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MODELING AND SOLUTION OF METHANE JET DIFFUSION FLAMES

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Abstract: *The aim of this work is to model a jet diffusion flame, to show the corresponding proof of existence of solutions, and to present numerical results. The model is based on the flamelet equations for the chemistry and on the mixture fraction for the flow. Numerical tests are carried out for Sandia Flame D and the results are found to compare well with available data found in the literature.*

Keywords: *diffusion flames, solution existence, LES, methane*

1 Introduction

Combustion corresponds to a complex sequence of chemical reactions between a fuel and an oxidizer, producing heat and sometimes light too. It is well known that combustion not only generates heat, which can be converted into power, but also produces pollutants such as oxides of nitrogen (NO_x), soot, and unburnt hydrocarbons (HC) (PETERS, 2006). In addition, unavoidable emissions of CO_2 are believed to contribute to the global warming. These emissions will be reduced by improving the efficiency of the combustion process, thereby increasing fuel economy.

The flames can be classified as premixed, nonpremixed and partially premixed, being laminar or turbulent. For example, the combustion in homogeneous charge spark-ignition engines or in lean-burnt gas turbines occurs under premixed conditions. In contrast, combustion in a diesel engine or in furnaces essentially takes place under nonpremixed or partially premixed conditions.

In diffusion (nonpremixed) flames the fuel and the oxidizer enter the domain in separate streams. If the fuel and the oxidizer velocities are small (low Reynolds) the mixture among fuel, oxidizer and products of combustion will be basically by diffusion, establishing a laminar diffusion flame. However, if the velocity is high, for high Reynolds, the mixture occurs due to the transport of mass characterizing the turbulent flux.

Most of the applications of technical interest in combustion involves nonpremixed turbulent flames, as in jet engines, diesel engines, steam boilers, furnaces, and hydrogen-oxygen rocket motors (WARNATZ *et al.*, 2001). The jet diffusion flame is an important example of nonpremixed flames.

When the burner dimensions are much larger than the fuel jet diameter, of a jet diffusion flame, the heat losses to the walls are usually small and the contribution due to radiation turns negligible; radiation turns more important in furnaces, spreading of buildings and forest fires (LAW, 2006).

When a chemically reacting flow is considered, the system at each point in space and time is completely described by specification of its pressure, density, temperature, velocity, and concentration of each species. These properties can change in time and space. These changes are the result of fluid flow, chemical reaction and molecular transport. A mathematical description of flames, therefore, has to account for each of these processes (WARNATZ *et al.*, 2001).

In this work we develop the flamelet model, we present results about the existence of solutions for the Lagrangian and the Eulerian flamelet models and show some numerical results for the Sandia Flame D.

2. Governing Equations and the Flamelet Model

The governing equations for combustion processes, in the gas phase, include the balance equations for mass, momentum, energy and chemical species (WILLIAMS, 1985).

We introduce the Lewis number as $Le_i = \kappa / c_p \rho D_i$, $i = 1, 2, ..., n$, where κ is the thermal conductivity, c_p is the specific heat capacity at constant pressure of the

mixture, ρ is the density of the fluid, and D_i is the diffusivity of each species i. For methane flames we consider that the diffusivity and the temperature of all species are the same, and therefore the Lewis number of all species is equal to one (PETERS, 1992).

The Favre averaging governing equations for a jet diffusion flame are the following:

Momentum

$$(1)\quad \frac{\partial\left(\overline{\rho}\widetilde{u}_i\right)}{\partial t}+\frac{\partial\left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j\right)}{\partial x_j}=-\frac{\partial\overline{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\frac{\mu_T}{R_e}\widetilde{\tau}_{ij}\right)$$

Species Mass Fraction

$$(2)\quad \frac{\partial\left(\overline{\rho}\widetilde{Y}_i\right)}{\partial t}+\frac{\partial\left(\overline{\rho}\widetilde{u}_j\widetilde{Y}_i\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_T}{P_e}\frac{\partial\widetilde{Y}_i}{\partial x_j}\right)+\dot{\widetilde{w}}_i$$

Mixture Fraction

$$(3)\quad \frac{\partial\left(\overline{\rho}\widetilde{Z}\right)}{\partial t}+\frac{\partial\left(\overline{\rho}\widetilde{u}_j\widetilde{Z}\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_T}{S_c}\frac{\partial\widetilde{Z}}{\partial x_j}\right)$$

