encit 2020

ABCM Associação Brasileira de Engenharia e Ciências Mecânicas

18th Brazilian Congress of Thermal Sciences and Engineering
November 16-20, 2020 (Online)

ENC-2020-0325
EFFECT OF DIFFERENT COMBUSTION MODELS AND CHEMICAL KINETICS INTERMEDIATE STEPS IN THE PREDICTION OF THE RADIATIVE TRANSFER IN TURBULENT METHANE-AIR FLAMES

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Abstract. *In this study, it is presented the numerical simulation of a turbulent natural gas flame with focus on the analysis of the radiative heat flux, using the CFD (Computational Fluid Dynamics) Ansys Fluent. The combustion process was solved with the Non-Premixed Combustion - Steady Laminar Diffusion Flamelet (SLDF) model, with detailed reaction mechanism, as well as with the Non-Premixed Combustion - Chemical Equilibrium (CE), with simpler reaction mechanisms, in order to evaluate the sensitivity of the problem with respect to the chemical kinetics. The turbulence was modeled through the k-ε standard model. For the radiation calculation, the weighted-sum-of-gray-gases (WSGG) was implemented as the spectral model and the discrete ordinates method (DOM) as the spatial-directional model. This work considered the correlation between the absorption coefficient and the temperature and the temperature self-correlation to account for the effects of turbulence-radiation interaction (TRI). The two models showed physically acceptable results, for instance, showing that the inclusion of TRI effects reduces the flame temperature and increases the radiative heat flux. The results for the SLDF model, with greater detail of the chemical kinetics, showed better results in comparison with experimental data. For the CE model, there was a shift in temperature, species concentration and radiative heat flux in comparison with both the experimental data and the SLDF solution.*

Keywords: *SLDF, chemical equilibrium, WSGG, turbulence-radiation interaction, CFD.*

1. INTRODUCTION

The problem under investigation consists of computing the radiation transfer in a natural gas turbulent flame, comparing the numeric results to experimental measurements. Considering the complexity of the involved phenomena in turbulent flames, solving the flow, the turbulence, the chemical kinetics and the thermal radiation with exactitude is not a possible task. In this way, the objective of this study is to establish the methodologies that lead to satisfactory accuracy, but with relative efficiency, focusing on combustion models and chemical kinetics.

The main contribution of this work is to test different approaches for modeling the gas combustion process, which vary the complexity of the chemical kinetics mechanisms, and thus attest the sensitivity of the calculation of the radiative heat flux to these factors.

Combustion and chemical kinetics were solved by Steady Laminar Diffusion Flamelet (SLDF) model, formalized by Peters (1984), which considers the flame as a group of laminar flames structures almost one-dimensional, providing good results in comparison to experimental data (Enami and Fard, 2012). Subsequently, it was switched to the Chemical Equilibrium model, under the assumption the chemistry can be modeled as being in chemical equilibrium, requiring simpler reaction mechanism, for evaluating the sensitivity of the problem to chemical kinetics. The chosen model for turbulence was the standard k-ε, which presented accurate results in Deon (2016).

The spectral model for the thermal radiation was the weighted-sum-of-gray-gases (WSGG). The WSGG model considers that the entire spectrum can be divided in a certain number of gray gases with constant pressure absorption coefficients, which can lead to accurate results in spite of its simplicity (Fonseca et al., 2018 and Rodrigues et al., 2019). The interaction of turbulence with radiation (TRI) was approximated using the RANS model proposed by Snegirev (2004), which considers a combined correlation between the absorption coefficient and the temperature and an auto-correlation of the temperature.

The comparison of numeric simulations was performed with data from experimental measurements of turbulent flames carried out at the Combustion Laboratory (LC) of UFRGS.

2. COMPUTATIONAL PROCEDURE

2.1 Physical system and domain

The flame under investigation was diffuse and surrounded by ambient air (free boundary). The fuel composition was CH_4 = 54.48 %, C_2H_6 = 3.6 %, C_3H_8 = 0.72 %, CO_2 = 40.3 %, N_2 = 0.9 %. Denoting by d the diameter of the burner and by L_f the flame length, the geometric domain of the computer simulation consists, longitudinally, of $30\times d$, corresponding to the burner length, plus $2.5\times L_f$, and $0.5\times L_f$ radially. This last dimension corresponds to the radial position defined for the radiative heat flux values generated on the software, between the available experimental measurement positions for comparison. The domain was set up in order to represent half of the real system and later to revolutionize the results around an axisymmetric axis, coaxial to the burner axis. The main reason for this simplification is the considerable reduction of computational time required to numeric calculation. Figure 1 shows this domain, specifying the boundary conditions, which include the fuel inlet, the burner wall and the ambient pressure.

