ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

EVALUATION OF TURBULENCE-RADIATION INTERACTIONS MODEL CORRELATIONS ON RANS SIMULATIONS OF A 2D AXISYMMETRIC TURBULENT NON-PREMIXED METHANE-AIR FLAME

Felipe Roman Centeno, frcenteno@mecanica.ufrgs.br
Guilherme Velasco, guilherme@mecanica.ufrgs.br
Francis Henrique Ramos França, frfranca@mecanica.ufrgs.br
Department of Mechanical Engineering - Federal University of Rio Grande do Sul - UFRGS
Sarmento Leite St., nº 425, Cep 90050-170, Porto Alegre, RS, Brazil

Cristiano Vitorino da Silva, cristiano@uricer.edu.br
Department of Mechanical Engineering – Universidade Regional Integrada do Alto Uruguai e das Missões - URI

Abstract. *Turbulence-radiation interactions effects are estimated using WSGG model based on new correlations for a turbulent non-premixed methane–air flame, evaluating the importance of the absorption coefficient – temperature correlation and the temperature self-correlation on the overall thermal behavior. Comparing results from the simulations (calculations with/without radiation, with/without TRI, with both absorption coefficient – temperature correlation and temperature self-correlation, and only with temperature self-correlation), it is verified that temperature, radiative heat source, and radiant fraction are importantly affected by thermal radiation, independently of the TRI correlation that is employed. The major conclusions of this investigation are: (i) for the currently studied flame, it is indispensable to consider thermal radiation in the calculations; (ii) the TRI effect can be properly modeled by the TRI approximation that considers the temperature self-correlation only.*

Keywords: *Radiation, WSGG model, Combustion, Turbulent non-premixed flames, Turbulence-Radiation Interactions*

1. INTRODUCTION

In diffusion flames the fuel and oxidant are initially separated and the combustion is controlled by diffusion. Since combustion problems involve a number of coupled phenomena, such as chemical kinetics, fluid flow, soot production and heat transfer, an accurate prediction of the thermal radiation heat transfer in participating medium, the dominant heat transfer mechanism in some combustion systems, is necessary to achieve appropriate solutions for this complex phenomena. Heat transfer can directly affect the chemical kinetics, in this way, accurate description of radiative heat transfer is a crucial element in simulations of turbulent combustion systems. On the other hand, its modeling is a difficult task due to the highly complex dependence of the absorption coefficient with the wavenumber, which is typically characterized by several thousands of spectral lines. Thus, the solution of the radiative transfer equation (RTE) is very expensive or even impossible without a model to solve the spectral problem. As a simplification, in the numerical models to predict the gas combustion processes, the RTE is frequently solved with the gray gas (GG) model, where the dependence of the absorption coefficient over the wavenumber is neglected. In order to provide better results, spectral or global models are commonly used. Among the global models, the weighted-sum-of-gray-gases (WSGG) (Hottel and Sarofim, 1967) is a method that is still widely used nowadays, especially in global simulation of combustion processes in which the RTE is solved together with fluid flow, chemical kinetics and energy equation. In the WSGG model the entire spectrum is represented by a few bands having uniform absorption coefficients, each band corresponding to a gray gas. The weighting coefficients account for the contribution of each gray gas, and correspond to the fractions of the blackbody energy in the spectrum region where the gray gases are located. In practice, those coefficients are obtained from fitting experimental data, such as those presented in Smith et al. (1982) and Smith et al. (1987). In a recent study, Demarco et al. (2011) assessed several radiative models (narrow band, wide band, gray gas and global models as the WSGG and the SLW) and stated that the WSGG formulation is also very efficient from a computational view and yields considerably improved predictions, but can lead to significant discrepancies in high soot loadings. Simplified radiative property models, such as the WSGG or GG models are often used in computational fluid dynamics (CFD) to simulate combustion problems. The main reason is that implementing more sophisticated models may become extremely time consuming when fluid flow/combustion/radiative heat transfer are coupled. As an example, Bidi et al. (2008) solved the RTE using the WSGG model to compute non-gray radiation effect of combustion gases in a cylindrical chamber, with the purpose of studying the radiation effect on the flame structure.

