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IMPLEMENTATION OF THE FLAMELET-GENERATED-MANIFOLD FOR PREMIXED TURBULENT FLAMES

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Abstract: *It is known that turbulent flows are computationally costly when performing numerical simulations. Adding combustion physics to the flow drastically increases the computational cost, which makes the use of modeling approaches mandatory. In the literature, different approaches have already been reported to solve turbulent flames with reasonable computational time. In the present study, a premixed flame (CH_4/air, = 0.71) in an adiabatic single jet 3D geometry is simulated. Combustion is modeled through the Flamelet-Generated-Manifold (FGM) technique, which solves a set of one-dimensional flames (flamelets) using detailed chemical kinetics and tabulates the results through control variables which must describe the physics of the multidimensional problem. For turbulent flows, the mean values of chemical terms are modeled assuming that a variable is described locally by a presumed Beta Probability-Density-Function ($\beta - PDF$). The result is a two-dimensional database, whose control variables are the progress variable and the variance of progress variable. The turbulent flow is modeled using Reynolds Averaged Navier-Stokes (RANS) with a second-order closure model ($k - \epsilon$ RNG). It was coupled with the database and solved in a stationary regime. The preliminary results have been compared to other (numerical and experimental) works of literature and the FGM has been presenting satisfactory results.*

Keywords: *Premixed flames,β-PDF, FGM, Turbulence.*

1. INTRODUCTION

In combustion, a combination of mathematical models and experimental tests for combustion processes are useful to optimize fuel-efficiency and minimize the pollutants. An experimental approach is in general extremely expensive. Therefore a way to minimize the costs is maximizing the usage of simulations in the design phase. However, it is a very challenging task to develop a precise model. The combination between turbulence, chemical reactions, and heat transfer become the problem very complex. This leads many authors to research for different approaches.

The simulation of a turbulent flow can be done by different techniques. Some authors have invested resources trying to solve a turbulent flow using the Direct Numerical Simulation (DNS)(Donini *et al.*, 2015a; Mukhopadhyay *et al.*, 2015; van Oijen *et al.*, 2005; Vervisch and Poinsot, 1998), however, this model is the most expensive and time-consuming, that is why much commercial software does not have this numerical technique implemented yet. Another possibility to implement turbulent flow is using the Large Eddy Simulation (LES) (Riley, 2006; Pitsch, 2006; Malalasekera *et al.*, 2010), which is an intermediate approach between the DNS and Reynolds Averaged Navier-Stokes (RANS)(Ramaekers *et al.*, 2005; Fiorina *et al.*, 2005). The LES implementation considers only the larger scales of turbulence that are set by the geometry or specific flow conditions, and to account for the influence of the neglected smaller scales by use of a model. The RANS is solved using mean variables and normally this formulation has lower CPU cost comparing with LES and DNS.

To solve a numerical turbulent flame is necessary to choose a model that describes the chemical kinetic. There are many formulations in the literature, for instance, the detailed chemical technique solves the kinetic on a molecular level. This approach captures with high precision the value of all species, but the computational time can be impracticable whether the project will have a complex and/or large geometries. The way to get around this problem is using a simplified mechanism. The first and well-known systematic reduction method is introduced by (Peters and Rogg, 1993). Assuming that many chemical species and reactions are steady state, the differential equation can be replaced by algebraic relation, which reduces the computational costs. The methodology has a good agreement in high temperature, however, in 'low' temperature the steady-state assumptions are less efficient because the number of slow chemical processes increase and

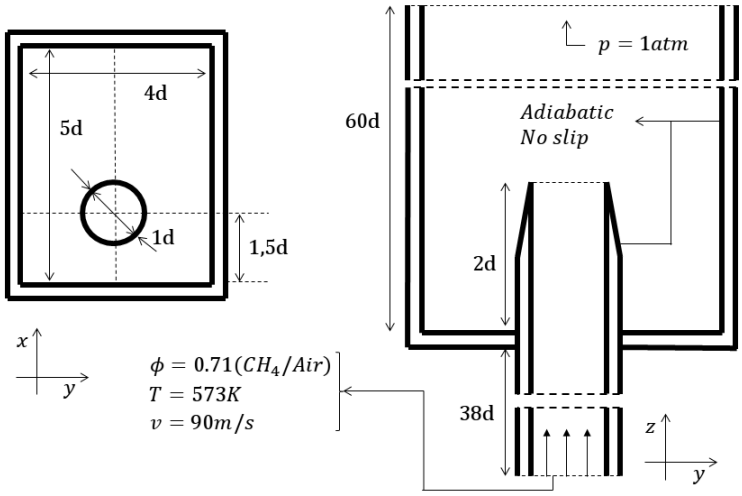


Figure 1: Burner configuration of the studied premixed flame.

less species can be assumed in steady state.

