

LES SOLUTION OF A METHANOL JET DIFFUSION FLAME

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Abstract. *The methanol has favorable combustion properties that include lower emissions of particulates and nitrogen oxides. Therefore, this work presents a model for the solution of methanol jet diffusion flames for low Mach-number. The model is based on the solution of the Lagrangian flamelet equations for the chemistry and on the mixture fraction for the flow. The governing equations are discretized using the second-order space finite difference method, using LES (Large-Eddy Simulation) with the Smagorinsky model for the turbulent viscosity. Numerical tests are carried out for methanol diffusion flames, and the results compare favorably with data from the literature.*

Keywords: *diffusion flames, methanol, flamelet, LES*

1. INTRODUCTION

Recently, a growing interest has been observed in the application of methanol as an alternative fuel that can be directly used in the Otto engines or fuel cells (Demirbas, 2008). Its potential as an alternative fuel is due to its favorable combustion properties, which include low emission of particulates and nitrogen oxides (Lindstedt and Meyer, 2002). Currently, the methanol is commonly used as an alcohol for producing biodiesel because of its low price, although other alcohols such as ethanol or the iso-propanol may yield a biodiesel fuel with better properties (Knothe, 2005).

The obtainment of efficient models to represent the combustion of hydrocarbons is currently a topic of great interest. Combustion scientists and engineers have explored computational methods to develop practical combustion systems, especially with regard to the decrease of the pollutants emission in the atmosphere (Griffiths, 1995). Therefore, chemical kinetic modeling has become an important tool for interpreting and understanding combustion phenomena. Its application requires as an input a valid chemical reaction mechanism (Leung and Lindstedt, 1995). A large amount of effort has been devoted to the development of reduced kinetic mechanisms, obtained from detailed kinetic mechanisms, specially for hydrocarbon combustion.

To model the combustion of the methanol it is necessary a good understanding of the mixing process and of the combustion process, since the reaction occurs when the fuel and the oxidant are mixed at molecular level (Pitsch and Fedotov, 2001). The majority of the applications of technical interest involves nonpremixed and turbulent flows. Turbulent flames are complex to model due to the strong coupling that exists between the chemical heat release and the turbulent motion. Nonpremixed flames are characterized by their internal structure and by the transport of fuel and oxidizer to the reaction zone where the products of combustion are formed (Mahalingam *et al.*, 1995). The flamelet model has been successfully used for numerical predictions of turbulent nonpremixed combustion (Pitsch and Peters, 1998).

LES, Large-Eddy Simulation, appears as a promising tool to capture combustion instabilities, and is a good candidate to capture unsteady turbulent mixing. Moreover, it may directly provide part of the description of turbulence/combustion interactions because zones of fresh and burnt gases, having different turbulence characteristics, are instantaneously identified at the level of the resolved grid.

The direct numerical simulation (DNS) of the governing equations for the combustion processes, without using any model for turbulence, requires refined meshes resulting in a prohibitive computational time. Therefore, LES is used in

this work to achieve good results, with computational cost appropriate to the research.

2. OBTAINING A REDUCED KINETIC MECHANISM FOR THE METHANOL

Based on a mechanism composed by 352 elementary reactions among 56 reactive species for high temperature ethanol oxidation given by [Marinov \(1999\)](#), we present a simplified mechanism for the methanol. Typically, the mechanisms for hydrocarbons are generated in a hierarchical way, starting with the hydrogen/oxygen system, adding the carbon monoxide subset, followed by the formaldehyde and larger $C_2 - C_n$ species ([Curran, 2009](#)). Consider the hydrogen-oxygen and the C_1 hydrocarbon submechanisms presented by [Marinov \(1999\)](#), with 129 reversible reactions among 31 species, for the methanol oxidation. For the methanol combustion, the C_2 hydrocarbon submechanism is, in principle, not necessary.

