

# ANALYTICAL/NUMERICAL SOLUTION FOR CONFINED JET DIFFUSION FLAME (SANDIA FLAME C)

A. L. DE BORTOLI<sup>†‡</sup>

<sup>†</sup>Graduate Program in Applied Mathematics, PPGMAp-UFRGS, Porto Alegre, P.O. Box 15080, Brazil  
dbortoli@mat.ufrgs.br

<sup>‡</sup>Graduate Program in Chemical Engineering, PPGEQ-UFRGS, Porto Alegre, Brazil

**Abstract**— The aim of the present work is the development of a method based on the momentum transfer law to obtain the solution of confined jet diffusion flames. The Reichardt's equation is used to approximate the flow/mixture fraction and it is discretized based on the second order finite difference technique. All thermochemical variables are determined by the mixture fraction as the Sandia Flame C, used to check the results, is close to equilibrium. The semi-analytical/numerical results compare reasonably with the experimental data indicating that the method contributes to solve some jet flames at low cost.

**Keywords**— Piloted diffusion flame, Flame C, Low Mach-number, Semi-analytical solution, Mixture fraction

## I. INTRODUCTION

A jet diffusion flame is an important example in non-premixed combustion, since the fuel and the oxidizer enter the chamber in separate streams. Combustion corresponds to a complex sequence of chemical reactions between a fuel and an oxidizer releasing heat and sometimes producing light too. Combustion is usually fast compared to molecular mixing, happening in layers thinner than the typical length scales of turbulence (Peters, 2000).

The length scale disparity in turbulent combustion inside a burner, for example, is very large: the burner has lengths of order  $1m$ , the containing energy eddies have diameters of order  $1 - 10cm$ , the small-scale mixing eddies are of order  $1 - 10mm$ , the flame thickness has dimensions which varies between  $10 - 100\mu m$ , and the molecular iterations characteristic lengths are very small, ranging from  $1 - 10nm$ .

Moreover, the time-scale disparity is also very large (Poinsot and Veynante, 2005) and, at least theoretically, all scales must be well predicted to obtain an adequate mathematical solution of a jet diffusion flame. Due to the exothermicity of combustion reactions, the temperature raises since the chemical reactions become faster, then the length scale is short.

Jets and jet flames seem to be simple; however, their structure is complex because a jet usually starts with a potential zone of 2 to 10 diameters length and ends with a turbulent plume which is very difficult to be simulated by the conventional numerical techniques, including RANS (Reynolds Averaged Navier-Stokes) and LES (Large-Eddy Simulation). The majority of jet and jet flame simulations found in the literature reveals a turbulent structure which is much coarser than that seen in the experiments.

To solve nonpremixed flames many approximate models are found in the literature (Williams, 1985; Liñán, 1991; Peters, 2000; Warnatz et al., 2001; Veynante and Vervisch, 2003; Fernández-Tarrazo *et al.*, 2006). A two-layer flame structure considers a very thin fuel consumption layer and a much thicker oxidation layer, hypothesis valid for stoichiometric and lean conditions and for moderately rich flames. Some models employ a formulation based on the mixture fraction for the flow and on the flamelet models for the chemistry. The basic idea of the flamelet modeling is that an instantaneous flame element embedded in a turbulent flow has a structure of a laminar flame (Peters, 2000). The flamelet equations correspond to a balance between the unsteady changes, the diffusive effects and the chemical reactions. Then the species mass fraction  $Y_i$  depend on the mixture fraction, on the scalar dissipation rate and on the time.

The initially chemical elements contained in the fuel are conserved during combustion; they can be calculated by the mixture fraction (Bilger, 1980; Law, 2006), a conserved scalar. The element mass fractions are not changed by reactive processes, they are changed by mixing and such is governed by diffusion. The mixture fraction axial decrease in a flame is similar to that of velocity decrease (Kuo, 2005); such velocity decrease depends on the mixing, which indicates the turbulent flow evolution.

The scalar dissipation rate turns an important quantity when analyzing turbulent combustion using flamelets (Peters, 2000). It can be seen as a diffusion coefficient acting on an infinitely fast chemistry model. For jet flames its mean value is of order  $10^0$ , and it may oscillate considerably.

When the burner dimensions are much bigger than that of 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; it is more important in furnaces, spreading of buildings and forest fires (Law, 2006).