The FGM technique can be an alternative to working around this problem (de Goey and ten Thije Boonkkamp, 1999; van Oijen and de Goey, 2000, 2002). A database is built through of a group of laminar one-dimensional flames solved with detailed chemical and it is associated with control variables (enthalpy, progress variable, mixture fraction). This database is called the $manifold$. After a CFD problem to be defined and conservation equations are adapted in therms of these controlling variable. During the solution, the manifold is accessed and retrieved at each iteration. This technique has had satisfactory results in both regime (laminar and turbulent flow). Furthermore, in some cases, this methodology can be hundred times faster than the detailed mechanism (van Oijen, 2002; Donini *et al.*, 2015b).

The present work was aimed to evaluate a three-dimensional configuration of a premixed flame using RANS coupled with FGM technique. The results were compared with an experimental test and a numerical similar approach. The results and comparison discussed in the present study serve as validation of the model, authorizing the modeling of systems with heat loss in future works.

2. PROBLEM DEFINITION

The Figure 1 represents a single jet computational domain. The geometry chosen is a tube injector (inner diameter $d = 10mm$) with a length of $40d$ and positioned outside of a combustion chamber. It has a rectangular cross section with lengths $5d \times 4d$ and a length of $60d$. The off-center arrangement is selected to obtain a pronounced recirculation on one side of the jet flow, thereby shaping a flow field in analogy to the inner recirculation zone of a FLOX (n.d.)® combustor (Lammel *et al.*, 2012).

In this work is performed with an inlet mean bulk velocity at $v = 90m/s$ with equivalent ratio at $\phi = 0.71$ (CH_4/Air) and temperature equals to $573K$. This condition was analyzed experimentally by Lammel *et al.* (2012). However, in Lammel *et al.* (2012) the walls were cooled to a constant temperature $T_{wall} = 800K$ and the present study is neglected the heat loss, i.e., walls are considered adiabatic. Donini (2014) also performed numerical simulations of this present configuration considering both situations (adiabatic/no adiabatic). The Reynolds number calculated at the inlet diameter to this configuration is approximately 25600. The high turbulence levels allows to assume $Le = 1$, i.e., the diffusion of temperature and species is dominated by turbulent mixing. To calculate the transport properties with reduced computational cost, the follow equations are considered (Smooke and Giovangigli, 1991):

$$\lambda/c_p = 2.58 \times 10^{-5}(T/298K)^{0.69} \tag{21}$$

$$\mu/c_p = 1.67 \times 10^{-8}(T/298K)^{0.51} \tag{22}$$

The $\lambda[W/mK]$ is the thermal conductivity, $c_p[J/kgK]$ is specific heat, $\mu[kg/ms]$ dynamic viscosity and $T[K]$ the temperature. At top of the domain is opened to atmosphere ($p = 1atm$). Furthermore, the velocities are smaller than the speed sound ($\approx 30\%$). Thereby, a reasonable approximation to calculate the density is (ideal-gas law):

$$\rho = \frac{p_{amb}\overline{M}}{RT}, \tag{23}$$

with $R[J/molK]$ the universal gas constant, $p_{amb}[Pa]$ ambient pressure and $\overline{M}[kg/mol]$ the average molar mass defined as $\overline{M} = (\sum_{i=1}^{N_s} Y_i/M_i)^{-1}$. Consider $Y_i[-]$ the mass fraction and $N_s[-]$ the number of species.

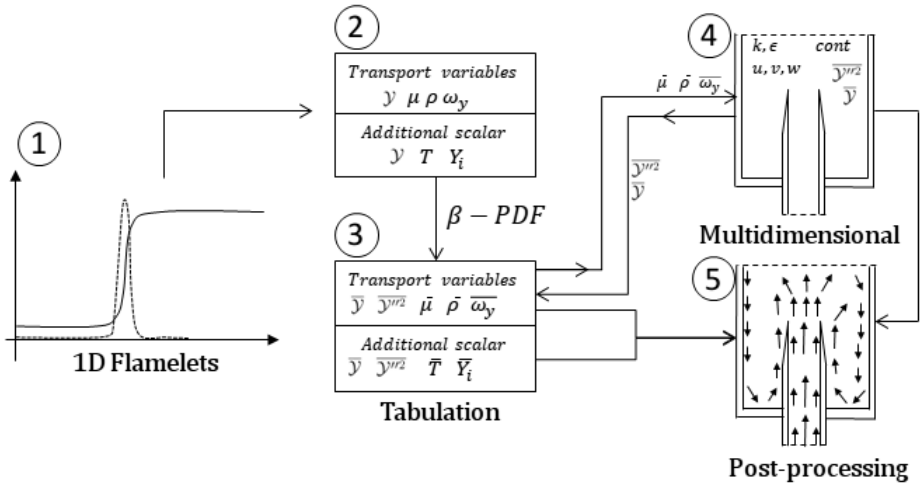


Figure 2: Flowchart of the implemented methodology.

