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IMPLEMENTATION OF FGM TECHNIQUE IN THE OPEN SOURCE PACKAGE OPENFOAM TO SOLVE A NON PREMIXED LAMINAR FLAME

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Abstract. *The present study solves a diffusive laminar jet flame through numerical simulation. The fuel used is pure methane and methane diluted in nitrogen. Due to the high computational cost even for laminar flames, the use of chemical kinetics simplification approaches become necessary. The Flamelet-Generated-Manifold technique is based on the flamelets and manifold approaches. The implementation of such technique in the open source tool OpenFOAM is performed on a multidimensional scope from an already built manifold. Results from literature are used to verify the implementation and evaluate the technique. Simulations using 1-step global mechanism are also performed in order to compare both chemical kinetics approaches. The FGM presented better results compared to the 1-step mechanism, getting closer to the detailed mechanism. The quality of the FGM results decreased when varying the fuel composition.*

Keywords: FGM, DRM19, OpenFOAM®, 1 step...

1. INTRODUCTION

According to MME, 2015, the burn of petrol derivatives, natural gas, coal, wood, and agro-industrial residues represent more than 80% of the energy consumed in Brazil. The combustion processes have great impact in industrial, transport and energy production sectors, being interesting to society to conduct studies in this subject. Among the different types of flames, the laminar non-premixed flames are the object of many fundamental researches aiming to understand better physical and chemical phenomena for complex reacting flows (Cao *et al.*, 2015, Xuan and Blanquart, 2013, Verhoeven, 2011, Smooke *et al.*, 2005, Santoro *et al.*, 1987, per example).

Although many analytic solutions for laminar non-premixed co-flow flames are available, the recurrent concern about increasing efficiency of combustion processes and reduction in pollutant emissions demands more sophisticated physical models. Among them, is worthy to highlight the usage of combustion numerical simulations considering the Finite Volume Method (for computational fluid dynamics simulations) using detailed chemical kinetics. Detailed kinetics for hydrocarbons oxidation describe the chemical process through elementary reactions as it really occurs in nature. In this way, hundreds of reactions and dozens of chemical species are necessary to exactly calculate the chemical kinetics in any combustion process. In addition, the system of non-linear differential equations to be solved is strongly stiff and coupled, making the problem computationally demanding even for laminar flames.

Global kinetic mechanisms are an alternative to reduce the computational time and commonly employed to solve practical problems. As it describes the chemical kinetics through only few reactions, its use is restricted to conditions for which their rates and constants were adjusted. While global mechanisms are computationally efficient, their solutions present deviations when compared with more detailed mechanism (Hoerlle and Pereira, 2014, Wang *et al.*, 2012). For that reason, their use for solving practical combustion problems are losing space and more advanced models for reduction of chemical kinetics mechanisms have been developed, as the Steady Laminar Diffusion Flamelet model (SLDF, Peters, 1984), the Intrinsic Low-Dimensional Manifold (ILDM, Mass and Pope, 1992), the Flamelet-Generated-Manifold (FGM, (Oijen and Goey, 2000)), the Lagrangian Flamelet Model (LFM, Pitsch, 2000) and the Flame Prolongation of ILDM (FPI, Gicquel *et al.*, 2000).

Several combustion practical problems have been solved with the FGM technique. In Oijen, 2002 the FGM was employed to solve a porous burner of ceramic-foam. Verhoeven, 2011 compared the FGM technique with detailed kinetic mechanism for laminar non-premixed co-flow flames. Formation of Polycyclic Aromatic Hydrocarbon, PAH, achieved with the FGM technique, was compared with experimental data by Verhoeven *et al.*, 2013. Fancello, 2014 studied flame stabilization in transient regime to solve gas turbines considering Large Eddies Simulations, LES, in the open source CFD package OpenFOAM[®]. All those studies reported a good agreement between the FGM technique and solution employing detailed kinetic mechanisms or experimental measurements. One has to note, however, that the FGM, even bringing information about detailed kinetic mechanisms, cannot be considered a correct solution.

The objective of this paper is to solve a non-premixed laminar flame using the FGM technique, which will be implemented in the open source package OpenFOAM[®]. To verify the implementation, Verhoeven, 2011 will be use as reference, in which the FGM technique was implemented on ANSYS[®]Fluent. A 1 step reaction mechanism will also be employed to solve the same flame in order to compare both chemical kinetics reduction approaches. Both approaches will be compared to results with the DRM19 mechanism from Verhoeven, 2011. Once verified the implementation, the same problem will be solved with different fuel composition in order to evaluate the FGM technique at a different condition.

