

STUDY OF THE EFFECTS OF PREFERENCIAL DIFFUSION IN ETHANOL LAMINAR REACTIVE FLOWS

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Abstract. *The present study evaluates the effects of preferential diffusion in axisymmetric confined reactive flow. The analysis of combustion reaction is conducted for two different fuels, methane and ethanol, with air as the oxidizing agent. A global, single step, irreversible with infinitely fast rate reaction is considered as a model for the chemical kinetic mechanism. The preferential diffusion effects are evaluated using a classical formulation proposed in the literature, which uses the generalized mixture fraction and excess enthalpy as conserved scalar, extending thus the classical formulation for non-unitary Lewis numbers. Temperature variation of thermophysical properties is considered in the developed model. The quantities of interest for the reactive flow are obtained using the Finite Volume Method in a structured mesh. The results are obtained for different Lewis numbers for fuel and oxidizer, and show the general behavior of the flow velocities, temperature, mass fraction and mixture fraction profiles influenced by this parameter. The results are compared with the unitary Lewis number case.*

Keywords: *preferential diffusion, Lewis number, confined laminar diffusion flame, flame-sheet model, finite volume method*

1. NOMENCLATURE

c_p	constant pressure specific heat
D	mass diffusion coefficient
g	gravitational constant
h_{RP}	enthalpy of reaction
H	excess of enthalpy
P	pressure
r	radial coordinate
t	time
T	temperature
u	axial velocity
v	radial velocity
x	axial coordinate
Y	mass fraction
Z	generalized mixture fraction

Greek Symbols

λ	thermal conductivity
μ	viscosity
ρ	specific mass
ω	reaction rate
Subscripts	
0	reference state
A_∞	air inlet
f	flame front
F	fuel
F_∞	fuel inlet
O	oxidizer

2. INTRODUCTION

Diffusion flames play an important role in practical combustion applications. Many combustion systems make use this type of flame, also named non-premixed (Williams, 1994), in the presence of turbulent flows. The term diffusion flame was introduced by Burke and Schumann (1928) to designate flames in which fuel and oxidant are initially separated, mixing occurs in a region where combustion occurs, forming a flame structure. In mixtures constituted by fuels with different molecular weight, the preferential mass diffusion of the light species, potentiated by the presence of heavy species, has an important influence on the flame. In addition, the preferential thermal diffusion of heavy species is augmented by the presence of light species. The importance of the mass and thermal diffusions are registered by the Lewis (rate between thermal and mass diffusivity) numbers effects (Fachini, 2007).

The experimental analysis of a confined axisymmetric methane laminar flame presented by Mitchell et al. (1980) has been used as a reference to the development of new experiments and to the validation of numerical solutions. Keyes and Smooke (1987) utilized the flame sheet model as a starting estimate for counterflow diffusion flame problem. They obtained a numerical solution for boundary layer equations and validated it using the experimental results of Mitchell et al. (1980). Xu and Smooke (1993) applied a primitive variable Newton's Method for the calculation of an axisymmetric

laminar diffusion flame based on the experiment of Mitchell et al. (1980). Ern et al. (1995) used the velocity-vorticity formulation and Riedel (1998) applied a solution obtained using the finite volume method with unstructured grid to analyze the same system (Mitchell et al., 1980). Tarhan and Selçuk (2003) applied the method of lines to the numerical simulation of a confined methane/air laminar diffusion flame, extended by Uygur et al. (2008) that presented a solution considering thermal radiation; all of them also based on the experiment of Mitchell et al. (1980).

The literature of ethanol flames is more restricted. Lyu and Chen (1991) used ethanol to the solution of a non-confined diffusion flame obtained by the fuel vaporization on the walls of a cylinder and on a flat plate, considering boundary layer approximation. Saxena and Williams (2007) presented the numerical and experimental solution of a counterflow ethanol diffusion flame. The numerical solution was obtained using of commercial software that considered several effects, like radiation heat transfer, the Soret effect, multicomponent diffusion and a detailed reaction mechanism.

Sauer (2012) conducted an analysis of a confined axisymmetric reactive laminar flame based on the Mitchell et al. (1980) experiment. A global, single step, irreversible with infinitely fast rate reaction is considered as a model for the chemical kinetic mechanism, consistent with the flame sheet approximation. Temperature variation of thermophysical properties was considered and the solution was obtained using the finite volume method in a structured mesh with a collocated grid arrangement. The analysis of the combustion reaction is conducted for two different fuels, methane and ethanol, with air as the oxidizing agent. The numerical results for methane were compared with experimental data (Mitchell et al., 1980) and with numerical results (Xu and Smooke, 1993; Tarhan and Selçuk, 2003). The ethanol results were compared with the ones obtained for methane and the main difference was observed for in the flame height, which was lower for ethanol which is an oxygenated fuel with a lower stoichiometric rate than methane.