A way to describe numerically the chemical kinetic of the present configuration is using the detailed chemistry. In this methodology, for each species involved, a Partial Differential Equation (PDE) has to be solved. This commonly results in hundreds of equations being necessary an enormous CPU power. Because of it, an alternative approach is needed to work around this high computational time. A viable solution is to apply a chemistry reduction method as FGM technique. it is implemented in the present work and detailed in the next section.

3. FGM METHODOLOGY

The basic idea of FGM is a chemistry reduction method that combines the advantages of chemistry reduction and flamelets method. Solving one-dimensional flame in detailed kinetic, the most important aspects of the internal structure of the flame fronts are captured and stored in function of a few of independent control variables, for which transport equations are solved during run-time. Here lies one the main strengths of FGM technique, a complete combustion phenomena can be represent solved few number of transport equations.

In the present work, the five steps to solve the turbulent premixed flame are shown in Figure 2. In the first part, only one unidimensional laminar flame is calculated using detailed kinetic with the purpose to obtain scalars that represent the characteristics of the flame as the temperature, density, specific heat, etc (**1d flamelets**). The scalars are tabulated as function of progress variable. They could be divide into two groups: the transport variables and additional scalars. The first group is accessed during the multidimensional solution, while the additional scalars are retrieved only on the post-processing step. How the flow is turbulent, it is necessary to determine the mean value of all scalars. Here, it is used an integration by presumed $\beta - PDF$. This allows having all scalars of interest in the function of two control variables: mean progress variable and the variance of the progress variable (**tabulation**). In the next step a turbulent flow (RANS) is solved with an additional transport equation (mean progress variable) and an algebraic expression to calculate the variance of progress variable. The mean values of variables of transport are iteratively retrieved from the database by a bi-linear interpolation. The simulation is finished when the convergence of the flow is achieved (**multidimensional**). In the final part, it is the post-processing. The fields of the multidimensional are rebuilt through of transport variables and additional scalars stored during the tabulation (**post-processing**).

3.1 Flamelet equations

The first step of the methodology was to solve the flat, freely-propagating, premixed, adiabatic flame in the $Chem1D$ software (van Oijen, 2002; Chem1D, n.d.). The $Chem1D$ solve differents types of the flames using finite volume in a one-dimensional domain. The system of conservation equations for the flamelets are described below:

$$\frac{\partial m}{\partial s} = 0 \tag{3.1}$$

The $m[kg/m^2 s]$ is mass burning rate and the $s[m]$ is the arc length perpendicular to the flame surface. The species transport equation is:

$$\frac{\partial (m Y_i)}{\partial s} - \frac{\partial}{\partial s}\left(\frac{\lambda}{c_p}\frac{\partial Y_i}{\partial s}\right) = \dot{w}_i \tag{3.2}$$

with $\dot{w}_i[kg/m^3s]$ is the source term.

The specific enthalpy is represent by $h[J/kg]$:

$$\frac{\partial(mh)}{\partial s} - \frac{\partial}{\partial s}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial s}\right) = 0 \tag{3.3}$$

The boundaries conditions used to solve the equations (3.1)-(3.3) are shown on the Table 1:

Unburnt Side ($Left$)	Burnt Side ($Right$)
$Y_i(-\infty) = Y_i$	$\frac{\partial Y_i}{\partial s}(\infty) = 0$
$h(-\infty) = h$	$\frac{\partial h}{\partial s}(\infty) = 0$

Table 1: Boundaries condition imposed to solve a free flame.

The m is an eigenvalue of the problem and the solution of the set of equations (3.1) - (3.3) is called a *flamelet*. The $Chem1D$ uses an exponential finite-volume discretization in space and the set the equations are solved using a fully implicit, modified Newton technique (Somers, 1994). The grid is adaptative to increase the resolution around the front flame.

3.2 Tabulation

After solving a flat flame using the equations (3.1) - (3.3), it is built a database through of FGM technique. It is based on the observation that multidimensional flames could be represented by as an ensemble of unidimensional flames. The solutions of the flamelets are stored in a manifold as a function of control variables. The complexity of the database will depend on the number of phenomena that will be considered (gradient pressure, heating lost, non-premixed flame). With each additional dimension will be necessary a new transport equation. These results give more accurate on the description of phenomena, but more computational time is necessary to achieve the final solution.

In this study, it will be considered only one control variable called progress variable ($\mathcal{Y}^*[-]$) and it is defined as:

$$\mathcal{Y}^* = \sum_{i=1}^{N_s} \alpha_i Y_i \tag{3.4}$$

The weighting factor $\alpha_i[-]$ chosen:

$$\alpha_{O_2} = -1 \tag{3.5}$$

$$\alpha_i = 0 \ \forall \ i \neq O_2 \tag{3.6}$$

It is emphasized that it is not a single choice. To prevent that a unique combination of control variables result in two equal results, the monotonicity of the function is required. Besides that, for the construction of the database care should be taken to ensure that $0 \leq \mathcal{Y} \leq 1$ and $\nabla\mathcal{Y} \neq 0$.