The present work develops an analytical/numerical method to approximate the solution of confined jet diffusion flames. The method is based on the solution of the diffusion Reichardt's equation, discretized by the finite difference technique.

## II. MODEL FORMULATION AND SOLUTION PROCEDURE

In a jet diffusion flame the jet is injected usually from a tube with diameter  $d$  and the pilot, used to stabilize the flame, has a diameter  $D$ , as shown in Fig. 1. Inside a burner the Mach is normally low, the pressure remains almost constant and the heat losses to the walls are small (Poinso and Veynante, 2005).

The complete set of governing equations includes the momentum (Navier-Stokes), mixture fraction, enthalpy, species mass fraction and state. Favre filtering, or density weighted Favre filtering, turns convenient when writing the governing equations. It helps to avoid terms such as  $\rho'u'$  that comes from the time-averaging method. The set of governing equations in nondimensionalized form can be derived by applying a spatial, density-weighted filter, resulting (De Bortoli, 2008) for:

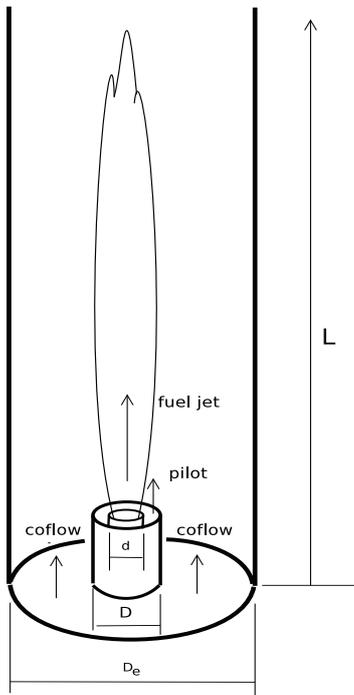


Figure 1: Cylindrical burner sketch

Momentum/ Navier-Stokes, mixture fraction, and enthalpy, respectively

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{1}{M^2} \frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \frac{\bar{\mu}_T}{R_e} \tilde{\tau}_{ij} \right) \quad (1)$$

$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\bar{\mu}_T}{S_c} \frac{\partial\tilde{Z}}{\partial x_j} \right) \quad (2)$$

$$\frac{\partial(\bar{\rho}\tilde{h})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{h})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\bar{\mu}_T}{P_r} \frac{\partial\tilde{h}}{\partial x_j} \right) \quad (3)$$

Species and mean species mass fraction, respectively

$$\frac{\partial Y_i}{\partial \tau} - \frac{a\chi}{2Le} \frac{\partial^2 Y_i}{\partial Z^2} = D_a Y_F Y_O e^{-\frac{Z_e(1-\theta)}{1-\alpha(1-\theta)}} \quad (4)$$

$$\tilde{Y}_i(x_j, t) = \int_0^1 Y_i(Z, t) \tilde{P}(Z; x_j, t) dZ \quad (5)$$

where  $\tilde{u}$  is the velocity,  $\bar{\rho}$  the density,  $t$  the time,  $\bar{p}$  the pressure,  $\tilde{\tau}$  the stress tensor,  $\tilde{Z}$  the mixture fraction,  $\tilde{h}$  the enthalpy, and  $\tilde{Y}_i$  the mass fractions:  $Y_F$  for the fuel and  $Y_O$  for the oxidizer.  $\chi$  is the scalar dissipation rate and  $\tau$  the nondimensional time.