The strategy to obtain the reduced mechanism is inspired in the work of [Peters \(1988\)](#). Initially, we obtain the reaction rate coefficient k of each elementary reaction through the modified equation of Arrhenius

$$k = AT^\beta \exp\left(-\frac{E}{RT}\right) \quad (1)$$

where A is the frequency factor, T the temperature, β the temperature exponent, E the activation energy, and R the gas constant. Then, it is estimated the magnitude of the reaction rate coefficients and it is defined the main chain for the process (see the Fig. 1).

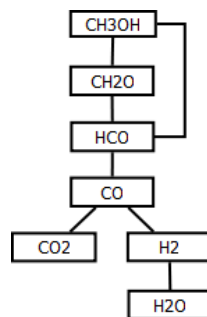
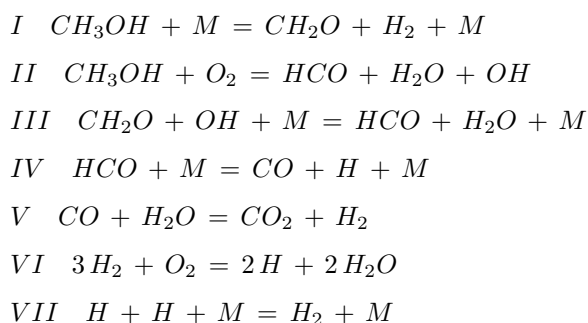


Figure 1. Diagram of the main chain for the methanol.

The hypotheses of steady-state and partial equilibrium are applied. In a homogeneous system, the assumption of steady-state is valid for those intermediate species that are produced by slow reactions and are consumed by fast reactions, so that their concentrations remain small. The partial equilibrium hypothesis is justified when the rate coefficients of forward and backward reactions are much larger than all the other reaction rate coefficients of the mechanism ([Peters, 1988](#)).

After applying the hypothesis of partial equilibrium, it remains the reactions of Table 1. The additional application of the steady-state assumption for the species $HCOH$ and CH_2 , results in the following reduced mechanism of seven-step among 10 species



where M is an inert needed to remove the bond energy that is liberated during recombination.

The reduced mechanism obtained for the methanol can be justified by an asymptotic analysis. For the set of elementary reactions presented in the Table 1, the balance equations can be written as

$$w_{H_2} = +w_1 + w_8 + w_{15} + w_{19} + w_{20} \quad (2)$$

$$w_H = -w_1 - w_2 + w_6 + w_{12} + w_{16} \quad (3)$$

$$w_{O_2} = +w_1 - w_3 - w_5 - w_{11} - w_{13} - w_{14} \quad (4)$$

$$w_O = +w_3 + w_{13} \quad (5)$$

$$w_{H_2O} = +w_2 + w_7 + w_{18} \quad (6)$$

$$w_{OH} = -w_2 + w_4 + w_9 + w_{11} + w_{14} \quad (7)$$

$$w_{HO_2} = -w_1 - w_4 + w_5 - w_9 - w_{17} - w_{23} \quad (8)$$

$$w_{H_2O_2} = +w_9 + w_{17} + w_{23} \quad (9)$$

$$w_{CO} = -w_3 - w_4 + w_5 + w_6 + w_7 + w_9 \quad (10)$$

$$w_{CO_2} = +w_3 + w_4 + w_8 \quad (11)$$

$$w_{CH_4} = -w_{17} + w_{21} + w_{22} \quad (12)$$

$$w_{CH_3} = -w_{13} - w_{14} - w_{15} - w_{16} + w_{17} - w_{21} - w_{22} \quad (13)$$

$$w_{CH_2} = -w_{11} + w_{16} + w_{18} \quad (14)$$

$$w_{CH} = +w_{15} \quad (15)$$

$$w_{CH_3O} = +w_{13} + w_{22} \quad (16)$$

$$w_{CH_3OH} = -w_{18} - w_{19} - w_{20} - w_{21} - w_{22} - w_{23} \quad (17)$$

$$w_{CH_2O} = +w_{10} - w_{12} + w_{14} + w_{20} \quad (18)$$

$$w_{CH_2OH} = +w_{21} + w_{23} \quad (19)$$

$$w_{HCO} = -w_5 - w_6 + w_{11} + w_{12} \quad (20)$$

$$w_{HCOH} = -w_{10} + w_{19} \quad (21)$$

$$w_{HCOOH} = -w_7 - w_8 - w_9 \quad (22)$$

where the plus sign refers to species that appear on the right side of an elementary reaction, while the minus sign refers to species on the left. For example, in the reaction 1. $H + HO_2 = H_2 + O_2$, $w_H = -w_1$ and $w_{H_2} = +w_1$, repeating this procedure for all other species and reactions of the mechanism.