The first condition ($0 \leq \mathcal{Y} \leq 1$) can be imposed using a simple normalization:

$$\mathcal{Y} = \frac{\mathcal{Y}^* - \mathcal{Y}^*_{min}}{\mathcal{Y}^*_{max} - \mathcal{Y}^*_{min}} \tag{3.7}$$

The second condition ($\nabla\mathcal{Y} \neq 0$) is guaranteed with an adequate definition for the progress variable. More information about how to choose the progress variable can be found in Ihme *et al.* (2012).

In Figure 3 shows ($1D$-condition) the temperature and the mass fraction of O_2 in relation to the progress variable and domain x. It is possible to note the monotonicity of O_2 and T as a function of $\mathcal{Y}$. When we observe the variables in relation of x, it is presents the flame front at position $x = 0$.

3.3 β-PDF function

The β-Probability Density Function (β-PDF) is a statistical approach used for describing mean scalars in turbulence flow as RANS and LES (Ottino *et al.*, 2016; Guo *et al.*, 2003). Normally, it is determined by two parameters (*mean* and *variance*) and it is normalized between 0 and 1. In equation 3.8 is possible to calculate the mean temperature. The other variables are obtained in the same manner.

$$\overline{T} = \int_0^1 T(\mathcal{Y})P(\mathcal{Y})d\mathcal{Y} \tag{3.8}$$

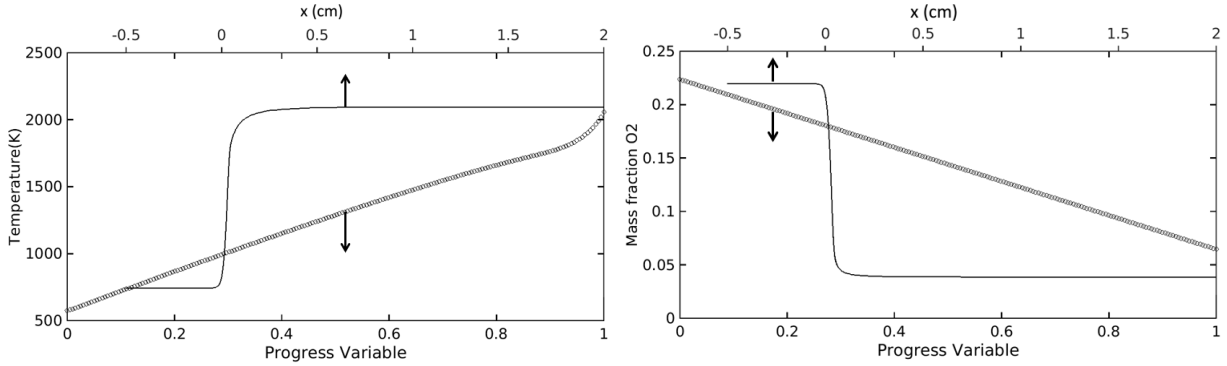
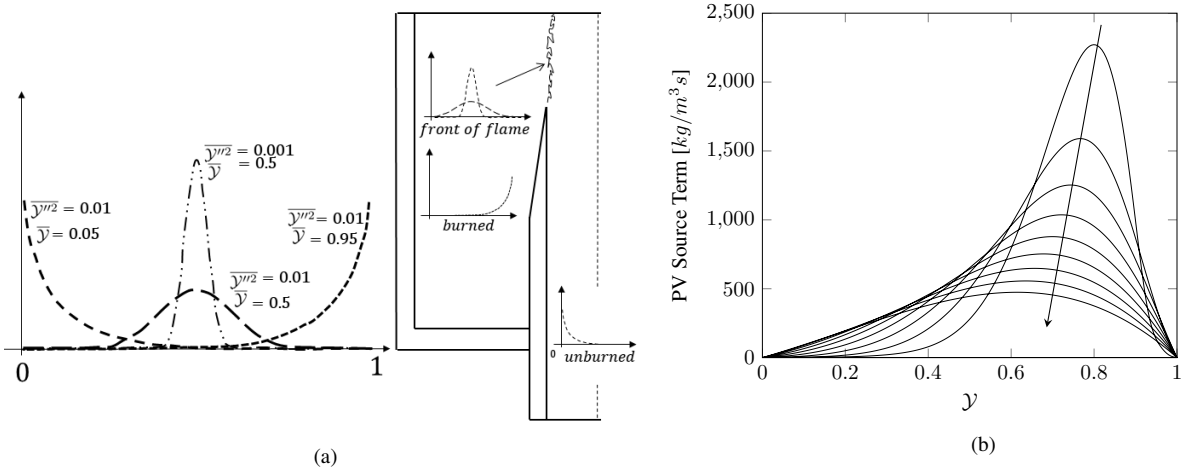


Figure 3: Profile of temperature (*left*) and O_2 (*right*) mass fraction as function of position (x) and the progress variable ($\mathcal{Y}$) for the 1D freely-propagating premixed flame.



