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COMPUTATION OF THE RADIATIVE HEAT TRANSFER IN A NON-PREMIXED TURBULENT FLAME USING THE GRAY GAS AND THE WSGG MODELS

Larissa Domingues Lemos
Felipe Roman Centeno
Francis Henrique Ramos França
Universidade Federal do Rio Grande do Sul, Department of Mechanical Engineering, Porto Alegre, Brazil
larissa.lemos@ufrgs.br; frcenteno@mecanica.ufrgs.br; frfranca@mecanica.ufrgs.br

Abstract. This work solves a numerical problem and analyses the comparison of numerical and experimental data for radiative heat flux. The problem consists of a non-premixed turbulent flame, the fuel is natural gas with a 40% CO_2 dilution and the ambient air is the oxidant. The chemical kinetics was solved with the steady laminar diffusion flamelet (SLDF) model. To generate the flamelet library, turbulence-chemistry interaction is taken into account through previously assumed probability density functions (PDF) of mean scalars. The spatial integration of the radiative transfer equation is carried out with the discrete ordinates method. This study considers the influence of two spectral gas modeling, the gray-gas 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). Turbulence is solved with k-ε Standard model, while the TRI methodology is based on correlation between the absorption coefficient and the temperature as well as the temperature self-correlation. The solution is obtained using ANSYS/Fluent code coupled with user-defined functions (UDFs).

Keywords: Turbulence-radiation interaction, gray-gas model, weighted-sum-of-gray-gases model, SLDF, CFD.

1. INTRODUCTION

Turbulent flames are present in several industrial applications. This is due to the participation of the turbulence together with the chemical reactions promoting the mixing of the reagents and the transport of heat. In addition, non-premixed flames are more commonly used because they allow significantly easier control than premixed flames. Since this is a complex problem involving highly nonlinear functions, the solution involves some methodologies to obtain accurate results. Studies have evidenced the inaccuracy of predictions of radiative heat flux and temperature when the turbulence-radiation interactions (TRI) is neglected (Miranda, *et al*., 2019) and (Centeno, *et al*., 2016).

The steady laminar diffusion flamelet (SLDF) was formalized by Peters (1984). The flamelets model treats a multidimensional flame as a group of structures of unidimensional laminar flames. Each flamelet is submitted to local conditions of flow, keeping its internal structure. In this way, the laminar structure of flamelets can be previously calculated from a database and then tabulated. The table contains the most important reactive scalars parametrized by a small number of control variables. The application of this methodology in several works has been shown to provide accurate results when compared with experimental data (Emami and Fard, 2012). In order to obtain the laminar flamelets, the chemical kinetic mechanism used is GRI-Mech 3.0 with 53 chemical species and 325 elementary reactions.

Simulations of turbulent reactive flows are not satisfactorily computed with the scalars mean fields, so it is necessary a model that consider the effect of their fluctuations. Probability Density Function (PDF) has provided reliable results in combustion problems (Ziani, *et al*., 2013). The probability density function can be interpreted as the fraction of time which a portion of fluid in determined spatial coordinate stays in the neighbourhood of a state. The advantage of PDF models is the dependency of probability function with the real fluctuations. In this model the mean and the variance are the key parameters of the probability function. The turbulence effects are incorporated in laminar flamelets through PDFs.

There are different turbulence models based on Reynolds-Average Navier-Stokes equations (RANS). Even with advanced methodologies as Large Eddy Simulation (LES), RANS approach is still being broadly employed. This is due its relative easiness of implementation and convergence. In this work the closure model is Standard *k-ε*, which showed accurate results for a turbulent diffusion jet flame according to recent work (Sukirt, *et al*., 2019).

The radiative heat transfer was calculated with the discrete ordinates method (DOM) for spatial integration. The gray-gas spectral model consider that the coefficient of absorption independent of wave number, that is, it is assumed 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 has proved its importance for radiative heat transfer (Krishnamoorthy e Rahman, 2018). The 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 modeling (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 (Fraga, *et al.*, 2019; 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 a non-premixed turbulent flame.

2. COMPUTATIONAL PROCEDURE

The problem was solved using ANSYS Fluent, academic version 19.0. 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 to 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:

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

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

The TRI effect was incorporated in the solution of the RTE, according to 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:

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

$$\frac{\partial \kappa_g}{\partial T} = p_{H_2O}\left(c_1 + 2c_2 T + 3c_3 T^2 + 4c_4 T^3 + 5c_5 T^4 \right) + p_{CO_2}\left(c_7 + 2c_8 T + 3c_9 T^2 + 4c_{10} T^3 + 5c_{11} T^4 \right)$$ (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).

