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FLUIDYNAMICAL ASPECTS OF n-HEPTANE-ALCOHOL DIFFUSION FLAMES

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Abstract

The paper presents fluidynamical aspects of diffusion flames generated by the burning of mixtures of n-heptane-methanol and n-heptane-ethanol. The analysis is based on a generalisation of the Shvab-Zel'dovich formulation already developed to study multicomponent fuel burning. The choice of these pairs of fuels is due to the fuels mixture used commercially. The configuration of the flow is that established by two opposing streams, the counterflow. This configuration was used because of its similarity to the flamelet configuration, used in turbulent combustion description. The results will be depicted in a such way that they will reveal some flame properties, like as temperature and scalar dissipation. The scalar dissipation, determined around the flame, can be related to the residence time of the reactants in the reaction region.

Keywords: diffusion flame, multicomponent fuels, flamelet

1. Introduction

Due to the importance of multicomponent fuel burning for electric generation and transport in general, from surface to space transportation, an extensive number of studies has been performed on combustion evolving those fuels. Despite of that fact, much more attention has to be dedicated to elucidate some questions. This analysis addresses some such questions related to fluidynamics aspects of diffusion flames generated by mixtures of alcohol and n-heptane.

Nowadays, rigorous restrictions on the combustion emissions into the ambient atmosphere have been driven detailed analyses on flames. Together with those analyses, several methods were proposed to reduce emissions. One them is the doping of the multicomponent fuel flames with substances that make the flame clean, for instance, the hydrogen is one of these substances. The influence of the hydrogen on burning of fuel mixtures has been studied for a long time (1; 2; 3; 4; 5; 6; 7; 8; 9). Another method is to change the combustion conditions based one the knowledge of the burning process. Following this aim, the present work focused on the fluidynamical details of diffusion flames established by n-heptane-methanol and n-heptane-ethanol burning.

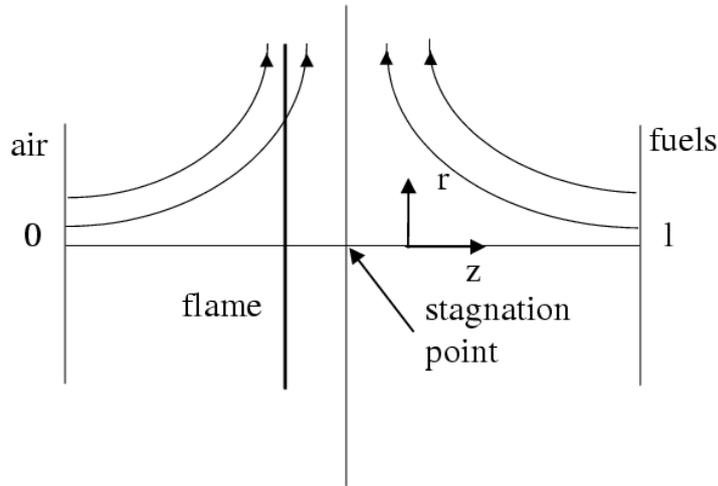


Figure 1: Schematic representation of the counterflow geometry.

The infinite reaction rate of the Burke-Schumann mechanism imposes conditions that all reactions take place inside an infinitely thin flame. A question arises when the reactions rates are considered finite. Does the burning of multicomponent-fuels occur in a single diffusion flame?

Experimental works pointed out that the burning of binary and ternary fuels mixtures (n-heptane, methanol, toluene) occur inside a determined region (10; 11; 12; 13). Also, numerical works on binary fuels (heptane-hexadecane, n-heptane-decane and heptane-octane) droplet combustion indicated that a single flame region is observed (14; 15; 16). More recently, results from theoretical analysis established the asymptotical conditions for the burning of multicomponent fuel to proceed in a single flame (17; 18; 19). Therefore, the assumption of single flame for multicomponent fuels is valid even for the analysed cases with finite reaction rate. Moreover, this fact justifies the usage of the developed model to describe multicomponent fuel combustion (20).

By making usage of the developed model to study the multicomponent fuel burning, some aspects of diffusion flames from n-heptane-methanol mixtures and n-heptane-ethanol mixtures.

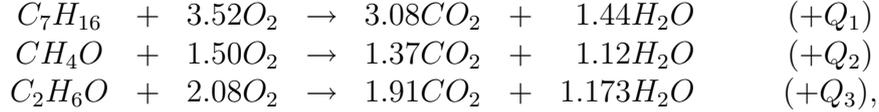
2. Flowfield Description

The analysis of multicomponent fuel diffusion flames will be performed based on the counterflow configuration, which is schematically presented in Figure 1. This configuration is broadly used in numerical and analytical analyses since the results can be verified experimentally due to the easy access into the flame. In addition, the particularities of the counterflow configuration permit several simplifications on the flow field description (21).