Energy

$$(4)\quad \frac{\partial\left(\overline{\rho}\widetilde{T}\right)}{\partial t}+\frac{\partial\left(\overline{\rho}\widetilde{u}_j\widetilde{T}\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_T}{P_e}\frac{\partial\widetilde{T}}{\partial x_j}\right)+\frac{\widetilde{h}_i\dot{\widetilde{w}}_i}{c_p}$$

where the '~' denotes the Favre averaged variables. Here, u_j is the velocity vector, τ_{ij} viscous stress tensor, Y_i mass fraction of each species i, $\dot{w}_i$ reaction rate of the species i, Z mixture fraction, T temperature and h_i specific enthalpy. The $\overline{\rho}$ and $\overline{p}$ denote the mean values of the density and pressure, respectively. The R_e is the Reynolds, S_c the Schmidt and P_e the Peclet numbers; the t is the time, μ_T eddy viscosity and c_p heat capacity.

The reaction rate of species i may be modeled as

$$(5)\quad \dot{\widetilde{w}}_i=\nu_i W_i A\frac{\widetilde{Y}_F}{W_F}\frac{\widetilde{Y}_O}{W_O}\rho^2 e^{-E/R\widetilde{T}},$$

where ν_i is the stoichiometric coefficient of the component i, W_i the molecular weight of species i, A the frequency factor, E the total activation energy, and R the gas constant.

The Eq. (3) does not contain source term, since Z represents the chemical elements originally contained in the fuel, and these are conserved during the combustion. We assume that the mixture fraction Z is a space and time function.

The combustion occurs in a fine layer of the stoichiometric surface if the *Damköhler* number is elevated. We introduce an orthogonal coordinate system x_1, x_2, x_3, t, where x_1 is normal to the surface $Z(x_\alpha, t)=Z_{st}$, according to Fig. 1. We change the coordinate x_1 by mixture fraction Z and x_2, x_3, t by Z_2, Z_3, τ, respectively. So, the temperature T and the mass fractions Y_i can be expressed as functions of the mixture fraction Z. By definition, the new coordinate Z is locally normal to the surface of stoichiometric mixture (PETERS, 1992).

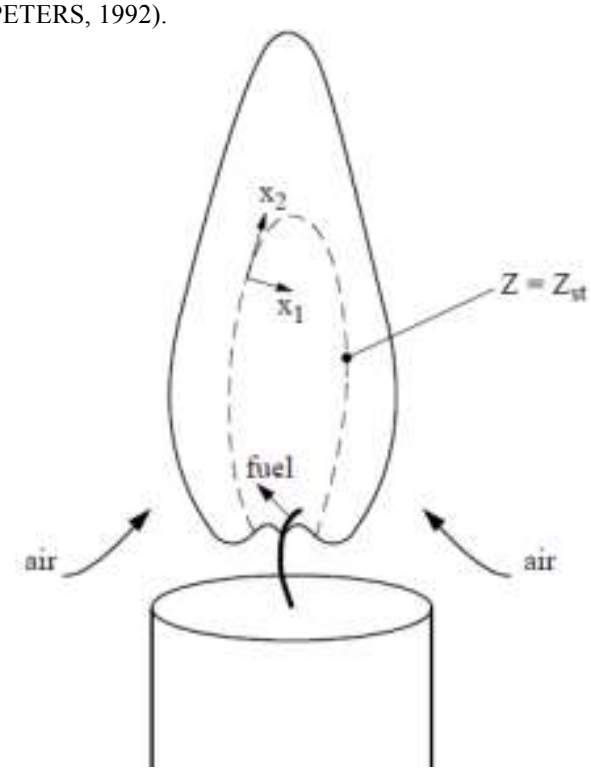


Figure 1. Orthogonal coordinate system to a surface of the stoichiometric mixture.

Consider the transformations

$$(6)\quad \frac{\partial}{\partial t}=\frac{\partial}{\partial\tau}+\frac{\partial Z}{\partial t}\frac{\partial}{\partial Z},$$

$$(7)\quad \frac{\partial}{\partial x_k}=\frac{\partial}{\partial Z_k}+\frac{\partial Z}{\partial x_k}\frac{\partial}{\partial Z},\ k=2,3,$$

$$(8)\quad \frac{\partial}{\partial x_1}=\frac{\partial Z}{\partial x_1}\frac{\partial}{\partial Z}.$$

After neglecting high order terms, results the equations for the mass fraction and the temperature in the mixture fraction space (in the flamelet form)

$$(9)\quad \rho\frac{\partial Y_i}{\partial\tau}-\frac{\rho}{Le_i}\frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2}=\dot{w}_i,$$

$$(10)\quad \rho c_p\frac{\partial T}{\partial\tau}-\rho c_p\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2}=\sum_{i=1}^{n}h_i\dot{w}_i,$$

where $\chi = 2D\left(\partial Z / \partial x_k\right)^2$ is the instantaneous scalar dissipation rate.

