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COMPARISON OF THE GRAY-GAS AND WEIGHTED-SUM-OF-GRAY-GASES MODELS IN A NON-PREMIXED METHANE -AIR FLAME CONSIDERING THE TURBULENCE- RADIATION INTERACTION

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Abstract. *This study considers the influence of two spectral gas modeling, the gray-gas **(**GG**)** and the weighted-sum-of-gray-gases (WSGG) models, on the solution of the radiative transfer in a turbulent flame considering or not the interaction between turbulence and radiation (TRI). The problem consists of a non-premixed turbulent methane flame surrounded by a low-velocity air coflow identified as Flame DLR-A. The model for the chemical kinetics is the steady laminar diffusion flamelet (SLDF). To generate the flamelet library, the turbulence-chemistry interaction is taken into account through previously assumed probability density functions (PDF) of the mean scalars. The spatial integration of the radiative transfer equation is carried out with the discrete ordinates method. Turbulence is solved with k-ε Standard model, while the TRI methodology is based on temperature self-correlation. The solution is obtained using ANSYS/Fluent code coupled with user-defined functions (UDFs).*

Keywords: *Turbulence-radiation interaction, gray gas model, weight-sum-of-gray-gases model, Flame DLR-A, SLDF, CFD*

1. INTRODUCTION

Turbulent flames are present in several industrial applications. Studies have evidenced the inaccuracy of predictions of radiative heat flux and temperature when the turbulence-radiation interactions (TRI) is neglected (Centeno, et al., 2016) and (Gupta, et al., 2013). The TRI analysis has proved its importance for radiative heat transfer (Krishnamoorthy e Rahman, 2018).

In the present study, the chemical kinetics was solved by steady laminar diffusion flamelet (SLDF) (Peters, 1984). The flamelets model applied to a multidimensional flame can be understood as a group of structures of unidimensional laminar flames. This way the laminar structure of the flamelets can be previously calculated and stored in a database. The turbulence effects are incorporated in laminar flamelets through probability density functions (PDFs). The PDFs have provided reliable results in combustion problems (Ziani *et al*.,2013), in which the mean and the variance are parameters of the probability function.

The turbulence model is based on Reynolds-average Navier-Stokes equations (RANS). This approach is often used due the relative simplicity of implementation and convergence. In this study, the closure model is the standard k-ε, which has shown accurate results for flame DLR-A (Deon, 2016).

The radiative heat transfer was calculated with the discrete ordinates method (DO) for spatial integration. The gray-gas (GG) spectral model consider that the coefficient of absorption independent of wave number, that is, it is ssumed to be constant for the entire spectrum. The gray-gas model in Cassol (2015) presented an absorption coefficient that depended on the local temperature and the concentrations of CO_2 and H_2O for each volume of the domain. This model will be applied in the present study for comparison with the weighted-sum-of-gray-gases (WSGG) model considering or not the TRI effects. The WSGG model considers a few gray gases with constant absorption coefficient plus transparent windows to represent the entire spectrum. The WSGG model assumes that each pressure absorption coefficient $\kappa_{p,i}$ is assumed to be independent of the temperature T and of the partial pressure p_a of the participating species.

The TRI analysis is made through the radiative transfer equation (RTE). The RTE is applicable only to instantaneous quantities, while the turbulence model employed in the present study provides only mean temporal quantities. In this way, it is necessary the decomposition of the variables in medium and fluctuating components that require modelling (Coelho, 2007). In the present analysis, the approximation used was proposed by Snegirev (2004). It considers the combined correlation between the absorption coefficient and the temperature as well as the temperature self-correlation. These two correlations of TRI interactions were considered the most important in reactive flows (Li

and Modest, 2002a; Li and Modest 2002b; Gupta, *et al*., 2013). Thus, the objective of this study is to evaluate the contribution of the spectral model for radiative transfer considering or not TRI effects in the DLR-A flame.

2. COMPUTATIONAL PROCEDURE

The problem was solved using ANSYS Fluent, academic version 18. The solution was built by setting a series of parameters for Standard *k-ε*, building the flamelets and creating a PDF Table (Ansys, 14.0 2011). This is a sequence of steps available on Fluent. The TRI effects need special implementation, so the radiative heat transfer solution made use of User Defined Functions (UDF's), programmed according to Ansys 14.0 (2011b). Several UDF's were programmed, and coupled to Ansys Fluent, including codes for variance of temperature, TRI modeling, gray-gas and WSGG modeling.