The species O , HO_2 , H_2O_2 , CH_4 , CH_3 , CH_2 , CH , CH_3O , CH_2OH , $HCOH$ and $HCOOH$ are assumed to be in steady-state, which leads to the following algebraic equations among the reaction rates w_κ : $w_1 = -w_4 + w_5$, $w_7 = w_3 - w_8$, $w_9 = -w_3$, $w_{10} = w_{19}$, $w_{11} = w_{16} + w_{18}$, $w_{12} = -w_{16}$, $w_{13} = -w_3$, $w_{14} = w_3 - w_{16}$, $w_{15} = 0$, $w_{17} = w_3 + w_{21}$, $w_{22} = w_3$ and $w_{23} = -w_{21}$.

Making the rates w_I , w_{II} , w_{III} , w_{IV} , w_V , w_{VI} and w_{VII} equal to

$$w_I = 0.5w_2 + w_3 - 0.5w_4 + w_{19} + w_{20} \quad (23)$$

$$w_{II} = -0.5w_2 + 0.5w_4 + w_{18} \quad (24)$$

$$w_{III} = 0.5w_2 - 0.5w_4 \quad (25)$$

$$w_{IV} = w_5 + w_6 \quad (26)$$

$$w_V = w_3 + w_4 + w_8 \quad (27)$$

$$w_{VI} = 0.5w_2 + w_3 + 0.5w_4 \quad (28)$$

$$w_{VII} = w_2 + w_3 + w_5 \quad (29)$$

Table 1. Methanol mechanism rate coefficients (units are mol, cm^3, s, K and cal/mol).

Reaction	A	β	E
1. $H + HO_2 = H_2 + O_2$	6.63E+13	0.00	2126
2. $H + OH + M = H_2O + M$	2.21E+22	-2.00	0
3. $CO + O_2 = CO_2 + O$	2.53E+12	0.00	47688
4. $CO + HO_2 = CO_2 + OH$	5.80E+13	0.00	22934
5. $HCO + O_2 = HO_2 + CO$	7.58E+12	0.00	410
6. $HCO + M = H + CO + M$	1.86E+17	-1.00	17000
7. $HCOOH + M = CO + H_2O + M$	2.09E+14	0.00	40400
8. $HCOOH + M = CO_2 + H_2 + M$	1.35E+15	0.00	60600
9. $HCOOH + HO_2 = CO + H_2O_2 + OH$	2.40E+19	-2.20	14030
10. $HCOH = CH_2O$	2.10E+19	-3.07	31700
11. $CH_2 + O_2 = HCO + OH$	1.29E+20	-3.30	284
12. $CH_2O + M = HCO + H + M$	3.31E+16	0.00	81000
13. $CH_3 + O_2 = CH_3O + O$	1.45E+13	0.00	29209
14. $CH_3 + O_2 = CH_2O + OH$	2.51E+11	0.00	14640
15. $CH_3 + M = CH + H_2 + M$	6.90E+14	0.00	82469
16. $CH_3 + M = CH_2 + H + M$	1.90E+16	0.00	91411
17. $CH_4 + HO_2 = CH_3 + H_2O_2$	1.12E+13	0.00	24640
18. $CH_3OH + M = CH_2 + H_2O + M$	2.84E+10	1.00	83871
19. $CH_3OH + M = HCOH + H_2 + M$	4.20E+09	1.12	85604
20. $CH_3OH + M = CH_2O + H_2 + M$	2.03E+09	1.00	91443
21. $CH_3OH + CH_3 = CH_2OH + CH_4$	3.19E+01	3.17	7171
22. $CH_3OH + CH_3 = CH_3O + CH_4$	1.45E+01	3.10	6935
23. $CH_3OH + HO_2 = CH_2OH + H_2O_2$	9.64E+10	0.00	12578