To avoid the large consume of CPU time in turbulent reacting flow simulations in certain conditions, the flow field and the chemistry are decoupled assuming the flame to be a infinitely thin frontier separating the fuel from the oxygen. The next approximation is to consider the flame as an ensemble of laminar diffusion flamelets (22). Because these flamelets are forced to move non stationarily by the turbulence, the flamelet flow configuration is represented well by the counterflow. Isolated flamelet can be studied numerically, experimentally and asymptotically by the laminar counterflow diffusion flames, Therefore, the choice for the counterflow configuration is to extract information from the results suitable for turbulent conditions.

According to Fig. 1, the oxidant stream comes out at $r = 0$ and the multicomponent fuel stream comes out at $r = 1$. Consequently, the subscript 0 is used to denote the condition at $r = 0$ and the subscript 1 is used to denote the condition at $r = 1$. The oxidant stream is constituted in a such way that Y_{O_0} is the oxygen mass fraction and $(1 - Y_{O_0})$ is the nitrogen mass fraction. The multicomponent-fuel stream comes with mass fractions Y_{i1} for the fuels and $(1 - \sum_{i=1}^n Y_{i1})$ for the nitrogen mass fraction.

The multicomponent fuels chemical reactions, given in terms of mass, proceed at one global step according to the following set of reactions,



which is considered to perform in a infinite rate.

The radiative energy transfer is included in the model by the approximation of optically thin transparent gas and released in the CO_2 and H_2O bands. The radiative energy loss is taken into account in the analysis through the term q_{rad} expressed by

$$q_{rad} = \sigma \theta^4 \left(X_{CO_2} \frac{\bar{l}_P}{l_{P_{CO_2}}} + X_{H_2O} \frac{\bar{l}_P}{l_{P_{H_2O}}} \right)$$

in which $\theta (\equiv T/T_0)$ is the nondimensional temperature, X_i denotes the mole fraction of species i ; T_0 is the reference temperature and is equal to the flow temperature at the boundary $r = 0$.

The Planck-mean absorption lengths l_P for CO_2 and H_2O can be found elsewhere (23; 24). The dimensionless emissivity σ that appears in the previous equation is given by

$$\sigma = \frac{4\sigma_B T_0^3 l}{\bar{l}_P c_p \rho_0 v_0}$$

where σ_B is the Stefan-Boltzmann constant, \bar{l}_P is the mean value between $l_{P_{CO_2}}$ and $l_{P_{H_2O}}$ evaluated at the flame position, l is the distance between the boundaries, c_p is the specific heat at constant pressure, ρ_0 and v_0 are the gas density and velocity at $r = 0$, respectively.

3. Results and Comments

The results correspond to n-heptane-methanol and n-heptane-ethanol counterflow diffusion flames. The characteristic of the counterflow problem is given by the following properties. The space between the two nozzles is set to $l = 2cm$, oxidant and fuel mass fluxes are equals, relating to the velocities $v = 0.5, 1, 2m/s$, and the temperature fixed at 373 K for all cases. The Lewis numbers are different from unity; the n-heptane, methanol, ethanol, oxygen, water vapour and carbon dioxide Lewis numbers are 1.7, 1.07, 1.28, 1.1, 0.85 and 1.2, respectively.

Here the n-heptane is labelled by species 1 and alcohol is labelled by species 2. The heat released by the n-heptane reaction is $4.495 \times 10^4 (J/kg)$, by the methanol reaction is $2.2479 \times 10^4 (J/kg)$ and by the ethanol reaction is $2.9167 \times 10^4 (J/kg)$

The results presented in this section are obtained by the numerical integration of the multicomponent-fuel diffusion flame problem (20). The numerical scheme is based on the finite difference. The first derivatives are represented by a backward difference in the part of the domain in which velocity v is positive, but by a forward difference in the other part of the domain in which mass flux is negative.

The condition $v > 0$ is found between the oxidant nozzle and the stagnation point, and the condition $v < 0$ is found between the stagnation point and the fuel nozzle.