The equations for the mixture fraction and the temperature may be conveniently written in the nondimensional form as

$$(11)\quad \frac{\partial Y_i^*}{\partial \tau^*} - \frac{a\chi^*}{2Le_i}\frac{\partial^2 Y_i^*}{\partial Z^2} = \nu_F D_a Y_F^* Y_O^* e^{-\frac{Z_e(1-\theta)}{1-\alpha(1-\theta)}},$$

$$(12)\quad \frac{\partial T^*}{\partial \tau^*} - \frac{a\chi^*}{2}\frac{\partial^2 T^*}{\partial Z^2} = \nu_F H_e D_a Y_F^* Y_O^* e^{-\frac{Z_e(1-\theta)}{1-\alpha(1-\theta)}},$$

where D_a is the Damköhler number, Z_e the Zel'dovich number and H_e the heat release rate.

In the following we discuss the existence of solutions for the mass fraction and the temperature equations in the flamelet form. The proof of the existence is given by Faedo-Galerkin method.

3. Existence of Solutions

Starting with the incompressible flamelet equations, an appropriate transformation (PITSCH, 2002) leads to the Lagrangian or to the Eulerian flamelet models for the mass fraction equation, as follows:

Lagrangian Flamelet Model

$$(13)\quad \rho\frac{\partial Y_i}{\partial \tau} - \rho\frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} - \dot{w}_i = 0$$

Eulerian Flamelet Model

$$(14)\quad \rho\frac{\partial Y_i}{\partial \tau} + \rho v\cdot\nabla Y_i - \rho\frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} - \dot{w}_i = 0$$

where the time τ is defined in the coordinate system attached to the stoichiometric surface.

In the Eulerian system both the velocity vector and the scalar dissipation rate are functions of time, space and mixture fraction. Moreover, the velocity and the scalar dissipation rate are fluctuating quantities in a turbulent flow field.

The equations (13) and (14) may be rewritten in a general form, respectively as

$$(15)\quad \frac{\partial u}{\partial t} - \nu\frac{\partial^2 u}{\partial Z^2} = f,$$

$$(16)\quad \frac{\partial u}{\partial t} + h\cdot\nabla u - \nu\frac{\partial^2 u}{\partial Z^2} = f.$$

To prove the existence of solutions for the Lagrangian and the Eulerian flamelet model equations, we consider a bounded open Lipschitz set Ω in R^3 and fixed $t^* > 0$. We consider also that $D(\Omega)$ is a space of functions C^∞ with compact support contained in Ω, H the closure of D in $L^2(\Omega)$ and V the closure of D in $H_0^1(\Omega)$ (TEMAM, 1977; ODEN, 1979; FOIAS *et al.*, 2001; DOERING & GIBBON, 2004). H and V are the Hilbert spaces associated, respectively, with the scalar products

$$(17)\quad (u,v) = \int_\Omega u(Z)v(Z)dZ,$$

$$(18)\quad ((u,v)) = \sum_{i=1}^{3}\left(\frac{\partial^i u}{\partial Z^i}, \frac{\partial^i v}{\partial Z^i}\right),$$

and H' is the dual space of H, V' is the dual space of V. As the scalar products of $f \in H$ and $u \in V$ in H is the same as the scalar product of f and u in the duality between V' and V, $\langle f,u\rangle = (f,u)$ for all $f \in H$ and $u \in V$. Moreover, for each $u \in V$, the form $v \in V \to ((u,v)) \in R$ is linear and continuous on V and there exists an element Au of V' such that $\langle Au, v\rangle = ((u,v))$ for all $v \in V$.

We intend to find a vectorial function $u : \Omega\times[0,t^*] \to R^3$ such that

$$(19)\quad \frac{\partial u}{\partial t} - \nu\Delta u = f \text{ in } Q = \Omega\times]0,t^*[,$$

$$(20)\quad u(Z,0) = u_0(Z), \text{ in } \Omega$$

for the Lagrangian case, and

$$(21)\quad \frac{\partial u}{\partial t} - \nu\Delta u + h\cdot\nabla u = f, \text{ in } Q = \Omega\times]0,t^*[,$$

$$(22)\quad u(Z,0) = u_0(Z), \text{ in } \Omega$$

for the Eulerian case, where the functions f and h are given and defined in $\Omega\times[0,t^*]$, and u_0 is given and defined in Ω.