2. PROBLEM DESCRIPTION AND NUMERICAL MODEL

Laminar non-premixed coflow flames are simulated at atmospheric conditions. The burner geometry is formed by two concentric tubes, a schematic of which is shown in Figure 1. The fuel is injected normal to the circular section of the inner tube with radius of $r_i = 12$ mm, surrounded by air in an annular tube section with radius of $r_o = 55$ mm. The domain length is 0,2 m for the pure methane flame and 0,1 m when the fuel is diluted to N_2 . The oxidant is standard dry air, both at 298 K. Parabolic velocity profile for the fuel injection is applied for all cases and follows the relation:

$$u = u_{\infty} \left(2 \frac{r}{D_c} - \left(\frac{r}{D_c} \right)^2 \right), \quad (1)$$

being r the radial coordinate, D_c the inner jet diameter and u_{∞} the maximum velocity of the parabolic profile (0,23 m/s). The air injection velocity is constant and equal to (0,23 m/s).

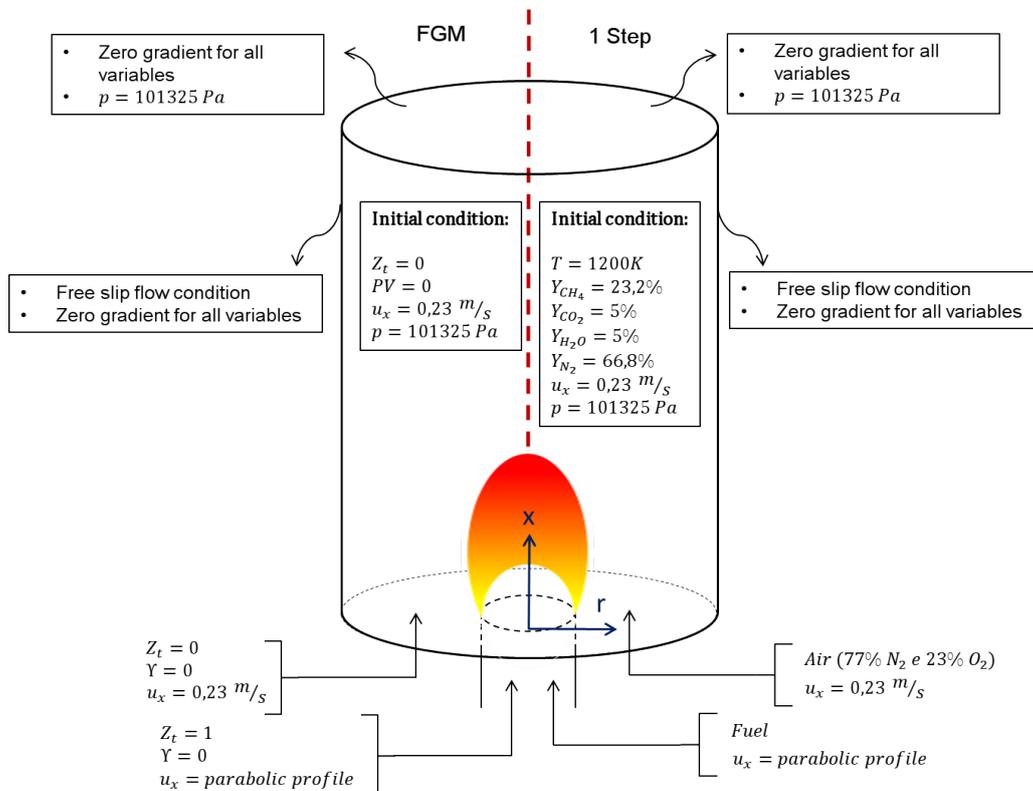


Figure 1: Schematic of diffusive flame burner used in numerical simulations.

The problem is modelled by an axisymmetric bidimensional computational domain. Pseudo-transient solutions were achieved by solving the system of conservation equations in radial coordinate system through the freely-available computational fluid dynamics software OpenFOAM[®]. The solver used is the *reactingFoam*, whose equations system account

for the conservation of total mass, momentum in axial and radial directions, mass of chemical species and energy (for the detailed kinetic approach) or control variables (for the FGM approach). Details about each chemical kinetic approach are given in next sections. The solver considers the PIMPLE method for the pressure-velocity coupling. To discretize the transport equations, a second order scheme is considered for both the diffusive and advective terms, and interpolation from cell centres to faces are given by central difference scheme. Due to the low Mach approximation, the mixture density is assumed to be a function of temperature only. The gases are assumed Newtonian and diffusion process is based on Fick's Law. The Soret, Dufour and viscous dissipation effects are neglected, buoyant effects are considered and no soot model is included.

