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COMPARISON BETWEEN MIXTURE FRACTION AND SPECIES TRANSPORT COMBUSTION APPROACHES THROUGH RADIATIVE TRANSFER ANALYSIS IN TURBULENT FLAMES

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Abstract. *The simulation of a turbulent methane-air flame was carried out using the Computational Fluid Dynamics Ansys Fluent, with different combustion models, in order to evaluate the sensitivity of the radiative transfer equation with respect to the rate of formation of the participating chemical species. The combustion was solved with three different mechanisms: the Non-Premixed Combustion - Steady Laminar Diffusion Flamelet (SLDF) model with detailed reaction mechanism; the Non-Premixed Combustion - Chemical Equilibrium (CE) model; and finally with the Species Transport - Eddy Dissipation (ED) model, both last based on simpler mechanisms of reactions. The turbulence was resolved through the k-ε standard model. For the radiation calculation, the weighted-sum-of-gray-gases (WSGG) was implemented as the spectral model, with the discrete ordinates method (DOM) to solve the spatial-directional part of the problem. This study considered the correlation between the absorption coefficient and the temperature as well as the temperature self-correlation to account for the effects of turbulence-radiation interaction (TRI). As main results, the three models presented better comparisons with experimental data with inclusion of TRI effects and for the CE and ED models there was a shift in temperature, species concentration and radiative heat flux profiles in comparison to SLDF model, corresponding to the model for which it is used the greater detail of the chemical kinetics.*

Keywords: *mixture fraction, SLDF, eddy dissipation, WSGG, turbulence-radiation interaction, CFD.*

1. INTRODUCTION

In the oil and gas industry, thermal radiation is most often the main heat transfer mechanism in combustion processes due to the formation of participating gases at high temperatures. In industrial applications, as well under natural conditions, turbulent flows are more common, and, combined with chemical reactions, benefits reactant mixing and heat transport. Therefore, the study of turbulent flames from gas combustion is of great importance, aiming improvements in energy efficiency, minimization of environmental impacts and guarantee of process safety.

The problem under investigation consists of computing the radiation transfer in a turbulent flame, comparing the numeric results to experimental measurements. Computational analysis of thermal radiation requires modeling the fluid flow, turbulence, chemical kinetics and combined heat transfer. The main objective of this study is to test different approaches for modeling the gas combustion process, which vary the complexity of the chemical kinetics mechanisms, thus assessing the sensitivity of the calculation of the radiative heat flux with respect to the choice of the chemistry kinetics.

Combustion and chemical kinetics were solved by the Steady Laminar Diffusion Flamelet (SLDF) model, which considers the flame as a group of almost laminar, one-dimensional structures, formalized by Peters (1984) and still present in recent contributions (Deon, 2016). Subsequently, it was switched to the Chemical Equilibrium and Species Transport models, both requiring simpler reaction mechanism, to evaluate the sensitivity of the problem to chemical kinetics. The chosen model for turbulence was the standard k-ε, which uses two conservation equations to determine turbulent viscosity. presenting accurate results in Pember et al. (1996); Gomes et al. (1997) and Deon (2016).

The discrete ordinates method (DOM) was used for the spatial-directional integration of the radiative transfer equation (RTE) (Modest, 2003; Bidi et al., 2008), based on a discrete representation of the directional dependence of the radiative intensity, while the spectral model was the weighted-sum-of-gray-gases (WSGG), which considers that the entire spectrum can be divided in a certain number of gray gases with constant pressure absorption coefficients (Smith et al., 1982; Gomes et al., 1997; Dorigon et al., 2013). The interaction of turbulence with radiation (TRI) was approximated using a combined correlation between the absorption coefficient and the temperature as well as an autocorrelation of the temperature proposed by Snegirev (2004) and employed in Krishnamoorthy, (2010a and 2010b).

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×*d*, corresponding to the burner length, plus 2.5×L_f, and radially of 0.5× L_f. This last dimension corresponds to the radial position for which there is experimental data of radiative heat flux. In turn, this data will be used for comparison with the results of the simulations carried out in the present study. The domain was set up in order to represent half of the real system; the full domain can then be obtained by simply revolutionizing the results around the 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 (3.1 m/s), the burner wall and the ambient pressure (air at 1 atm).