Consider now the Lagrangian flamelet model equations. Assuming that u is a classical solution, we have that $u \in C^2(\overline{Q})$. If v is an element of D, then

$$(23)\quad \left(\frac{\partial u}{\partial t}, v\right) + \nu((u,v)) = (f,v).$$

Due to continuity, this equation is valid for each $v \in V$. Therefore, we obtain a weak formulation of this problem, that is, given f and u_0 with $f \in L^2(0,t^*;V')$ and $u_0 \in H$, we will find u satisfying

(24) $u \in L^2\left(0,t^*;V\right),$

(25) $\frac{d}{dt}(u,v)+\nu((u,v))=\langle f,v\rangle,\ \forall\, v \in V,$

(26) $u(Z,0)=u_0(Z).$

After rewriting this problem in a convenient way, we obtain the following result:

Theorem: Let $f \in L^2\left(0,t^*;V'\right)$ and $u_0 \in H$. Then, there exists at least one function u that satisfies

(27) $u \in L^2\left(0,t^*;V\right),\ u' \in L^2\left(0,t^*;V'\right),$

(28) $u'+\nu Au = f \text{ in } \left]0,t^*\right[,$

(29) $u(Z,0)=u_0(Z).$

The proof of the theorem follows the Faedo-Galerkin method (LORENZZETTI & DE BORTOLI, submitted to *Combustion and Flame*). The result of the existence of solutions for the Eulerian Flamelet model equations is found in a similar manner.

4. Numerical Solution via Large Eddy Simulation

The solution of the Navier-Stokes equations for turbulent flows demands a great amount of computational time, because the resolution of the small scales in turbulent flows needs far more grid points than does the analogous laminar flow. In practice, a full solution of the Navier-Stokes equations for turbulent reacting flows is not yet possible (WARNATZ *et al.*, 2001).

The Navier-Stokes solution of turbulent flows is itself time-dependent and there is not a steady solution, different from laminar flow solutions. If one estimates that at least 1000 time steps are needed to represent a turbulent combustion process, the number of computational operations needed in the calculation easily exceeds 10^{14}, assuming 100 operations per grid point. So, the overall time for the computation increases with the fourth power of the Reynolds number.

The usual numerical tools used for the solution of combustion problems are *Reynolds Averaged Navier-Stokes* (RANS), *Direct Numerical Simulation* (DNS) and *Large Eddy Simulation* (LES). Turbulence models based on RANS equations employ turbulent transport approximations with an effective turbulent viscosity that is by orders of magnitude larger than the molecular viscosity. If steady state versions of these equations are used, this tends to suppress large scale instabilities, which occur in flows with combustion even more frequently than in nonreacting flows. If those instabilities are to be resolved in numerical simulations, it is necessary to resort to more advanced, but computationally more expensive, methods such as DNS or LES (PETERS, 2006).

The LES is a very attractive tool for numerical simulations of fluid flows. The idea is to explicitly compute the largest structures of the flow field, typically the structures larger than the computational mesh size, whereas only the effects of the small ones are modeled (VEYNANTE & VERVISCH, 2003). LES for reacting flows allows more precise computations of turbulent flames but also opens new perspectives to compute the interaction between combustion and acoustics, especially combustion instabilities, which are a serious problem in many combustion devices. LES is especially well adapted to the study of these phenomena, which are controlled by large scale vortices, explicitly captured in LES (WESTBROOK *et al.*, 2005).

LES modifies the Navier-Stokes equations to obtain a new system of equations which is more amenable to approximate, while retaining all the most energetic features of the unperturbed problem. The classical idea is to use a filter which allows for the separation of large and small length scales in the flow field. Applying the filtering operator to the Navier-Stokes equations provides a new equation governing the large scales, except for one term involving the small velocity scales. Modeling this term in an appropriate manner (procedure commonly referred to as closure problem) we can arrive at a set of equations with only the large velocity, and pressure, scales as the unknowns (GUERMOND *et al.*, 2004).

In the following we indicate some numerical results for jet diffusion flames obtained using LES and we compare them with available experimental data found in the literature.