In these equations  $R_e = u_0 d / \eta$  is the Reynolds,  $S_c = \frac{\eta}{D_i} = 0.7$  (where  $\eta$  is the kinematic viscosity and  $D_i$  the diffusivity of each specie) the Schmidt,  $P_r = \frac{\eta}{D_T} = 0.7$  (where  $D_T$  is the thermal diffusivity) the Prandtl,  $D_a = \frac{AaY_O(1-\alpha)\rho_{st}e^{-Z_e/\alpha}}{\chi_{st}W_{O_2}(1-\alpha)(1-\theta)} \sim 1000$  the Damköhler,  $L_e = \frac{S_c}{P_r} = 1$  the Lewis and  $Z_e = \frac{E(T_b - T_u)}{RT_b^2} \sim 10$  the Zel'dovich numbers;  $\alpha = \frac{T_b - T_u}{T_b} \sim 0.8$  and  $\theta = \frac{T - T_u}{T_b - T_u}$  (Steiner and Bushe, 1998).  $u_0$  is the velocity,  $E$  the activation energy,  $A$  the pre-exponential coefficient,  $T_u$  and  $T_b$  the unburnt and burnt temperatures, respectively,  $W_F$  the molecular weight of the fuel and  $W_{O_2}$  of the oxidizer,  $\chi_{st}$  the scalar dissipation rate and  $\rho_{st}$  the density at stoichiometric condition.  $a = 2\Delta Z Z_{st}(1 - Z_{st})$  appears after the nondimensionalization of the species mass fraction equation and  $Z_{st} = \frac{Y_{O_{2,2}}}{\frac{\mu_{O_2} W_{O_2}}{\mu_F W_F} Y_{F_1} + Y_{O_{2,2}}}$  is the mixture fraction at stoichiometric condition, where  $\mu_F$ ,  $\mu_{O_2}$  are the reaction coefficients and  $Y_{F_1}$  and  $Y_{O_{2,2}}$  correspond to the initial mass fraction quantities of fuel and oxidizer, respectively.

The temperature can be obtained from the enthalpy through a simple Newton iteration  $\tilde{h} = \sum_{i=1}^n \tilde{Y}_i h_i(\tilde{T})$ . The reaction rate, in nondimensional form, can be approximated by  $\dot{w} \sim D_a Y_F Y_O e^{-\frac{Z_e(1-\theta)}{1-\alpha(1-\theta)}}$  (De Bortoli, 2008).

The exponential source term, of the Arrhenius type approximation, depends strongly on the temperature which modifies considerably the density, affecting the stability of a numerical procedure. At low Mach numbers the spatial variations in pressure are small compared with the pressure itself and may be neglected in the equation of state, where  $p$  may be approximated by a constant (Liñán, 1991) when obtaining the density.

Instead of solving the set of equations (1-5), one solves a simplified momentum equation. Reichardt discovered that the velocity profiles under consideration can be approximated successfully by a Gauss function, or by its integral, the error function (Schlichting and Kestin, 1968). In two-dimensional frictionless flow the momentum equation is given by

$$\frac{\partial}{\partial x} \left( \frac{\bar{p}}{\rho} + (\bar{u})^2 \right) + \frac{\partial}{\partial y} (\bar{u}\bar{v}) = 0 \quad (6)$$

Reichardt made the assumption that  $\bar{u}\bar{v} = -\lambda(x) \frac{\partial \bar{u}^2}{\partial y}$ ,  $\lambda(x)$  is the momentum transfer length, which states that the flux of the x-component of momentum is proportional to the transverse gradient of momentum. Eliminating  $\bar{u}\bar{v}$  and with the assumption of constant pressure one obtains the Reichardt's fundamental equation

$$\frac{\partial \bar{u}^2}{\partial x} = \lambda(x) \frac{\partial^2 \bar{u}^2}{\partial y^2} \quad (7)$$

In this way, the distribution of momentum in free turbulent flow is governed by a generalized heat conduction equation type. The distribution of momentum can be approximated by

$$\bar{u}^2 = c_1 + \frac{c_2}{b} \exp \left[ - \left( \frac{y}{b} \right)^2 \right] \quad (8)$$

where  $c_1$  and  $c_2$  are constants and  $b$  is the half jet diameter, which depends on the axial distance from the jet origin. Then, to satisfy the Eq. (7), the momentum transfer length must be equal to  $\lambda(x) = \frac{b}{2} \frac{db}{dx}$ .

As for jet diffusion flames almost in equilibrium the jet is governed essentially by mixing, one proposes to employ here the Reichardt's equation in axisymmetric coordinates with  $\lambda$  depending on  $x$  as well as on  $r$ ;  $\lambda(x, r)$ , resulting

$$\frac{1}{\lambda(x, r)} \frac{\partial \bar{u}^2}{\partial x} = \frac{\partial^2 \bar{u}^2}{\partial r^2} + \frac{1}{r} \frac{\partial \bar{u}^2}{\partial r} \quad (9)$$