2.1 Mathematical equations

The gray-gas spectral model consider that the coefficient of absorption independent of wave number and it is possible assume a constant value for the entire spectrum. The modeling considering the dependency of the participating at the absorption coefficient leads to sufficiently accurate estimations, Cassol (2015). The present study will compare the gray-gas model with the absorption coefficient dependent of the temperature and partial pressure of the absorbing species according Eq.(1):

$$\kappa_i = p_i\left(c_0 + c_1 T + c_2 T^2 + c_3 T^3 + c_4 T^4 + c_5 T^5\right) \tag{1}$$

where κ_i is the absorption coefficient for *i* participating species, the value of constants *c* was provided in Cassol et al., (2015) based on an emission-based average integrating the spectral line generated from HITEMP2010 database. In this particular case, the species are water vapor and carbon dioxide. It follows that the equation for the absorption coefficient κ_g for the entire spectrum can be written by:

$$\kappa_g = p_{H_2O}\kappa_{p,H_2O} + p_{CO_2}\kappa_{p,CO_2} \tag{2}$$

The WSGG model considers that the pressure absorption coefficient $\kappa_{p,i}$ of each gray gas *j* can be assumed independent of the temperature *T* and of the partial pressure p_a of the participating species. The WSGG model introduces the weighting factor a_j, which represents the blackbody energy fraction that is emitted in the spectrum locations related to each gray gas, and can be expressed as a polynomial function of the temperature (Smith et al., 1982, Dorigon *et al*.,2013):

$$a_j = \sum_{k=1}^{j+1} b_{j,k} T^{k-1} \tag{3}$$

where $b_{j,k}$ are the polynomial coefficients. The correlations for $\kappa_{p,I}$ and $b_{j,k}$ used at this study was proposed by Dorigon *et al*., (2013), using the HITEMP2010 database, for mixtures of carbon dioxide and water vapor. The absorption coefficient for mixtures is determined by:

$$\kappa_j = \kappa_{p,j}\, p\left(Y_{CO_2} + Y_{H_2O}\right) \tag{4}$$

in which Y_{CO2} and Y_{H2O} are the mole fractions, and *p* is the total pressure. With this expression the absorption coefficient is computed locally as a function of the mole fractions of the participating species.

Modest (1991) demonstrated that the WSGG can be applied with any solution method of the radiative transfer equation (RTE), which can be written as:

$$\frac{dI_j}{dS} = -\kappa_j I_j + \kappa_j a_j I_b \tag{5}$$

The TRI effect was incorporated in the solution of the RTE, according Lemos *et al*., (2017) and Centeno *et al*., (2016) in the emission term. The second term at the right side of Eq. (5) can be written, considering the time average of the RTE, as:

$$\overline{\kappa T^4} = \bar{\kappa}\overline{T^4}\left(1 + C_{TRI1}6\frac{\overline{T'^2}}{\bar{T}^2} + C_{TRI2}4\frac{\overline{T'^2}}{\kappa}\frac{\partial\kappa}{\partial T}\bigg|_{\bar{T}}\right) \tag{6}$$

Equation (6) is an approximation proposed by Snegirev (2004); the variance of temperature was determined by a transport equation, incorporated at the ANSYS Fluent through user defined function (UDF). The gray gas model coupled with TRI, according to Eq.(6), leads to a derivative for the absorption coefficient:

$$\frac{\partial\kappa_g}{\partial T} = p_{H_2O}\left(c_1 + 2c_2T + 3c_3T^2 + 4c_4T^3 + 5c_5T^4\right) + p_{CO_2}\left(c_7 + 2c_8T + 3c_9T^2 + 4c_{10}T^3 + 5c_{11}T^4\right) \tag{7}$$

However, in the WSGG model coupled with TRI, the derivative for the absorption coefficient leads to a derivative of only the weighting factor Eq.(8), since the pressure absorption coefficient is assumed constant in each gray gas band (Centeno *et al*., 2016).