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

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

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

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

2.2 Studied flame

The fuel of the flame consists of 60% of natural gas and 40% of CO_2. The fuel mixture result of 54.48% CH_4, 40.3% CO_2, 3.6% C_2H_6, 0.72% C_3H_8, and 0.9% N_2. The steel tube of fuel has internal diameter D = 16.55 mm. The oxidant is ambient air at temperature of 300K. The fuel velocity, 3.1 m/s corresponds to a Reynolds number equal to 4487. The temperature of the fuel is 300K. The geometrical domain consists, longitudinally, of a length of 49.65 cm prior to fuel jet exit and more 214.6 cm from it, and 52.85 cm in radial distance from the flame axis, as shown in Figure 1. The radial distance corresponds to half flame length.
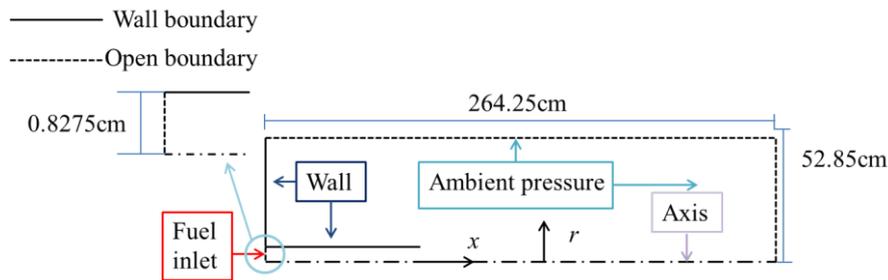
Figure 1. Axisymmetric representation of the geometrical domain and boundary conditions.

Simulations were performed using the commercial CFD code ANSYS Fluent, version 19.0.0, adopting the SIMPLE scheme for pressure-velocity coupling. The mesh is two-dimensional with rectangular non-uniform size elements, has 117,968 elements with refinement concentrated in the region near the fuel jet. The convergence criterion for all equations require residuals less than 10^{-5}. The angular discretization used for discrete ordinates method was 80 directions.

3. RESULTS

In this work five cases are considered, in the first case, identified as NR, the radiative heat lost is neglected. The second and third cases the gray-gas and WSGG models are considered but the influence of TRI is disregard, GG-NTRI and WSGG-NTRI respectively. The fourth and fifth cases consider the gray-gas and WSGG models with the TRI effects included, they are identified GG-TRI and WSGG-TRI. The Table 1 describes the five cases. The results are compared between the numerical solution for temperature, velocity and mixture fraction. The available experimental data is for radiative heat flux, compared with the cases GG-NTRI, WSGG-NTRI, GG-TRI and WSGG-TRI.

Table 1. Cases considered in this study.

Case	Method to model the radiative heat transfer	TRI on emission term
NR	Absent	Absent
GG-NTRI	Gray-Gas	Absent
WSGG-NTRI	WSGG	Absent
GG-TRI	Gray-Gas	Present
WSGG-TRI	WSGG	Present

The temperature contour for the case disregarding the radiative heat transfer is shown in Figure 2, this figure is presented to observe that the flame is completely inside the domain. The temperature decrease when the radiative heat transfer is considered, according to Figure 3. The TRI effects leads to another little decrease of the temperature at axis line. The Figure 4 presents the temperature in one position, for x equal to 0.55m. The difference in temperature is not very pronounced between cases GG-NTRI and GG-TRI and between WSGG-NTRI and WSGG-TRI. Is possible observe the difference when the radiative heat transfer is neglected, NR, and between the gray-gas and WSGG models.
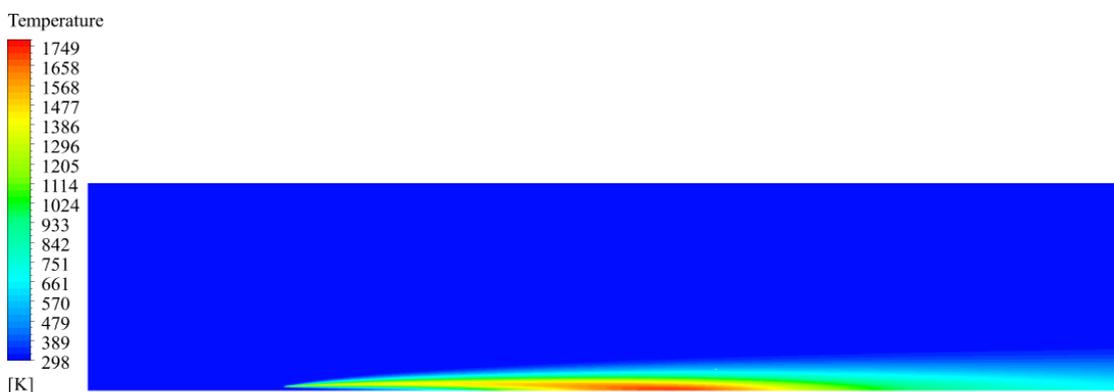