Several researchers have studied new WSGG correlations for application in combustion systems. Taking into account that a limitation of the WSGG is that its correlations coefficients are established for particular ratio of partial pressures for CO_2 and H_2O mixtures, Krishnamoorthy (2010a) obtained new WSGG parameters computed from total emissivity correlations encompassing the range of the H_2O/CO_2 ratios encountered within Sandia Flame D. With the same motivation, Johansson et al. (2011) modified the WSGG to account for various ratios of H_2O and CO_2

ISSN 2176-5480

concentrations, covering from oxyfuel combustion of coal, with dry or wet flue gas recycling, as well as combustion of natural gas. Dorigon et al. (2013) obtained new WSGG temperature dependent weighting factors polynomial coefficients and absorption coefficients fitted from HITEMP2010 molecular spectroscopic database (Rothman et al., 2010), which is the latest database available. Dorigon et al. (2013) tested those new coefficients against line-by-line (LBL) calculations in one-dimensional problems and found good agreement; also, Centeno et al. (2013) tested those coefficients against classical ones (Smith et al., 1982) in an axisymmetric cylindrical combustion chamber and found better agreement with experimental data.

Another complexity in turbulent combustion simulations is the so-called turbulence-radiation interactions (TRI). Turbulence and radiation are physical phenomena of high complexity even when analyzed independently. In turbulent reactive flows, temperature and species concentration fields can undergo high levels of fluctuations, leading to variations on the radiative field. In this manner, in this sort of flow it is not possible to deal with these phenomena in an independent way, but it is necessary to deal with them in a coupled form. The first theoretical investigation on TRI (Foster, 1969) had already shown that radiative properties of a turbulent flame would be incorrectly predicted if turbulent fluctuations were neglected from calculations, especially for high optical thickness mediums.

Numerical simulations of TRI can be decoupled or coupled. Decoupled calculations consider temperature and species concentrations distributions as inputs, i.e., they are taken from previous CFD solutions or from experimental data. Coupled calculations consider simultaneously all flow mechanisms, such as turbulence, heat transfer and combustion, so they are considerably more complex than the former. Decoupled calculations are presented in Hall and Vranos (1994), where results obtained from time-averaged RTE solution were compared to those obtained from a stochastic method for an one-dimensional problem; Krebs et al. (1994) studied TRI effect on radiation intensity from CO_2; in another work (Krebs et al., 1996), the investigation was focused on propane-air flames with the objective of analyzing the influence of temperature and species concentration fluctuations; Coelho (2002) and Coelho (2004) evaluated the accuracy of OTFA (Kabashnikov and Kmit, 1979) by comparing results obtained with this approximation and results from exact solutions of RTE. The first coupled calculation of radiative transfer in reactive flow to investigate TRI was reported in Song and Viskanta (1987), in which properties functions were prescribed for the combustion gases. Nowadays, some coupled researches can be found in the literature, in which most of them are focused on analyzing the most important TRI correlations (temperature self-correlation, absorption coefficient-temperature correlation, absorption coefficient self-correlation, absorption coefficient-radiation intensity correlation). Some examples of coupled investigations are reported in Li and Modest (2002a) and in Habibi et al. (2007a) for RANS simulations, and in Poitou et al. (2012) and in Gupta et al. (2013) for LES simulations. Results pointed that both absorption coefficient-temperature correlation and temperature self-correlation are the most important TRI terms in reactive flows (Li and Modest, 2002a, 2002b; Gupta et al., 2013; Habibi et al., 2007b). Furthermore, it was found in Gupta et al. (2013) and in Modest and Mehta (2006) that the absorption TRI term (correlation between absorption coefficient and radiation intensity fluctuations, which is neglected in OTFA) is important only for optically thick medium.

This work presents a numerical RANS simulation of turbulent non-premixed methane-air flame in a cylindrical combustion chamber taking into account radiation effect of non-gray gases by means WSGG correlations generated from HITEMP 2010 database (Dorigon et al., 2013) and including TRI (Snegirev, 2004). The TRI approximation adopted for the current investigation (Snegirev, 2004) takes into account both absorption coefficient-temperature correlation and temperature self-correlation, while the approximation employed in Krishnamoorthy (2010a, 2010b) takes into account the temperature self-correlation only, so the objective of this work is evaluating the importance of these two TRI correlations on the radiation modeling and, consequently, on the thermal behavior of the combustion chamber. For evaluation of the proposed solution, the case described in Garréton and Simonin (1994) was studied, since detailed spatial distributions measurements are available for major gas species concentrations as well as of the temperature field.