Such equation admits a solution of the following form

$$\bar{u}^2 = u_0^2 e^{-c_1 b^q} e^{-c_2 (r/b)^2} \quad (10)$$

To satisfy the Eq. (9), the momentum transfer length needs to be equal to  $\lambda(x, r) = \frac{b}{2} \frac{db}{dx} \frac{[c_2 (\frac{r}{b})^2 - \frac{c_1}{2} q b^q]}{c_2 [1 - c_2 (\frac{r}{b})^2]}$ . The constants  $c_1$  and  $c_2$  can be determined considering that  $\bar{u} = u_0$  for  $x = 0$ ,  $r = 0$  and  $\bar{u} \sim 0.1u_0$  for  $r = 0$ ,  $x \sim 70d_0$ , where  $d_0$  is the fuel jet diameter.

The mixture fraction is assumed to be equal to the velocity obtained from Eq. (9) because one considers the existence of two jet invariants (Kuo, 2005):

- conservation of momentum  $I_u = \int_0^\infty u^2 r dr = \frac{1}{\eta} (u_0^2 r_0^2 / 2)$

- conservation of mass of fuel specie  $I_Z = \int_0^\infty u Z r dr = \frac{1}{\eta} (u_0 r_0^2 / 2)$

Moreover, the relation  $\frac{Z \cdot x}{I_Z} = \frac{U \cdot x}{I_u}$ , results in  $Z = U$  for  $u_0 = 1$ .

All thermochemical variables are determined by the mixture fraction since the Sandia Flame C is close to equilibrium. Consider a one-step global reaction given by  $\mu_F [C_m H_n] + \mu_{O_2} [O_2] \rightarrow \mu_{CO_2} [CO_2] + \mu_{H_2O} [H_2O]$

if  $Y_{O_2} = 0$ , then (Peters, 2000)

$$Y_F = Y_{F_1} (Z - Z_{st}) / (1 - Z_{st}) \quad (11)$$

$$T = T_0 + Q Y_{O_2,2} (1 - Z) / (C_{pO_2} \mu_{O_2} W_{O_2}) \quad (12)$$

and if  $Y_F = 0$ , then

$$Y_{O_2} = Y_{O_2,2} (1 - Z / Z_{st}) \quad (13)$$

$$T = T_0 + Q Y_{F_1} Z / (C_{pF} \mu_F W_F) \quad (14)$$

where  $Q$  is the heat release,  $T_0$  the mixing temperature (without combustion) and  $C_p$  the specific heat. As the elements mass fraction does not change during combustion (are conserved) one can obtain the burned quantities for:

-  $Z \leq Z_{st}$

$$Y_{CO_2,b} = m W_{CO_2} Y_{F,1} Z / W_F \quad (15)$$

$$Y_{H_2O,b} = n W_{H_2O} Y_{F,1} Z / W_F \quad (16)$$

-  $Z \geq Z_{st}$

$$Y_{CO_2,b} = m \frac{W_{CO_2}}{W_F} Y_{F,1} Z_{st} \frac{1 - Z}{1 - Z_{st}} \quad (17)$$

$$Y_{H_2O,b} = n \frac{W_{H_2O}}{2W_F} Y_{F,1} Z_{st} \frac{1 - Z}{1 - Z_{st}} \quad (18)$$

where  $W_*$  are the corresponding molecular weights.

Observe that the solution (10) corresponds to a general/possible form of the analytical solution of Eq. (9), where  $b$ , the half of the jet diameter, depends on  $x$  at some exponent  $q$ .

### III. RESULTS

The jet flame was chosen because it seems to be representative of the class of nonpremixed flames. A burner commonly employed in practice consists in surrounding a high velocity jet of gas fuel with an annular pilot flame. Here, one employs a duct of cylindrical cross section with diameter  $D_e = 1$  and the fuel is injected from a tube of diameter  $d$ . The Sandia Flame C ( $R_e = 13400$ ) is used to compare the results; it 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 (Barlow and Frank, 2003). The domain spans a region of  $110D \times 10D$  in the axial and the radial directions, respectively. One employs a uniform mesh containing  $300 \times 100$  points. In the following, some results for flame C are compared with the corresponding experimental data (Barlow and Frank, 2003). The velocity/mixture fraction result shown in Fig. 2 indicates the axial decreasing behavior, since