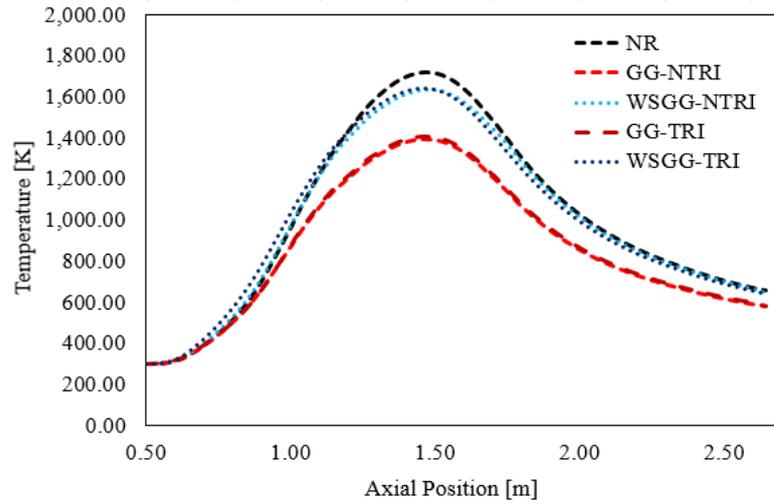Figure 2. Temperature profile of the flame in case NR.

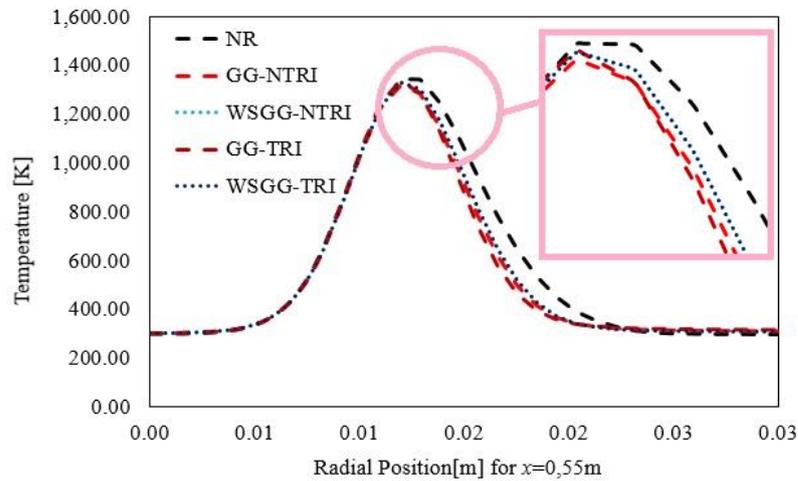Figure 3. Temperature at axial position.

Figure 4. Temperature at radial position.

