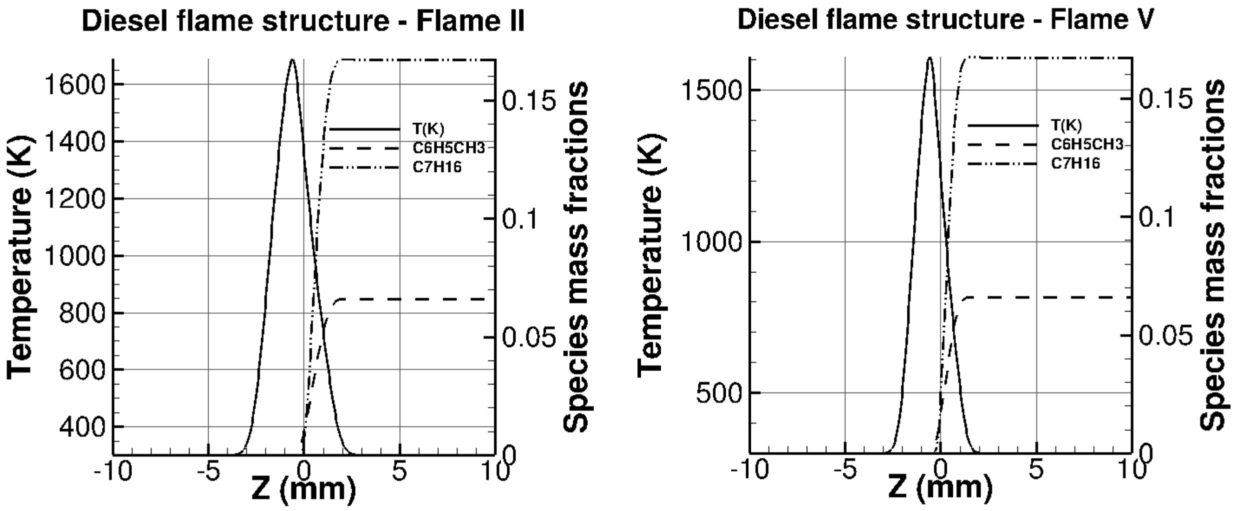

Figura 9: Counterflow diffusion Diesel flame structure - Flame II (left), Flame V (right)

toluene). Therefore, this was the mixture chosen to represent diesel chemistry and analyse the flame structure in the counterflow configuration.

A typical counterflow diffusion diesel flame structure was presented and analysed. Then, the influence of both equivalence ratio and injection velocity (strain rate) was also analysed.

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## 7. RESPONSIBILITY NOTICE

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