# Analytical, Numerical and Experimental Results for Piloted Jet Diffusion Flame (Sandia Flame D)

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**Abstract:** The aim of this work is to obtain and compare analytical/numerical results with experimental data for a confined jet diffusion flame. All thermochemical variables are determined by mixture fraction as the Sandia Flame D, used to check the results, is close to equilibrium. The developed method, based on the low Mach number formulation, allows to decrease the time needed to obtain reasonable results for confined jet diffusion flame. The analytical/numerical results compare reasonably with the experimental data indicating success obtaining the solutions.

keywords: Piloted diffusion flames, Sandia Flame D, Low Mach number, Flamelets.

# 1 Introduction

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 [10].

Many applications of technical interest in combustion are based on nonpremixed or diffusion flames. A jet diffusion flame is probably the most common configuration in nonpremixed combustion, since the fuel and the oxidizer enter the chamber in separate streams.

Turbulent nonpremixed flames are located where the fuel and the oxidizer meet; they are more sensitive to turbulence and stretch. In turbulent combustion only a thin region around the reacting zone is governed by molecular transport; the turbulent transport is dominant in the outer inert mixing region.

Combustion involves a large range of time and length scales; the length scales 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 the 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 [12] and, at least theoretically, all scales must be well predicted to obtain an adequate mathematical solution of a jet diffusion flame.

To solve nonpremixed flames many models are found in the literature [5], [8], [10], [13]. 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 instantaneos

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flame element embedded in a turbulent flow has a structure of a laminar flame [10]. The flamelet equations correspond to a balance between the unsteady changes, the diffusive effects and the chemical reaction. 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 [3] [7], 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 [6]; such velocity decrease depends on the mixing, which indicates the turbulent flow evolution.

## 2 Model formulation

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 Figure 1. Inside a burner the Mach is normally low, the pressure remains almost constant and the heat losses to the walls are small [12].

Simplified models, such as the flamelet model, are currently employed for the solution of non-premixed combustion situations of technical interest. The flamelet equations describe the balance between the unsteady changes, the diffusive effects and the chemical reactions. The flamelets require that the reaction zone be embedded within the smallest scales of turbulence. As the flame surface is assumed to be smallest than the Kolmogorov length scale, the region is locally laminar.

The definition of a conserved scalar, the mixture fraction, which relates the quantities of fuel and oxidizer, turns convenient when using the flamelet model. It measures the reactants mixing and is mainly related to the large scales of motion. For very fast chemistry, high Damköhler, the reaction can be approximated by a fast one-step reaction. But, the fast chemistry model can not account for any effect of turbulence in the chemistry, for extinction or ignition phenomena. In this way, consider the following one-step reaction for fuel  $C_m H_n = CH_4 = [F]$ .

$$\nu_F[F] + \nu_{O_2}[O_2] \Rightarrow \nu_{CO_2}[CO_2] + \nu_{H_2O}[H_2O] + heat$$
(1)

The mixture fraction is given by

$$Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}} \tag{2}$$

Here  $\nu = \frac{\nu_{O_2} W_{O_2}}{\nu_F W_F}$  is called the stoichiometric mass ratio where  $\nu_i$  is the stoichiometric coefficient of species i,  $Y_i$  the mass fraction of species i:  $Y_{O_2,2}$  the mass fraction of oxygen in the oxidizer stream,  $Y_{F,1}$  the mass fraction of fuel in the fuel stream and  $W_i$  the molecular weight of species i.