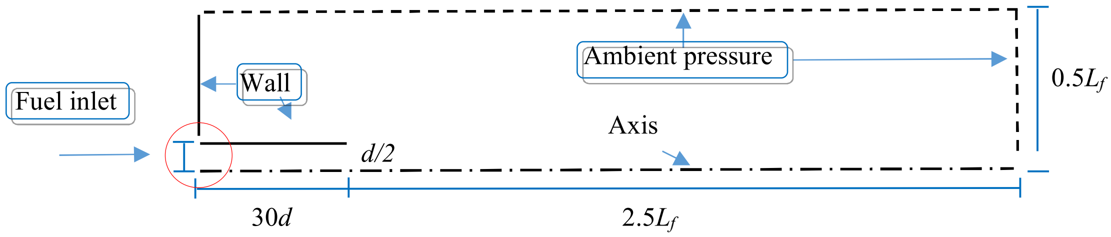


Figure 1. Geometric domain and boundary conditions. Available from: Sandia National Laboratories, 2017 – adapted by the authors.

For the numeric solution, the domain was discretized with greater refinement in the flame formation region, which corresponds to the output of the burner (30*d*) onwards. The conservation equations related to reactive flows was solved through the Finite Volume Method – FVM for each element resulting from the discretization of this domain.

2.2 Mathematical and physical modeling

Due to the property fluctuations caused by turbulence, the conservation equations need to be solved through Favre decomposition, which expresses the instantaneous value of a scalar in an average value and a fluctuation; 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 mass conservation results in:

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

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

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

where τ is 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. 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 standard 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 Pope (1978) and Morse (1980).

The chemical species mass is conserved according to the equation:

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

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:

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

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}:

$$S_{rad} = -\nabla\cdot\vec{q}_r \quad (6)$$

2.3 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 the space and in the wavenumber spectrum. With the RTE, it is possible to determine the increase in intensity due to emission and due to scattering in the direction of the intensity path as well as the effects of intensity attenuation due to absorption and scattering in other directions. The variation in the intensity due to scattering is neglected in this study, as there is no significant formation of particulates.

2.3.1 Radiative Transfer Equation

The spectral radiative transfer equation for a medium that emits and absorbs energy along a given path is given by:

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

where $I_\eta(\xi)$ and $I_{\eta b}(\xi)$ are the spectral intensity travelling along the path and the spectral intensity of the blackbody at the medium temperature in position ξ; 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.

2.3.2 Application of the WSGG Model in the Radiative Heat Flow 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 wavenumber 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:

$$\kappa_{\eta,a} = \kappa_{\eta,CO_2} + \kappa_{\eta,H_2O} \quad (8)$$

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; p_a is the total partial pressure of the species, $p_a = p_{H2O} + p_{CO2}$.

The total emission of the medium along a given path of length *S,* for an isothermal and homogeneous medium, is defined for the WSGG model 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 emission 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 the above equation, $a_i(T)$ represents the fraction of the blackbody emission in the $\Delta\eta_i$ bands of the spectrum. 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 emission 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 carried out using 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 were obtained 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 emission curves in relation to those calculated from the line-by-line integration of the spectral lines through HITEMP2010.

2.3.3 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 over the regions of the spectrum corresponding to each 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).

2.3.4 Turbulence-radiation interaction (TRI)

Experiments show that the radiative transfer of a turbulent flame would be incorrect if based solely on the average temperature field; disregarding the TRI interactions lead to considerably underestimated values for radiation heat transfer [Amin and Foster, 1973; Coelho, 2002; Li and Modest, 2002]. 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. On the other hand, it was observed a decrease in the average temperature in regions of high temperature, and that emission was 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 also the temperature autocorrelation [Li e Modest, 2002a e 2002b; Gupta et al., 2013]. Accordingly, the relation below was incorporated in the emission term of the RTE:

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

Equation (15) is an approximation proposed by Snegirev (2004), and can be derived from decomposing the temperature and the medium absorption coefficient in mean and fluctuating components considering the time average of the RTE after integration into the spectrum. 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 was implemented by a user defined function (UDF) in C language in Ansys Fluent, which, together with another UDF for the WSGG model and the parameters available in 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).

2.4 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 cover all the directions, with the solid angles summing up 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 Modest (2003).

In this study, 80 angular discretization were used, which was found to be sufficient according to mesh quality tests carried out in Lemos (2020), with an average percentage deviation of less than 1% in relation to greater discretization.