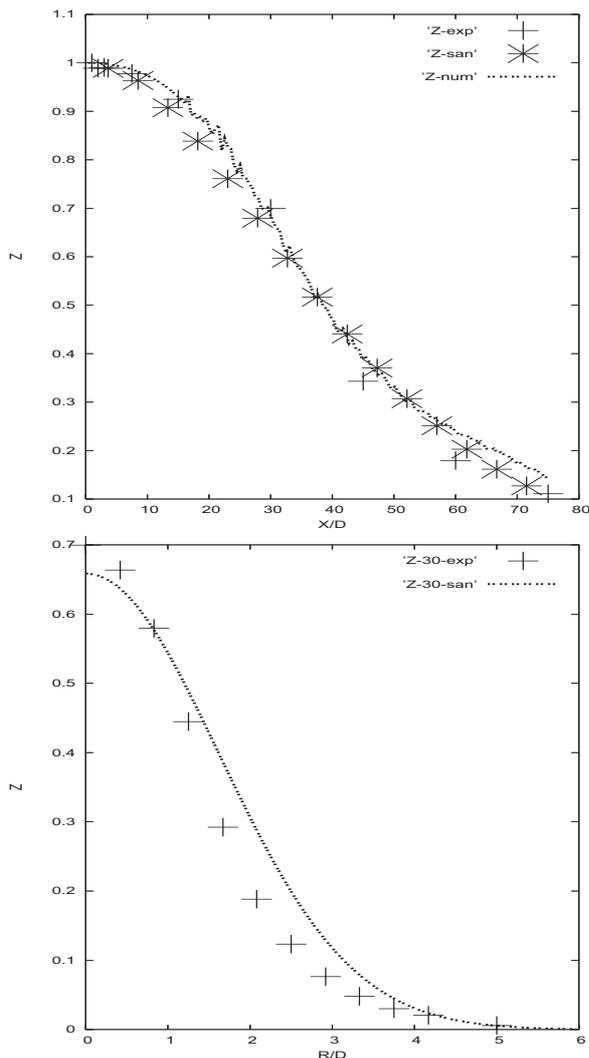


Figure 2: Comparison of the axial and radial (at  $X/D = 30$ ) mixture fraction profiles for flame C with experimental data (Barlow and Frank, 2003)

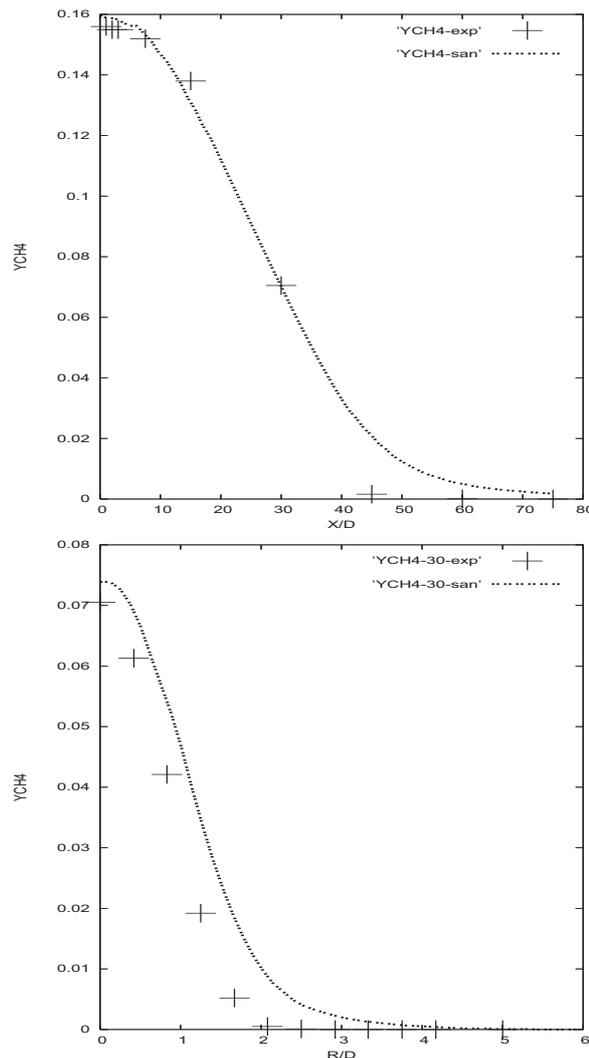


Figure 3: Comparison of the axial and radial (at  $X/D = 30$ ) fuel  $CH_4$  mass fraction profiles for flame C with experimental data (Barlow and Frank, 2003)

this flame is governed by hydrodynamics. The reaction occurs at a very thin zone, not affecting the mean flow. The radial velocity distribution can be reasonably approximated by a Gaussian function. If we solve the LES set of equations (1-5) the mixture fraction is better predicted for  $X/D$  between 10–30, as shown in Fig. 2 for a mesh containing  $199 \times 41 \times 41$  cells; however, its cost is at least  $10^2$  times the cost for solving the Eq. (9).