2.1 Detailed kinetic mechanism approach

Chemical kinetic modelling consist in solve the production and consumption rates of chemical species present in elementary reactions. The semi-detailed kinetic mechanism *DRM19* (Kazakov and Frenklach (1994)), formed by 21 chemical species and 84 elementary reactions, is considered for the detailed kinetic simulation to reduce computational time. In addition to the conservation of the total mass and the momentum in axial and radial directions, a transport equation for the mass of each chemical species is solved in the detailed kinetic approach, where the sink term is evaluated by the Arrhenius rate equation. To complete the system of equations, the energy transport equation is solved in terms of the total specific enthalpy of the mixture. Finally, the set of differential equations is accompanied by two state equations: the ideal gas law and the caloric equation of state. Chemical species diffusivity, thermal and transport properties were evaluated in OpenFOAM® as follows: Schmidt number S_c and the Lewis number L_e are considered to be equal to unity for simplicity, thermal conductivity λ and dynamic viscosity μ are mixture averaged. The thermal conductivity λ is given by the modified correlation of Eucken (Equation 3, (Assael *et al.*, 1996)) and the dynamic viscosity μ is calculated through Sutherland equation (Equation 2, (Sutherland, 1893)). The specific heat C_p is calculated through the NASA polynomials.

$$\mu_i = \frac{A_{s_i} \sqrt{T_i}}{1 + T_{s_i}/T_i}, \quad (2)$$

$$\lambda_i = \mu_i (p, T) C_v \left(1.32 + \frac{1.77 R_i}{C_v} \right), \quad (3)$$

2.2 Flamelet-Generated Manifolds approach

The Flamelet-Generated Manifold technique, introduced by Oijen and Goey, 2000, was developed by combining two methods of chemical kinetic reduction: the flamelets model and the Intrinsic Low-Dimensional Manifold (ILDM) from Mass and Pope, 1992. The FGM is based on the observation that multidimensional flames could be represented by a several unidimensional flames (called flamelets) that describe all the flame composition space. Details about flamelets equations are found in Verhoeven, 2011. In this technique, the solutions of the flamelets (thermal, chemical and transport scalars that represent the combustion process) are stored in a manifold as function of control variables. The manifold is further used in computational fluid dynamics codes to reconstruct a multidimensional flame. In this way, the technique solves only transport equations for the control variables besides the conservation equation of each chemical specie and energy that are solved in conventional flame simulations. The reduced number of equations to be solved in the FGM results in only a fraction of the total computational time of the conventional combustion models with detailed kinetic mechanism.

Control variables have a function which parametrize the scalars of interest and are able to represent the physical phenomena. For adiabatic laminar non-premixed flames the minimum necessary control variables are the mixture fraction Z_t and the progress variable γ . The mixture fraction Z_t is a scalar that is only transported by advection and diffusion and assumes value 1 in the fuel inlet and 0 in the oxidizer inlet. The progress variable γ describes the chemical kinetic and need to be monotonous in composition space. In this work, γ was defined by following Verhoeven, 2011 definition:

$$\gamma = \alpha_{CO_2} Y_{CO_2} + \alpha_{H_2O} Y_{H_2O} + \alpha_{H_2} Y_{H_2}, \quad (4)$$

where the weight α_i is defined as the inverse of the molar weight of specie i ($\alpha_i = 1/MW_i$).

Finally, the system of equations consist of conservation equations for mass, momentum in axial and radial directions and one for each control variable. The transport equations for Z_t and γ are, respectively, given by

$$\vec{\nabla} (\rho \vec{u} Z_t) = \vec{\nabla} \left(\frac{\lambda}{Le_{Z_t} c_p} \vec{\nabla} Z_t \right), \quad (5)$$

$$\vec{\nabla}(\rho\vec{u}\gamma) = \vec{\nabla}\left(\frac{\lambda}{Le_{\gamma}c_p}\vec{\nabla}\gamma\right) + \dot{\omega}_{\gamma}, \quad (6)$$

where $\lambda/Le_{Z_t,\gamma}c_p$ is the diffusion term, with $Le_{Z_t,\gamma} = 1$. λ is the mixture conductivity and c_p is the specific heat at constant pressure. The source term of the γ transport equation $\dot{\omega}_{\gamma}$ is given by the net source term \dot{w}_i of the species i considered in the progress variable definition, and is given by

$$\dot{\omega}_{\gamma} = \alpha_{CO_2}\dot{w}_{CO_2} + \alpha_{H_2O}\dot{w}_{H_2O} + \alpha_{H_2}\dot{w}_{H_2}. \quad (7)$$

In multidimensional simulations, the manifold is constantly accessed by the FGM algorithm. During the iterative process, thermodynamics and transport properties are retrieved from the manifold to solve the equation system. After the solution is achieved, the flame can be reconstructed in a post-processing step with the fields of the control variables. The manifold is read by an algorithm of search and bilinear interpolation as function of Z_t and γ .