2. PROBLEM STATEMENT

The physical system consists of the natural gas combustion chamber that was analyzed in Centeno et al. (2013), Silva et al. (2007) and Magel et al. (1996), a test case proposed in Garréton and Simonin (1994). The cylindrical chamber has length and diameter of 1.7 m and 0.5 m, respectively, as shown in Fig. 1. Natural gas is injected into the chamber by a duct aligned with the chamber centerline. The burner provides the necessary amount of air and natural gas as required by the process. In all cases a fuel excess of 5% (equivalence ratio of 1.05) was prescribed. For a fuel mass flow rate of 0.01453 kg/s at a temperature of 313.15 K, this requires an air mass flow rate of 0.1988 kg/s, at a temperature of 323.15 K. The fuel enters the chamber through a cylindrical duct having 0.06 m diameter, while air enters the chamber through a centered annular duct having a spacing of 0.02 m. For such mass flow rates, the fuel and air velocities are 7.23 and 36.29 m/s, respectively. The Reynolds number at the entrance, approximately 1.8×10^4, points that the flow is turbulent. The inlet air is composed of oxygen (23% in mass fraction), nitrogen (76%) and water vapor (1%), while the fuel is composed of 90% of methane and 10% of nitrogen. The burner power is 600 kW. The fan and the other external components are not included in the computational domain, although their effects are taken into account through the inlet flow conditions. Buoyancy effects are neglected due to the high velocities.

ISSN 2176-5480

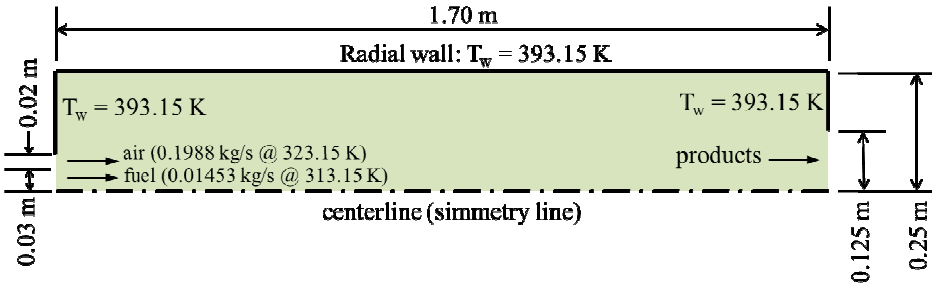

Figure 1. Combustion chamber geometry

3. MATHEMATICAL FORMULATION

The proposed work is stated as: considering a steady turbulent non-premixed methane-air flame in a cylindrical chamber, compute temperature, species concentrations and velocity fields, and verify the influence of different TRI correlations on the process.

3.1 Governing equations

Considering the conservation equation for steady incompressible flow in 2D axisymmetric coordinates for the generic variable ϕ, Eq. (1), the mass, momentum in the axial and radial directions, k-ε turbulence model, energy and chemical species conservation equations can be determined by choosing ϕ, Γ_ϕ, and source term S^ϕ from Table 1.

$$\frac{\partial}{\partial z}\left(\rho u\phi - \Gamma_\phi \frac{\partial \phi}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\rho v\phi - r\Gamma_\phi \frac{\partial \phi}{\partial r}\right) = S^\phi \tag{1}$$

On Table 1, the following variables are used: z and r are the axial and radial coordinates (in m), u and v are the velocities in these respective directions (in m/s), w is the angular velocity (in m/s), ρ is the density of the gaseous mixture (in kg/m³), μ is the gaseous mixture dynamic viscosity and μ_t is the turbulent viscosity (both in Ns/m²), defined as $\mu_t = C_\mu \rho k^2/\varepsilon$. The term $p^*=p-(2/3)k$ is the modified pressure (in Pa), C_μ is an empirical constant of the turbulence model (C_μ = 0.09), p is the combustion chamber operational pressure (p = 101325 Pa (Spalding, 1979)), and k (in m²/s²) and ε (in m²/s³) are the turbulent kinetic energy and its dissipation. Also, $C_{1,\varepsilon}$ and $C_{2,\varepsilon}$ are empirical constants of the turbulence model ($C_{1,\varepsilon}$ = 1.44 and $C_{2,\varepsilon}$ = 1.92), σ_k and σ_ε are the Prandtl numbers of the kinetic energy and dissipation, respectively (σ_k = 1.0 and σ_ε = 1.3). Pr_t and Sc_t are the turbulent Prandtl and Schmidt numbers, R_α (in kg/(m³.s)) is the volumetric rate of formation or destruction of the α-th chemical species (CH_4, O_2, CO_2, CO, H_2O) (this term is briefly discussed in the next section). T is the temperature of the gaseous mixture (in K). $\overline{MM}_\alpha$ (in kg/kmol) , $c_{p,\alpha}$ (in kJ/(kg.K)), h_α^0 (in J/kg) and $T_{ref,\alpha}$ (in K) are the molecular mass, the specific heat, the formation enthalpy and the reference temperature of each α-th chemical species. S_{rad} (in W/m³) is the radiative heat source term, computed as the negative divergence of the radiative heat flux (discussed later on this work).