The velocity vectors in Figure 5 was obtained for the case NR, it is possible observe the flow nearly aligned with the axis. The combustion occurs due to mixing of fuel and ambient air, and for this reason, the boundary of the domain is open. The difference between the cases are present on Figure 6, where the velocity is considered for one position x equal to 0.55m. The difference in velocity is not very pronounced, appearing only when the flame distance increase, which implies a low value of magnitude.
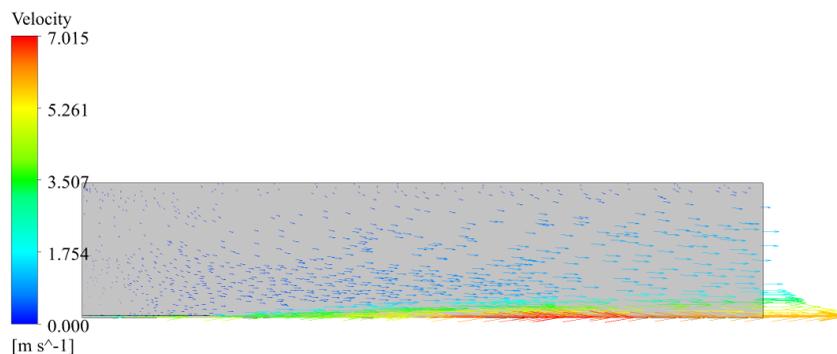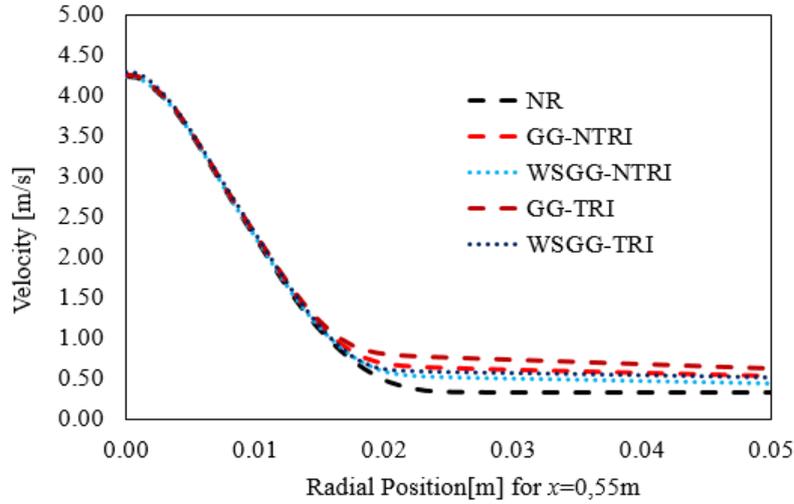

Figure 5. Velocity vectors for case NR.

Figure 6. Velocity at radial position.

The mixture fraction is the key parameter for chemical kinetics, Figure 7 present the numerical solution obtained for the five cases. The difference between the solutions is small, that indicate a low impact on the prediction of chemical species related to the method to model the radiative heat transfer. Figure 7 shows that even the case NR is close to the other cases, so, even neglecting the radiative heat transfer, the chemical species are not considerably affected.
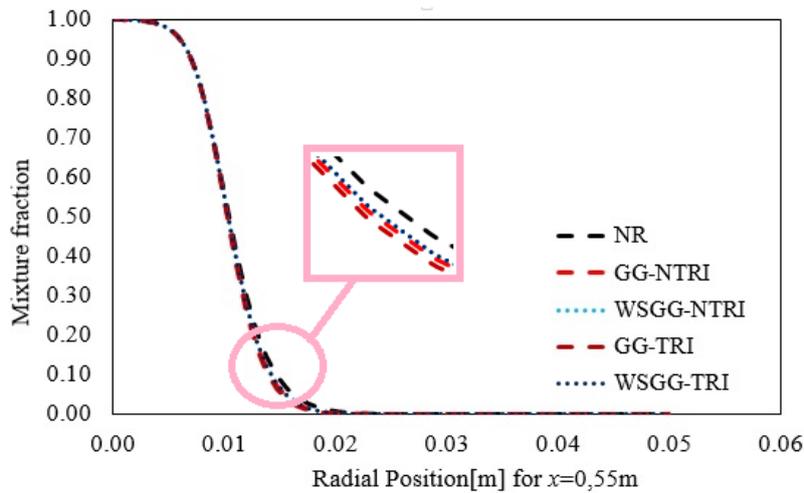

Figure 7. Mixture fraction at radial position.

Figure 8 shows the experimental data for radiative heat flux, obtained by Llanos 2018, including the deviation bars, calculated by random analysis, related to the measurements and the numerical solution for the four cases. The results are obtained at the boundary opposite the axis. The radiative heat flux calculated in case GG-TRI, the gray-gas considering TRI reaches to 778.00 W/m², while the peak of experimental data is 467 W/m², this is the case with the largest discrepancy between the results. The gray-gas overestimates the radiative heat flux, so when the TRI is considered, the result obtained for radiative heat flux moves away from the experimental data. The case WSGG-TRI present the closest numerical result to the experimental data, this is the case which WSGG model and TRI effects on emission term are considered. For considering the deviation between the numerical solution and the experimental data, was used the Eq. (10).