$$\overline{\kappa T^4} = \bar{\kappa}\overline{T^4}\left(1 + C_{TRI1}6\frac{\overline{T'^2}}{\bar{T}^2} + C_{TRI2}4\frac{\overline{T'^2}}{a_j(\bar{T})\bar{T}}\frac{\partial a_j}{\partial T}\bigg|_{\bar{T}}\right) \tag{8}$$

The derivative of the weighting factor for the WSGG model can be writing by:

$$\frac{\partial a_j}{\partial T} = \sum_{k=1}^{j+1}(k-1)b_{j,k}T^{k-2} \tag{9}$$

This is the difference between the TRI modeling for gray-gas and WSGG models.

2.2 DLR-A Flame

The flame consists of a fuel mixture of 22.1% CH_4, 33.2% H_2 and 44.7% N_2, supplied by a vertical stainless steel tube with internal diameter D = 8 mm with a thinned rim at the exit, and a 350 mm long straight cross-section prior to exit. The fuel velocity, 42.15 m/s, corresponds to a Reynolds number equal to 15200 based on internal diameter of the pipe, so turbulent flow can be considered. The stoichiometric mixture fraction is Z_{st} = 0.167; its adiabatic flame temperature is T_{ad} = 2130 K. The geometrical domain consists, longitudinally, of a length of 40 cm prior to fuel jet and air coflow exit and more 200 cm from it, and 40 cm in radial distance from the flame axis, as shown in Figure 1.

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. In this work the original geometrical configuration and experimental conditions were adopted, as reported by DLR Institute of Combustion Technology.

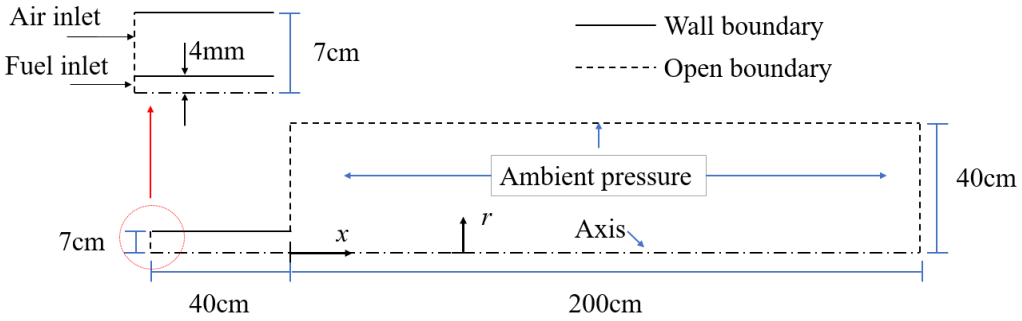

Figure 1. Axisymmetric representation of the geometrical domain and boundary conditions.

The Sandia National Laboratories produced experimental data for flame DLR-A. There are measurements of temperature and mole fractions of N_2, O_2, CO_2, H_2O, H_2, CO, OH, and NO at axial positions (x/D = 2.5 up to x/D = 120) and radial positions (x/D = 5, 10, 20, 40, 60, 80), including both mean and root mean square (rms) values. There is no available data for the radiative heat flux.

3. RESULTS

The first analysis consists of a study of the number of direction at discrete ordinates. The considered mesh, which is two-dimensional with rectangular non-uniform size elements, has 18,599 elements with refinement concentrated in the region near the fuel jet. The convergence criterion for all equations required residuals less than 10^{-5}. The evaluation of the directions was made without TRI influence, and using the WSGG model (Figure 2).

The error $\delta(\%)$ between the solutions was calculated using Eq. (10):

$$\delta(\%) = \frac{\left|q''_{R2} - q''_{R1}\right|}{\max(q''_{R2})} \times 100\% \tag{10}$$

where q''_{R2} is the radiative heat flux for the highest number of directions, while q''_{R1} is obtained for the lower number of directions that is under comparison. The mean errors, $\delta(\%)$, are presented on Table 1.