(a) (b)

Figure 4: (a) Probability density function shapes for the β-distribution. (b) Progress variable source term at different variances.

To determinate the probability function, a suitable probability distribution $P(\mathcal{Y})[-]$ was considered and it can be calculated, as follow:

$$P(\mathcal{Y}) = \frac{\mathcal{Y}^{\alpha-1}(1-\mathcal{Y})^{\beta-1}}{\int_0^1 \mathcal{Y}^{\alpha-1}(1-\mathcal{Y})^{\beta-1}d\mathcal{Y}} \tag{3.9}$$

The coeficients $\alpha[-]$ and $\beta[-]$ which must both be positive ($\alpha \geq 0$ and $\beta \geq 0$). They can be determined from the mean and variance of $\mathcal{Y}$:

$$\gamma = \left[\frac{\overline{\mathcal{Y}}(1-\overline{\mathcal{Y}})}{\overline{\mathcal{Y}''^2}} - 1\right] \ , \quad \alpha = \overline{\mathcal{Y}}\gamma \ , \quad \beta = (1-\overline{\mathcal{Y}})\gamma \, .$$

The $\overline{\mathcal{Y}''^2}[-]$ is defined as variance of progress variable. On the Figure 4a presents the influence of first moment ($\overline{\mathcal{Y}}$) and second moment ($\overline{\mathcal{Y}''^2}$) on the probability profile. The shape of $\beta - PDF$ is very flexible and looks like either a Gaussian function. The extreme condition are completely burnt gases ($\overline{\mathcal{Y}} = 1$) and unburnt gases ($\overline{\mathcal{Y}} = 0$). In this situation the shape is a Dirac delta function.

The nine values of the progress variable (PV) variances were considered for each scalar, varying from 10^{-4} to 0.6 equally spaced. The result of source term of progress variable after convolved for different level of variances shown in Figure 4b. The arrow represents the direction in which the variance of the progress variable increases.

The calculation of the variance is simplified using the algebraic expression (3.10) adopted by Knudsen *et al.* (2012) and Vreman *et al.* (2009).

$$\overline{\mathcal{Y}''^2} = \frac{a^2\Delta^2}{12}\left(\left(\frac{\partial\overline{\mathcal{Y}}}{\partial x}\right)^2 + \left(\frac{\partial\overline{\mathcal{Y}}}{\partial y}\right)^2 + \left(\frac{\partial\overline{\mathcal{Y}}}{\partial z}\right)^2\right) \tag{3.10}$$

where Δ and a are the filter width ($\Delta = \Delta x \Delta y \Delta z$) and a constant, respectively. The a value is equal the unity.

The final step of implementation is database, as shown in table 2. The first column is presented the PV mean value and the second one is the PV variance. In the other columns are the average scalars are stored.

$\overline{\mathcal{Y}}$	$\overline{\mathcal{Y}'^2}$	$\overline{T}$	$\overline{c_p}$	...
0.000	0.0001	573	1136	...
0.005	0.0001	579	1138	...
0.010	0.0001	586	1141	...
...	...	...	...	...
1.000	0.6000	2057	1434	...

Table 2: FGM database structure for the current work.

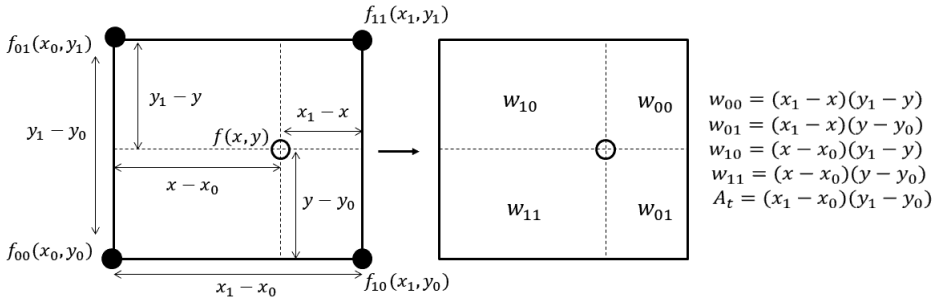


Figure 5: Illustration of bi-dimensional interpolation.

