# COMPARISON OF DIFFERENT WSGG APPROACHES IN NUMERICAL SIMULATION OF A NON-PREMIXED TURBULENT METHANE-AIR FLAME

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Abstract. The Steady Laminar Diffusion Flamelet (SLDF) and the Weighted-Sum-of-Gray-Gases (WSGG) models are employed to solve numerically the Flame DLR-A, a non-premixed turbulent methane flame surrounded by a lowvelocity air coflow, using ANSYS/Fluent code. The SLDF model allows for the separation of the interaction between chemical reactions and the flow field. Therefore, the laminar flamelet solutions can be pre-calculated and tabulated in a database, containing the mean reactive scalars, like temperature and species mass fractions, parameterized by few control variables, which in this study are the mixture fraction, its variance and dissipation rate. To generate the flamelet library, the turbulence-chemistry interaction is taken into account through presumed probability density functions (PDF) of these mean scalars. This approach efficiently reduces the computational time needed to achieve convergence of the solution. Radiation is taken into account through the WSGG model, in which the highly complex wavelength dependence of a non-gray gas is replaced by a small number of gray gases, for which the heat transfer rates are calculated independently. This study presents a comparison between Smith's classical (Fluent) and correlations based on the HITEMP2010 database for the WSGG model (UDF). The coupling between the new WSGG correlations and the numerical code is made by a user-defined function (UDF). The numerical results are compared to experimental measurements in order to show the agreement level between the correlations for the WSGG model and the experimental data. The results show reasonable agreement with the measurements for temperature and species mass fractions for both approaches. However for the radiative heat flux distribution, the WSGG/Fluent tends to overpredict the radiation absorption in comparison with the WSGG/UDF.

Keywords: flamelet, ANSYS/Fluent, Weighted-Sum-of-Gray-Gases, radiation

# **1. INTRODUCTION**

Due to security reasons, non-premixed flames are certainly the most found in practical applications, especially in industrial applications. Despite the theoretical complexity introduced by turbulence, its participation in conjunction with chemical reactions tends to be quite advantageous, taking into account that it benefits the mixture of reactants and heat transport. However, the numerical simulation of turbulent flames is still a challenge to computational fluid dynamics due to the presence of rapid and random fluctuations in flow properties such as velocity, temperature and density. It still remains one of the most challenging problems of classical physics yet, and the inclusion of chemical reactions, and radiation makes the solution for the problem even more complex. Because of these factors, a series of approaches aiming at reducing the computational time is required to obtain accurate results.

The flamelet concept is one of these alternatives to reduce the chemical kinetics. The flamelet model assumes that a multidimensional turbulent flame can be seen as an ensemble of quasi-unidimensional laminar flame structures, named flamelets. This approach allows for the decoupling of the chemical reactions and the turbulent flow field (Peters, 1984 and 1986). Each flamelet is subjected to local flow field conditions, resulting in their convection and stretching. Therefore, the local flame structure can be described only by local flow parameters, usually the mixture fraction and its scalar dissipation rate. The laminar flamelet structure can be pre-calculated and tabulated into a flamelet library, a databank containing the main reactive scalars, parameterized by a few number of control variables. Once the values of these parameters are known from the flow field, one can find the thermo-chemical quantities from the flamelet library. (Deon and Pereira, 2015).

The model has been applied to predict flow variables in many applications, both for laminar and turbulent flames (Lentini and Puri, 1995; Pitsch, 2000; Coelho and Peters, 2001; Claramunt, 2005; Odedra and Malalasekera, 2007; Lee and Choi, 2009; Ziani et al., 2013).

In order to solve the radiation the WSGG model is used. The WSGG model was first proposed by Hottel and Sarofim, 1967. The basic assumption is that the entire spectrum can be divided into a few gray gases with constant absorption coefficient plus one transparent window. Each gray gas covers a defined region of the spectrum that is not necessary continuous. The WSGG model was implemented by Bidi, Hosseini and Nobari, 2008, in order to verify the radiation effect on temperature and species concentrations fields in turbulent diffusive flames, revealing its important

influence. Bordbar et al., 2014, compared the model with the Line-by-line (LBL) benchmark solution in 1D and 3D test cases with defined temperature and participating species profiles. Dorigon et al., 2013, generated the correlations for concentrations of water vapor and carbon dioxide for partial pressure ratios of 2/1 and 1/1 using the HITEMP2010 spectral database, testing the WSGG solution against the LBL benchmark for a set of 1D test cases. Centeno et al., 2014, in a 2D axisymmetric turbulent methane/air flame investigated the turbulence-radiation interaction. In the present work the correlations obtained by Dorigon et al., 2013 are coupled with Fluent, by means of user-define-functions (UDF), to modify the treatment of radiation model.