Lewis number influence on diffusion flames in conditions far from the extinction has been studied for a long time. The Lewis number is involved in the stoichiometric reactants fluxes conditions at the flame, thus any change of the reactants Lewis numbers represent modifications on the corresponding mass flux to the flame, forcing it to establish in different location (Sibulkin and Malory, 1982). In addition, the difference between the mass diffusion and the thermal diffusion of each reactant influences the flame temperature (Takagi and Xu, 1994).

Law and Chung (1982) and Chung and Law (1984) observed the preferential diffusion effects on the temperature field and flame extinction. Lee and Chung (1991) analyzed the effect of streamwise and preferential diffusion on cylindrical Burke-Schumann flame using perturbation method and Green's function technique. Liñan et al (1994) carried out direct numerical simulations of diffusion controlled combustion with non-unity Lewis numbers for the reactants and products, thus accounting for the differential diffusion effects of the temperature and concentration fields. Liu et al (2000) studied the thermal effects of radiation heat loss and Lewis numbers on diffusion flame extinction, particularly at small stretch rates. It was shown that departure of the fuel Lewis numbers from unity has a much stronger effect on the flame location than the oxidizer Lewis numbers. Shamim (2006) numerically investigates this interaction with a particular emphasis on the effect of unequal and non-unity fuel and oxidizer Lewis numbers in a transient diffusion flame. The unsteadiness is simulated by considering the flame subjected to modulations in reactant concentration.

An extension of the Shvab-Zel'dovich formulation was used by Fachini (2007). This extended formulation is based on the Burke-Schumann kinetic mechanism. The model was applied to a diffusion flame generated by the burning of mixtures of n-heptane and hydrogen diluted in nitrogen in a counterflow configuration. It was revealed by the results, the effects of the potentiated preferential hydrogen mass diffusion in compositions in which nitrogen and n-heptane are the majority species, and the potentiated preferential n-heptane thermal diffusion in compositions in which nitrogen and hydrogen are the majority species, on the flame properties. Caldeira and Fachini (2010) numerically studied the combustion of an infinite linear array of gaseous fuel pockets in a stagnant oxidizing environment under microgravity conditions. The gas pocket combustion was described using the generalized Shvab-Zel'dovich formulation with nonunitary Lewis number. A nonstaggered grid is used and the SIMPLEC algorithm is employed to solve the modified pressure-velocity coupling. Nonunitary Lewis number and interaction effects on flame behavior and on the fuel consumption were analyzed. The combined effect of nonunitary Lewis number with gas pocket interaction revealed that the flame behavior, the fuel consumption, and the burning time were modified in relation to the unitary Lewis number condition. Moreover, the influence of the oxidant Lewis number on the flame behavior was more effective than the fuel Lewis number. The results also showed that the pocket has a limited capacity to furnish fuel to the flame, but the oxidant environment has an unlimited capacity to supply the oxidant to the flame.

The present work describes a confined laminar flame for methane and ethanol considering preferential diffusion effects. Conservation equations are considered by the use of the finite volume method and variable properties. The flame-sheet method is used to simplify the chemical reactions of the system. The formulation applied to evaluate the effects of preferential diffusion was introduced by Liñan (1991). It is based on combining the conservation equations in a way to eliminate the reaction terms similar to the method used by Burke and Schumann (1928) for unity Lewis numbers. The results of the methane and ethanol flame are compared and analyzed.

3. MATHEMATICAL MODEL

The reactive flow in multicomponent systems is described by the mass conservation, the species conservation, the momentum conservation and the energy conservation equation. These conservation laws can be shown mathematically as the equation of continuity, momentum equation, equation of energy and equation of chemical species.

The equations below in transient state treat the fluid as a continuum. The equations of continuity and species are the exact representation of the law of mass conservation to mixtures in multicomponent systems. In order to simplify the governing equations, the heat flux due to radiation is neglected because of low absorptivity of gases considered in this work. The effects of viscous dissipation and pressure work will also be neglected in the energy conservation equation considering the hypothesis of flow at low speed, the Soret and Dufour effects will also be omitted. In addition, the specific heats of all chemical species are considered constants and the diffusion velocities follow the Fick's law.

The equations of continuity, of momentum conservation in axial and radial directions, species conservation and energy conservation are written respectively in the cylindrical axisymmetric coordinate system, and in dimensionless form, by:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u)}{\partial x} + \frac{1}{r} \frac{\partial(\rho r v)}{\partial r} = 0 \quad (1)$$