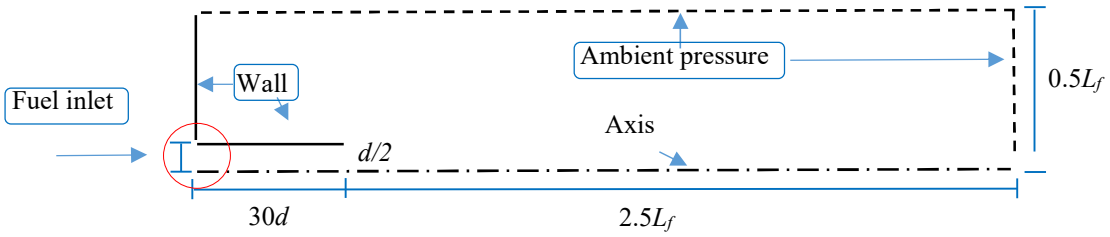

Figure 1. Geometric domain and boundary conditions. Available from: Sandia National Laboratories, 2017 – adapted by Author.

For the numeric solution, the domain was discretized with greater refinement in the flame formation region. The conservation equations related to reactive flows was solved for each element of the domain, through the Finite Volume Method – FVM.

2.2 Mathematical equations

Due to property variations caused by turbulence, the conservation equations in the combustion need to be solved through Favre decomposition, which expresses the instantaneous value of a scalar in an average value and a fluctuation, in which this average value is defined by weighting the value instantaneous by the density ρ of the fluid. For the case in study, the equation for total mass result in:

$$\nabla \cdot (\bar{\rho}\,\tilde{u}) = 0 \tag{1}$$

for a flow with velocity u. The bar denotes the terms in which it is applied a simple time average, while the tilde denotes the Favre average. For the momentum, the equation carries the advective terms, pressure forces and the gravitational field forces, giving rise to the buoyant effects:

$$\nabla \cdot (\bar{\rho}\,\tilde{u}\,\tilde{u}) = -\nabla\bar{\rho} + \nabla \cdot \left(\tilde{\tau} - \bar{\rho}\,\widetilde{u''u''}\right) + \bar{\rho}\,g \tag{2}$$

being τ the stress tensor, dependent of the fluid molecular dynamic viscosity μ and representing the forces of viscous origin; g is the gravity acceleration. Additional tensors from turbulent fluctuations correlations include turbulent viscosity μ_t and turbulent kinetic energy k. In this way:

$$-\bar{\rho}\,\widetilde{u''u''} = \mu_t[\nabla\tilde{u} + (\nabla\tilde{u})^T] - \frac{2}{3}\bar{\rho}\,\tilde{k}I \tag{3}$$

It is assumed the Stokes hypothesis for a Newtonian fluid and an analogy to stresses in laminar flows. I is the identity matrix tensor. The terms μ_t and k depend on the adopted turbulence model. In this study, it was used the standart k-ε model, which involves conservation equations for turbulent kinetic energy k and its dissipation rate ε, with modified constants for free jet according to Morse (1977) and Pope (1978).

The chemical species mass is conserved according to the equation:

$$\nabla \cdot \left(\bar{\rho}\,\tilde{u}\,\tilde{Y}_k\right) = \nabla \cdot \left(\bar{\rho}\,\overline{\mathcal{D}_k}\nabla\tilde{Y}_k - \bar{\rho}\,\widetilde{u''Y_k''}\right) + \overline{\dot{\omega}}_k \tag{4}$$

for $k = 1, N_{k-1}$. Y_k is the chemical specie k mass fraction, $\mathcal{D}_k$ is an average coefficient of specie mass diffusion into the mixture, corresponding to the mass diffusion flux caused by species concentration gradients (Fick's law), and $\dot{\omega}_k$ is the species mass production/destruction rate. For the energy conservation, the more conventional implementation form in CFD codes is in term of mixture total enthalpy h:

$$\nabla \cdot \left(\bar{\rho}\,\tilde{u}\,\tilde{h}\right) = \nabla \cdot \left(\overline{\frac{\lambda}{C_p}\nabla h} - \bar{\rho}\,\widetilde{u''h''}\right) - \nabla \cdot \left[\overline{\sum_{k=1}^{N_k}\left(1 - \frac{1}{Le_k}\right)\frac{\lambda}{C_p}h_k\nabla Y_k}\right] + \overline{\dot{S}_h} \tag{5}$$

h_k is the specific enthalpy of specie k, λ is the thermal conductivity and C_p is the constant pressure specific heat, both referring to mixture, Le_k is the Lewis number, which relates the mixture thermal diffusivity to species mass diffusivity, and $\dot{S}_h$ is the source term of heat generation rate, corresponding to the negative divergent of the radiative heat flux S_{rad}

$$S_{rad} = -\nabla \cdot \vec{q}_r \tag{6}$$

3. THERMAL RADIATION

A participating medium absorbs, emits and scatters thermal radiation. To determine the radiative transport in a participating medium, the radiative transfer equation (RTE) must be solved in space and in spectrum. Thus, it is possible to determine the increase in intensity due to emission and due to scattering in the direction of the intensity path and the effects of intensity attenuation due to absorption and scattering in other directions. The variation as a result of scattering is neglected in this work, as there is no significant formation of particulates.

3.1 Radiative Transfer Equation

The spectral radiative transfer equation that defines the radiative energy intensity, dI_η, in a medium that emits and absorbs energy along a given path is given by:

$$\frac{dI_\eta(\xi)}{d\xi} = -\kappa_\eta(\xi)I_\eta(\xi) + \kappa_\eta(\xi)I_{\eta b}(\xi) \tag{7}$$

where $I_\eta(\xi)$ and $I_{\eta b}(\xi)$ are the spectral intensity and spectral intensity of the blackbody at position ξ along the path and κ_η is the spectral absorption coefficient of the medium. To solve with computational efficiency the problem of the highly complex spectral variation of the absorption coefficient, a number of gas models have been proposed in the literature. One of the most widely used is the weighted-sum-of-gray-gases (WSGG) model.

3.1.1 Application of the WSGG Model in the Radiative Heat Flux Solution

The WSGG model consists of the representation of the spectral variation of the absorption coefficient by a small number of gray gases, in which each gray gas has an absorption coefficient that can be considered constant (covering a fixed portion $\Delta\eta_i$ in the spectrum) and independent of temperature and partial pressure of the participating species. These two considerations decouple the dependence of the absorption coefficient with the wave number and the thermodynamic state (temperature and concentration of the participating species).

This study considers a mixture of water vapor and carbon dioxide as participating species, as they are the main products of the combustion. The absorption coefficient of the mixture, denoted by $k_{n,a}$, can be obtained by simply adding the absorption coefficients of each component:

$$\kappa_{\eta,a} = \kappa_{\eta,CO_2} + \kappa_{\eta,H_2O} \tag{8}$$

where the absorption coefficient is given by the product between the absorption coefficient at a given pressure and its pressure p, that is, $\kappa_{\eta,c} = p_c\kappa_{p\eta,c}$, c = H_2O or CO_2. It follows that

$$\kappa_{p\eta,a} = \frac{p_{CO_2}\kappa_{p\eta,CO_2} + p_{H_2O}\kappa_{p\eta,H_2O}}{p_a} \tag{9}$$

where p_{H2O} and p_{CO2} are the partial pressures of H_2O and CO_2, and p_a is the total partial pressure of the species, $p_a = p_{H2O} + p_{CO2}$.

An important definition for the WSGG model is the total emittance of the medium along a given path of length S. The total emittance for an isothermal and homogeneous medium is given by:

$$\varepsilon(T, p_a S) = \frac{\int_{\eta=0}^{\infty} I_{\eta b}(\eta, T)[1 - \exp(-\kappa_{p\eta,a} p_a S)]d\eta}{\sigma T^4 / \pi} \tag{10}$$

where $p_a S$ is the pressure path. $I_{\eta b}$ is given by the Planck distribution:

$$I_{\eta b}(\eta, T) = \frac{2C_1\eta^3}{\exp(C_2\eta/T) - 1} \tag{11}$$

C_1 and C_2 are constant. Integrating Eq. (10) on the spectrum under the WSGG model assumptions, the total emittance becomes:

$$\varepsilon(T, p_a S) = \sum_{i=1}^{I} a_i(T)\left[1 - \exp(-\kappa_{p,i} p_a S)\right] \tag{12}$$

In this equation, $a_i(T)$ is the fraction of the blackbody emission in the $\Delta\eta_i$ bands of the spectrum, correlating emittance data and absorption coefficients. Temperature-dependent coefficients $a_i(T)$ can be used to solve general radiation problems, that is, considering variations in temperature and partial pressures of the participating species.