The problem under investigation in this study concerns the use of the steady flamelet modeling approach in a nonpremixed turbulent flame of methane enriched with hydrogen and diluted with nitrogen, surrounded by a low-velocity air coflow, named Flame DLR-A, due to the laboratory which conducted it experimentally, the DLR Institute of Combustion Technology from Stuttgart (Bergmann, 1998). It can be found in several numerical approaches (Pitsch, 2000; Kim et al., 2005; Lee and Choi, 2009; Emami and Fard, 2012; Ziani et al., 2013). Results are compared to those obtained by measurements and other numerical simulations.

## 2. PROBLEM CHARACTERIZATION

A non-premixed turbulent flame of a mixture of methane (CH<sub>4</sub>), hydrogen (H<sub>2</sub>) and nitrogen (N<sub>2</sub>) surrounded by a low-velocity coflow of air (TNF Workshop, 1998) has been proposed by the DLR Institute of Combustion Technology from Stuttgart (Bergmann, 1998), and was subsequently conducted experimentally by two other laboratories, the Sandia National Laboratory from Livermore (Meier et al., 2000), and the Technisque Universität Darmstadt (Schneider et al., 2003).

In the experiments, it was used as fuel a mixture of 22.1% CH<sub>4</sub>, 33.2% H<sub>2</sub> and 44.7% N<sub>2</sub> (by volume), supplied by a vertical stainless steel tube with internal diameter, *D*, equal to 8 mm, with a thinned rim at the exit, and a 350 mm long straight cross-section prior to exit. Its bulk velocity, 42.15 m/s, corresponds to a Reynolds number equal to 15,200 based on internal diameter of the pipe. Its stoichiometric mixture fraction,  $Z_{st}$ , is equal to 0.167 and the adiabatic flame temperature,  $T_{ad}$ , to 2,130 K.

The air flow is provided by a forced-draft vertical wind tunnel, and has a velocity of 0.3 m/s. In the case of DLR Institute of Combustion Technology and Technisque Universität Darmstadt, dry air is discharged by a circular nozzle, with an internal diameter of 140 mm. In the case of Sandia National Laboratory experiments, air stream has 0.8% water vapor by volume and its outlet nozzle is square and 300 mm wide, with the fuel pipe centered on it. This difference between the air coflow suppliers, however, may not be significant, since its velocity is very low, being the room air the responsible for providing most of the oxidant needed by the flame.

Fuel and oxidant streams and the environment are maintained at the temperature of 292 K. Ambient pressure is reported to be 95.3 kPa on DLR Institute of Combustion Technology, and 99.0 kPa in the case of Sandia National Laboratory, and no information is available for Technisque Universität Darmstadt.

The present study adopted the original geometrical configuration and experimental conditions, i.e., as reported by DLR Institute of Combustion Technology.

#### **3. NUMERICAL MODELING**

#### 3.1 Flow modeling

The Reynolds-Averaged Navier-Stokes (RANS) equations for conservation of total mass and momentum flow was, assuming the Stokes hypothesis for a Newtonian fluid in steady-state was employed for solving the problem numerically,

$$\nabla \cdot (\overline{\rho} \ \widetilde{\boldsymbol{u}}) = 0 \tag{1}$$

$$\nabla \cdot (\overline{\rho} \ \widetilde{\boldsymbol{u}} \ \widetilde{\boldsymbol{u}}) = -\nabla \widetilde{p} + \nabla \cdot \left[ \mu \left( \nabla \widetilde{\boldsymbol{u}} + (\nabla \widetilde{\boldsymbol{u}})^T - \frac{2}{3} \nabla \widetilde{\boldsymbol{u}} \ \boldsymbol{I} \right) - \overline{\rho} \ \widetilde{\boldsymbol{u}'' \boldsymbol{u}''} \right] + \overline{\rho} \ \boldsymbol{g}$$
(2)

where  $\boldsymbol{u}$  is the flow velocity vector,  $\boldsymbol{\rho}$  is the mixture density,  $\boldsymbol{p}$  is the system pressure,  $\boldsymbol{g}$  is the gravity vector,  $\boldsymbol{\mu}$  is the dynamic molecular (or laminar) viscosity and  $\boldsymbol{I}$  is the identity matrix.