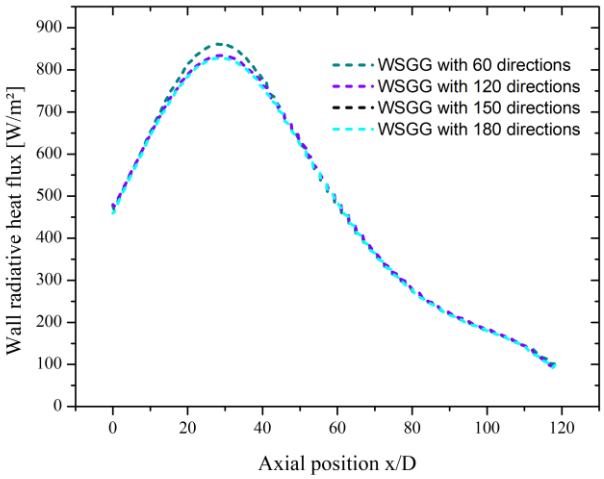

Figure 2. Test of the number of directions in the discrete ordinates method in the computation of the radiative heat flux on the control surface around the flame.

Table 1. Comparison between the numbers of directions for discrete ordinates method

Number of directions	δ% (mean)
60	-
120	1.23
150	0.68
180	0.15

According to Fig. 2, the solution obtained with 60 directions considerably overestimated the radiative heat flux, while, for the solutions with 120 directions or above, the results almost overlap. Table 1 shows the decrease of the error between the solutions when the number of directions was increased. The selected number of directions was 150, since there is only 0.68 % of deviation with the results for the mesh with 180 elements. The radiant fraction was calculated according to Houf and Schefer (2007), where the radiations are integrated along a surface around the flame. The surface creates a cylinder of radius R concentric to the axis of the flame, the radiant fraction is given by:

$$X_R = \frac{2\pi R \Delta y}{\dot{m} LCV} \sum_{i=1}^{n} q''_R \tag{11}$$

where Δy is the difference between the positions where the radiative heat flux is measured, n is the number of measures, $\dot{m}$ the fuel flow and LCV is the lower calorific value.

Next, the DLR-A flame was simulated with the WSGG model and gray-gas model using 150 directions. Figure 3 shows the temperature at the center line of the domain compared with experimental data. The deviation of gray-gas

solution, described by Equation (9), was on average 6.63%, with maximum deviation of 19.29%. For the WSGG model, the deviation was on average 5.58% and maximum 16.02%. The highest error was on the last point, at x/D= 120. Therefore, in general the temperature along the centerline presented good agreement between the numerical and the experimental results.

$$\delta(\%) = \frac{\left|T_{\exp} - T_{num}\right|}{T_{\exp}} 100 \tag{12}$$

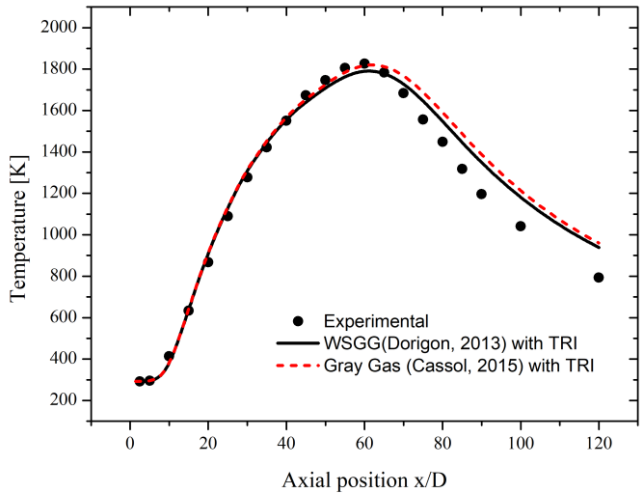

Figure 3. Temperature at centerline of domain, comparison between experimental and numerical solutions.