The results will be presented in three parts. The first part displays the rules of the preferential mass diffusion of alcohol and thermal diffusion of n-heptane, via the Lewis number of the fuels, on the temperature and reciprocal scalar dissipation χ_f^{-1} (the unit is second) at the flame. The definition of χ_f is $(k/\rho c_p)(1/l^2)[\nabla^2(Z/Z_1)]^2|_{r=r_f}$, in which Z is the mixture fraction ($\equiv s_1 Le_O Y_1/Y_{O0} Le_1 + s_2 Le_O Y_2/Y_{O0} Le_2 - Y_O/Y_{O0} + 1$); r_f is the flame position, s_i is the oxygen mass to burn stoichiometrically a unit fuel i mass, Le_i is the Lewis number of fuel i , Y_i is the fuel i mass fraction and Y_O is the oxygen mass fraction. For the n-heptane reaction, s_1 is equal to 3.52, for the methanol reaction, $s_2 = 1.5$ and for the ethanol reaction $s_2 = 2.08$.

The second part exhibits the influence of the radiative heat loss on those flame properties. The radiative heat loss depends directly on the hot gases volume. Thereby, the increase of the velocity v_0 reduces that volume, and consequently reduces radiative heat loss.

The third part shows the influence of velocity v_0 on the temperature and reciprocal scalar dissipation of n-heptane-methanol and n-heptane-ethanol diffusion flames.

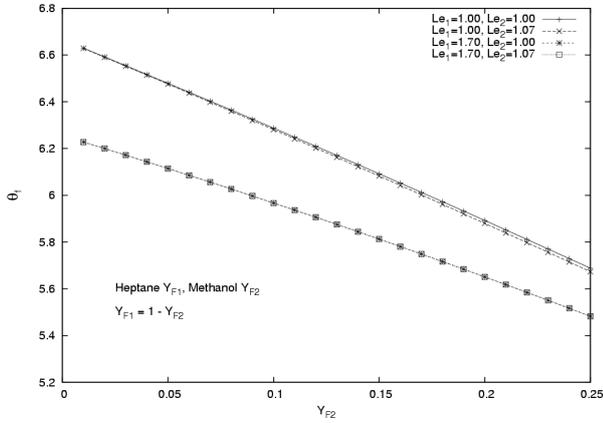
3.1. Lewis Number Effects

Figures (2) display the temperature of the diffusion flame established by the burning of mixtures of n-heptane-methanol and n-heptane-ethanol. From Figs. (2a,b,c), the results confirm the dependence of the flame temperature on the Lewis numbers of the fuels. By decreasing the Lewis number with the choice of methanol as the second fuel, the diffusive transport relatively to the conductive transport is larger than that for the ethanol. The consequence is such that the flame temperature for the n-heptane-methanol mixtures is larger than the flame temperature for the n-heptane-ethanol mixtures, even for $Q_{ethanol} > Q_{methanol}$. Since the alcohol Lewis number is close to one, numerical simulations considering Lewis number unity do not compromise seriously the results. However, this consideration can not be assumed by the n-heptane Lewis number.

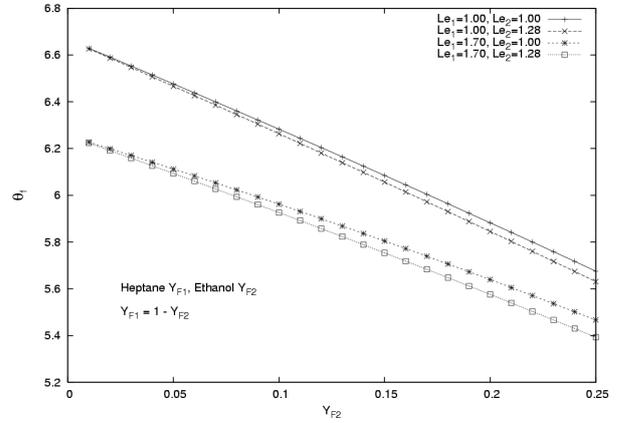
The model considers the reaction region infinitely thin, because the reaction rate is assumed as infinitely fast. Thereby, the residence time of the reactants inside the flame is infinitely small. Although the chemical reaction is under this condition, the reciprocal scalar dissipation χ_f^{-1} can be used as a measurement of the residence time of the reactants in the flame. The results depicted by Figs. (3a,b) reveal that χ_f^{-1} is strong dependent on the Lewis number of the fuels.. Thereby, the reciprocal scalar dissipation χ_f^{-1} for the mixture n-heptane-methanol is smaller than that for the mixture n-heptane-ethanol, as seen in (3c). The dependence of χ_f^{-1} on Le_2 is via the thermal conductivity k , the density ρ and the gradient ∇Z . Thus, decreasing Le_2 , changing ethanol by methanol, the flame temperature θ_f increases, according to Figs. (2), ρ decreases and k increases. The consequence is an decrease of χ_f^{-1} . This result is important if the burning conditions are close to that of the extinction: as smaller χ_f^{-1} is, as closer the flame becomes to a unstable condition (extinction). Therefore, from Fig. (3c), it is seen that diffusion flames generated by the burning of n-heptane-methanol mixtures is more unstable than that n-heptane-ethanol mixtures.