The manifold is the same considered by Hoerlle *et al.*, 2015 for pure methane simulations. The manifold were constructed by solving a series of one-dimensional counterflow flames for varying strain rate from near equilibrium to extinction. It was assumed unity Lewis number and the relations proposed by Smooke (1991) for the conductivity ($\lambda = 2.58 \times 10^{-5}c_p(T/298)^{0.69}$) and viscosity ($\mu = 1.67 \times 10^{-8}c_p(T/298)^{0.51}$) of the mixture as function of temperature (T) and specific heat at constant pressure (c_p) are used. As those relations were determined for oxidation of methane in air, it is not expected higher difference in relation to the conventional approach considered in the detailed kinetic approach.

3. THE FGM TECHNIQUE IN OPENFOAM®

In this work, the FGM technique code, already implemented by Fancello, 2014 in OpenFOAM®, was adjusted for non-premixed flames. The solution procedure consists in solving the cold flow, whose resultant Z_t field is used as initial condition for ignition. The ignition is given by prescribing values of γ which corresponds to the maximum value found for the source term \dot{w}_{γ} in the manifold. The location of ignition is chosen just in the burner exit, position where one may find Z_t values close to its stoichiometric value. The FGM algorithm (Figure 2) is executed until convergence and thus the temperature and specie mass fractions fields are post-processed through search and interpolation functions in the manifold.

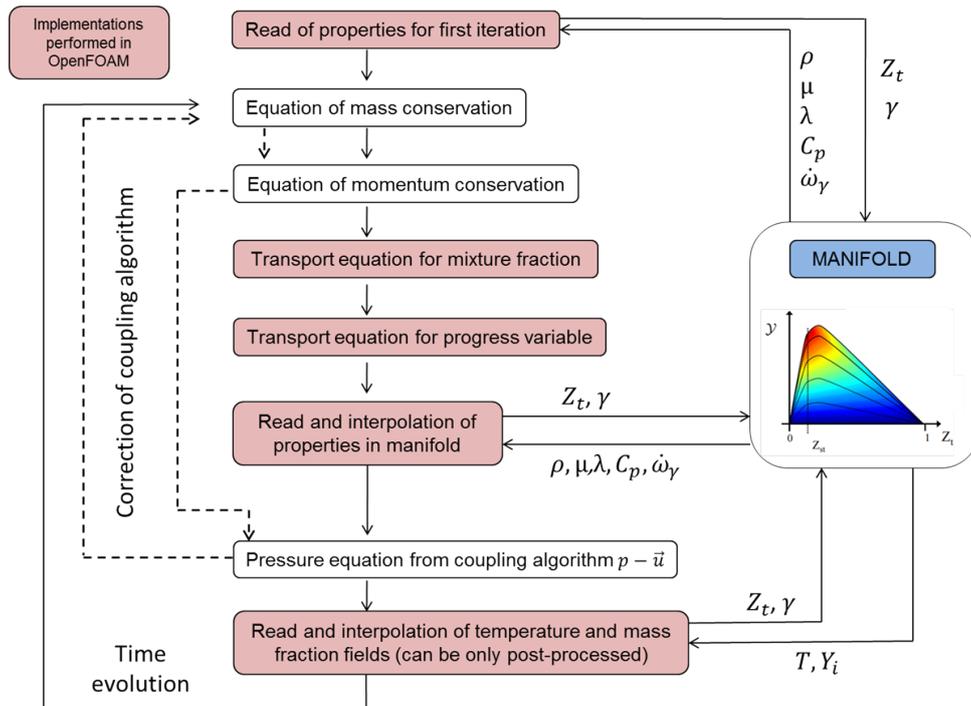


Figure 2: Solution algorithm of the multidimensional simulation in OpenFOAM®, showing the steps implemented in the present work in red color.