2.5 Combustion Modeling

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

2.5.1 Non-Premixed Combustion - Mixture Fraction Approach

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 regarding 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 overwhelms molecular diffusion.

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, the flamelets. Physically, flamelets are the smallest scale that is not perturbed by viscosity. This approach allows the dissociation of the convective and reactive parts of the flow, even in turbulent flows. Each flamelet is subjected to local conditions in the flow, resulting in its advection and stretching, but without destroying its laminar internal structure (Deon, 2016). In addition 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 mechanisms 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.

Chemical Equilibrium (CE). 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, it was chosen the mechanism JL (1988) with four intermediate steps, totalizing 7 species.

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 Deon (2016).

2.5.2 Species Transport

Switching the combustion model to Species Transport, the ANSYS Fluent solve the conservation equations for each chemical species. The total mass fraction of each specie, Y_a, is estimated through the solution of equations for N-1 species, in which N is the total number of fluid phase chemical species that are present in the system. Since the sum of species mass fractions must be the unit, the mass fraction N_{th} is determined as 1 minus the sum of N-1 mass fractions that are solved. To minimize the numerical error, the selected N_{th} species must be those with the highest general mass fraction, as the case of N_2 when the air is the oxidizer.

Eddy Dissipation (ED). The Eddy-dissipation model was based on Magnussen and Hjertager, 1976; it assumes the reaction rates as controlled by turbulence. It is responsible for turbulence-chemical kinetics interaction under the assumption that, in this condition, the fuel reacts quickly, allowing neglecting detailed chemical reactions mechanism, and admitting instantaneous reaction after mixing. The production rate of specie k due to reaction r, $\dot{\omega}_{k,r}$, is given by the lesser of the two expressions:

$$\dot{\omega}_{k,r} = v'_{k,r} M_{w,k} A \rho \frac{\varepsilon}{k} \min\left(\frac{Y_R}{v'_{R,r} M_{w,R}}\right) \tag{17}$$

$$\dot{\omega}_{k,r=} v'_{k,r} M_w A B \rho \frac{\varepsilon}{k} \frac{\sum Y_P}{\sum_k^N v''_{k,r} M_{w,k}} \tag{18}$$

where $v'_{k,r}$ are the stoichiometric coefficients, Y_P is the products mass fraction, Y_R is the reactants mass fraction and A and B are constants, equals to 4 e 0,5, respectively. In this model the chemical reaction is governed by $\frac{k}{\varepsilon}$, which represents the mixture in a scale of time, and combustion starts whenever turbulence is present in the flow ($\frac{k}{\varepsilon}$ >0). This avoids the computationally heavy Arrhenius calculations (finite rate option) for chemical kinetics; as these calculations determine the reaction mechanism parameters, for correct estimates only one or two intermediate steps must be used. To include detailed chemical kinetics mechanisms, Ansys Fluent offers the Eddy-Dissipation-Concept (EDC) model, but this model is more appropriate for the approach Large-Eddy Simulation (LES) of turbulence, in which the smallest chemical kinetics scales are modeled.

3. RESULTS AND DISCUSSION

Table 1 shows the results for the maximum temperatures reached for the three models of combustion and chemical kinetics. It also presents the comparison of the effects in the temperature of including the calculation of thermal radiation in the simulation with and without TRI. When enabling the WSGG radiation model, the maximum temperatures for all the models decreases around 10%, in relation to the case that do not consider radiation effects. Including TRI effects, the maximum temperatures decrease more on average 4% compared to the case with only WSGG radiation model without TRI effects.

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

Model	Maximum temperatur e without radiation effects (K)	Maximum temperature with radiation effects (K)	Maximum temperature with radiation and TRI effects (K)
ED	1940	1767 (↓ 9%)	1661 (↓ 6%)
CE	1681	1499 (↓ 11%)	1460 (↓ 3%)
SLDF	1674	1526 (↓ 9%)	1488 (↓ 2%)

These results are also shown in Figure 1 in order to analyze the behavior of the temperature contours for the three models in 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 temperature peak region, about 1 m from the burner outlet. Despite the little difference between the maximum temperature values of the models SLDF and CE, there was a shift in the peak of the curve with the CE model in relation to the SLDF model, showing a first consequence of the simplification in the chemical kinetics mechanism. The Eddy Dissipation model was the one that most distanced itself from the others, which presented lower temperatures and greater smoothing at the peak of the curves.