The total emittance is computed with the line-by-line (LBL) integration of Eq. (10) in the spectrum range between $0 < \eta < 30{,}000$ cm^{-1}. The LBL integration can be considered exact for the numerical approximation of integration of each line. The integrations are made based on HITEMP2010, a high resolution spectral database that provides spectroscopic parameters to generate the transition lines, and which is established for high temperature applications, including combustion gases such as H_2O, CO_2, CO and OH.

The coefficients used in the present study are valid for temperatures between 400 K and 2500 K, and were proposed in the work by Dorigon et al. (2013) for four gray gases and a mixture of carbon dioxide and water vapor with partial pressure ratio, obtained performing the adjustment of the total emissivity curves in relation to those calculated from the line-by-line integration of the spectral lines through HITEMP2010.

3.1.2 Global Radiative Heat Transfer Solution

Applying the WSGG model, the total radiation intensity in a certain direction can be quantified by simply adding the partial intensities I_i related to each gray gas:

$$I(\xi) = \sum_{i=1}^{I} I_i(\xi) \tag{13}$$

where the partial intensity I_i, in W/m^2, is obtained from the integration of RTE under the region of the spectrum corresponding to gray gas i:

$$\frac{dI_i(\xi)}{ds} = -\kappa_{p,i} p_a(\xi) I_i(\xi) + \kappa_{p,i} p_a(\xi) a_i(\xi) I_b(\xi) \tag{14}$$

In the above equation, the partial pressure of the participating species, $p_a(\xi)$, the temperature dependent coefficient, $a_i(\xi)$, and the total blackbody intensity, are evaluated for local conditions, that is, for temperature and concentration of the species participating in point ξ. Thus, although the WSGG model assumes that the absorption coefficient is constant, the method can be applied to non-isothermal and non-homogeneous media (Dorigon et al., 2013).

3.1.3 Turbulence-radiation interaction (TRI)

Experiments showed that the radiative properties of a turbulent flame would be incorrect if the turbulent fluctuations were neglected and that disregarding the TRI interactions led to underestimated values for radiation heat transfer (Amin and Foster, 1973; Coelho, 2002; Li and Modest, 2002). Moreover, numerical studies from Habibi et al., (2007a) and (2007b) indicated that radiation does not affect the structure of the flame, in the sense that the fields of velocities, temperatures and concentrations of species are very little affected even with the inclusion of the TRI interactions, obtaining the result of the decrease in the average temperature in regions of high temperature, and concluding that emission is the dominant process in optically thin flames.

The most important terms for modeling the TRI effects are the correlation between the absorption coefficient and the temperature and the temperature autocorrelation (Li and Modest, 2002a and 2002b; Gupta et al., 2013). Accordingly, the relation below was incorporated in the emission term of the RTE:

$$\overline{\kappa T^4} = \overline{\kappa}\,\overline{T^4}\left(1 + C_{TRI1}\,6\frac{\overline{T'^2}}{\overline{T}^2} + C_{TRI2}\,4\frac{\overline{T'^2}}{\kappa}\left.\frac{\partial \kappa}{\partial T}\right|_{\overline{T}}\right) \tag{15}$$

Equation (14) is an approximation proposed by Snegirev (2004), and derives from decomposition of temperature and absorption coefficient in medium and floating components considering the time average of the RTE. The variance of the temperature fluctuation due to turbulence is included in the problem with an additional transport equation, solved together with the governing flow equations.

The modeling of the additional TRI equation is implemented by a routine in C language in Ansys Fluent, which together with the routine of the WSGG model and the parameters available by the CFD, compute the radiation emitted by the flame.