It is worth to recall that this analysis does not provide the extinction condition, but only fluidynamical information about the flow conditions around the flame; the extinction is the interaction of the flow conditions and the chemical reactions. Therefore, since the chemical reaction is considered infinitely fast, the extinction will never occur.

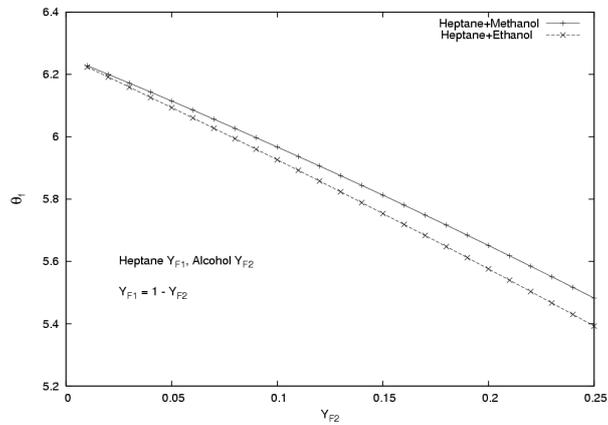
3.2. Radiation Effect



(a)

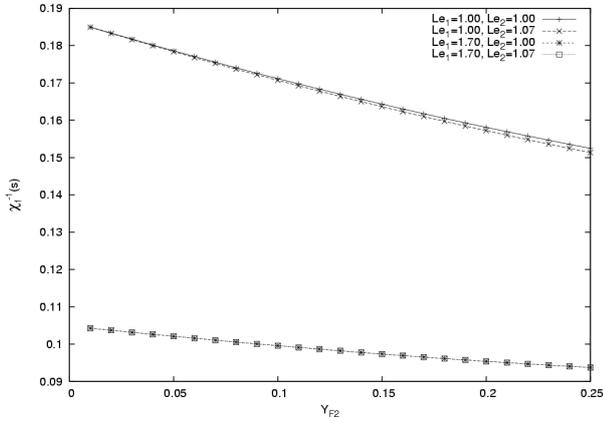


(b)

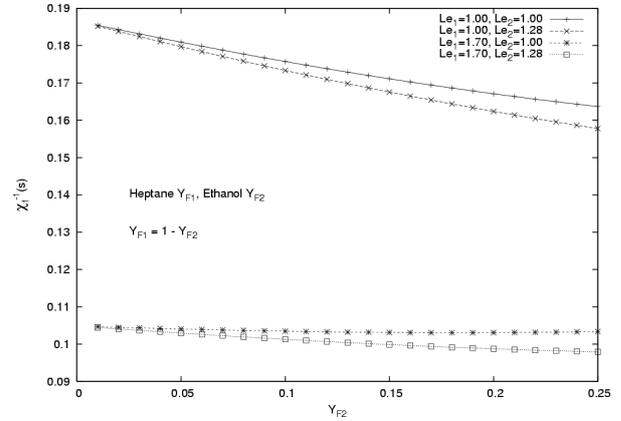


(c)

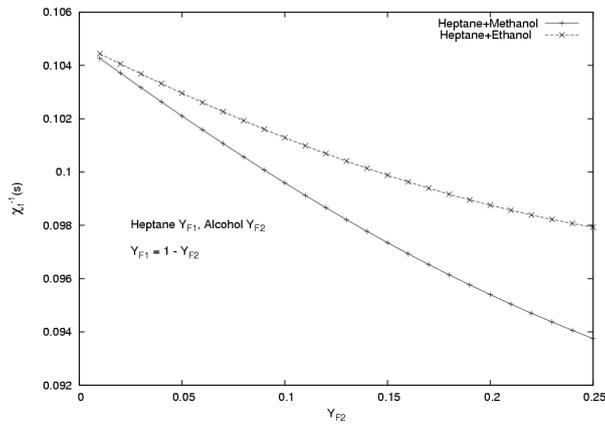
Figure 2: a) Shows flame temperature θ_f as a function of the methanol mass fraction. b) Shows flame temperature θ_f as a function of the ethanol mass fraction. The results are displayed for four combinations of Lewis numbers $(Le_1, Le_2) = (1, 1), (1, 1.07 \text{ or } 1.28), (1.7, 1), (1.7, 1.07 \text{ or } 1.28)$. c) Shows flame temperature θ_f as a function of the mass fraction of methanol and ethanol. The results are displayed for Lewis numbers $(Le_1, Le_2) = (1.7, 1.07), (1.7, 1.28)$.