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u u)}{\partial x} + \frac{1}{r} \frac{\partial(\rho r u v)}{\partial r} = & -\frac{\partial P}{\partial x} + \frac{1}{\text{Pr}} \left[\frac{1}{r} \frac{\partial}{\partial x} \left(r \mu \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial u}{\partial r} \right) \right] + \\ \frac{1}{\text{Pr}} \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial x} \right) + \frac{1}{3} \frac{1}{r} \frac{\partial}{\partial x} \left(r \mu \frac{\partial u}{\partial x} \right) - \frac{2}{3} \frac{1}{r} \frac{\partial}{\partial x} \left(r \mu \left[\frac{\partial(rv)}{\partial x} \right] \right) \right\} + \frac{1}{Fr} \rho \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u v)}{\partial x} + \frac{1}{r} \frac{\partial(\rho r v v)}{\partial r} = & -\frac{\partial P}{\partial r} + \frac{1}{\text{Pr}} \left[\frac{1}{r} \frac{\partial}{\partial x} \left(r \mu \frac{\partial v}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial r} \right) \right] + \\ + \frac{1}{\text{Pr}} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial x} \left(r \mu \frac{\partial u}{\partial r} \right) \right] + \frac{1}{\text{Pr}} \left\{ -\frac{2}{3} \frac{1}{r} \frac{\partial}{\partial r} \left[\mu \frac{\partial(rv)}{\partial x} \right] + \frac{2}{3} \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \frac{\partial u}{\partial x} \right] \right\} + \\ + \frac{1}{\text{Pr}} \left[-\frac{2\mu v}{r^2} + \frac{2}{3} \frac{\mu}{r^2} \frac{\partial}{\partial r} (rv) + \frac{2}{3} \frac{\mu}{r} \frac{\partial u}{\partial x} \right] \end{aligned} \quad (3)$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u Y_k)}{\partial x} + \frac{1}{r} \frac{\partial(\rho r v Y_k)}{\partial r} = \frac{1}{Le_k} \left[\frac{1}{r} \frac{\partial}{\partial x} \left(r \rho \alpha \frac{\partial Y_k}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho \alpha \frac{\partial Y_k}{\partial r} \right) \right] + \omega_k \quad (4)$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \frac{1}{r} \frac{\partial(\rho r u \rho c_p T)}{\partial x} + \frac{1}{r} \frac{\partial(\rho r v \rho c_p T)}{\partial r} = \frac{1}{r} \frac{\partial}{\partial x} \left(r \rho \alpha \frac{\partial T}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho \alpha \frac{\partial T}{\partial r} \right) - \sum_{k=1}^N h_{f_k}^0 \omega_k \quad (5)$$

The dimensionless parameters present in the equations above are Froude number, Prandtl number, and Lewis number, represented respectively by:

$$Fr = \frac{u_a^2}{g R_o}, \quad \text{Pr} = \frac{\mu_a c_{p_a}}{\lambda_a}, \quad Le = \frac{\lambda_a}{c_{p_a} \rho_a D_a} \quad (6)$$

3.1 Flame Sheet Model

The flame sheet model, which was introduced by Burke and Schumann (1928) and later used by several researchers, makes the assumption that the chemical reaction is confined to thin reaction zone where fuel and oxidizer cannot coexist. This assumption results in the absence of fuel in oxidizer side and of oxidizer in fuel side of the flame. Fuel and oxidizer flow toward the reaction zone in stoichiometric proportions, this condition for the reactants to be completely consumed. In the flame sheet model the reactions are described by a single one-step irreversible reaction corresponding

to an infinitely fast conversion of reactants into stable products. Although the analysis of Burke and Schumann were restricted to the unitary Lewis number (same diffusion rate between heat and mass), it is possible to generalize this formulation to different Lewis numbers by the method presented by Liñan (1991).

In Liñan (1991), the Eqs. (4) and (5) are linearly combined in order to eliminate the reaction terms. Through this method appear the Eqs. (7) and (8) that represent the generalized mixture fraction and excess enthalpy conservation equation, as following:

$$\frac{\partial(\rho Z)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Z) = \frac{1}{Le(Z)} \nabla \cdot [\rho D \nabla(Z)] \quad (7)$$

$$\frac{\partial(\rho H)}{\partial t} + \nabla \cdot (\rho \mathbf{v} H) = \nabla \cdot [\rho D \nabla(H)] - \frac{N(Z)}{Le(Z)} \nabla \cdot [\rho D \nabla(Z)] \quad (8)$$

The stoichiometric mixture fraction which sets the flame position is defined as:

$$Z_f = \left(1 + \frac{s_o Y_{F_{\infty}}}{Y_{O_{\infty}}} \frac{Le_O}{Le_F} \right)^{-1} \quad (9)$$

Using the flame position defined by Eq. (9) it is possible to generate expressions for the temperature and mass fractions fields on the fuel and oxidizer side. These expressions to the variables of interest are written, on the fuel side, as,

$$H + \left(1 + \frac{1}{S} \right) (1 - Z) = (1 + S) Le_F c_p (T - T_0) \frac{1}{Y_{F_{\infty}} h_{RP}} \quad (10)$$

$$Y_F = \frac{Y_{F_{\infty}} Z (S + 1) - 1}{S} \quad \text{and} \quad Y_O = 0 \quad (11)$$

$$Le(Z) = Le_F \quad \text{and} \quad N(Z) = (Le_F - 1)(S + 1) \frac{1}{S} \quad (12)$$

and on the oxidizer side,

$$H + (1 + S)Z = (1 + S) Le_F c_p (T - T_0) \frac{1}{Y_{F_{\infty}} h_{RP}} \quad (13)$$

$$Y_F = 0 \quad \text{and} \quad Y_O = Y_{O_{\infty}} [1 - (1 + S)Z] \quad (14)$$

$$Le(Z) = Le_O \quad \text{and} \quad N(Z) = (1 - Le_O)(S + 1) \quad (15)$$

and S is the generalized stoichiometric air-fuel rate, defined by:

$$S = \frac{s_o Y_{F_{\infty}}}{Y_{O_{\infty}}} \frac{Le_O}{Le_F} \quad (16)$$

The variations of thermophysical properties with temperature are given by the following expressions,

$$\rho = \frac{\rho_0 T_0}{T} \quad \text{and} \quad \mu = \rho \alpha = T^m \quad (17)$$

where $\rho_0 = 1.1707 \text{ kg/m}^3$, $T_0 = 298.15 \text{ K}$, $m = 0.7$ are reference values for air (Murty, 1975).