5. Numerical Results

The jet flame is chosen because it represents the class of nonpremixed flames. To build a burner one can surround a high velocity jet of gas fuel with an annular pilot flame of lower velocity (LEWIS & VON ELBE, 1961).

Those experimental flames which are well-defined and well-documented are used for comparison of the numerical values. Among the piloted flames, it seems that flame D is preferred (BARLOW & FRANK, 2003), (SCHNEIDER *et al.*, 2003), (PITSCH & STEINER, 2000), (SHEIKHI *et al.*, 2005), when doing the comparisons because high Reynolds number is desired for model validation. Sandia flame D consists of a main jet with a mixture of 25% of methane and 75% of air. This jet is placed in a coflow of air and the flame is stabilized by a pilot.

Consider the burner as shown in Fig. 2. The duct has a cylindrical cross section with $D_e = 1$ and a cylindrical tube that injects fuel with $d = 0.025$; the tube of the coflow has a diameter $D = 0.0267$ and the burner length is $L = 11$. The number of grid points was taken as $199 \times 51 \times 51$ for flame D in the (x, y, z) directions, respectively; x corresponds to the axial direction.

Fig. 3 top shows the comparison between the experimental and the numerical instantaneous mixture fraction profiles along the burner centerline. The mixture fraction measures the reactants mixing and is mainly related to the large scale motions of the flow. The solution shows the axial decreasing behavior of the mixture fraction. The numerical result for the velocity along the burner centerline (see Fig. 3 below) is also in reasonable agreement with the experimental data. In order to avoid spurious oscillations in the vicinity of strong gradients, mainly close to the jet exit, a TVD (Total Variation Diminishing) scheme is applied for the advection of Z .

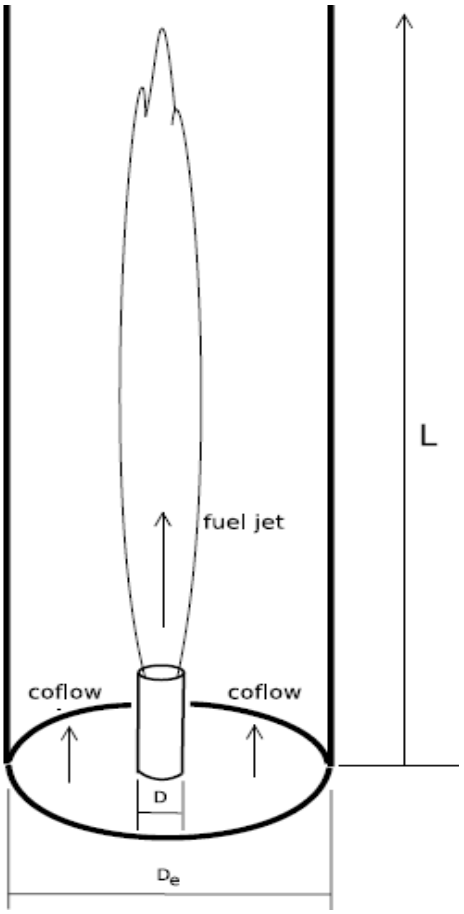


Figure 2. Burner sketch

Fig. 4 presents the comparison for the temperature and the fuel CH_4 mass fractions along the burner centerline. The numerical result agrees with the experiment, but the temperature is overpredicted mainly at $x/D = 40$. The fuel CH_4 mass fraction is in very good agreement with the experimental data.

Finally, Fig. 5 shows the CO_2 and the H_2O mass fractions along the burner centerline. The carbon dioxide mass fraction is reasonably well predicted, while the water vapor maximum value is underpredicted. Away from the centerline the flow field is smoother, with smaller gradients and, consequently, low fluctuations.