(a)



(b)



(c)

Figure 3: a) Shows reciprocal scalar dissipation χ_f^{-1} as a function of the mass fraction of methanol. b) Shows reciprocal scalar dissipation χ_f^{-1} as a function of the mass fraction of ethanol. The results are displayed for four combinations of Lewis numbers $(Le_1, Le_2) = (1, 1), (1, 1.07 \text{ or } 1.28), (1.7, 1), (1.7, 1.07 \text{ or } 1.28)$. c) Shows reciprocal scalar dissipation χ_f^{-1} as a function of the mass fraction of methanol and ethanol. The results are displayed for Lewis numbers $(Le_1, Le_2) = (1.7, 1.07), (1.7, 1.28)$.

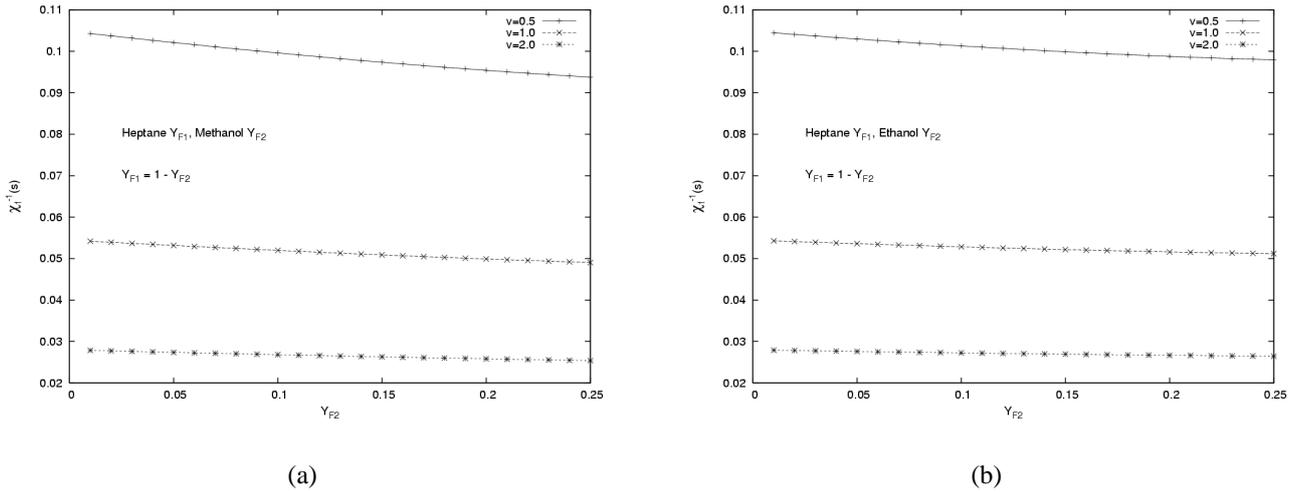


Figure 4: a) Shows flame temperature θ_f as a function of the mass fraction of methanol, for four combinations of Lewis numbers. b) Shows flame temperature θ_f as a function of the mass fraction of ethanol, for four combinations of Lewis numbers.

The model included the radiative heat loss with the hypothesis of transparent gas. This hypothesis does not permit the radiative heat to be absorbed by the gas and re-emitted to the flame. The results show a slight change in the flame temperature and the scalar dissipation with the inclusion of the radiative heat loss. Therefore, the results from Figs. (2c) and (3c) represent well those properties.

3.3. Flow Velocity Effect

The flow velocity has no important effect on the flame temperature θ_f because the infinitely fast chemical reaction can be not modified. The flow velocity has a strong influence on the thickness of the viscous layer around the the plan that has the stagnation point. It is inside this viscous layer that the flame is established. Also, it is from that layer that the radiative heat is emitted. Thus, increasing the velocities of the opposed flows, the viscous layer becomes thinner and the hot gas volume, from which the radiative heat is lost, decreases. In these cases the reduction of the viscous layer thickness produces only a small variation on the flame temperature, via a reduction in the radiative heat loss. However, the decrease in the viscous layer thickness produces an increases in the gradient of Z that causes an important reduction in χ_f^{-1} , as seen in Fig. (4). Therefore, the flow velocities in the counterflow configuration is the main factor to lead to flame to extinction.

4. Conclusion

In this work, it was seen that Lewis numbers, mainly for the heavy fuels, have to be included in the model to study multicomponent fuels diffusion flames. Moreover, the reciprocal scalar dissipation χ_f^{-1} , a factor of measuring the residence time of the reactants in the flame, is strongly influenced by the flow velocities.

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