In Eq. (2) the Reynolds stresses term is closed following the Boussinesq hypothesis, i.e., assuming that the turbulent stresses can be treated in an analogous way to the stresses in laminar flows (Wilcox, 1998),

$$-\overline{\rho}\,\widetilde{\boldsymbol{u}^{\prime\prime}\boldsymbol{u}^{\prime\prime}} = \mu_t [\boldsymbol{\nabla}\widetilde{\boldsymbol{u}} + (\boldsymbol{\nabla}\widetilde{\boldsymbol{u}})^T] - \frac{2}{3}\overline{\rho}\,\widetilde{\boldsymbol{k}}\,\boldsymbol{I}$$
(3)

where  $\mu_t$  is the turbulent (or eddy) dynamic viscosity and k is the turbulence kinetic energy.

Modeling k and  $\mu_t$  depends on the turbulence closure model. In this study was employed the Standard k- $\varepsilon$  model, proposed by Launder and Spalding (1972), with a modified value for constant  $C_{\varepsilon 1}$ , which controls the generation of the turbulent kinetic energy dissipation rate, from 1.44 to 1.60, according to proposal made by Morse (1977) and Pope (1978).

#### 3.2 Steady laminar diffusion flamelet model

In non-premixed flames, combustion occurs in a thin layer in the vicinity of the surface of the stoichiometric mixture fraction. In general, non-premixed combustion is called to diffusive flamelets in counter-flow configuration, in which fuel and oxidant are injected one against the other through opposed axisymmetric nozzles. As the distance between the nozzles is decreased or increased the flow rate of the jets, the flame is deformed in order to compress it longitudinally and stretch it in the transverse direction, distancing it from the chemical equilibrium condition, until it is completely extinguished.

The equations that describe the flamelet structure in a counter-flow configuration is based on the mixture fraction, *Z*. If assumed that its local gradient is sufficiently high, and under certain simplifying assumptions, can be said that the fluid thermo-chemical state is related to it (Peters, 1984 and 1986). The mixture fraction depending on the fuel composition and the characteristics of the phenomenon that are aimed to be captured: the oxidizer stream is equal to 0 and the fuel equal to 1, and by presenting any monotonic behavior over the spatial resolution of the flamelet. For fuels composed by hydrocarbons it is usual to use the mixture fraction as defined by Bilger (1988)

$$Z = \frac{2(Y_c - Y_{c,2})/W_c + 0.5(Y_H - Y_{H,2})/W_H - (Y_o - Y_{o,2})/W_o}{2(Y_{c,1} - Y_{c,2})/W_c + 0.5(Y_{H,1} - Y_{H,2})/W_H - (Y_{o,1} - Y_{o,2})/W_o}$$
(4)

where  $Y_i$  and  $W_i$  are the mass fractions and atomic weights corresponding to atoms of carbon (C), hydrogen (H) and oxygen (O) present in the mixture. Sub-indices 1 and 2 refer to streams of pure fuel and oxidant, respectively.

In the steady laminar diffusion flamelet model species and energy equations are rewritten in the mixture fraction space, assuming unity Lewis number and using the Crocco-type coordinate transformation and a subsequent asymptotic analysis of the order of magnitude for individual terms, leading to

$$\frac{1}{2}\rho \chi \frac{\partial^2 Y_k}{\partial Z^2} + \dot{\omega}_k = 0 \quad for \quad k = 1, N_k - 1$$
(5)

$$\frac{1}{2}\rho \chi \frac{\partial^2 T}{\partial Z^2} - \frac{1}{c_p} \sum_{k=1}^{N_k} h_k \dot{\omega}_k + \frac{1}{2} \frac{\rho \chi}{c_p} \left( \frac{\partial c_p}{\partial Z} + \sum_{k=1}^{N_k} c_{p,k} \frac{\partial Y_k}{\partial Z} \right) \frac{\partial T}{\partial Z} = 0$$
(6)

where T is the temperature,  $\chi$  is the scalar dissipation rate,  $Y_k$  is the mass fraction of a species k,  $\dot{\omega}_k$  is its mass production rate,  $h_k$  is its specific enthalpy, and  $c_{p,k}$  and  $c_p$  are the  $k^{th}$  species specific heat and the mixture-averaged specific heat, respectively.