3.2 Boundary and Initial Conditions

The combustion system used in this study and represented in Fig. 1 is based on the experiment performed by Mitchell et al. (1980). Such a system consists essentially in two concentric pipes with ratios R_O and R_F , where air and fuel flow respectively. When the two gases are outside of the pipes a diffusion flame, with a well-defined shape, forms, as well as in the experiment the burner is confined by a cylinder with solid walls.

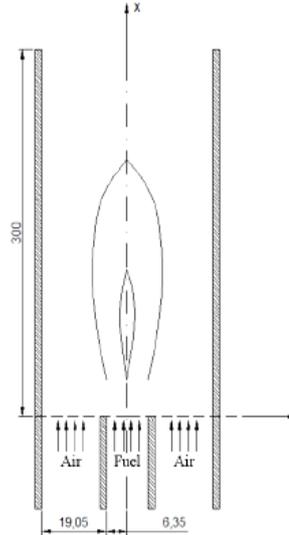


Figure 1. Schematic diagram of the axisymmetric burner (dimensions: mm). Adapted of Mitchell et al (1980).

Thus, the governing equations in the mathematical model are subject to the following boundary conditions

$$u = u_F, \quad v = 0, \quad H = 0, \quad Z = 1, \quad x = 0, \quad 0 < r < R_F \quad (18)$$

$$u = u_O, \quad v = 0, \quad H = 0, \quad Z = 0, \quad x = 0, \quad R_F < r < R_O \quad (19)$$

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial H}{\partial x} = \frac{\partial Z}{\partial x} = 0, \quad P = P_a, \quad x = \frac{L}{R_O}, \quad 0 < r < R_O \quad (20)$$

$$\frac{\partial u}{\partial r} = v = \frac{\partial H}{\partial r} = \frac{\partial Z}{\partial r} = \frac{\partial P}{\partial r} = 0, \quad r = 0, \quad 0 < x < L \quad (21)$$

$$u = v = \frac{\partial H}{\partial r} = \frac{\partial Z}{\partial r} = 0, \quad r = R_O, \quad 0 < x < L \quad (22)$$

In the instant $t = 0$ the entire domain is considered containing only air.

4. NUMERICAL APPROACH

A code was developed in FORTRAN. Conservation equations were discretized with the finite volume method. The physical domain was transformed to a computational using a structured non-uniform mesh. For the conserved scalar evaluation and its derivatives on the interfaces of elementary volumes is used the WUDS interpolation function. As the conservation equations are resolved using primitive variables, it is necessary a treatment for pressure-velocity coupling, which is done by SIMPLEC method in a mesh arrangement co-located.

The code developed in this study is based on the code developed by Sauer (2012) for unitary Lewis number. Sauer's results were validated using the experimental results of Mitchell et al. (1980). In the present study the solution for excess of enthalpy and generalized mixture fraction equations to Sauer's code, removing the unitary Lewis number assumption. To verify the developed code, the results, for unitary Lewis number, were compared with Sauer's results.

A grid convergence study was also conducted for the specific case of $Le_O = 0.75$ and $Le_F = 0.75$. The examined meshes were 40x40, 80x80 and 160x160 points. It was compared the axial velocity component and the temperature profiles obtained with each grid. The gains on result within the same order of magnitude every time a finer mesh is selected. However computational times for 40x40 grid is measured in minutes, for 80x80 grid in hours and for 160x160 grid in weeks. Thus, the 80x80 grid was selected for the present work.

5. RESULTS

Numerical results obtained for methane and ethanol as fuels are presented. These fuels were chosen due the large literature available for methane, which includes experimental data, and due to the high availability of ethanol in Brazil. For the methane-air flame the profiles of fuel and oxidizer mass fraction and the temperature profiles are compared with the experimental results of Mitchell et al. (1980).

Different cases are evaluated for both fuels studied by varying the Lewis number of fuel and oxidizer. Different Lewis numbers represent different physical properties, for example if the fuel is doped with an inert component.

The results were achieved in a cluster with 260 physical cores and 672 logical cores. Although a transient simulation is conducted only steady state results are presented.