3.4 Bi-linear interpolation

To retrieve the data from the database is used a bi-linear interpolation. Consider a point in a bi-dimensional domain coordinate (x,y), which has a value $f(x, y)$ that needs to be interpolated, as shown in Figure 5. The rectangle formed by these four points could be divided into four sub-rectangles. The area of main rectangle and sub-rectangles were defined as A_t and $w_{01}, w_{10}, w_{01}, w_{11}$, respectively. After five hours and fifteen minutes was possible to show:

$$f(x, y) = \frac{w_{00} f_{00} + w_{01} f_{01} + w_{10} f_{10} + w_{11} f_{11}}{A_t} \tag{3.11}$$

During the run-time, the fields of $\overline{\mathcal{Y}}$ and $\overline{\mathcal{Y}'^2}$ are calculated. With each pair ($\overline{\mathcal{Y}}$,$\overline{\mathcal{Y}'^2}$) is possible to obtain the value of each scalar of interest. if there is no exact value in the database, a bi-linear interpolation is used. The algorithm was developed using User-Defined Functions (UDFs).

3.5 Multidimensional simulation

In addition to the RANS methodology (mass($cont$), momentum(u,v,w), turbulence ($k-\epsilon\ RNG$)), a transport equation to the progress variable was solved ($\overline{\mathcal{Y}}$), as shown in equation 3.12.

$$\frac{\partial}{\partial x_i}\left(\rho \overline{v}\overline{\mathcal{Y}} - \frac{1}{Le_{\mathcal{Y}}}\frac{\overline{\lambda}}{\overline{c_p}}\frac{\partial \overline{\mathcal{Y}}}{\partial x_i}\right) = \overline{\dot{w}}_{\overline{\mathcal{Y}}} \tag{3.12}$$

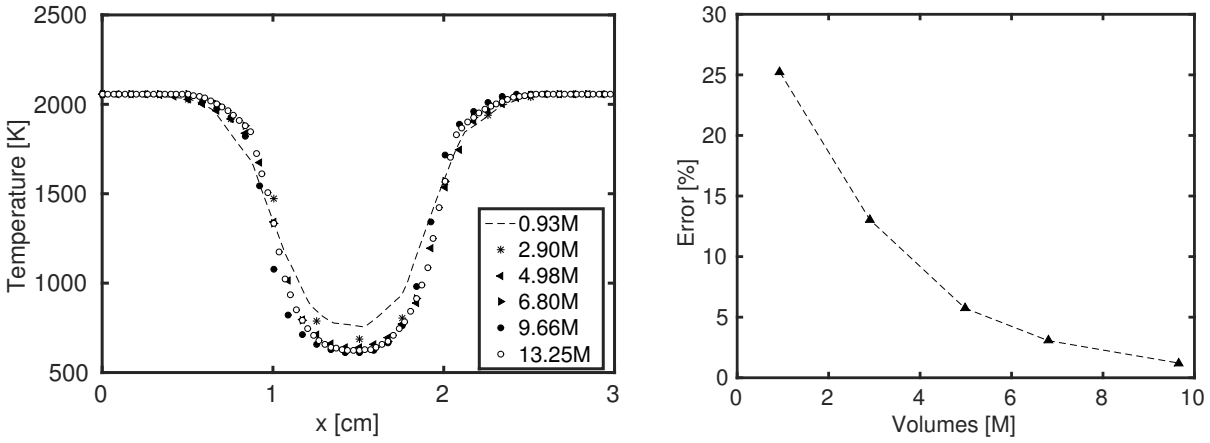
where the boundaries conditions were:

$$Inlet: \quad \overline{\mathcal{Y}} = 0\ , \quad Walls/Outflow: \quad \frac{\partial \overline{\mathcal{Y}}}{\partial x_i} = 0$$

The boundary conditions of the transport equations for k and ϵ were left standard of software.The boundaries condition of momentum were defined:

$$Inlet: \ w = 90[m/s], u = v = 0[m/s]\ , \quad Walls: No\ slip\ , \quad Outflow: p = 1atm$$

The system of seven equations has been implemented into the commercial CFD code (Fluent, n.d.). The implementation of FGM technique was performed by UDFs. During the solution, the control variables $\overline{\mathcal{Y}}$ and $\overline{\mathcal{Y}'^2}$ were read at each iteration and the manifold was accessed to retrieve of look-up table ($\overline{c_p}$, $\overline{\lambda}$, $\overline{\rho}$, etc). When the convergence was obtained ($\times 10^{-5}$), the pos-processing was performed. Through of control of variables was possible to rebuild the multidimensional flame.



(a) (b)

Figure 6: (a) Temperature distribution for different numbers of volumes in a line positioned at $z = 4cm$. (b) Relative error in relation to the mesh with 13.25 millions of volumes ($x = 1.5cm$, $y = 2cm$, $z = 4cm$).

The mesh evaluation was made with six different quantities of volumes ($0.93, 2.90, 4.98, 6.80, 9.66$ and 13.25 millions). The type of element was the tetrahedral, considering a fixed size of the element in the entire domain. Figure 6a presents the distribution of temperature in a line $4cm$ away from the injector tube. It can be observed that the mesh influence on the temperature profile. In Figure 6b presents the relative error in relation to the most refined mesh $|mesh - mesh_{13.25M}|/mesh_{13.25M}$ at the central point in $z = 4cm$. It is visible that the error becomes lower than 3% to the mesh $9.66M$. From hereon, the presents results of $3D$ model will be present with the mesh of 9.66 millions of volumes.