The scalar dissipation rate,  $\chi$ , is a parameter that quantifies the influence of multidimensional effects on the flow field. It has the dimension  $s^{-1}$ , and can be interpreted as a characteristic diffusion time of the flamelet. It is commonly obtained from asymptotic solutions. In this numerical code, it is employed the formulation from Kim and Williams (1997),

$$\chi = \frac{a_s}{4\pi} \frac{3(\sqrt{\rho_{\infty}/\rho} + 1)^2}{2\sqrt{\rho_{\infty}/\rho} + 1} exp\{-2[erfc^{-1}(2Z)]^2\}$$
(7)

where  $erfc^{-1}$  is the inverse of complementary error function,  $\rho_{\infty}$  is the density of the oxidant stream and  $a_s$  is the characteristic strain rate of the flamelet, used as boundary condition for solving the flamelet equations,

$$a_s = 0.5 \, V \, d^{-1} \tag{8}$$

where V is the relative velocity of the streams issuing from the fuel and oxidant jets and d is the distance between the jets nozzles. Thus, the scalar dissipation rate varies along the flamelet, and a characteristic value must be chosen to parameterize the results. In this study it is based on the position in which the mixture fraction is stoichiometric,  $\chi_{st}$ .

Defined the appropriate conditions for the problem, i.e., the boundary conditions for temperature, pressure and species mass fractions at the streams output of fuel and oxidant, the flamelet equations are solved for a wide range of  $\chi_{st}$ , which can be obtained by varying the strain rate parameter  $a_s$ , starting from low values, near the chemical

equilibrium condition,  $\chi_{st} \rightarrow 0$ , until the flame extinguishment. The solutions for species mass fractions and temperature are stored as functions of mixture fraction and stoichiometric scalar dissipation rate.

The influence of turbulent fluctuations on thermo-chemical quantities are taken into account by using a probability density function (PDF) and the beta-function distribution, first introduced on combustion literature by Janicka and Kollman (1979). Assuming statistical independence between the variables that comprise the PDF, can be computed the averaged values for temperature, mixture density and species mass fractions. These solutions are stored as functions of a few number of control variables, namely, the mean mixture fraction,  $\tilde{Z}$ , its variance,  $\tilde{Z''}$ , the mean stoichiometric scalar dissipation rate,  $\tilde{\chi}_{st}$ , and the mean system total enthalpy,  $\tilde{H}$ . The variances for  $\chi_{st}$  and H are not needed because the effect of their fluctuations over the thermo-chemical quantities mean values is commonly assumed negligible.

The averaged scalar dissipation rate is obtained through an algebraic equation, which is related to fluctuations of mixture fraction variance and flow turbulence scales, as follows

$$\widetilde{\chi_{st}} = C_{\chi} \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z^{\prime\prime 2}}$$
<sup>(9)</sup>

where  $C_{\chi}$  is a constant, equal to 2.

The system total enthalpy,  $\tilde{H}$ , in turn, is determined by a simplified expression for the balance of energy, as follows

$$\nabla \cdot \left(\overline{\rho} \ \widetilde{\boldsymbol{u}} \ \widetilde{H}\right) = \nabla \cdot \left(\frac{k_t}{c_p} \nabla \widetilde{H}\right) + \overline{S_H}$$
(10)

where  $S_H$  is a volumetric source term that accounts for the heat transfer to the walls or due to thermal radiation, and  $k_t$  is the turbulent thermal conductivity, that in the case of the Standard *k*- $\varepsilon$  turbulence model is usually given by

$$k_t = c_p \,\mu_t \, P r_t^{-1} \tag{11}$$

where  $Pr_t$  is the turbulent Prandtl number, which by default is equal to 0.85 for two-equation RANS models.