Modeling of thermal radiation in turbulent flames has received continuing attention in the literature. Despite the recognized importance of the turbulence-radiation interaction (TRI) (Lemos et al., 2020), numerical simulations using current radiation models available in commercial CFDs most often neglect TRI effects (Deon et al., 2015; Deon et al., 2016). In general, the characteristics and limitations of the TRI models are intrinsically related to the different approaches for the treatment of turbulence itself. As such, TRI models have been presented and analyzed in the framework of RANS approach (Snegirev, 2004; Centeno et al., 2016; Yi et al., 2017), of the large eddy simulation (Gupta et al., 2013; Fraga et al., 2017), and of the direct numerical simulation (Silva Freire et al., 2002; Wu et al., 2005). For a more general overview of the developments of TRI in the literature, it can be recommended the works by Modest (2005); Coelho (2007); and Coelho (2012).

3.2 Discrete Ordinates Method – DOM

The discrete ordinate method is based on a discrete representation of the directional dependence on radiative intensity. Thus, the solution to the problem of radiative transport is found by solving the RTE for a set of discrete directions that total the solid angle 4π. The RTE is then written for each discrete directional ordinate and its integral terms are replaced by numerical squares added for all discrete directions. More details and information about the DOM are found in Centeno (2014).

In this work, 80 angular discretization were used, a number considered sufficient to obtain the solution, according to tests carried out in Lemos (2020), with an average percentage deviation of less than 1% in relation to greater discretization.

4. COMBUSTION MODELING

Among the available models in ANSYS Fluent, the Non-Premixed Combustion - with Steady Laminar Diffusion Flamelet (SLDF) and Chemical Equilibrium approaches were analyzed.

4.1 Non-premixed combustion

This model is available only for turbulent flows. This modeling allows thermochemistry to be reduced by a single parameter: the mixture fraction, which is based on atomic elements conservation in chemical reactions.

The mixture fraction f defines the thermochemical state of the flow by a scalar quantity that is conserved, taking on firstly the value 0 in the oxidizer flow, 1 in the fuel flow and values between 0 and 1 during the flow. It can be written in terms of atomic mass fraction:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \tag{16}$$

where Z_i are the atomic masses of elements i that are present in the fuel and oxidizer flows. Thus, combustion is simplified as a mixture problem, avoiding difficulties about non-linear average rates of chemical kinetics reactions. The species conservation equation can be reduced to a single equation for the mixture, under the assumption of equal diffusivities, acceptable to turbulent flows in which turbulent convection overcomes the molecular diffusion.

4.1.1 Steady Laminar Diffusion Flamelet (SLDF)

The Steady Laminar Diffusion Flamelet (SLDF) model is the option of mixture close to chemical equilibrium, representing the flame by a group of almost one-dimensional laminar elements called flamelets. Physically, flamelets are the smallest scale that are not perturbed by viscosity. This approach allows the dissociation of the convective and reactive parts of the flow, even if turbulent. Each flamelet is subjected to local conditions in the flow, resulting in its convection and stretching, but without destroying its laminar internal structure (Deon, 2016).

In addiction with some other variable that can account for the departure of equilibrium condition, like temperature, density, and species mass fractions, the mixture fraction for this model must be able to describe the flame local structure, requiring detailed chemical kinetics mecanisms codes, such as GRI-Mech3.0, used in the present study, with 53 species and 325 chemical reactions. The variables are solved, tabulated and stored on a data base to be recovered during the simulation.

4.1.2 Chemical Equilibrium

Once mixed, the chemistry can also be modeled as being in chemical equilibrium – the situation in which the ratio between chemical reactants and products remains constant over time – with the species concentrations being determined from the mixture fraction using this assumption, being not necessary the inclusion of a large number of reactions and dissociations intermediate steps, as the SLDF model. For these simulations, was chosen the mechanism JL_(1988) with four intermediate steps, totalizing 7 species.

4.2 Probability Density Function (PDF)

The turbulence effects are incorporated into results obtained for temperature, density and species mass fractions from laminar flamelets or chemical equilibrium solution through Probability Density Function (PDF), which provides a statistic description of flow scalars fluctuations. The model that is part of CFD code employed is the Beta Distribuction Function, which can be found in more detail in (Ren et al, 2018).

5. RESULTS AND DISCUSSION

Figure 2 shows the flames formed by the combustion of methane without considering radiation effects using the three different approaches. The contours follow the decreasing color scale from red to green. When enabling the WSGG radiation model without TRI, the maximum temperatures for the chemical equilibrium and flamelets models decrease from 1682 K to 1500 K and from 1674 to 1526 K, respectively. Implementing the TRI model, these temperatures drop further to 1460 K and 1488 K. These results are presented in Table 1. As expected, the temperatures dropped with the inclusion of the radiation calculation and reduced even more including TRI effect.