4. RESULTS

4.1 Flamelet

In Figure 7 is presented a one-dimensional (flat, freely-propagating, premixed, adiabatic) comparison between a detailed kinetic and FGM technique. This implementation was done considering CH_4/air with $\phi = 0.9$ with inlet temperature equal $298K$ and $1atm$. The chemical reaction mechanism is the $Grimech3.0$ (Smith *et al.*, 2012) and unity Lewis number. The $Chem1D$ was used for the simulation. Furthermore, the results were compared with Donini (2014). A good agreement can be seen between all domain. This result is a good indication that the FGM technique could describe very well the present condition and good sign that the progress variable is suitable to solve this configuration.

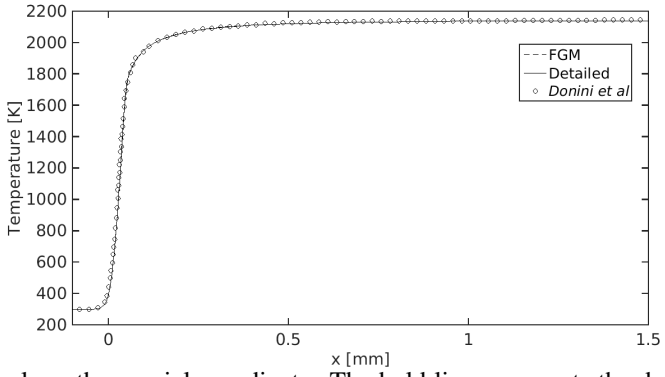


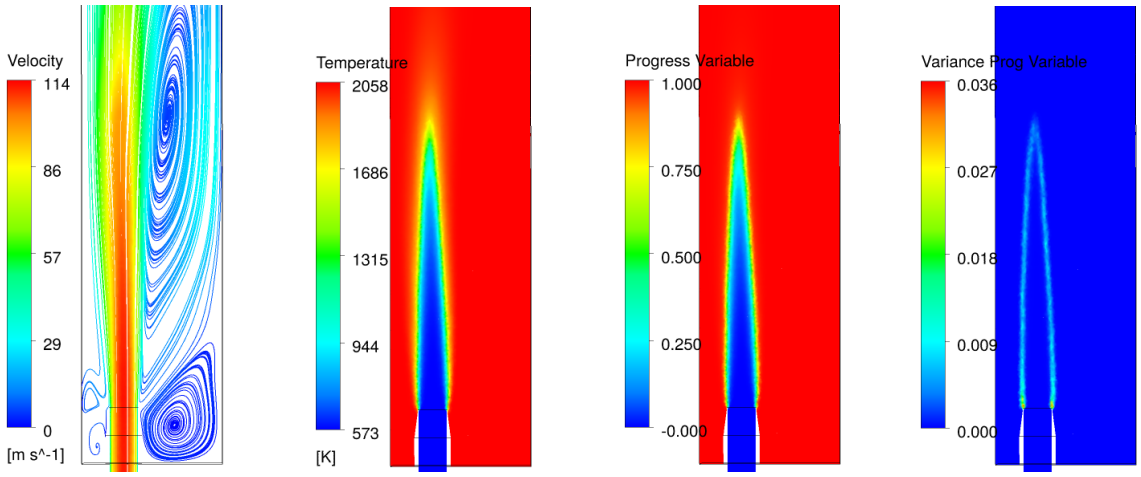
Figure 7: Temperature profile along the spacial coordinate. The bold line represents the detailed chemistry calculation, dashed lines are FGM technique and the circle represent the Donini (2014) results.

4.2 3D burner

In Figure 8 shown an overall of the burner. The velocity is presented in a set of streamlines projected on a cross-section, as shown in Figure 8 (a). It can be observed a maximum velocity of $114\,m/s$ and two large recirculation. These recirculations practically did not affect the temperature profile, which presented a symmetrical line form (Figure 8

(b)). In additional, it was possible to observe that the temperature did not decrease after the front of the flame (constant temperature ($2058K$)). It occurred because a strong assumption, i.e., the heat loss did not model.

The solution of progress variable ($\overline{\mathcal{Y}}$) had a similar behavior of temperature (Figure 8 (c)). It can be observed $\overline{\mathcal{Y}} = 0$ to unburned gases and $\overline{\mathcal{Y}} = 1$ after flame front. The maximum variance of progress variable is close of nozzle exit (Figure 8 (d)). Furthermore, the contour of variance creates the form of the front of the flame. This region is the maximum gradient of progress variable. The analysis of temperature in the domain was evaluated in two lines located at $4cm$ and $10cm$ from



(a) (b) (c) (d)

Figure 8: Cross section of (a) Velocity streamlines (b) Temperature (c) Progress variable (d) Variance progress variable.

the nozzle exit (Figure 9). The results were compared with a numeric simulation (Donini, 2014) and an experiment was done by Lammel *et al.* (2012). The comparison between the present work and Donini (2014) had a reasonable agreement. The difference found may have been caused by some difference in implementation that has not been explicitly declared (interpolation, range variance values, PDF implementation).