The stoichiometric mixture fraction  $Z_{st}$  happens when  $Y_{O_2} = \nu Y_F$ . If  $Z < Z_{st}$  fuel is deficient and the mixture is called lean. Then, combustion terminates when all fuel is consumed, in the burnt gas which is indicated by the subscript "b". The remaining oxygen mass fraction in the burnt gas and the temperature is [1] [10]

$$Y_{O_2,b} = Y_{O_2,2} \left( 1 - \frac{Z}{Z_{st}} \right)$$
(3)

$$T \simeq T_0 + (T_{ad} - T_0) \frac{Z}{Z_{st}}$$
 (4)

Similarly, if  $Z \ge Z_{st}$  oxygen is deficient and the mixture is called fuel rich. Combustion terminates when all oxygen is consumed,  $Y_{O_2} = 0$ , leading to

$$Y_{F,b} = Y_{F,1} \frac{(Z - Z_{st})}{(1 - Z_{st})}$$
(5)

$$T \simeq T_0 + (T_{ad} - T_0) \frac{(1 - Z)}{(1 - Z_{st})}$$
(6)

where  $T_{ad}$  is the adiabatic flame temperature and  $T_0$  the mixing temperature (without combustion). As the elements mass fraction does not change during combustion (are conserved) one can obtain the burned quantities for:

 $Z < Z_{st}$ 

$$Y_{CO_2} = m \frac{W_{CO_2}}{W_F} Y_{F,1} Z$$
(7)

$$Y_{H_2O} = n \frac{W_{H_2O}}{2W_F} Y_{F,1} Z$$
(8)

$$Z \ge Z_{st}$$

$$Y_{CO_2} = m \frac{W_{CO_2}}{W_F} Y_{F,1} Z_{st} \frac{1-Z}{1-Z_{st}}$$
(9)

$$Y_{H_2O} = n \frac{W_{H_2O}}{2W_F} Y_{F,1} Z_{st} \frac{1-Z}{1-Z_{st}}$$
(10)

The set of governing flamelet equations in nondimensionalized form results in:

$$\frac{\partial Y_i}{\partial \tau} - \frac{a\chi}{2L_e} \frac{\partial^2 Y_i}{\partial Z^2} = \pm \nu_F D_a Y_F Y_0 e^{-\frac{Z_e}{T}}$$
(11)

$$\frac{\partial T}{\partial \tau} - \frac{a\chi}{2} \frac{\partial^2 T}{\partial Z^2} = \nu_F H_e D_a Y_F Y_0 e^{-\frac{Z_e}{T}}$$
(12)

where the signal plus corresponds to producing species, and the less if they are consumed.

In these equation  $Y_F$  is mass fraction for the fuel and  $Y_O$  the mass fraction for the oxidizer,  $\tau$  the nondimensional time, T the temperature,  $Ze \sim 10^1$  the Zel'dovich number,  $D_a \sim 10^3$  the Damköler number,  $H_e \sim 10$  the heat released,  $\chi \sim 10^0$  the scalar dissipation rate,  $L_e = 1$  the Lewis number, and  $a = 2\Delta Z Z_{st}(1 - Z_{st})$  appears after the nondimensionalization of the species mass fraction equation, where  $\Delta Z = 1$  is the mixture fraction variation range. For  $L_e \neq 1$  the analysis turn more complex [11], what is left for a future work.

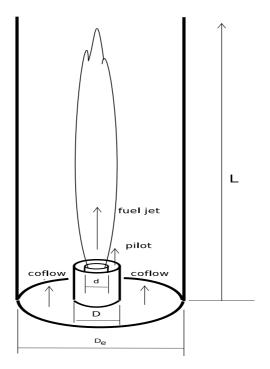


Figura 1: Burner sketch

The steady flamelet equations (for mass fraction and temperature) may be written as

$$A\frac{\partial^2 \psi}{\partial Z^2} + Be^{-Ze/T} = 0 \tag{13}$$

In order to find an analytical solution for Eq.(13) the exponential term  $e^{-Ze/T}$  is approximated as  $e^{-Ze\frac{T_{ad}-T}{T_{ad}}} \sim e^{-Ze\frac{T_{ad}-(c+kZ)}{T_{ad}}}$ , where for  $Z < Z_{st}$ ,  $c = T_0$  and  $k = \frac{T_{ad}-T_0}{Z_{st}}$  and for  $Z \ge Z_{st}$ ,  $c = T_0 + \frac{T_{ad}-T_0}{1-Z_{st}}$  and  $k = \frac{T_{ad}-T_0}{1-Z_{st}}$ . The analytical solution of Eq.(13) turns