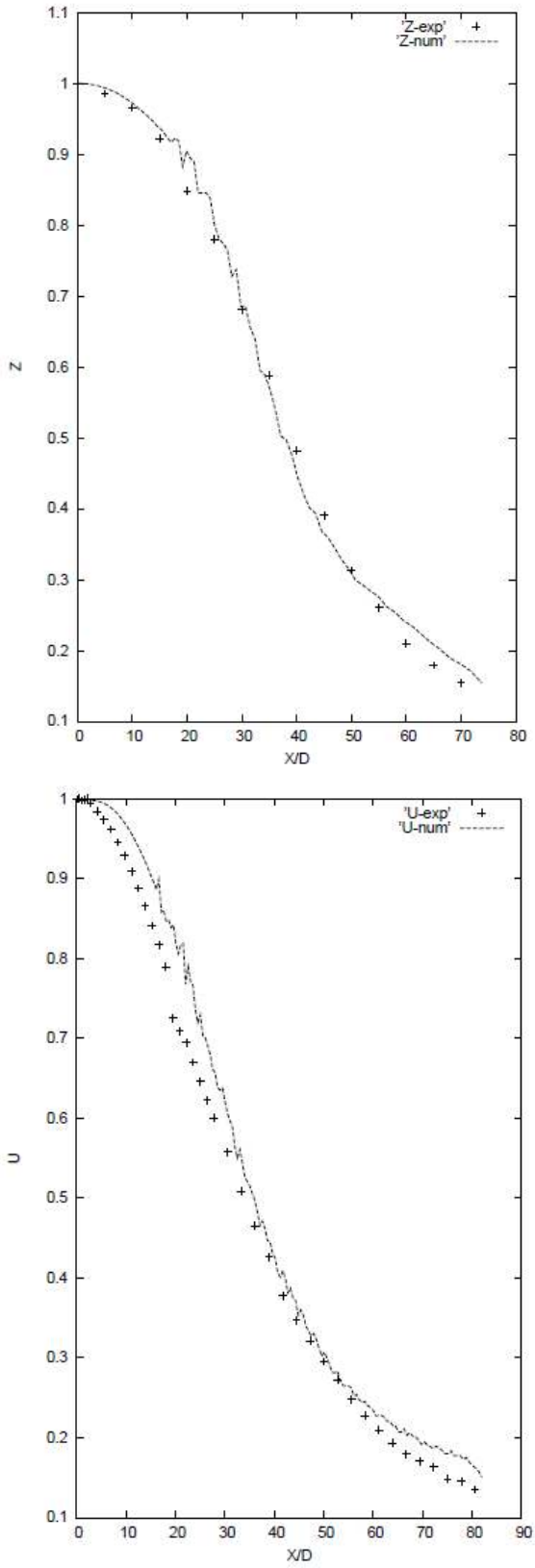
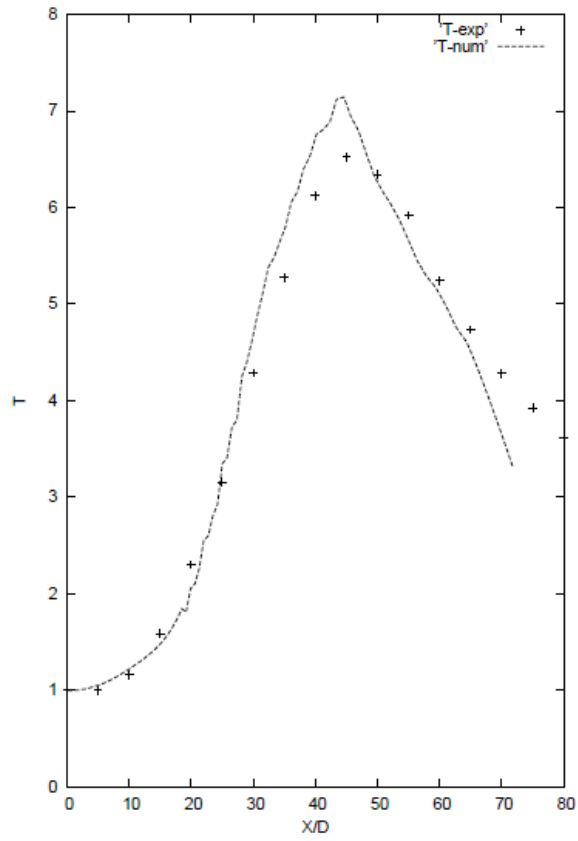


Figure 3. Comparison with experimental data (BARLOW & FRANK, 2003) for the mixture fraction (top) and velocity (below) profiles along the burner centerline.