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

where $q_{R\,\exp}^{''}$ is the radiative heat flux for experimental data, while $q_{Rnum}^{''}$ is obtained for numerical solution. The mean, maximum and minimum errors, $\delta(\%)$, are presented on Table 2.
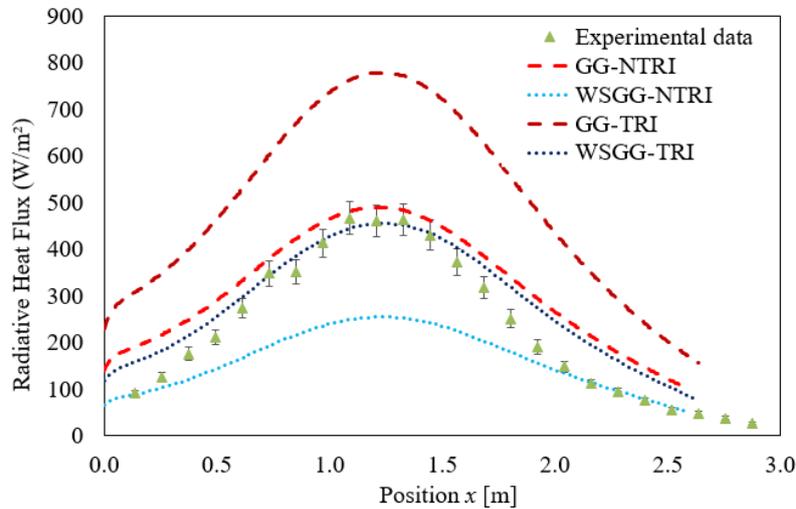

Figure 8. Radiative heat flux, comparison between experimental data and the four cases studied.

Table 2. Comparison between the experimental and numerical solution.

Case	δ%(mean)	δ%(maximum)	δ%(minimum)
GG-NTRI	14.25	21.63	1.93
WSGG-NTRI	19.12	46.89	0.29
GG-TRI	53.28	68.81	8.29
WSGG-TRI	11.21	21.96	1.05

According to Table 2, the minor deviation occur in WSGG-TRI, due the radiative heat flux close to experimental data in the peak of temperature, resulting in δ%(mean) equal to 11.21%, in this case, the deviation increase only in points far from the peak temperature. The δ%(minimum) occurs to WSGG-NTRI, due the lowest values in the radiative heat flux. The case GG-NTRI presents consistent results, δ%(mean) equal to 14.25%, despite being a simpler modeling. However, including TRI modeling the δ%(mean) for GG-TRI reaches to 53.28%, due the gray-gas overestimates the radiative heat flux. The difference between the upper and lower experimental points and the numerical solution for radiative heat flux may be due to the turbulence of the flame. In the upper part, according to Llanos 2018, there is a variation of visible flame height due to the buoyancy phenomenon. This variation in the upper part, according Llanos 2018, is understood as a lower flame presence, therefore, the upper part of the experimental results for the radiative heat flux may be affected by the temporal variation of the flame length.

The increase of radiative heat flux for the gray-gas model with TRI is in average 24.83% and maximum of 37.1%. For WSGG model, TRI modeling increase in average is 27.1% and the maximum is 44.9% at radiative heat flux. 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 25% in average and 40% in maximum for both methodologies, which indicates that the TRI methodology produced equivalent effects for the models. The implementation of a new TRI modeling for the RTE emission term, proposed by Fraga *et al.*, (2019), may approximate the numerical result of the experimental one and may be object of study in future works. More information on experimental measurements can be found in Llanos (2018).

4. CONCLUSIONS

The present study applied the steady laminar diffusion flamelet model for modeling the kinetics of a non-premixed turbulent flame, where the fuel is natural gas with a 40% CO_2 dilution and the ambient air is the oxidant. 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. For the employed models, chemical species and temperature were minor influenced by TRI, while it is influence on radiative heat flux was important.

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 radiative heat flux compatible with available experimental data. For this case, the mean deviation between the numerical solution and the experimental data is nearly 11.2%.

5. ACKNOWLEDGEMENTS

6. REFERENCES

Ansys. Fluent 14.0, 2011a. "Theory Guide", Ansys Inc.

Cassol, F.; Brittes R.; Centeno, F.R.; Vitorino, C.S.; França, F.H.R., 2015; "Evaluation of the gray gas model to compute radiative transfer in non-isothermal, non-homogeneous participating medium containing CO_2, H_2O and soot", *The Brazilian Societey of Mechanical Sciences and Engineering*, Vol. 37, pp. 163-172.