The geometric parameters of the physical system and the operating conditions are presented below,

Geometric Parameters:

$$R_O = 2.54 \text{ cm}, R_F = 0.635 \text{ cm}, L = 30 \text{ cm}$$

Fuel Side:

$$u_F = 4.5 \text{ cm/s}, v_F = 0 \text{ cm/s}, P = 1 \text{ atm}, T = 298.15 \text{ K}, Y_F = 1.0$$

Oxidizer Side:

$$u_F = 9.88 \text{ cm/s}, v_F = 0 \text{ cm/s}, P = 1 \text{ atm}, T = 298.15 \text{ K}, Y_{O_2} = 0.232, Y_{N_2} = 0.768$$

5.1 Methane Diffusion Flame

The solution for the methane-air flame is obtained considering the following global reaction:



The results shown in Fig. 2 and 3 for the mass fractions of CH₄ and O₂ indicate that as Le_O increases in relation to the case of Sauer (2012), the oxidant spreads more easily, so that the availability of oxidant for the flame is greater. The opposite effect occurs when the Le_O decreases, i.e, there is less oxidant available for the flame and therefore the flame is shorter.

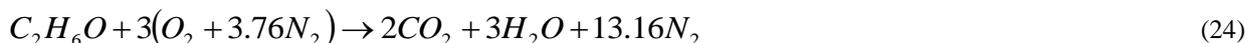
Similar effects are observed when the Le_F varies, when this decreases in relation to the case of Sauer (2012), it means the fuel spreads more easily, which makes the availability of fuel to the flame increase. The opposite effect occurs when Le_F decreases.

The flame height can be defined as the axial position in which is located the highest temperature along the centerline. This method used to determine the flame height is the same used by Sauer (2012), once the results are compared with experimental data, this method appears simpler than consider the position in which Y_F=Y_O=0. Fig. 5 shows the various flame heights for different cases. It is observed that when the Le_O decreases, the maximum temperature increases and the flame height gets smaller when compared with the case of Sauer (2012), the opposite occurs when the Le_O increases. Another fact to be noted is that the flame height obtained experimentally had approximately 5.8 cm height but in all cases simulated the flame heights were overrated.

The results in Figs 2 to 4, when compared with the experimental data, indicate the ability of this study in capturing the trend of experimental results, despite the mass fraction profiles of CH₄ and O₂ provide values with discrepancy greater than 100% in all positions considered.

5.2 Ethanol Diffusion Flame

Considering the same system configuration used for the methane burning, the profiles of the quantities of interest for ethanol burning are obtained. The overall reaction for ethanol-air flame is given by



A very important feature of ethanol is that it is an oxygenated fuel, this becomes important when we want to evaluate the distribution in the flame of the profiles of mass fraction and temperature. The results in Fig. 5 and 6 show the flame heights of ethanol and methane for different Lewis numbers. If a comparison is made between the Fig. 5 and Fig. 6, it is possible to verify that for every Lewis number case presented, the ethanol flame height is always lower than the methane. Besides the Lewis number influence flame height, another fact justifies the ethanol flame height be smaller than the methane flame, this fact is the stoichiometric coefficient, *s_O*, for the ethanol is 2.087, while the value of that term for the methane combustion reaction is equal to 4.0.

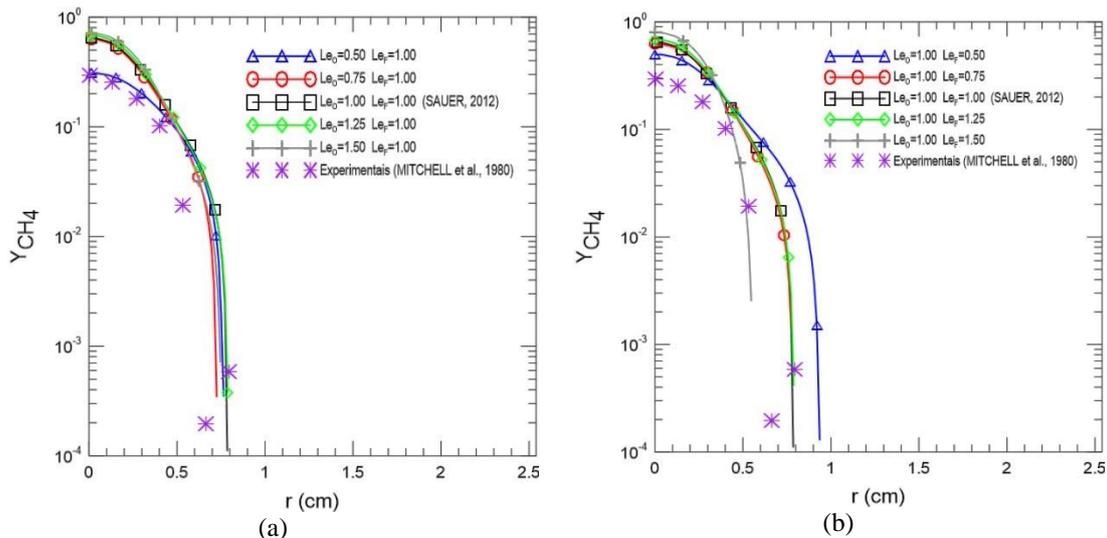


Figure 2. Mass fraction profiles of CH₄ in $x=1.2$ cm: (a) Variation of Le_O and keeping $Le_F = 1.0$; (b) Variation of Le_F and keeping $Le_O = 1.00$