The discrepancy between the numerical (present) and experimental results was already expected. In the present implementation the heat lost between the gas and the walls of the domain was not considered. In Lammel *et al.* (2012), the walls were maintained at a temperature of $800K$, this condition reduces the flow temperature in almost all of the line analyzed.

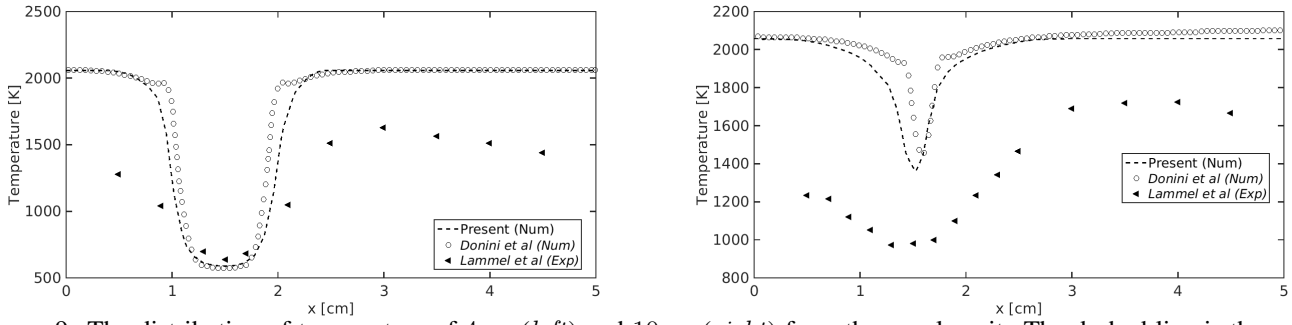


Figure 9: The distribution of temperature of $4cm$ (*left*) and $10cm$ (*right*) from the nozzle exit. The dashed line is the result of present work. The circle result of the simulation of Donini (2014). The Lammel *et al.* (2012) is represented by left-pointing triangle.

The profile of axial velocity is shown in the Figure 10. It was not so affected when the heat lost is neglected ($4cm$). When we move away from the nozzle ($10cm$), the influence of the heat lost on the walls become more important to the flow and the numerical do not have a good agreement.

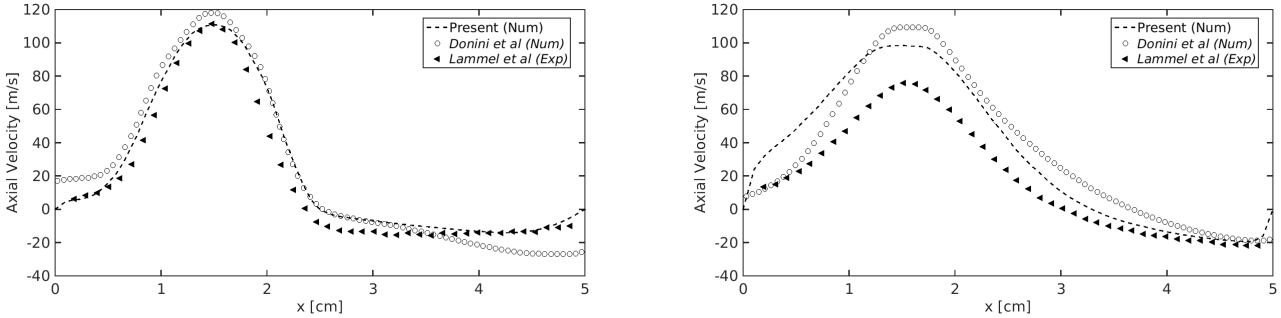


Figure 10: The distribution of axial velocity of $4cm$ $(left)$ and $10cm$ $(right)$ from the nozzle exit. The dashed line is the result of present work. The circle result of the simulation of Donini (2014). The Lammel *et al.* (2012) is represented by left-pointing triangle.

5. CONCLUSION

In the present work, the FGM method has been applied to premixed turbulent flame. The domain tested was a three-dimensional single jet. When the velocities and temperature fields were confronted with an identical implementation used in this work, the results had a good agreement. In the comparison with experimental results is possible to verify some discrepancies mainly on temperature fields. The difference in the results was attributed the boundary condition imposed on the walls. This suggests that the present methodology could be continued and expanded to a configuration with heat loss. In FGM technique, it could be done adding a new control variable (h). This would bring the possibility of examining combustion issue more complex and solve industrial problems.

6. ACKNOWLEDGEMENTS

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