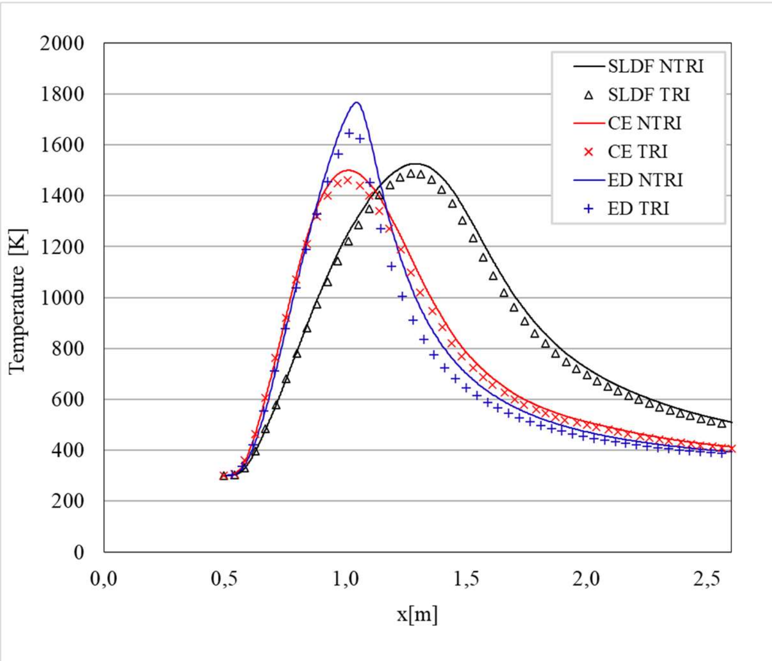
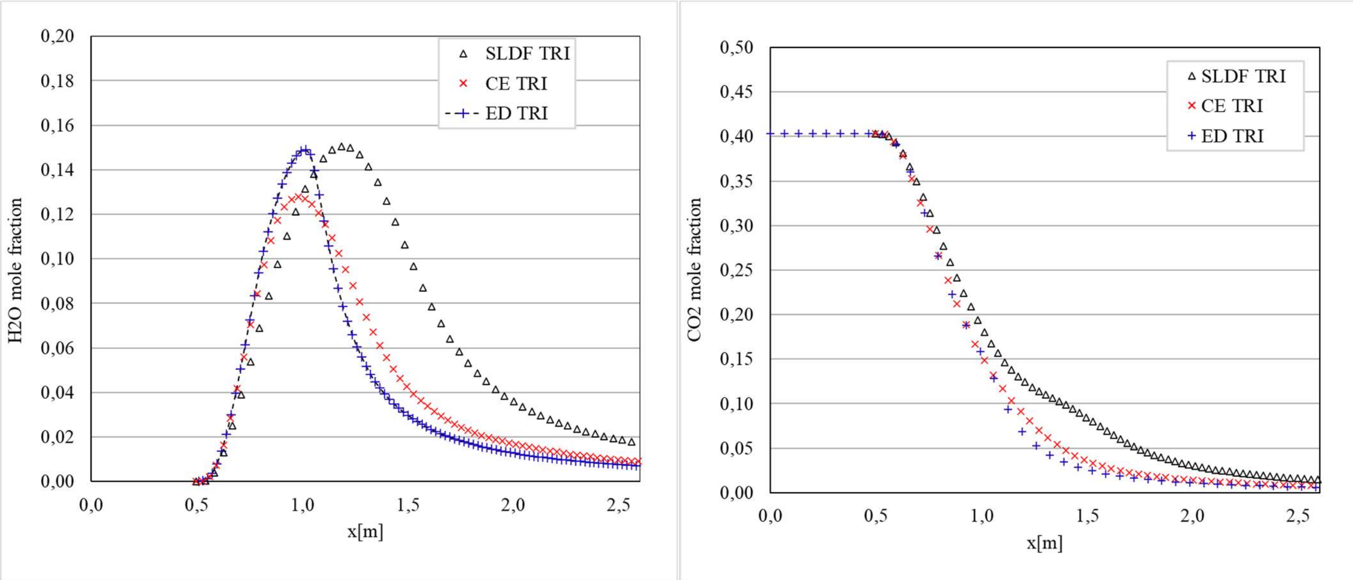


Figure 1. Graph of temperatures in the center line.