one obtains the following linear combinations

$$w_{CH_3OH} = -w_I - w_{II} \quad (30)$$

$$w_{CH_2O} = w_I - w_{III} \quad (31)$$

$$w_{HCO} = w_{II} + w_{III} - w_{IV} \quad (32)$$

$$w_{CO} = w_{IV} - w_V \quad (33)$$

$$w_H = w_{IV} + 2w_{VI} - 2w_{VII} \quad (34)$$

$$w_{H_2} = w_I + w_V - 3w_{VI} + w_{VII} \quad (35)$$

$$w_{H_2O} = w_{II} + w_{III} - w_V + 2w_{VI} \quad (36)$$

$$w_{OH} = w_{II} - w_{III} \quad (37)$$

$$w_{CO_2} = w_V \quad (38)$$

$$w_{O_2} = -w_{II} - w_{VI} \quad (39)$$

The stoichiometry of these balance equations corresponds to the reactions $I - VII$.

3. MATHEMATICAL FORMULATION AND SOLUTION PROCEDURE

The mathematical model is based on the numerical solution via LES of the equations of momentum, mixture fraction, energy and chemical species. It is assumed that inside the burner the Mach-number is low, the pressure remains almost constant, the heat losses to the walls are small and the contribution due to the radiation is negligible (Peters, 2006; Poinso and Veynante, 2001).

The mass fraction of each species is determined using the Lagrangian flamelet model. The flamelet equations describe the reactive-diffusive structure in the vicinity of the flame surface as a function of the mixture fraction, instead of space

coordinates (Peters, 2006). Initially, it makes a coordinate transformation applied to the flame surface, and then an analysis of the magnitude of the terms is used to show that the derivatives of the reactive scalars in the tangential directions can be neglected when compared to the derivatives in the normal direction. For the coordinates transformation, it is assumed that the fuel consumption layer is located at stoichiometric conditions, such that the surface of the flame is defined as the stoichiometric mixture surface $Z(x_j, t) = Z_{st}$. If the gradient of the local mixture fraction is sufficiently high, the combustion occurs in a thin layer in the vicinity of stoichiometric surface.

The variables are Favre averaged or density weighted as $\tilde{f} = \overline{\rho f} / \bar{\rho}$, where the “bar” denotes the standard LES filtering (Steiner and Bushe, 1998) and ρ is the density. The set of governing equations in nondimensionalized form (Watanabe *et al.*, 2007; Andreis, 2011) is given by

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{1}{Ma^2} \frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\frac{1}{Re} \bar{\sigma}_{ij} \right) + \tilde{S}_{u_i}, \quad i, j = 1, 2, 3 \quad (40)$$

$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re S_c} \frac{\partial\tilde{Z}}{\partial x_j} \right) + \tilde{S}_Z, \quad j = 1, 2, 3 \quad (41)$$

$$\frac{\partial(\bar{\rho}\tilde{h})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{h})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Pr} \frac{\partial\tilde{h}}{\partial x_j} \right) + \tilde{S}_h, \quad j = 1, 2, 3 \quad (42)$$

$$\frac{\partial\tilde{Y}_i}{\partial\tau} = \frac{a\tilde{\chi}}{2Le} \frac{\partial^2\tilde{Y}_i}{\partial\tilde{Z}^2} \pm \tilde{w}_i + \tilde{S}_{Y_i}, \quad i = 1, 2, \dots, n \quad (43)$$