Centeno, F.R.; Brittes R.; França F.H.R, 2016. "Application of the WSGG model for the calculation of gas-soot radiation in a turbulent non-premixed methane-air flame inside a cylindrical combustion chamber". *International Journal of Heat and Mass Transfer*, Vol. 93, p. 742–753.

Deon, D.L., 2016. Estudo numérico de chamas turbulentas não pré-misturadas através de modelos baseados no conceito de flamelets, M.Sc. thesis, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brasil.

Dorigon, L.J., Duciak, G., Brittes, R., Cassol, F., Galarça, M., França, F.H.R., 2013; "WSGG correlations based on HITEMP 2010 for computation of thermal radiation in non-isothermal, non-homogeneous H2O/CO2 mixtures", *IJHMT*, Vol. 64, pp. 863-87.

Emami, M.D.; Fard, A.E., 2012. "Laminar Flamelet Modeling of a Turbulent CH4/H2/N2 Jet Diffusion Flame Using Artificial Neural Networks", *Applied Mathematical Modelling*, Vol. 36, p 2082-2093.

Fraga, G.C.; Centeno, F.R.; Petry, A.P.; Coelho, P.J., França, F.H.R., 2019. "On the individual importance of temperature and concentration fluctuations in the turbulence-radiation interaction in pool fires", *IJHMT*, Vol. 136, pp. 1079-1089.

Gupta, A; Haworth, D.C.; Modest, M.F., 2013; Turbulence-radiation interactions in large-eddy simulations of luminous and nonluminous nonpremixed flames, Proceedings of the Combustion Institute, Vol. 34, pp.1281-1288.

Krishnamoorthy, G.; Rahman, M.A., 2018; "Assessing the role of turbulence-radiation interactions in hydrogen-enriched oxy-metane flames", *International Journal of Hydrogen Energy*, Vol.43, p. 5722-5736.

Lemos, L.; Centeno, F.R.; França, F.H.R., 2017. "Effects of turbulence-radiation interactions in a non-premixed turbulent methane-air flame" In *Proceedings of the 21st International Congress of Mechanical Engineering - COBEM2017*. Curitiba, Brazil.

Modest, M.F., 1991. "The Weighted-Sum-of-Gray-Gases model for arbitrary solution methods in radiative transfer" Journal of Heat Transfer, Vol. 113, pp. 650-656.

Li, G.; Modest, M.F., 2002a; "Aplication of composition PDF methods in the investigation of turbulence-radiation interactions", *Journal of Quantitative Spectroscopy and Radiative Transfer*, 73, pp.461-472.

Li, G.; Modest, M.F., 2002b; Importance of Turbulence-Radiation Interactions in turbulent reacting flows, ASME International Mechanical Engineering Congress and Exhibition, Lousina, USA.

Llanos, L.A.Q.,2018. *Estudo experimental de estabilidade e emissão de radiação térmica em chamas não pré-misturadas de gás natural diluídas com dióxido de carbono*. M.Sc. thesis, Universidade Federal do Rio Grande do Sul, Porto Alegre.

Miranda, F.C., Coelho, P.J., Mare, F., Janicka, J., 2019. "Study of turbulence-radiation interactions in large-eddy simulation of scaled Sandia flame D", Journal of Quantitative Spectroscopy & Radiative Transfer, Vol 228, pp.47-56.

Peters, N., 1984. "Laminar Diffusion Flamelet Models in Non-Premixed Turbulent Combustion" Progress in Energy and Combustion Science,Vol 10, p. 319-339.

Smith, T.F., Shen, Z.F. and Friedman, J.N., 1982. "Evaluation of coefficients for the weighted sum of gray gases model". Journal of Heat Transfer, Vol. 104(4), pp. 602-608.

Sukirt, T., Gaikwad, P., Sreedhara, S., 2019. "Reynolds-Averaged Navier–Stokes Simulations of Turbulence-Radiation Interaction in a Turbulent Diffusion Jet Flame". Journal Of Thermophysics And Heat Transfer, Vol 33, pp.875-880.

Ziani, L.; Chaker, A.; Chetehouna, K.; Malek, A; Mahmah, B., 2013. "Numerical simulations of non-premixed turbulent combustion of CH4-H2 mixtures using the PDF approach" International Journal of Hydrogen Energy, Vol 38, p. 8597-8603.

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