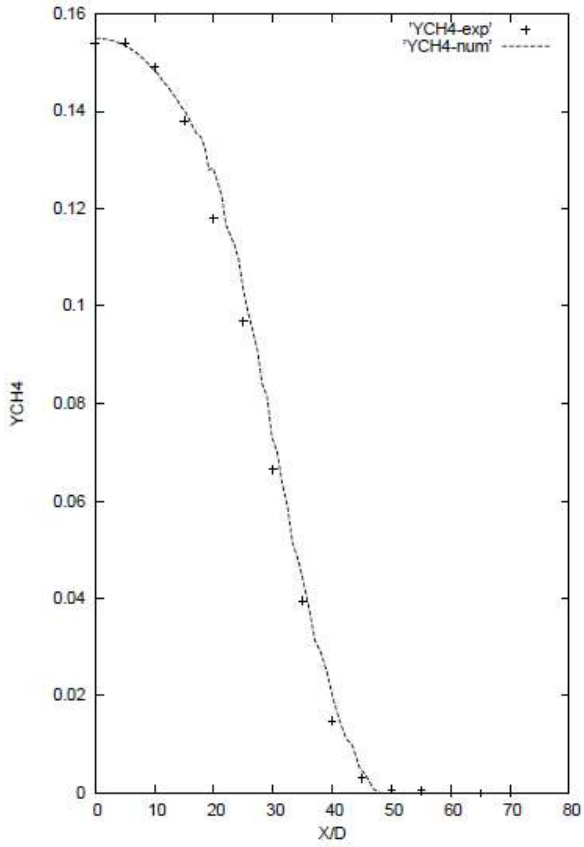
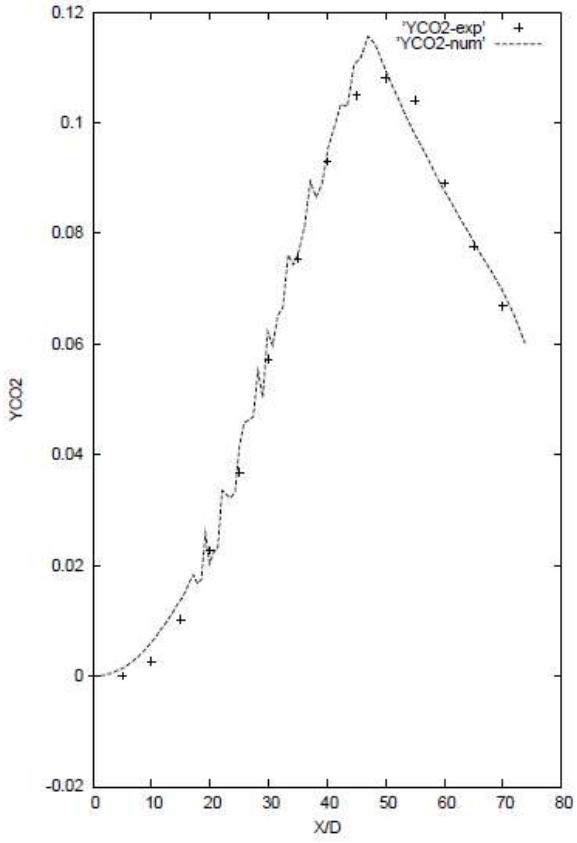


Figure 4. Comparison with experimental data (BARLOW & FRANK, 2003) for the temperature (top) and fuel CH_4 (below) mass fractions along the burner centerline.



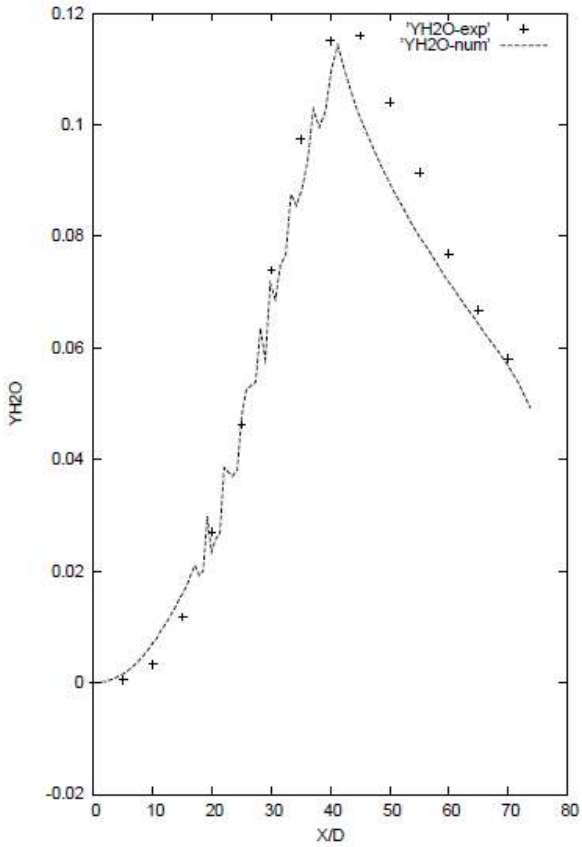


Figure 5. Comparison of the CO_2 (top) and H_2O (below) mass fraction profiles along the burner centerline with experimental data (BARLOW & FRANK, 2003).