For mixture fraction two additional transport equations are needed for solving its mean and variance values.

$$\nabla \cdot \left(\overline{\rho} \ \widetilde{\boldsymbol{u}} \ \widetilde{\boldsymbol{Z}}\right) = \nabla \cdot \left(\frac{\mu + \mu_t}{Pr_t} \nabla \widetilde{\boldsymbol{Z}}\right)$$
(12)

$$\boldsymbol{\nabla} \cdot \left( \overline{\rho} \, \widetilde{\boldsymbol{u}} \, \widetilde{Z^{\prime\prime 2}} \right) = \boldsymbol{\nabla} \cdot \left( \frac{\mu + \mu_t}{P r_t} \boldsymbol{\nabla} \widetilde{Z^{\prime\prime 2}} \right) + C_g \, \mu_t \left( \boldsymbol{\nabla} \widetilde{Z} \right)^2 - C_d \, \overline{\rho} \, \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z^{\prime\prime 2}} \tag{13}$$

where  $C_q$  and  $C_d$  are constants, equal to 2.86 and 2.0, respectively.

The mass production rates,  $\dot{\omega}_k$ , were solved according to GRI-Mech 3.0 chemical reaction mechanism, which consists of 325 elementary chemical reactions and contains 53 species, with variable thermodynamic and transport properties for each chemical species.

#### 3.3 Numerical methods and convergence criteria

The simulations were performed by ANSYS Fluent, version 17.0.0, adopting second order for all spatial discretizations, and the SIMPLE scheme for pressure-velocity coupling. The convergence criteria for all the computed properties were established for residuals lower than  $1 \ 10^{-5}$ , except for the radiative transfer equation, for which were adopted residuals lower than  $1 \times 10^{-6}$ .

#### 4. RADIATION MODELING

#### 4.1 The weighted-sum-of-gray gases (WSGG) model

The WSGG model was first proposed by Hottel and Sarofim, 1967. Figure 1 shows a representation of the model, in which the medium is divided into a few number of partial gray gases with absorption coefficient  $k_{p,i}$ , and transparent windows.

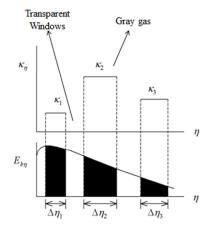


Figure 1. Representation of a medium composed of three gray gases.

An important assumption of the model is that the total emittance of a gas along a path S can be approximated by

$$\varepsilon(s) = \sum_{j=0}^{J} a_j(T) \left[ 1 - e^{-\kappa_{p,j} p S} \right]$$
(14)

where  $\kappa_{p,j}$  is the pressure absorption coefficient,  $a_j(T)$  the weighting factor and j is the number of gray gases (usually 3 or 4). The weighting factor represents, physically, the blackbody energy fraction that is emitted for each gray gas, and can be expressed as a polynomial function of temperature as (Smith et al., 1982)

$$a_i(T) = \sum_{k=1}^{J+1} b_{i,k} T^{k-1}$$
(15)

where  $b_{i,k}$  are the polynomial coefficients.

## 4.2 The weighted-sum-of-gray gases (WSGG) model, implemented by UDF

The implementation of the WSGG model in the code Fluent is made by user-defined-functions (UDF's). UDF's are small routines written on C programming language that can be coupled with Fluent in order to modify the models or change variables treatments. In the specific case of the WSGG, two UDF's were necessary: for the absorption coefficient and the medium emissivity weighting factor (Ansys, 2011).

In this case for an absorbing, non-scattering medium the spectral radiative transfer equation (RTE) is written with the discrete ordinates method as

(16) 
$$\frac{\partial I_{\eta}}{\partial S} = -\kappa_{\eta} I_{\eta} + \kappa_{\eta} I_{b\eta}$$

where  $I_{\eta}$  is the spectral intensity,  $I_{b\eta}$  the blackbody spectral intensity and  $\kappa_{\eta}$  is the spectral absorption coefficient. The negative term on the right side of Eq. (16) is the attenuation on the intensity by the medium absorption, while the positive term accounts for the increase in the intensity by the medium emission.