Based on the Burke-Schumann analytic solution (Peters, 2000; Poinso and Veynante, 2005), the fuel mass fraction is reasonably well predicted, as shown in Fig. 3; the oxidizer mass fraction is well predicted, but it tends to dissipate a little in the radial direction for high  $R/D$ , as shown in Fig. 4.

Figure 5 shows the temperature profile along the flame centerline. The temperature increases consid-

erably at  $X/D \sim 45$ , at reaction zone, and decreases after it due to the thermal expansion. The corresponding radial profile indicates that the flame can be reasonably approximated using a Gaussian function, as by Reichardt suggested. The temperature distribution can also be represented in terms of the velocity distribution (Schlichting and Kestin, 1968).

Finally, Fig. 6 shows the radial mass fraction of the product  $CO_2$  at  $X/D = 45$  and 60. Both profiles compare reasonably with the corresponding experimental data. Although the use of only one equation, Eq. (9), the flame spreading seems to be adequately captured with an enormous decrease of the computational time compared to that needed to solve the set of equations (1-5).

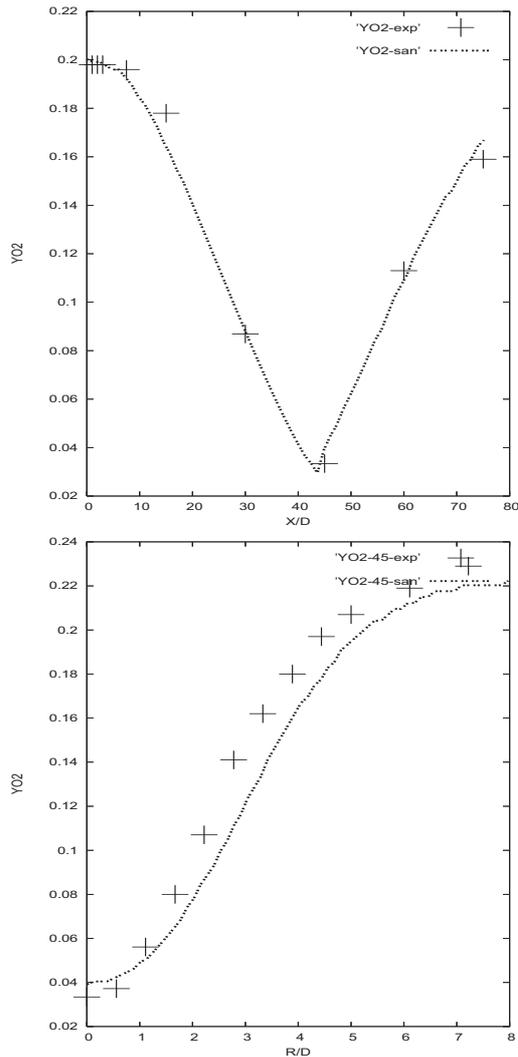


Figure 4: Comparison of the axial and radial (at  $X/D = 45$ ) oxidizer profiles for flame C with experimental data (Barlow and Frank, 2003)

#### IV. CONCLUSIONS

The present work developed an analytical/numerical method for the solution of a piloted jet diffusion flame. The numerical solution of the Reichard's equation is based on the corresponding analytical solution with  $\lambda$  in equation (9) depending on  $x$  as well as on  $r$ .

Many numerical works found in the literature employ more than one million points to obtain reasonable results for jet diffusion flames. Here, the analytical/numerical solution is cheaply obtained (less than 1 min in an Intel Acer Aspire 5570-2792 Dual Core Notebook). One observes that the appropriate model simplification results in a mathematical equation, based on the momentum transfer law, whose solution reduces the time needed when solving some confined jet diffusion flames.