6. Conclusion and Perspectives

6.1 Conclusions

In this work we have obtained the model for the solution of jet diffusion flames and we have indicated the corresponding proof of existence of solutions for the Lagragian and Eulerian flamelet model equations, based on the Faedo-Galerkin method. In addition, we showed some numerical results for a turbulent piloted methane-air diffusion flame, the Sandia Flame D (LORENZZETTI *et al.*, submitted to *The 3rd Southern Conference on Computational Modeling*).

The LES results for the nonpremixed reacting flow, for Sandia Flame D, compare well with the available data found in the literature. The method, based on the low Mach number with a density relaxation, helps to obtain good results. We spend about 240 minutes to obtain the results in an Acer Aspire 5570-2792 Intel Pentium dual-core notebook of 1.60 Ghz and 1MB L2 cache.

The authors show that the appropriate choose of the mathematical model helps the development of proofs for the existence of solutions for diffusion flames. Such and the comparison of numerical and experimental values with experimental data correspond to the main contributions of the present paper.

6.2 Perspectives

Before obtaining the solutions for piloted methanol and ethanol diffusion flames, we intend to solve for a higher Reynolds jet.

The incompressible two-dimensional Navier-Stokes equations in the Cartesian coordinate system (x, y) can be expressed in conservative form (GOKARN *et al.*, 2006) as

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}=\frac{\partial E_v}{\partial x}+\frac{\partial F_v}{\partial y}, \tag{30}$$

where $Q=\begin{pmatrix}0\\u\\v\\Z\end{pmatrix}$, $E=\begin{pmatrix}u\\u^2+p\\uv\\uZ\end{pmatrix}$, $F=\begin{pmatrix}v\\vu\\v^2+p\\vZ\end{pmatrix}$,

$E_v=\begin{pmatrix}0\\\nu\,\partial u/\partial x\\\nu\,\partial v/\partial x\\D\,\partial Z/\partial x\end{pmatrix}$, $F_v=\begin{pmatrix}0\\\nu\,\partial u/\partial y\\\nu\,\partial v/\partial y\\D\,\partial Z/\partial y\end{pmatrix}$.

Here, Q is the vector of unknown variables. The velocity field corresponds to the stream-wise velocity u and cross-stream velocity v. The pressure field is modified to account for the density of a fluid with kinematic viscosity. To couple the equations, the vector Q can be modified, allowing the use of preconditioning techniques which have shown to improve the convergence for time-marching methods. In this way we write

$$Q_v=(p,u,v,Z)^T, \tag{31}$$

which is incorporated in Eq. (30) using the chain rule. The new equations can be conveniently solved for steady-state solutions using preconditioning techniques. The system turns

$$\Gamma_p\frac{\partial Q_v}{\partial \tau}+\Gamma\frac{\partial Q_v}{\partial t}+\frac{\partial(E-E_v)}{\partial x}+\frac{\partial(F-F_v)}{\partial y}=0 \tag{32}$$

where $\Gamma_p=\begin{pmatrix}1/\beta & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 1\end{pmatrix}$, β is the artificial compressibility parameter, t is the physical time and τ is the pseudotime.

The set of equations (32) is discretized using a second order finite difference scheme for the physical time, an integrated using a second order Runge-Kutta method for the pseudotime, and second order explicit finite difference scheme for all spatial terms.

Based on this model we intend to find solutions like the one showed in Fig. 5, where u_i is the central stream velocity and u_0 is the outer stream velocity. After solving this flow we intend to introduce the chemical model in order to obtain the solution of diffusion flames of methane, methanol and ethanol (LORENZZETTI *et al.*, work in progress), as a natural sequence to understend the ethanol nonpremixed combustion.

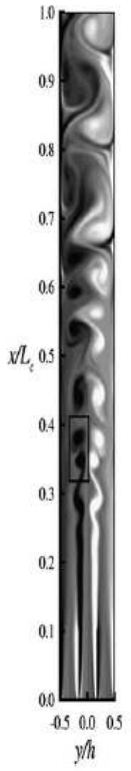


Figure 5. Instantaneous spanwise vorticity contours of the shear layer evolution for $u_i/u_0 = 3$ at $t = 40s$ (GOKARN *et al.*; 2006).

7. Acknowledgements

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