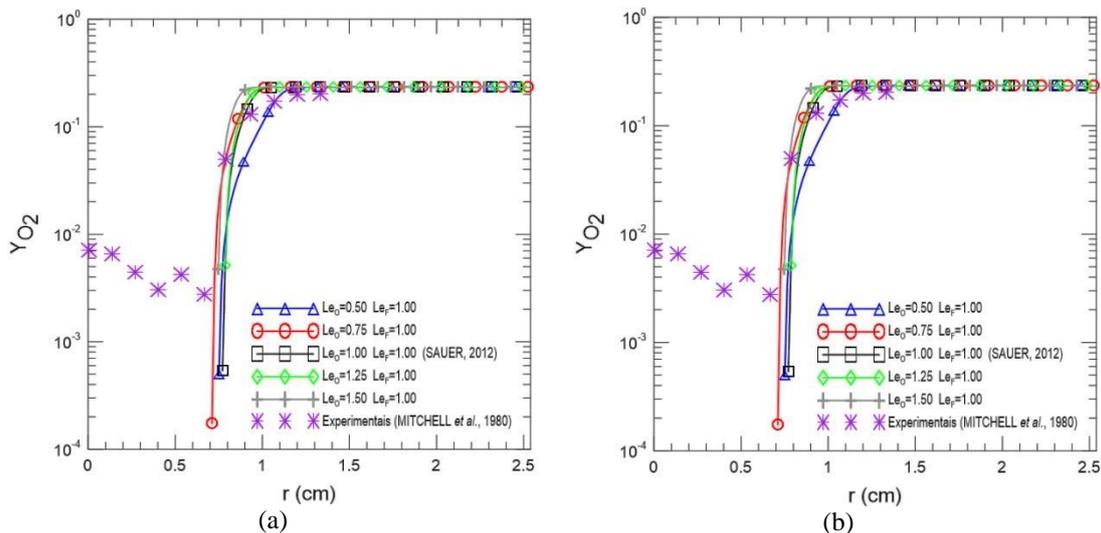


Figure 3. Mass fraction profiles of O₂ in $x=1.2$ cm: (a) Variation of Le_O and keeping $Le_F = 1.0$; (b) Variation of Le_F and keeping $Le_O = 1.00$

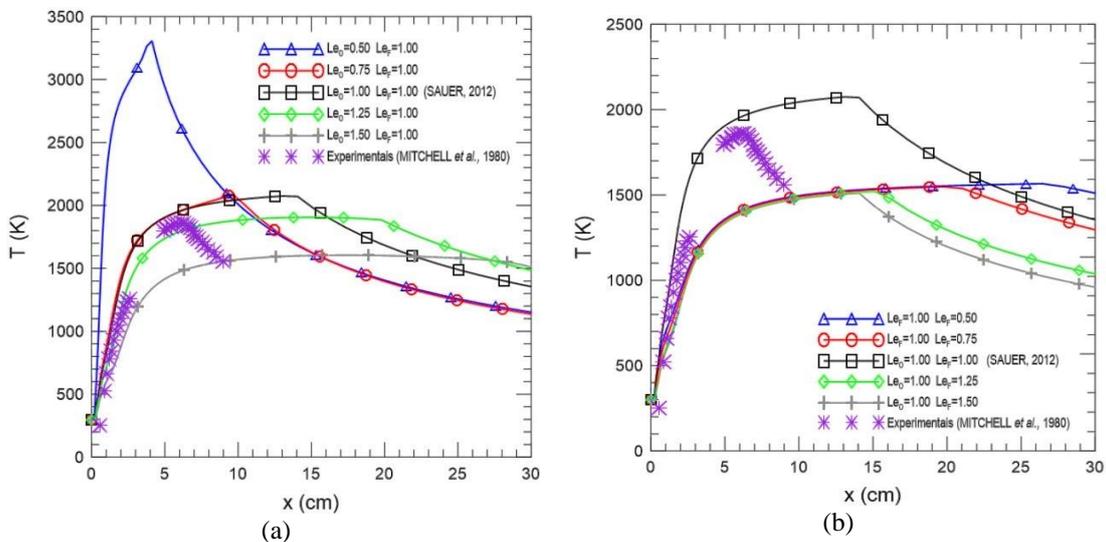


Figure 4. Temperature profiles of the methane flame along the centerline ($r=0$): (a) Variation of Le_O and keeping $Le_F = 1.0$; (b) Variation of Le_F and keeping $Le_O = 1.00$