where u_j is the velocity vector, t the time, x_j the spatial coordinate, p the pressure, Z the mixture fraction, $h = \sum_{i=1}^n Y_i h_i(T)$ the enthalpy, T the temperature, Y_i the mass fraction of the species i , and τ the time defined in the coordinate system attached to the stoichiometric surface. $\bar{\sigma}_{ij} = \bar{\mu}_t \left(2\tilde{S}_{ij} - 2/3\delta_{ij}\tilde{S}_{kk} \right)$ is the viscous stress tensor, $\tilde{S}_{ij} = 1/2(\partial\tilde{u}_i/\partial x_j + \partial\tilde{u}_j/\partial x_i)$ the rate of strain tensor, δ_{ij} the Kronecker symbol, $a = \Delta Z Z_{st}(1 - Z_{st})$, $\Delta Z \sim 2Z_{st}$, Z_{st} the stoichiometric mixture fraction, $\tilde{\chi} = 2D(\partial\tilde{Z}/\partial x_j)^2$ the scalar dissipation rate, D the diffusivity, $\tilde{w}_i = W_i \sum_{k=1}^r \nu_{ik}\tilde{w}_k$, W_i the molecular weight of species i , ν_{ik} the stoichiometric coefficient of the species i in the reaction k , and \tilde{w}_k the reaction rate of reaction k . The Smagorinsky model for the turbulent viscosity $\bar{\mu}_t$ is employed. In these equations Ma is the Mach, Re the Reynolds, S_c the Schmidt, Pr the Prandtl, and Le the Lewis numbers.

According to Watanabe *et al.* (2007), the source terms S_i due to interactions between gaseous and disperse phase may be expressed using the total number of droplets existing in the control volume of the gaseous phase calculations. The fuel droplets are treated in a Lagrangian manner. As the density of the droplets is much larger than that of the continuous phase, only the drag and the gravity effects are significant. Moreover, the effect of fluid shear on the fluid force acting on the droplets, the droplet breakup, their collision, and dense particulate effects are neglected (Ham *et al.*, 2003). The source terms \tilde{S}_{u_i} , \tilde{S}_Z , \tilde{S}_h and \tilde{S}_{Y_i} are given by

$$\tilde{S}_{u_i} = -\frac{1}{V} \sum_{i=1}^N \left(f_1 \frac{m_d}{\tau_d} (u_i - u_{d,i}) + \frac{dm_d}{dt} u_{d,i} \right) \quad (44)$$

$$\tilde{S}_Z = -\frac{\phi}{\phi + Y_{O_2}} \left(\frac{1}{V} \sum_{i=1}^N \frac{dm_d}{dt} \right) \quad (45)$$

$$\tilde{S}_h = -\frac{1}{V} \sum_{i=1}^N \left(\frac{1}{2E_c} \frac{d}{dt} (m_d u_{d,i} u_{d,i}) + Q_d + \frac{dm_d}{dt} h_{v,s} \right) \quad (46)$$

$$\tilde{S}_{Y_i} = \begin{cases} -\frac{1}{Y_{F,u} V} \sum_{i=1}^N \frac{dm_d}{dt}, & \text{se } i = F \\ 0, & \text{se } i \neq F \end{cases} \quad (47)$$

where V is the cell volume, N the number of droplets, m_d the droplet mass, $\tau_d = \rho_d d_d^2 / (18\mu)$ the particle response time, ρ_d the droplet density, d_d the droplet diameter, μ the gaseous phase viscosity, $u_{d,i}$ the droplet velocity, $\phi =$

$Z(1 - Z_{st})/[(1 - Z_{st})Z_{st}]$ the equivalence ratio, Y_{O_2} the mass fraction of oxygen in the oxidizer stream, $Y_{F,u}$ the mass fraction in the original fuel stream, E_c the Eckert number, $Q_d = f_2 m_d Nu c_p (T - T_d)/(3Pr T_d)$ the heat transfer from the convection, f_1 and f_2 the corrections of the Stokes drag and heat transfer for an evaporating droplet, respectively (Watanabe *et al.*, 2007), Nu the Nusselt number, $c_p \sim 1400 J/(kgK)$ the specific heat of the gas mixture, T_d the droplet temperature, and $h_{V,S}$ the enthalpy of the vapor at the droplet surface.