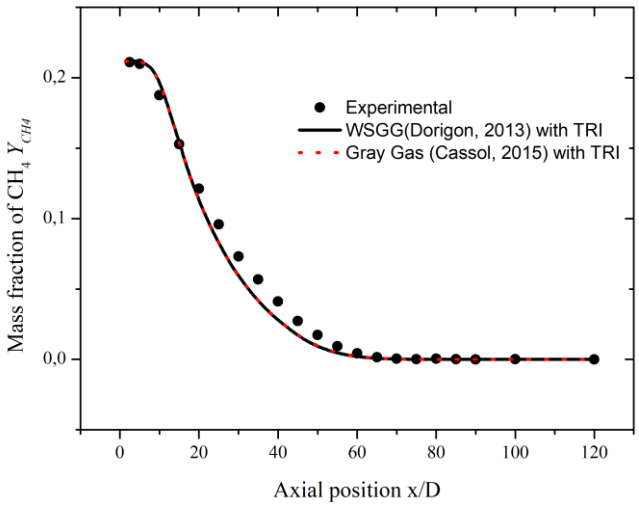

Figure 4. Mass fraction of CH_4 at centerline of domain, comparison between experimental and numerical solutions.

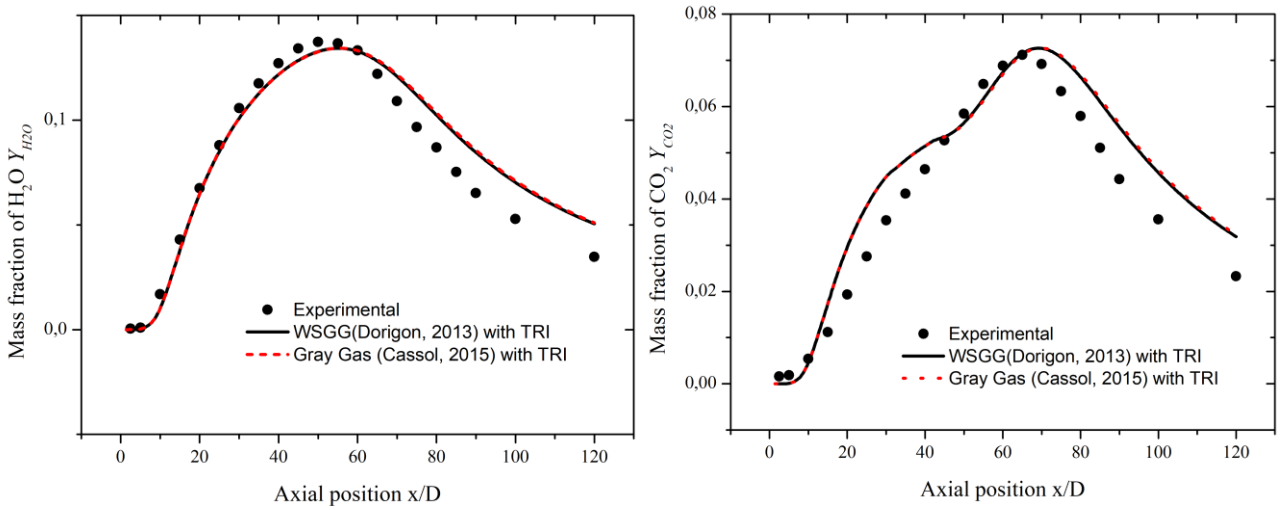

Figure 5. Mass fraction of H_2O and CO_2 at centerline of domain, comparison between experimental and numerical solutions.

The species CH_4, H_2O and CO_2 are compared with experimental results leading to good agreement. The solutions with and without TRI are close, as discussed after the radiative heat flux results. The results for species are compatible with Deon (2016).

The radiative heat flux considering or not the TRI effects are shown on Figure 6. The results are obtained at the boundary opposite the axis.

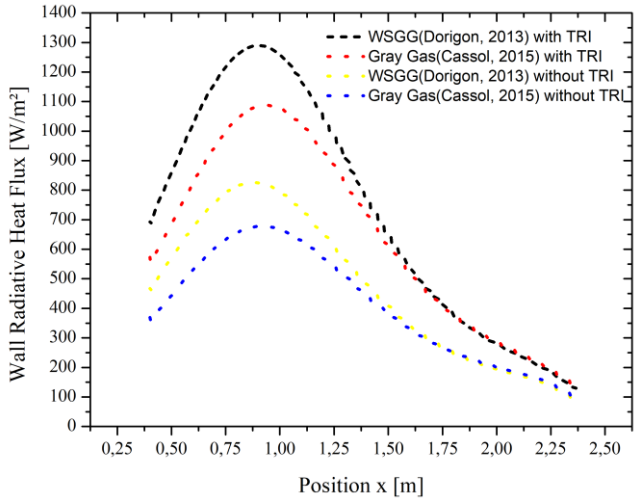

Figure 6. Radiative heat flux, comparison between gray-gas model and WSGG model with and without TRI effects.