In Figure 3, the database for density and viscosity are used as example, in which the colorful curves represent different flamelets simulated. The color transition in a single flamelet corresponds to different values assumed by such property as

function of Z_t and γ combination. Other properties, as well as temperature and specie mass fraction fields, are obtained in the same way. The steps of reading and interpolation of properties presented in the schematic algorithm of Figure 2 are more detailed by Figure 3. After solving equations 5 and 6, the data pair (Z_t, γ) is used as inlet parameter for the search and interpolation system of the manifold. Then, the closest 4 data points are found in the manifold and a bi-linear interpolation is used to find the property or field of interest.

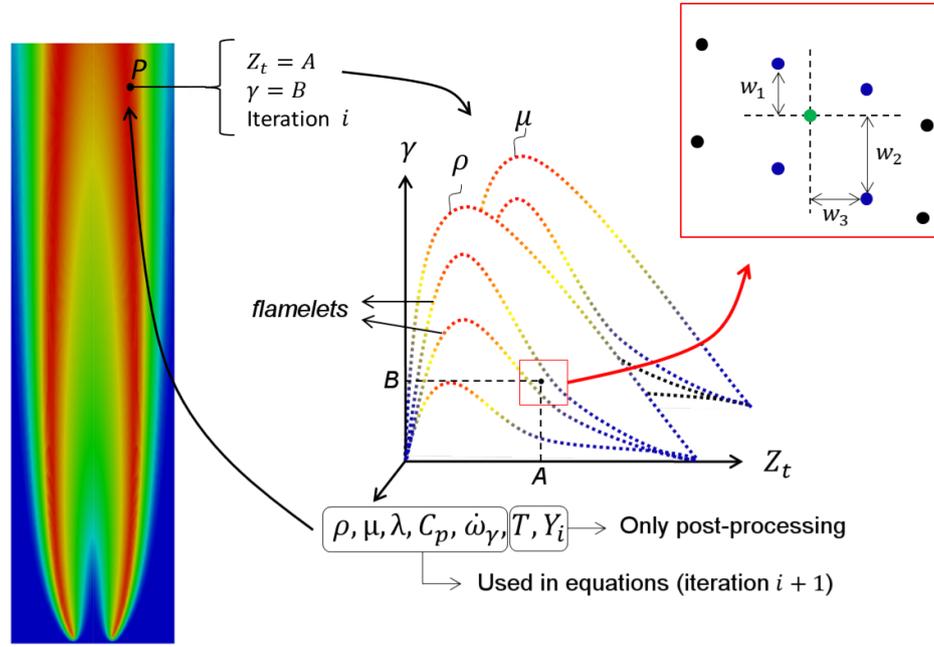


Figure 3: Search and interpolation system of the manifold. Properties are function of the data pair (Z_t, γ) , are obtained through a bi-linear interpolation and are used in the next iteration on the transport and conservation equations. The temperature and specie mass fraction fields are obtained analogously in the flame reconstruction (post-processing step).

4. RESULTS AND DISCUSSION

Different flame configuration were simulated and each case and its respective nomenclature can be found in Table ?? below.

Table 1: Nomenclature and configuration of flame simulations simulated and referred in the present work (NA = non applicable; CL = Combustion Laboratory)

Name in the work	Fuel	Method	Author
Detailed - Verhoeven	55% CH_4 e 45% N_2	Detailed	(Verhoeven, 2011)
FGM - Verhoeven	55% CH_4 e 45% N_2	FGM	(Verhoeven, 2011)
FGM	55% CH_4 e 45% N_2	FGM	Present work
1 step	55% CH_4 e 45% N_2	1 STEP	Present work
DRM19	100% CH_4	Detailed	CL - UFRGS
FGM1	100% CH_4	FGM	Present work
1 step	100% CH_4	1 STEP	Present work

The results obtained at Verhoeven, 2011 are used as reference to verify the FGM implementation in OpenFOAM[®]. The mesh used has 100.000 volumes for both simulations (FGM and detailed mechanism). A mesh independence study was performed and a coarser mesh could be used, however it was chosen to use the exact same mesh of Verhoeven, 2011's work. Besides her FGM results, Verhoeven reported a detailed mechanism results whose comparison to FGM ones shown good agreement of temperature and some specie mass fraction profiles. In the present work, temperature and CO mass fraction profiles are used to verify the implementation. Additionally, the same problem is simulated using a 1 step simplified mechanism to compare both reduction techniques approaches.

As presented in Figures 4a and 4b, the temperature profiles found with FGM technique in the present work and their

in Verhoeven, 2011 work presented great agreement, while the CO mass fraction shown in Figures 4c and 4d presented very small deviations at regions with high gradients for axial position $H = 0.04 m$. Such results leads to the conclusion that the implementation of the FGM technique in the OpenFOAM[®] package was successful.