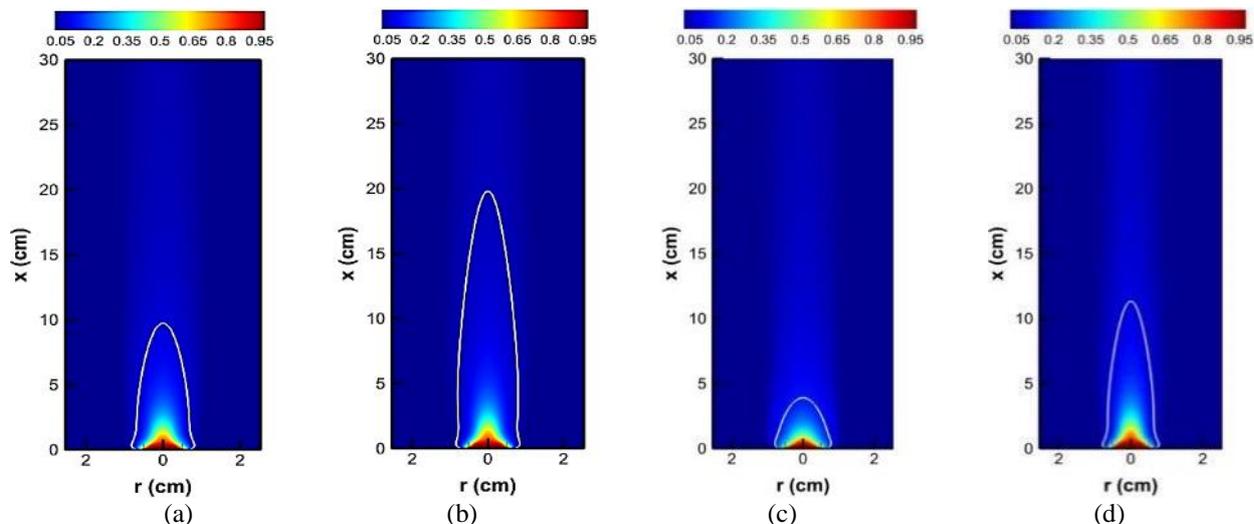


Figure 5. Comparison of mixture fraction profiles: (a) Methane - $Le_O = 0.75$ and $Le_F = 1.00$;
 (b) Methane - $Le_O = 1.00$ and $Le_F = 0.75$; (c) Ethanol - $Le_O = 0.75$ and $Le_F = 1.00$;
 (d) Ethanol - $Le_O = 1.00$ and $Le_F = 0.75$

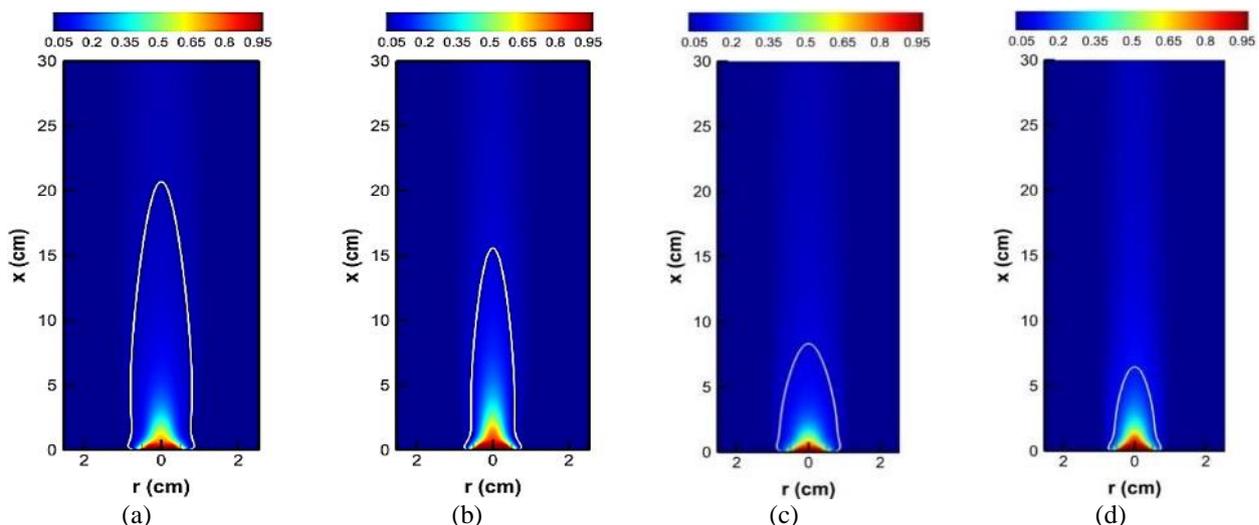


Figure 6. Comparison of mixture fraction profiles: (a) Methane - $Le_O = 1.25$ and $Le_F = 1.00$;
 (b) Methane - $Le_O = 1.00$ and $Le_F = 1.25$; (c) Ethanol - $Le_O = 1.25$ and $Le_F = 1.00$;
 (d) Ethanol - $Le_O = 1.00$ and $Le_F = 1.25$

6. CONCLUSIONS

The Lewis number as was studied is an important parameter in the study of preferential diffusion on diffusion flames, concluded that this number has significant influence in several features of the flame, causing significant changes in both shape and height, as well as in the temperature field due to inequality between heat and mass diffusion. Another fact that can be concluded is that the inclusion of the non-unitary Lewis number in the flame sheet model doesn't solve the significant difference of the profiles shown in the results when compared with the experimental data of Mitchell et al. (1980), which means the need for further studies in order to have results closer to the experimental data.