In order to analyze the behavior of the temperature contours in both models, Figure 3 shows the temperature along the center line, which comprises the central point of the exit of the burner to the end of the domain extension. It can be seen from the figure that the largest differences occur in the peak region, about 1 m from the burner outlet. Despite the little difference between the maximum temperature values, there was a shift in the peak of the curve with the CE model in relation to the SLDF model, showing an important effect of simplifying the chemical kinetics mechanism.

Table 1. Maximum temperatures reached for the models, considering or not the radiation and TRI effects.

Model	Maximum temperature without radiation effects	Maximum temperature with radiation effects	Maximum temperature with radiation and TRI effects
CE	1682 K	1500 K	1460 K
SLDF	1674 K	1526 K	1488 K

Since the participating species H_2O and CO_2, at high temperature, are the main responsible for the effects of absorption and radiation emission, Figures 4 and 5 show the concentrations, in mole fraction, of H_2O and CO_2 in the mixture. The molar fractions of water vapor for the CE and SLDF models followed similar behavior in relation to the displacement of the peak temperatures, where their maximum concentrations also varied, being underestimated with the

CE model. The peak in the concentration of CO_2 was also underestimated for the CE model, but became similar along the rest of domain. These results also explain the shift in the peak temperatures.

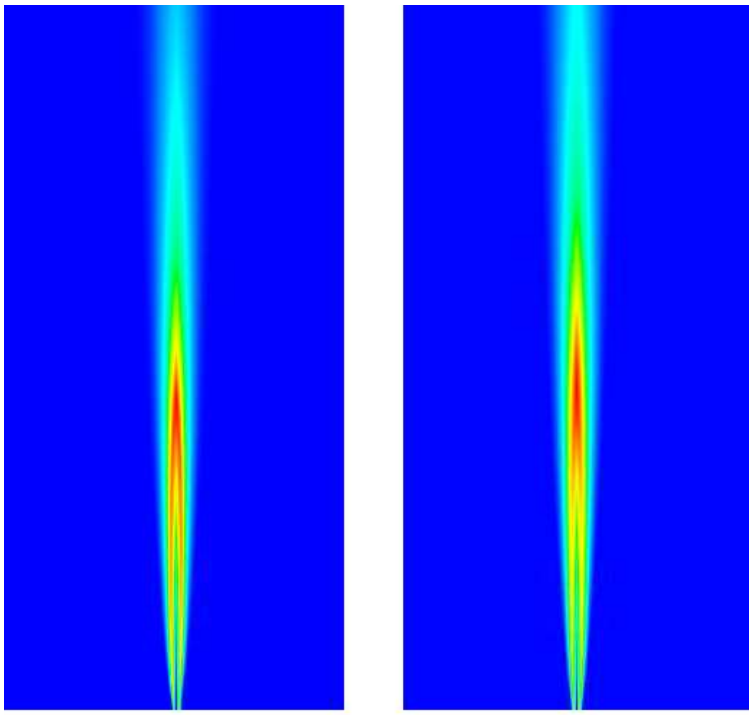

Figure 2. Contours of flame temperatures formed by the combustion of methane. a) Chemical equilibrium - T_{max} = 1682 K; and c) Flamelets - T_{max} = 1674 K.

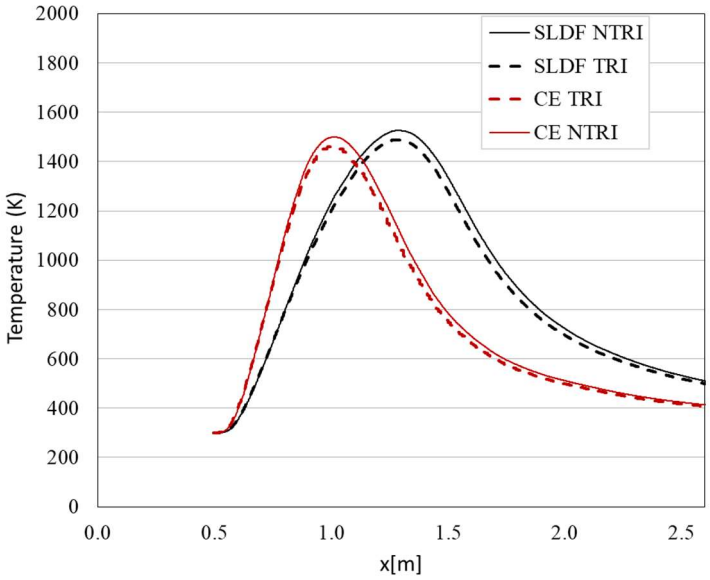

Figure 3. Temperature variation along the center line.