Was used in the UDF the correlations proposed by Dorigon et al., 2013, with the HITEMP2010 database, for mixtures of carbon dioxide and water vapor. Table 1 presents the coefficients for a gas mixture of  $H_2O$  and  $CO_2$  with a pressure ratio of 2/1, respectively.

Table 1. WSGG coefficients for four gray gases for an H<sub>2</sub>O /CO<sub>2</sub> mixture with partial pressures ratio of  $\frac{H_2O}{CO_2} = 2$ .

j	$\kappa_{p,j}(\mathrm{m}^{-1}\mathrm{atm}^{-1})$	$\begin{array}{c} b_{j,1} \\ \times \ 10^{-1} \end{array}$	$b_{j,2} \  imes 10^{-1}  ({ m K}^{-1})$	$b_{j,3} \times 10^{-2}  (\mathrm{K}^{-2})$	$b_{j,4} \  imes 10^{-3}  ({ m K}^{-3})$	$b_{j,2} \times 10^{-4}  ({ m K}^{-4})$
1	0.192	0.5617	7.8440	-8.5630	4.2460	-7.4400
2	1.719	1.4260	1.7950	-0.1077	-0.6972	1.7740
3	11.370	1.3620	2.5740	-3.7110	1.5750	-2.2670
4	111.016	1.2220	-0.2327	-0.7492	0.4275	-0.6608

Modest, 1991, demonstrated that the WSGG can be applied with any solution method of the RTE, which can be rewritten as

$$\frac{\partial I_j}{\partial S} = -\kappa_j I_j + \kappa_j a_j I_b \tag{17}$$

where  $\kappa_j$  is the absorption coefficient and  $I_j$  the radiation intensity of the gray gas *j*. For a mixture of carbon dioxide (CO<sub>2</sub>) and water vapor (H<sub>2</sub>O), the absorption coefficient is given by

$$\kappa_j = \kappa_{p,j} (Y_{CO_2} + Y_{H_2O}) p \tag{18}$$

in which  $Y_{CO_2}$  and  $Y_{H_2O}$  are the mole fractions and p the total pressure. With this expression the absorption coefficient is computed locally as a function of the mole fractions of the participating species, providing more accuracy in the solution.

#### 4.3 The weighted-sum-of-gray gases (WSGG) on Fluent

In the WSGG / Fluent, the heat fluxes due to radiation were computed also through the discrete ordinates method. The absorption coefficient of the gray gas is based on Smith *et al.*, 1982. However the Fluent considers the absorption coefficient the same in all bands.

### 5. MESH, FLAMELET LIBRARY AND DISCRETE ORDINATES METHOD REFINEMENT EVALUATION

The geometrical domain comprises, longitudinally, 40 cm prior to fuel jet and air coflow exit and more 200 cm since it, and 40 cm, radially, as shown in Fig. 1, together with the boundary conditions.



Figure 1. Geometrical domain and boundary conditions (Deon and Pereira, 2015).

In Deon and Pereira, 2015 results for independence with respect to the mesh refinement level is shown, the authors used a two-dimensional mesh composed by rectangular non-uniform size elements, with refinement concentrated at the region near the fuel jet. For each mesh tested the mean values for longitudinal velocity, mixture fraction and temperature along the axis were obtained. The mesh used in the present work is the same mesh used by Deon and Pereira, 2015 - a mesh with 25,031 elements.

Deon and Pereira, 2015 it was also evaluated the refinement level of the databank generated to store the chemical properties from the flamelet solutions. The authors generated four databanks, varying the amount of grid points for each controlling variable and was observed that the results dependence from the databank refinement level is practically undistinguishable. In the present study the same databank as Deon and Pereira, 2015 was used - with 86 grid points in  $\tilde{Z}$ , 34 in  $\tilde{Z}^{\prime\prime 2}$ , 130 in  $\chi_{st}$  and 35 in  $\tilde{H}$  to carry the computations.

An evaluation for the number of directions for the discrete ordinates method in the solution for radiative transfer equation (RTE) was developed. Several values of directions was tested. Sixty directions were initially tested, not showing satisfactory values for the radiative heat flux on the walls. The direction of number was gradually increased up to 250 directions that showed good results.