7. ACKNOWLEDGEMENTS

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8. REFERENCES

- Burke, S.P. and Schumann, T.E.W., 1928. "Diffusion flames". *Industrial & Engineering Chemistry*, Vol. 20, No. 10, pp. 998–1004.
- Caldeira, A., B. and Fachini, F., F., 2010. "Nonunitary lewis number effects on the combustion of a linear array of gaseous fuel pockets". *Numerical Heat Transfer*. Vol. 58, Part. A, pp. 784–801
- Chung, S. H. and Law, C. K., 1984. "Burke-Schumann Flames with Streamwise and Preferential Diffusion". *Combustion Science and Technology*, Vol. 37, pp. 21-46.
- Ern, A., Douglas, C.C. and Smooke, M.D., 1995. "Detailed chemistry modeling of laminar diffusion flames on parallel computers". *International Journal of High Performance Computing Applications*, Vol. 9, No. 3, pp. 167–186.
- Fachini, F., F., 2007. "Extended Shvab-Zel'dovich formulation for multicomponent-fuel diffusion flames". *International Journal of Heat and Mass Transfer*. Vol. 50, pp. 1035-1048.
- Keyes, D.E. and Smooke, M.D., 1987. "Flame sheet starting estimates for counterflow diffusion flame problems". *Journal of Computational Physics*, Vol. 73, No. 2, pp. 267–288.
- Law, C. K., and Chung, S. H., 1982. "Steady State Diffusion Flame Structure with Lewis Number Variation". *Combustion Science and Technology*, Vol. 29, pp. 129-145.
- Lee, S. R. and Chung, S. H., 1991. "Effect of Streamwise and Preferential Diffusion on Cylindrical Burke-Schumann Flames". *Journal of Mechanical Science and Technology*, Vol. 5, pp. 45-52.
- Liñan, A., 1991. *The Structure of Laminar Diffusion Flames*. California Institute Technology, Pasadena, CA, USA.
- Liñan, A., Orlandi, P., Verzicco, R. et al, 1994. "Effects of Non-Unity Lewis Numbers in Diffusion Flames". *Proceedings of the Summer Program 1994*, Center for Turbulence Research, pp. 5-18.
- Liu, F., Smallwood, J. G., Gulder, L. O. et al., 2000. "Asymptotic Analysis of Radiative Extinction in Counterflow Diffusion Flames of Non-Unity Lewis Numbers". *Combustion and Flame*, Vol. 121, pp. 275-287.
- Lyu, H.Y. and Chen, L.D., 1991. "Numerical modeling of buoyant ethanol-air wick diffusion flames". *Combustion and Flame*, Vol. 87, No. 2, pp. 169–181.
- Mitchell, R., Sarofim, A. and Clomberg, L., 1980. "Experimental and numerical investigation of confined laminar diffusion flames". *Combustion and Flame*, Vol. 37, pp. 227–244.
- Murty, K.A., 1975. *Introduction to Combustion Phenomena*. Gordon & Breach.
- Riedel, U., 1998. "A Finite Volume Scheme on Unstructured Grids for Stiff Chemically Reacting Flows". *Combustion Science and Technology*, Vol. 135, No. 1-6, pp. 99-116.
- Sauer, V. M., 2012. *Análise de Escoamentos Reativos de Biocombustíveis em Dutos*. M.Sc. dissertation, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil.
- Saxena, P. and Williams, F.A., 2007. "Numerical and experimental studies of ethanol flames". *Proceedings of the Combustion Institute*, Vol. 31, No. 1, pp. 1149–1156.
- Shamim, T., 2006. "Effect of Unequal Fuel and Oxidizer Lewis Numbers on Flame Dynamics". *International Journal of Thermal Science*, Vol. 45, pp. 1213-1223.
- Sibulkin, M. and Malary, S., 1982. "Diffusion Flame Calculations for Nonunity Lewis Number". *Combustion Science and Technology*, Vol. 28, pp. 85-88
- Takagi, T. and Xu, Z., 1994 "Numerical analysis of laminar diffusion flames – effects of preferential diffusion of heat and species", *Combustion and Flame*. Vol. 96, pp 50-59.
- Tarhan, T. and Selçuk, N., 2003. "Numerical simulation of a confined methane/air laminar diffusion flame by the method of lines". *Turkish Journal of Engineering and Environmental Sciences*, Vol. 27, pp. 275–290.
- Uygur, A.B., Selçuk, N. and Tuncer, I.H., 2008. "A non-iterative pressure based scheme for the computation of reacting radiating flows". *International Journal of Thermal Sciences*, Vol. 47, No. 3, pp. 209–220.
- Williams, F.A., 1994. *Combustion Theory: Second Edition*. Westview Press, second edition.
- Xu, Y. and Smooke, M.D., 1993. "Application of a primitive variable newton's method for the calculation of an axisymmetric laminar diffusion flame". *Journal of Computational Physics*, Vol. 104, No. 1, pp. 99–109.

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