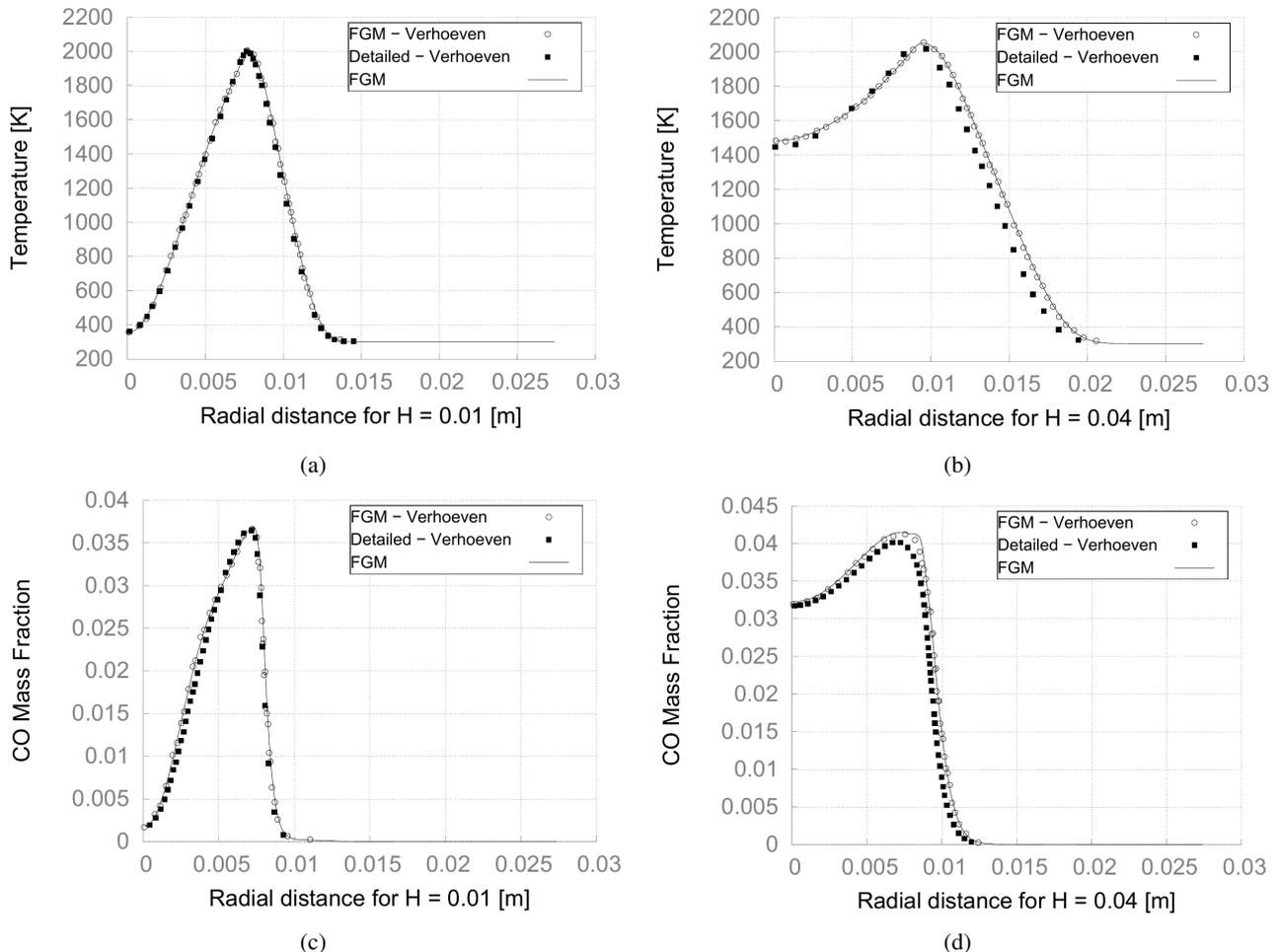


Figure 4: Radial profiles of temperature and CO mass fraction for different burner axial positions. Results from present work (FGM and 1 step) compared to Verhoeven, 2011 results (FGM - Verhoeven and Detailed - Verhoeven).

Once the FGM implementation is verified, a different fuel composition was analysed to evaluate the FGM technique in a different case ($100\% CH_4$). The burner length increased from $0,1 m$ to $0,2 m$. In this second case, 1 step simplified mechanism simulations are also performed to compare both chemical kinetics reduction techniques approaches. A simulation using the DRM19 mechanism was also performed by a Combustion Laboratory member using ANSYS[®] Fluent.