The Lagrangian equations for the droplets are given by

$$\frac{dm_d}{dt} = -\frac{S_h}{3S_c} \frac{m_d}{\tau_d} \ln(1 + B_M) \quad (48)$$

$$\frac{du_{d,i}}{dt} = \frac{f_1}{\tau_d} (u_i - u_{d,i}) + g_i \quad (49)$$

$$\frac{dT_d}{dt} = \frac{Q_d}{m_d c_{p,d}} + \frac{L_V}{m_d c_{p,d}} \frac{dm_d}{dt} \quad (50)$$

where S_h is the Sherwood number, B_M the mass transfer number, g_i the acceleration of gravity, $c_{p,d}$ the specific heat of the liquid, $L_V = hv^0 - (c_p - c_{p,d})T_d$ the latent heat of vaporization at T_d , $hv^0 \sim 10^5 J/K$, and $c_{p,d} \sim 2000 J/(kgK)$.

The set of governing equations are discretized using the finite difference second order method. Central schemes are preferred since they are not dissipative; such property is desired to avoid damping of the small scales of turbulence, which are important in reactive flows. For the simulation of diffusion flames, the method for low Mach-number seems to be appropriate. In this formulation, density comes from the state relation and it is necessary to write an equation to obtain the pressure gradients needed to correct the velocities. The pressure gradient is obtained after solving a Poisson's equation for pressure.

4. NUMERICAL RESULTS

After checking the accuracy of an in house Fortran90 code developed for solving jet diffusion flames of methane (Lorenzetti *et al.*, 2012), new results are obtained for methanol jet diffusion flames. The dimensions of the burner are $L = 1$, $h = 0.06 L$, $l = 0.1 L$, $d = 0.008 L$ and $D = 0.01 L$ (see Fig. 2(a)) (Gokarn *et al.*, 2006). A mesh of $489 \times 65 \times 65$ cells was considered. The Reynolds number is maintained at 3500, and the no-slip velocity condition was specified at all surfaces.

Figures 2(b) and 2(c) show the maps of mixture fraction and temperature obtained at 0.4 seconds for the methanol flame. The plots elucidate that fluid is entrained from the fast and slow feed streams into the shear layer. The developed code using LES capture the dynamical evolution of the mixing layer and the mechanisms of entrainment and mixing enhancement. The flow is initially symmetric and eventually the wall effects break down the symmetry (Gokarn *et al.*, 2006). In the scale indicated in Fig. 2(c), the value 1 corresponds to the ambient temperature. The adiabatic temperature of a methanol flame is approximately 2065 K. Intermittency in the jet arises from the action of large-scale turbulent eddies produced by the jet entraining quiescent fluid from the surroundings (Lawn, 2009).

Figures 2(d) and 2(e) show the maps for the products CO_2 and H_2O , obtained at 0.4 seconds. The regions of higher temperature (white color) correspond to regions of higher mass fraction of combustion products. These regions correspond to those near the stoichiometric surface, where there are ideal conditions of burning, being $Z_{st} \sim 0.14$ for methanol flames. The maximum mass fraction obtained in the work from Yalamanchili *et al.* (2005) is approximately 0.12 for CO_2 and 0.14 for H_2O ; our results are in agreement with those of Yalamanchili *et al.* (2005).

5. CONCLUSIONS

In this paper we developed a reduced kinetic mechanism for the methanol, and the method for the numerical simulation of jet diffusion flames. The main advantage of the obtained reduced reaction mechanism is the decrease of the work required to solve the system of equations for jet diffusion flames. The model, based on the flamelet equations for the chemistry and on the mixture fraction for the flow using LES, is appropriate for solving jet diffusion flames. Obtained