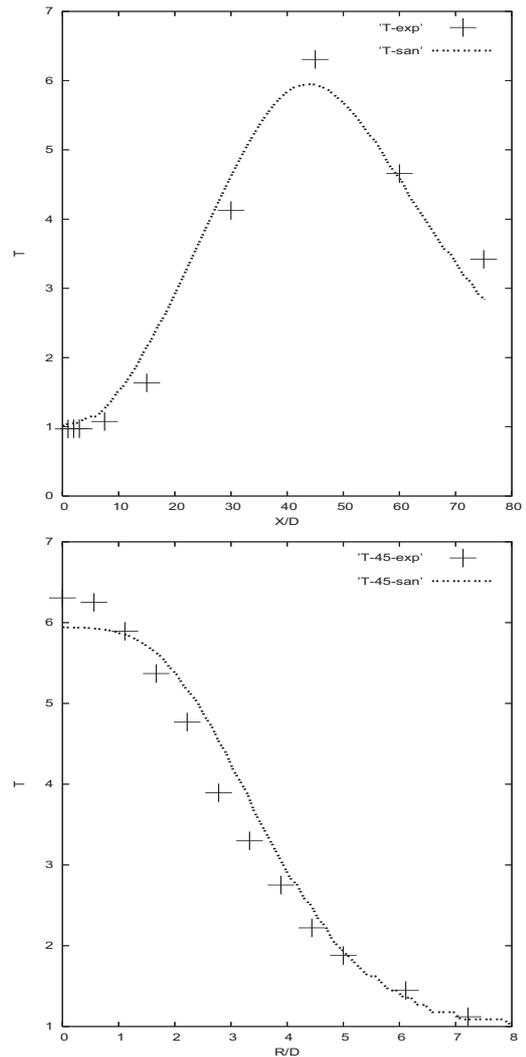


Figure 5: Comparison of the axial and radial (at  $X/D = 45$ ) temperature profiles for flame C with experimental data (Barlow and Frank, 2003)

#### V. ACKNOWLEDGEMENTS

This research is being developed at UFRGS, Federal University of Rio Grande do Sul, under the sponsorship of CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico); process 304600/2006-7. The author gratefully acknowledges the financial support from CNPq.

#### REFERENCES

- Barlow, R. and J. Frank, *Piloted CH<sub>4</sub>/Air Flames C, D, E and F*, Release 2.0, [www.ca.sandia.gov/TNF](http://www.ca.sandia.gov/TNF) (2003).
- Bilger, R.W., "Turbulent Flows with Nonpremixed Reactants in Turbulent Reacting Flows," in *Device and Materials Modeling in PEM Fuel Cells*, Eds. P.A. Libby and F.A. Williams, Springer-Verlag, 65-113 (1980).

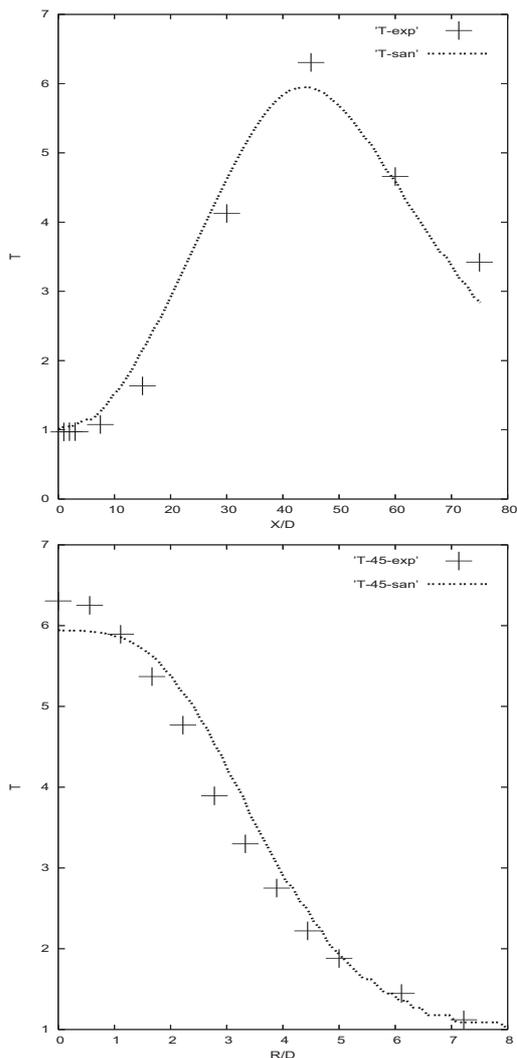


Figure 6: Comparison of the axial and radial (at  $X/D = 45$ ) temperature profiles for flame C with experimental data (Barlow and Frank, 2003)