The radiative heat flux calculated by gray-gas model not considering TRI effects has the maximum value in 678.01 W/m², the position is equivalent to x/D = 63. Figure 3 shows the temperature at center line and the maximum temperature of the flame is about x/D = 60, in this way the peak of the radiative heat flux is localize according the expected, at position of maximum temperature. The radiative heat flux calculated by gray-gas considering TRI reaches to 1086.97 W/m², the difference between radiative heat flux with and without TRI for gray-gas model, can be calculated by Eq. (7). The increase of radiative heat flux for the gray-gas model with TRI is in average 21.1% and maximum of 37.8%.

The radiative heat flux provided by the WSGG model, the yellow curve, is localized between the solutions obtained by gray-gas model with and without TRI. In this way the WSGG model predict a peak of 825.40 W/m², about 18% bigger than the prediction of the gray-gas model without TRI. Comparing the difference between the results, TRI modeling increase in average is 19.9% and the maximum is 36.1% at radiative heat flux for the WSGG model.

The methodology for obtaining these results is essentially the same, however for gray-gas the absorption coefficient is a direct derivative, Eq (7), while for the WSGG the derivative in Eq. (6) leads to derivative of weighting factor, Eq. (9). The inclusion of TRI modeling increases about 20% in average and 36% in maximum for both methodologies, which indicates that the TRI methodology produced equivalent effects for the models.

An important parameter, the radiant fraction X_R , calculated by Eq. (11), are present on Table 2.

Table 2. Comparison between the numbers of directions for discrete ordinates method

Model	X_R(%)
WSGG with TRI	5.0
WSGG	3.36
Gray gas with TRI	4.6
Gray gas	2.93

There is not any experimental measure for radiative heat flux for DLR-A flame. However, the Sandia Flame D, a similar flame, has known 5% for radiant fraction according Gupta, *et al*., (2013). The WSGG model with TRI leads to consistent results, the gray-gas model with TRI also approaching, but the maximum radiative heat flux for gray-gas model is 20.46% lower.

The comparison for species calculated with different radiative models does not present any differences. This can be understood due the radiant fraction being about 5%, so the impact of thermal radiation is about 5% on the source term of the energy equation. In this way, chemical kinetic dominate the source term of energy equation, still which occurs the increasing of radiative heat flux due TRI modelling, it is not able to modify the temperature and species for the DLR-A flame.

According to Lemos, *et al*., (2017) the gray-gas with constant absorption coefficient coupled with TRI leads to underestimation of the radiative heat flux. In this study, both spectral models consider the absorption coefficient dependency of temperature and participating gases concentration, therefore highlighting the need of modelling the influence of temperature and participant gases concentration at the absorption coefficient as well as considering the TRI effects. Ultimately, the WSGG spectral model predicted the radiative heat flux more accurately, according to the results obtained for radiant fraction.

4. CONCLUSIONS

The present study applied the steady laminar diffusion flamelet model for modeling the kinetics of a non-premixed turbulent $CH_4/H_2/N_2$-air flame. The turbulence effects are incorporated in laminar flamelets through probability density functions. The employed turbulence model was the standard k-ε. The radiative heat transfer was calculated with discrete ordinates method for the spatial integration, while the employed spectral models were the gray-gas and the WSGG models. Measured and simulated mean value of temperature along the flame centerline presented a satisfactory agreement. The number of directions was evaluated with WSGG model and indicated the need of 150 directions for this particular test case.

The WSGG model, in which absorption coefficient dependency of temperature and participating gases concentration coupled with TRI effects on emission term at the RTE, led to radiant fraction compatible with available data. The WSGG model predicted the radiative heat flux more accurately, with a radiant fraction of 5.0%, while the gray-gas model led to a radiation fraction of 4.6%.

5. ACKNOWLEDGEMENTS

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