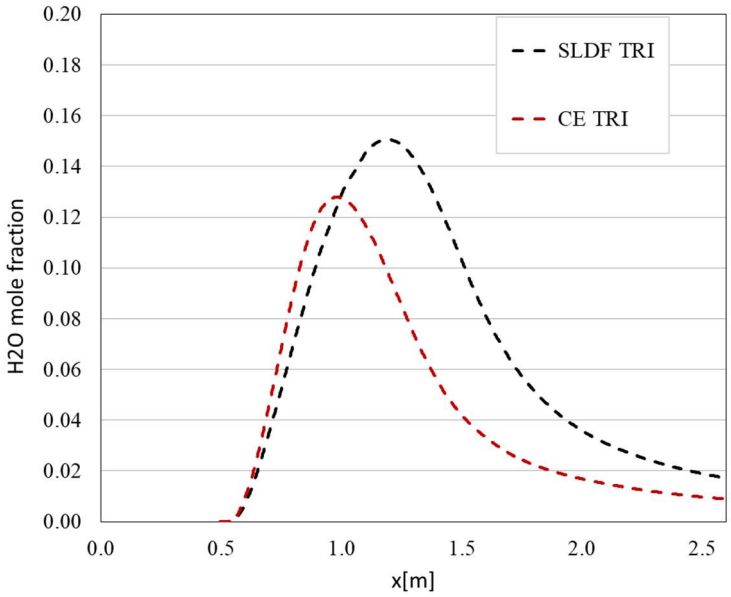

Figure 4. H_2O variation along the center line.

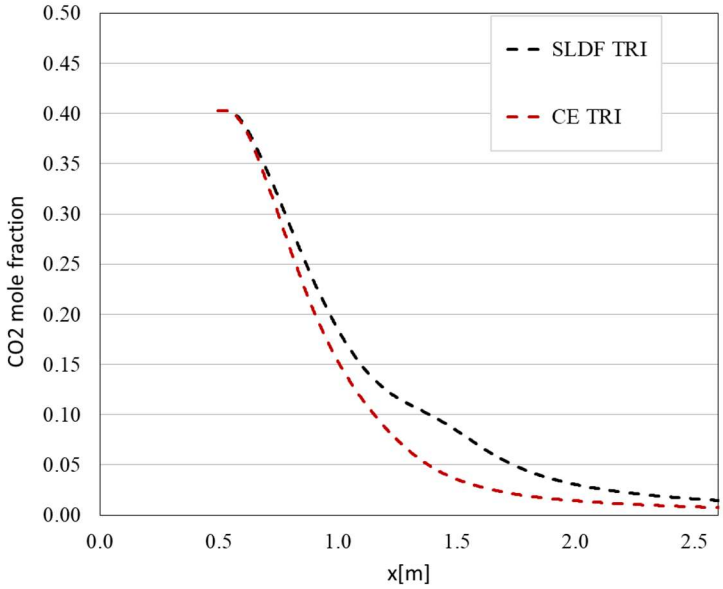

Figure 5. CO_2 variation along the center line.

The radiative heat flux is plotted in Figure 6 in comparison with the experimental data, which was measured along a line parallel to the flame main axis at a radial distance of $0.5 \times L_f$. As seen, for all cases the radiative heat flux increases to a maximum value around the half length of the flame, at about 1.0 m, then decreases continuously as the point of measurement moves away of the flame. There was a significant discrepancy between the radiative fluxes obtained from using the different chemical models, which results mostly from the differences in the temperature and participating species fields for each case. It can also be seen in the figure that the computed radiative were considerably lower than the experimental data for the case without considering TRI effects, which is known to considerably increase the radiative transfer.