## 6. RESULTS AND DISCUSSION

The results for mean values are presented along the flow centerline. In the graphs are shown together the experimental measurements and the numerical results for both methods: WSGG/Fluent and WSGG/UDF for the mean temperature and mass fractions of  $CH_4$ ,  $CO_2$  and  $H_2O$ , since these parameters are the most relevant in the radiative heat transfer.

Figure 3 shows the results for the mean temperature and mean mixture fraction of  $CH_4$ ,  $CO_2$  and  $H_2O$ .

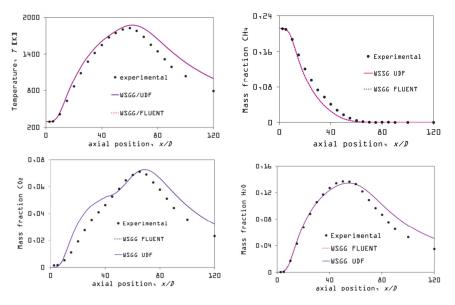


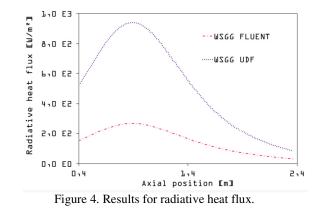
Figure 3. Results for mean temperature and mass fractions of species CH<sub>4</sub>, CO<sub>2</sub>, and H<sub>2</sub>O.

In general, the numerical results with both methods show acceptable agreement to experimental measurements. According to Figure 3 it is possible to see that both WSGG approaches have similar deviations. The maximum temperature are localized around x/D = 60 which is the middle of domain. The behavior for CH<sub>4</sub> mass fraction are as expected, all the fuel is consumed until the maximum peak of temperature and then is close to zero in the rest of domain. The higher deviation occurs for the mass fraction of CO<sub>2</sub> in comparison to experimental results, nevertheless are lower than 10%. The results with the WSGG/Fluent and WSGG/UDF for the mass fraction of H<sub>2</sub>O show fair agreement with the experimental results especially for the points before the peak of temperature (x/D = 60). Table 2 shows the temperature and mass fraction of species average error of the models in relation to the experimental data.

	Average Errors (%)		
	WSGG/FLUENT	WSGG/UDF	
Temperature	5.75	5.55	
$CH_4$	5.38	5.32	
CO <sub>2</sub>	8.82	8.64	
$H_2O$	5.28	4.95	

Table 2. Average errors in relation to experimental results.

The average errors in relation to experimental results do not show significant variations as seen in Table 2. However the difference between the two radiation modeling approaches appears on the radiative heat flux, as can be seen in Figure 4, where the solutions for WSGG/Fluent and WSGG/UDF are compared to each other, since the lack of experimental data. Considering that numerical solutions for temperature and mass fractions are according experimental data, and only radiative heat flux on the wall appears a different behavior, is possible to assign this result for the different treatment by the UDF coupling. According Figure 4, the radiative heat flux computed with UDF is clearly bigger than calculated for WSGG/Fluent. When UDF computes the absorption coefficient, it is considered the concentration of the participating species, but the WSGG/Fluent considers the entire medium as a gray gas with constant absorption coefficient. In this way a higher quantity of radiant energy is absorbed when using WSGG/Fluent approach. Furthermore, using UDF is possible to divide the medium into 4 gray gases (this number already showed enough in other works, Ziemniczak, 2014), giving a better spectral modeling treatment. The mean deviation between WSGG/Fluent and the WSGG/Fluent and the importance in apply a UDF for WSGG.



## 7. CONCLUSION

The present study investigated the performance of the steady laminar diffusion flamelet model for a non-premixed turbulent  $CH_4/H_2/N_2$ -air flame considering the heat transfer by radiation with the WSGG model. Measured and predicted averaged values for species mass fractions show fair agreement with experimental results.

In conclusion the steady laminar diffusion flamelet model showed to be a useful tool in the numerical simulation for a turbulent reacting jet. The analysis of radiation showed that the WSGG modeled through UDF has better accuracy since the absorption coefficient is calculated as function of the concentration of the participant species while the WSGG on Fluent considers the entire medium as only a gray gas over predicting the radiative heat flux.

## 8. ACKNOWLEDGEMENTS

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