$$\psi(Z) = -\frac{BT_{ad}^2}{AZe^2k^2}e^{-Ze\frac{T_{ad}-(c+kZ)}{T_{ad}}} + C_1Z + C_2$$
(14)

where for  $\psi(0) = 0$  and  $\psi(1) = 0$ , results

$$C_2 = \frac{BT_{ad}^2}{AZe^2k^2}e^{-Ze\frac{T_{ad}-c}{T_{ad}}}$$
(15)

$$C_1 = -C_2 + \frac{BT_{ad}^2}{AZe^2k^2}e^{-Ze\frac{T_{ad} - (c+k)}{T_{ad}}}$$
(16)

which can be used to compare the results in the mixture fraction space.

#### 3 Results

The jet flame was chosen because it seems to be representative of the class of nonpremixed flames. Consider that the burner shown in figure 1 has a duct of 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 lengths is L = 11. The Sandia Flame D (*Reynolds* = 23000) 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.

Figura 2 left presents the comparison between analytical and numerical solutions for the product  $CO_2$  mass fraction in the mixture fraction space. Figure 2 right shows the behavior of mixture fraction along the burner centerline compared to the experimental data [2]. The solution indicates the axial decreasing behaviour of the mixture fraction; the results are in good agreement. The line of the mixture fraction contains the error bars which indicate the upper and lower bounds of the experimental error. Such is also done for the  $H_2O$  mass fraction.

Figura 3 presents the comparison between the numerical and the experimental mass fraction of the product  $H_2O$  along the burner centerline with experimental data of [2]. Although the mean  $H_2O$  is underpredicted at stoichiometric region, it remains inside the experimental uncertainty. The good mixture fraction results, obtained from a Navier-Stokes equation type, conduct to good product results.

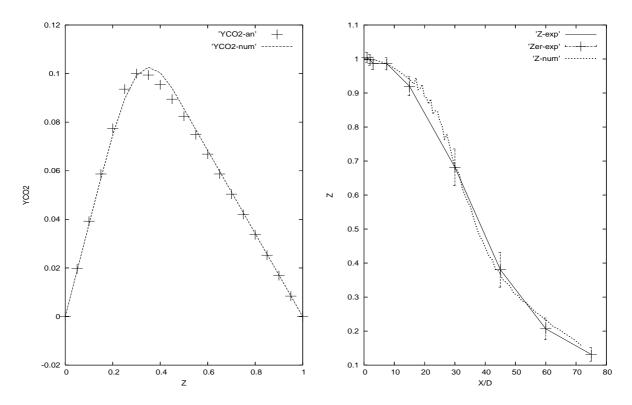


Figura 2: Analytical/numerical result for the product  $Y_{CO_2}$  mass fraction in the mixture fraction space (left) and the mixture fraction distribution (experimental and numerical) along the burner centerline (rigth); Zer corresponds to the error range of Z.

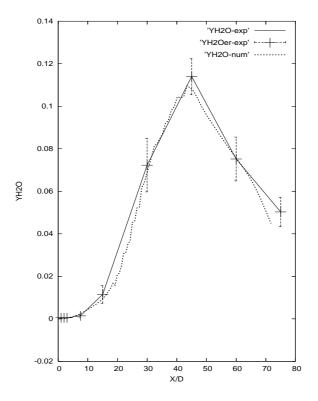


Figura 3: Product  $H_2O$  along the burner centerline; comparison with experimental data;  $YH_2Oer$  corresponds to the error range of the  $H_2O$  mass fraction.

## 4 Conclusions

In the present work we have compared analytical/numerical results with experimental data for a piloted jet diffusion flame. One observes that the appropriate model simplification results in a mathematical equation, which can be analytically treated. The numerical method was based on the flamelet equations for the chemistry and on the mixture fraction for the flow.

The analytical and numerical results for the non-premixed flow, for Sandia flame D, compare reasonably with the available experimental data found in the literature. The analytical solution ability to approximate a non-premixed jet flame corresponds to the main contribution of the present work.

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