In this second case, temperature profiles for 1 step mechanism presented closer curves to detailed ones (Figures 5a and 5b) when compared to the simulations with methane diluted to N_2 . Such bad results of the 1 step mechanism for the case with dillution may be due to fact that the reaction rates coefficients used are adjusted for pure methane fuels, in which the flame velocity was the main objective of mechanism development (Westbrook and Dryer, 1981). This is a big limitation of global mechanisms, which have reaction rates coefficients adjusted to specific conditions.

For pure methane, the temperature profiles obtained with FGM and 1 step mechanism compare in a similar way to the detailed results, as Figures 5a and 5b show. The evident difference between the FGM and 1 step mechanism can be seen in the CO_2 mass fraction profiles shown in Figures 5c and 5c, being the FGM the method which presented better results. Analysing the temperature contours of Figure 6, one can realize that the 1 step mechanism presented temperature values around $50K$ lower at regions with high gradients. However, even tough the FGM presented closer magnitude values for temperature in relation to detailed mechanism results, bigger flame lengths are observed. Inferior results from simplified reduced mechanisms compared to FGM technique also were reported by Hoerlle *et al.*, 2015.

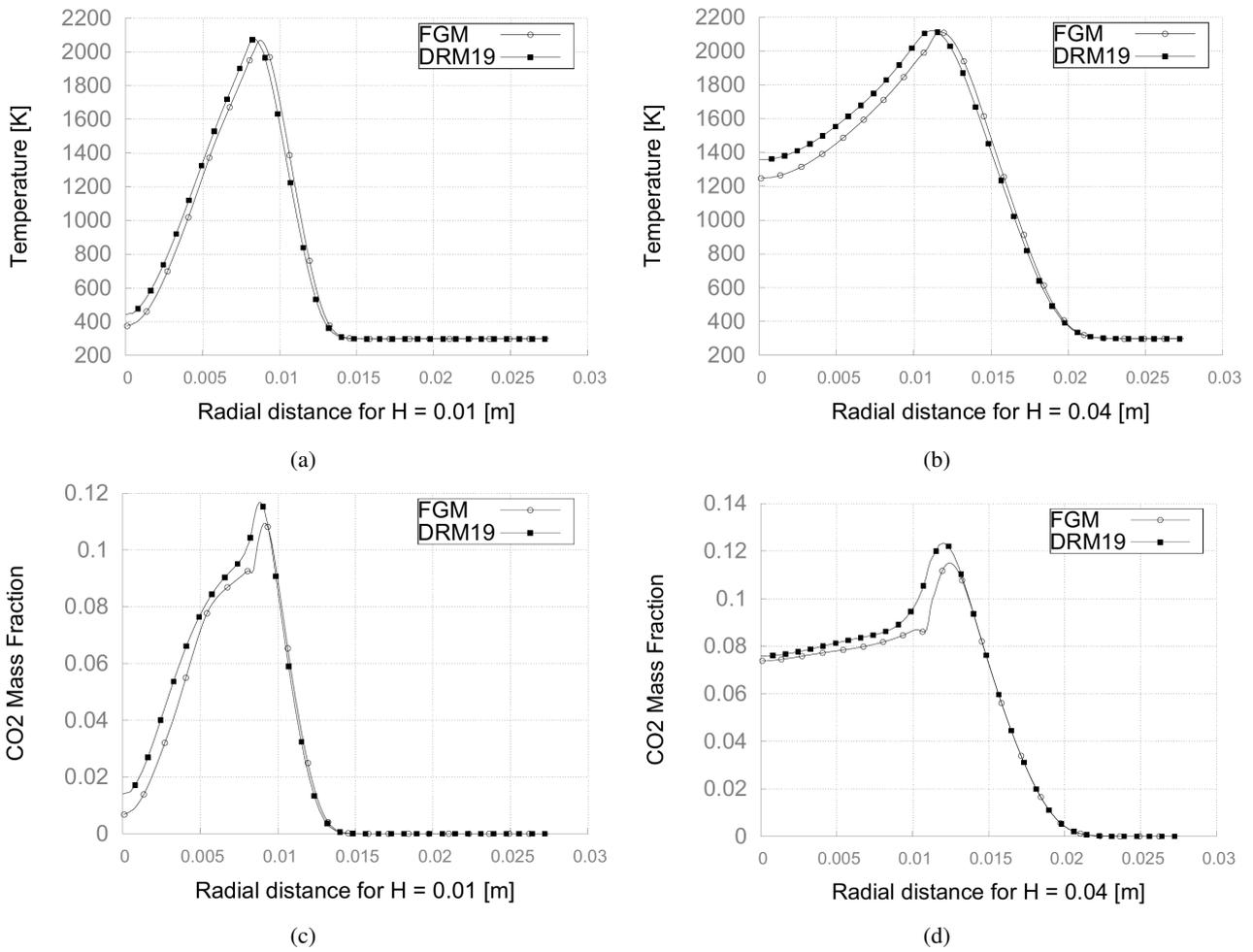
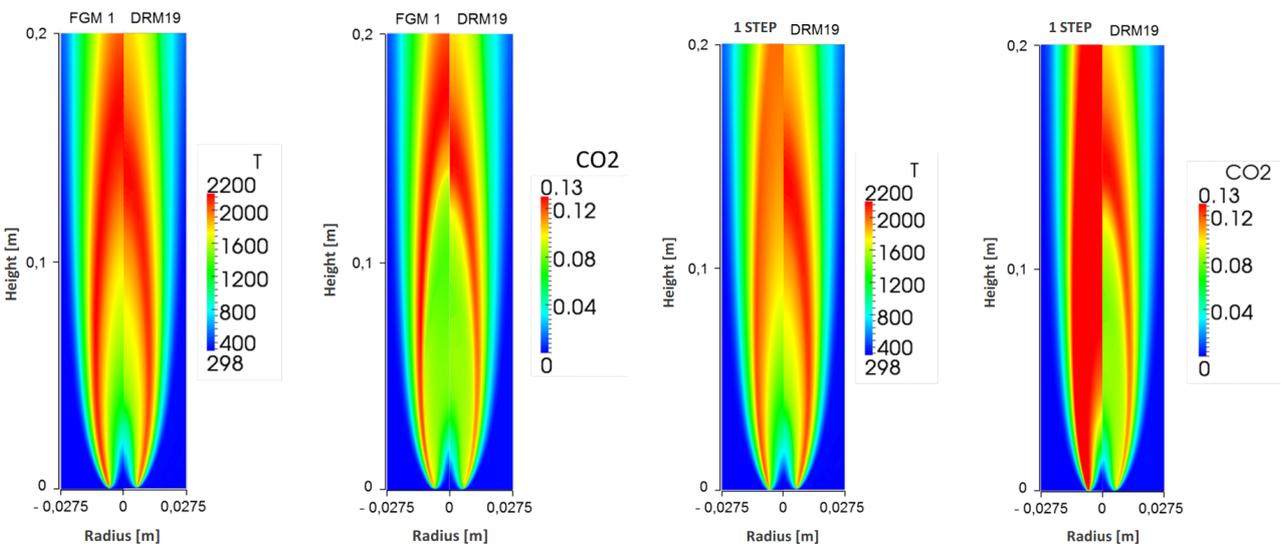