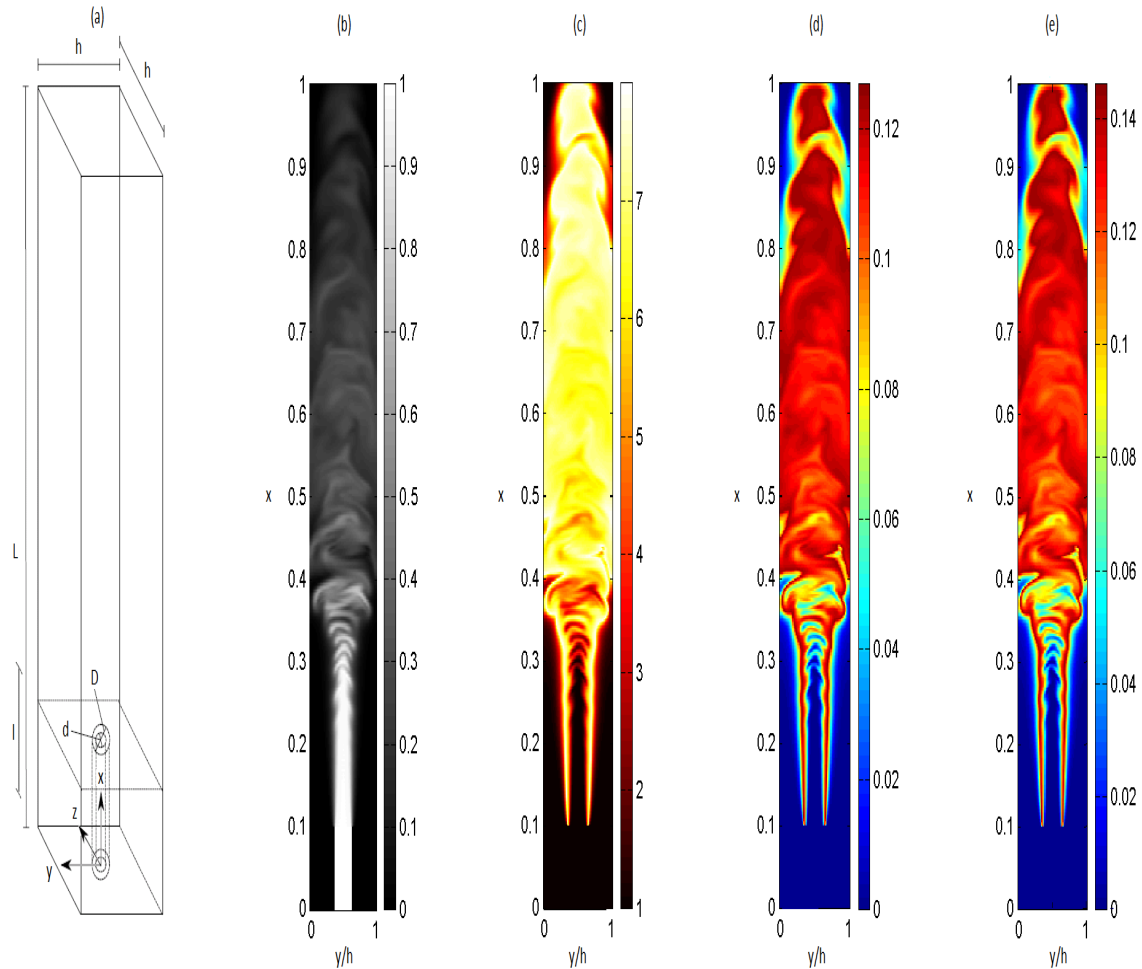


Figure 2. Geometry (a) and maps of (b) mixture fraction, (c) temperature, (d) CO_2 and (e) H_2O mass fractions for methanol diffusion flame at 0.4 seconds.

results are in agreement with data found in the literature.

Due to the hierarchical structure of biofuel mechanisms, this work is part of the steps to obtain reduced kinetic mechanisms for biodiesel flames.