Since the participating species H_2O and CO_2 are the main responsible for the effects of absorption and radiation emission, Figures 2 and 3 show the concentrations, in mole fraction, of H_2O and CO_2 in the mixture. The molar fractions of water vapor for the CE, ED and SLDF models followed similar behavior in relation to the displacement of the peak temperatures, where their maximum amount also varied, being underestimated in the CE model. The amount of CO_2 was again underestimated for the CE and for ED model but got similar along the rest of domain. These results may explain the shift in peak temperatures. One observation is that these last graphs do not bring the comparison between the cases with and without TRI effects, as the result curves were superimposed, confirming what was seen in section 2.3.4 about optically thin flames - characteristic of the flame of this and the aforementioned studies - for which the term chemical source is much larger than the term radiative source, explaining the small impact on the flame structure.



a) b)

Figure 2. a) H_2O concentration in the center line. b) CO_2 concentration in the center line.

The curves of the radiative heat flux are plotted in Figure 3 in comparison to 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 species concentration fields for each case. For instance, since the eddy dissipation model led to the highest temperature in the flame, the radiative heat flux from this model was the highest. It can also be seen that the computed radiative were considerably lower than the experimental data for the case without considering TRI effects (NTRI), which is known to considerably increase the radiative transfer.

Therefore, the inclusion of TRI increased the radiative heat flux, which led to the numerical solutions to move towards the experimental results in Figure 3. However, there is still an important overall discrepancy between the numerical solutions and the experimental data.

4. CONCLUSIONS

A turbulent methane-air flame was simulated with different combustion models and levels of chemical kinetics. As seen, for the three models 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, since turbulence foments the heat transport, meaning an increase in the emission of thermal radiation (heat loss by the flame) and a consequent decrease in temperature.

The TRI effects had less impact on the species concentration in comparison to case without TRI. For the radiative heat flux, with the inclusion of TRI, as expected, the curve approximated of the experimental data in all cases.

As to assess the sensitivity of the radiative heat transfer with respect 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 in the simulation of flame radiation, representing as one of the main points the different chemical kinetic mechanisms used, with their respective number of intermediate steps and species involved in the reactions. One major challenge for future analyses will be establishing the role of the different aspects of modeling (turbulent transport, combustion kinetics, gas spectral model and turbulence-radiation interactions) on the global deviation with the experimental data.

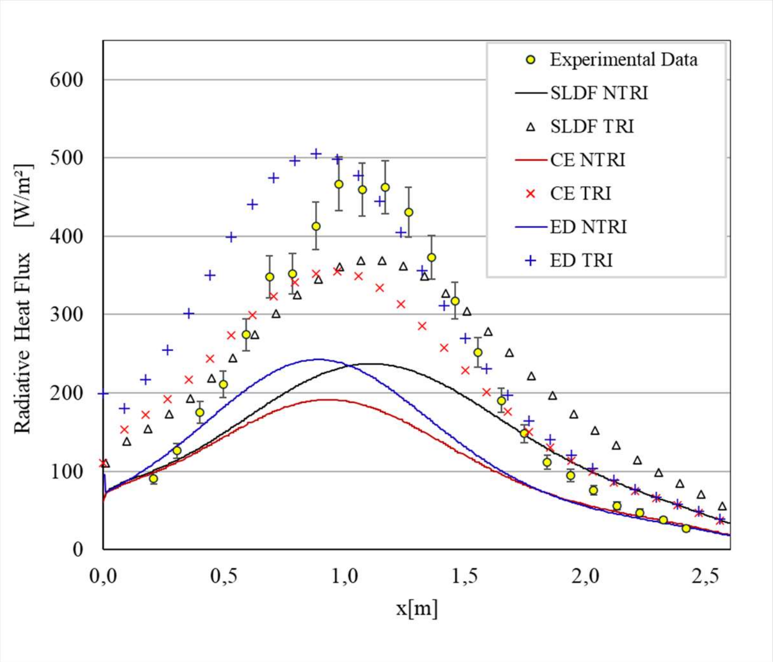


Figure 3. Radiative heat flux experimental and for the three models at a radial position of $0.5L_f$.

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