Figure 5: Radial profiles of temperature and CO_2 mass fraction for the second case studied (pure CH_4). Results from present work (FGM and 1 step) compared to results obtained from detailed simulation (skm-DRM19) performed by UFRGS Combustion Laboratory member.



(a) FGM1 (left) and *skm*-DRM19 (right)

(b) 1 step (left) and *skm*-DRM19 (right)

Figure 6: Temperature contour for the second case studied (pure CH_4).

5. CONCLUSION

In the present work, the implementation of the FGM method for multidimensional flames was realized in the OpenFOAM[®] package. A non-premixed laminar coflow flame was used as study case. The results obtained were compared to Verhoeven, 2011 ones, in which the same implementation was performed in ANSYS[®]Fluent code. The curves analysed in the verification had great agreement to Verhoeven's ones, verifying the implementation of the technique in OpenFOAM[®]. Simulations using a 1 step mechanism for the same problem were also performed, in which the results presented considerable deviations from the detailed mechanism DRM19. Once the implementation was verified, a second case was studied by changing the fuel composition (100% CH_4), also comparing FGM and 1 step mechanism results to DRM19 ones. The FGM results did not agree as well as in the first case. Temperature profiles for both reduction techniques (FGM and 1 step mechanism) presented similar behavior, with slightly better results for FGM at regions of high gradients. However, for CO_2 mass fraction profiles, the FGM technique presented much better results than the 1 step mechanism ones. Besides the better agreement for the CO_2 mass fraction curves, a big advantage of FGM lies in its possibility to reconstruct any specie profile contained in the detailed mechanism used in the flamelets simulated to generate the manifold.

6. ACKNOWLEDGEMENTS

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