6. ACKNOWLEDGEMENTS

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7. REFERENCES

- Andreis, G.S.L., 2011. *Solução via LES de chamas difusivas de metano, metanol e etanol*. Tese de doutorado, Universidade Federal do Rio Grande do Sul.
- Curran, H.J., 2009. "Detailed chemical kinetic mechanisms for combustion". *Proceedings of the European Combustion Meeting*, pp. 1–6.
- Demirbas, A., 2008. *Biodiesel: A Realistic Fuel Alternative for Diesel Engines*. Springer-Verlag London Limited.
- Gokarn, A., Battaglia, F., Fox, R.O. and Hill, J.C., 2006. "Simulations of mixing for a confined co-flowing planar jet".

Computers & Fluids, Vol. 35, pp. 1228–1238.

- Griffiths, J.F., 1995. “Reduced kinetic models and their application to practical combustion systems”. *Progress in Energy and Combustion Science*, Vol. 21, pp. 25–107.
- Ham, F., Apte, S.V., Iaccarino, G., Wu, X., Herrmann, M., Constantinescu, G., Mahesh, K. and Moin, P., 2003. “Unstructured LES of reacting multiphase flows in realistic gas turbine combustors”. *Center for Turbulence Research, Annual Research Brief, NASA Ames/Stanford University*, pp. 135–159.
- Knothe, G., 2005. *The Biodiesel Handbook*, AOCS Press, chapter Introduction: What is biodiesel?
- Lawn, C.J., 2009. “Lifted flames on fuel jets in co-flowing air”. *Progress in Energy and Combustion Science*, Vol. 35, pp. 1–30.
- Leung, K.M. and Lindstedt, R.P., 1995. “Detailed kinetic modeling of C1-C3 alkane diffusion flames”. *Combustion and Flame*, Vol. 102, pp. 129–160.
- Lindstedt, R.P. and Meyer, M.P., 2002. “A dimensionally reduced reaction mechanism for methanol oxidation”. *Proceedings of the Combustion Institute*, Vol. 29, pp. 1395–1402.
- Lorenzetti, G.S., De Bortoli, A.L. and Marczak, L.D.F., 2012. “A numerical method for the solution of confined co-flowing jet diffusion flames”. *Latin American Applied Research*, Vol. 42, No. 1, pp. 27–32.
- Mahalingam, S., Chen, J.H. and Vervisch, L., 1995. “Finite-rate chemistry and transient effects in direct numerical simulations of turbulent nonpremixed flames”. *Combustion and Flame*, Vol. 102, pp. 285–297.
- Marinov, N.M., 1999. “A detailed chemical kinetic model for high temperature ethanol oxidation”. *International Journal of Chemical Kinetics*, Vol. 31, No. 3, pp. 183–220.
- Peters, N., 1988. *Dynamics of Reactive Systems. Part I: Flames*, Progress in Astronautics and Aeronautics, chapter Systematic reduction of flame kinetics: principles and details, pp. 67–86.
- Peters, N., 2006. *Turbulent Combustion*. Cambridge University Press.
- Pitsch, H. and Fedotov, S., 2001. “Investigation of scalar dissipation rate fluctuations in non-premixed turbulent combustion using a stochastic approach”. *Combustion Theory and Modelling*, Vol. 5, pp. 41–57.
- Pitsch, H. and Peters, N., 1998. “A consistent flamelet formulation for nonpremixed combustion considering differential diffusion effects”. *Combustion and Flame*, Vol. 114, pp. 26–40.
- Poinsot, T. and Veynante, D., 2001. *Theoretical and Numerical Combustion*. R. T. Edwards, Inc.
- Steiner, H. and Bushe, W.K., 1998. “LES of nonpremixed turbulent reacting flows with conditional source term estimation”. *Center for Turbulence Research, Annual Research Briefs*, pp. 23–34.
- Watanabe, H., Kurose, R., Hwang, S.M. and Akamatsu, F., 2007. “Characteristics of flamelets in spray flames formed in a laminar counterflow”. *Combustion and Flame*, Vol. 148, pp. 234–248.
- Yalamanchili, S., Sirignano, W.A., Seiser, R. and Seshadri, K., 2005. “Reduced methanol kinetic mechanisms for combustion applications”. *Combustion and Flame*, Vol. 142, pp. 258–265.

8. RESPONSIBILITY NOTICE

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