Therefore, the inclusion of TRI increased the radiative heat flux, which led to improvement in the accuracy in comparison to the experimental results in Figure 6. An important point to consider is that the computational domain for all the models was configured to be adapted in order to capture the main gradients during combustion simulation. This step was carried out before coupling the radiation mechanism, which smoothes out the gradients. This adaption consists on refining those cells in which there were the largest gradients due to combustion reactions, increasing, therefore, the

mesh elements number before considering the radiation effects, making the simulation more accurate. The adaption of mixture fraction, temperature, axial and radial velocity, CO_2 and H_2O mass fractions, density, turbulent kinetic energy, among others parameters, provides a rise of 47 % in elements number (41.600 to 61.337) for the SLDF model and 34 % (41600 to 55926) for the CE model.

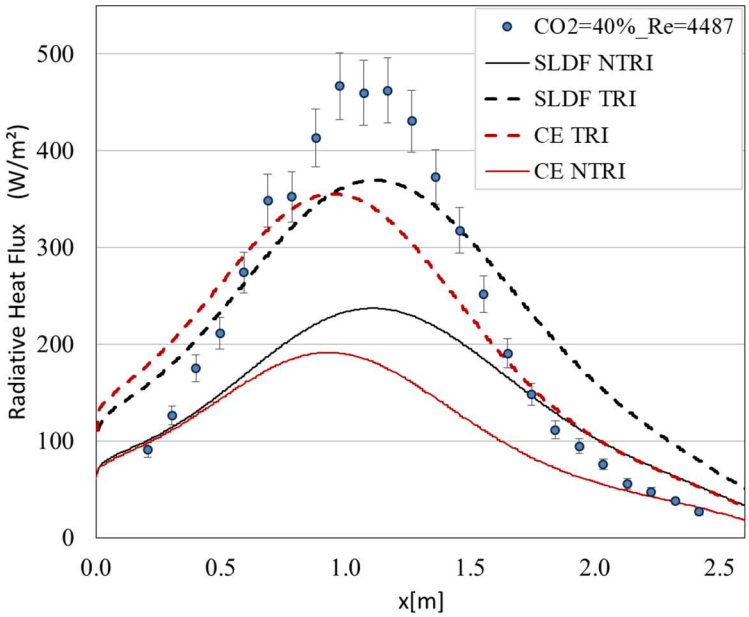

Figure 6. Radiative heat flux experimental and for the four models at a radial position of $0.5L_f$.

6. CONCLUSIONS

A turbulent methane flame was simulated with different combustion models and detailed levels of chemical kinetics, in order to assess the sensitivity of the radiative heat flux to these different chemical models. The problem showed high sensitivity to changes and simplifications, mainly in the behavior of temperature and flow, making it clear the importance of selecting different combustion models and chemical kinetics in the simulation of flame radiation.

As presented, temperatures dropped with the inclusion of the radiation calculation, even when it is not considered the turbulence-radiation interaction (TRI) effects in the solution of the governing equations. Including TRI effects reduced even more the temperature of the flame, but had less impact on the concentration species in relation to case without TRI. For the radiative heat flux, with the inclusion of TRI, as expected, the curve approximated of the experimental data.

The mesh adaptation for the SLDF model led to a greater refinement than for the CE model. This may have been caused by the greater number of species present in the SLDF and the simplification by chemical equilibrium of the CE model, causing greater variations in the mixture fraction. To assess the quality of the numerical solutions presented in this article, a verification process based on the grid convergence index (GCI) could also be applied.

The CE model can solve more detailed mechanisms of chemical kinetics than that of four steps used, but a different numerical adjustment is needed from what was being used, because for this model with more detailed mechanisms, convergence was not possible with the numerical parameters used in the simulation. Another suggestion is to simulate the case by changing the combustion model for Species Transport - Eddy Dissipation, which solves conservation equations for each chemical species and considers reaction rates as governed by turbulence, which allows neglecting a detailed reaction mechanism and assume an instant reaction after mixing. Finally, in order to use a more detailed turbulence mechanism, it would be necessary to use the Large-Eddy Simulation (LES) model instead of the RANS Reynolds averages. This would allow to use the Eddy Dissipation Concept (EDC), which allows precise calculations of Arrhenius reactions for intermediate reaction steps.

7. ACKNOWLEDGEMENTS

AGF thanks CAPES due to its financial support. LDL thanks CNPq due to its financial support. LGPR thanks CAPES due to its financial support. FHRF thanks CNPq for research grant 302686/2017-7.

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