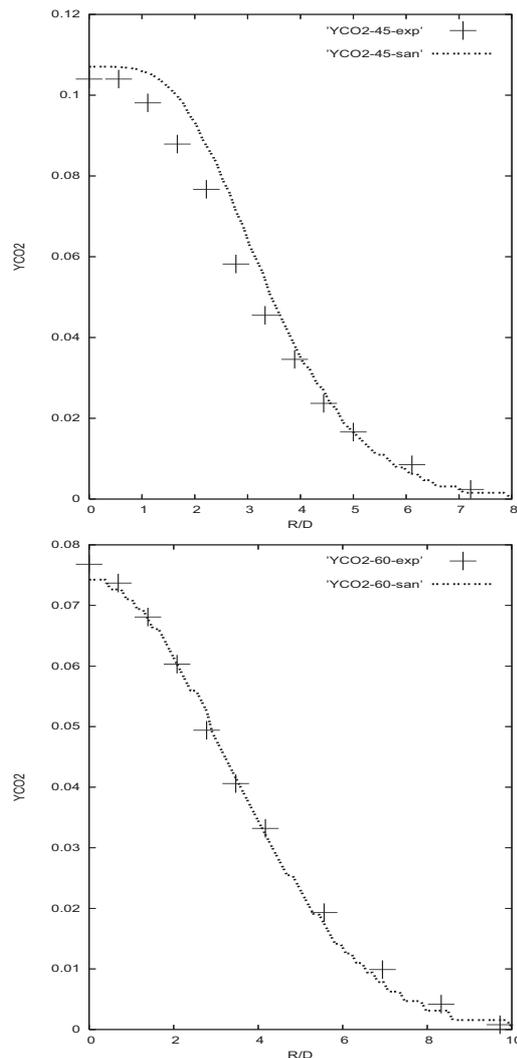


Figure 7: Comparison of the radial  $CO_2$  mass fraction at  $X/D = 45$  and at  $X/D = 60$  profiles for flame C with experimental data (barlow and Frank, 2003)

De Bortoli, A.L., “Large Eddy Simulation of a Confined Jet Diffusion Flame Using a Finite Difference Method,” *Progress in Computational Fluid Dynamics*, **8**, 379-383 (2008).

Fernández-Tarrazo, E., A.L. Sánchez, A. Liñán and F.A. Williams, F.A., “A Simple One-Step Chemistry Model for Partially Premixed Hydrocarbon Combustion,” *Combustion and Flame*, **147**, 32-38 (2006).

Kuo, K.K., *Principles of Combustion*, John Wiley & Sons (2005).

Law, C.K., *Combustion Physics*, Cambridge University Press (2006).

Liñán, A., “The Structure of Diffusion Flames,” *Fluid Dynamical Aspects of Combustion Theory*, Long-

man Scientific and Technical, United Kingdom (1991).

Peters, N., *Turbulent Combustion*, Cambridge University Press (2000).

Poinsot, T. and D. Veynante, *Theoretical and Numerical Combustion*, 2<sup>nd</sup> Edition, Edwards (2005).

Schlichting, H. and J. Kestin, *Boundary Layer Theory*, McGraw-Hill (1968).

Steiner, H. and W.K. Bushe, “LES of Nonpremixed Turbulent Reacting Flows with Conditional Source Term Estimation,” *CTR - Annual Research Briefs*, 23-34 (1998).

Veynante, D. and L. Vervisch, “Turbulent Combustion Modeling,” *Lecture Series du Von Karman Institute* (2003).

Warnatz, J., U. Maas and R.W. Dibble, *Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation*, 3<sup>rd</sup> Edition, Springer-Verlag (2001).

Williams, F.A, *Combustion Theory*, 2<sup>nd</sup> Edition, Addison-Wesley, Redwood City, CA (1985).

Received: June 2, 2008

Accepted: September 25, 2008

Recommended by Subject Editor: Eduardo Dvorkin