In addition to the conservation laws presented in Table 1, an equation of state is required to calculate the mixture density. Considering the mixture of fuel, oxidant and products as an ideal gas, the equation of state may be written as $\rho = p/\bar{R}T\sum_\alpha y_\alpha/\overline{MM}_\alpha$, where $\bar{R}$ is the universal gas constant ($\bar{R}$ = 8.314 kJ/(kmol.K)), y_α (in kg_α/kg_{tot}) is the mean mass fraction of each α-th chemical species. Also, it is important to note that in the present work all quantities (as u, v, h, T, c_p, y_α, ρ, R_α, S_{rad}, etc.) are time-averaged (mean), but they are not written with an overbar (usual in RANS simulations) in order to not confuse with molar quantities (which are denoted with an overbar).

3.2 Combustion kinetic

As a basic assumption, it is considered that the combustion process occurs at finite rates with methane oxidation taking two global steps: $2CH_4 + 3\left(O_2 + 3.76N_2\right) \rightarrow 2CO + 4H_2O + 11.28N_2$ and $2CO + 1\left(O_2 + 3.76N_2\right) \rightarrow 2CO_2 + 3.76N_2$. The rate of formation or destruction, $R_{\alpha,c}$, of each α-th species in each c-th reaction (in this formulation there are two reactions, so c = 2) is obtained by the combined Arrhenius-Magnussen's model (Eaton et al., 1999; Turns, 2000), in which the rate of formation or destruction of the chemical species are taken as the least one between the values obtained from Arrhenius kinetic rate relation or Magnussen's equations (Eddy Breakup) (Magnussen and Hjertager, 1977). This formulation was succesfully employed in Silva et al. (2007), Nieckele et al. (2001) and Centeno et al. (2013), where all model parameters are described in detail.

ISSN 2176-5480

The above mentioned two-equation chemistry assumption was employed in the current study for economy of the CPU time. While the two-equation chemistry assumption (and even one-equation) has been used with great success in combustion modeling, it should be recognized that detailed reaction mechanisms effects may be very important in several practical applications, especially those involving flame ignition and extinction, or those involving predictions of minor species such as soot, NO and other radicals, which are not the aim of the present work. Also, it was an assumption in the present work that the presently studied flame has negligible amount of soot.

The average volumetric rates of formation or destruction of the α-th chemical species, R_α, which appears in both the energy and species mass fraction equations, are then computed from the summation of the volumetric rates of formation or destruction in all the c-th reactions where the α–th species is present, i.e., $R_\alpha = \sum_c R_{\alpha,c}$.

Table 1. Generic variable, diffusive coefficient, source terms for the conservation equations

Equation	ϕ	Γ_ϕ	S^ϕ
Continuity	1	0	0
Axial momentum	u	$(\mu+\mu_t)$	$-\frac{\partial p^*}{\partial z}+\frac{\partial}{\partial z}\left(\mu_t\frac{\partial u}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial v}{\partial z}\right)$
Radial momentum	v	$(\mu+\mu_t)$	$-\frac{\partial p^*}{\partial r}+\frac{\partial}{\partial z}\left(\mu_t\frac{\partial u}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial v}{\partial r}\right)-\frac{(\mu+\mu_t)v}{r^2}+\frac{\rho w^2}{r^2}$
Turbulent kinetic energy	k	$\left(\mu+\frac{\mu_t}{\sigma_k}\right)$	$\left[\mu_t\left(2\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}\right)^2+2\left(\frac{\partial v}{\partial r}\right)^2+2\left(\frac{v}{r}\right)^2\right)\right]-\rho\varepsilon$
Turbulent kinetic energy dissipation	ε	$\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)$	$C_{1,\varepsilon}\left[\mu_t\left(2\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}\right)^2+2\left(\frac{\partial v}{\partial r}\right)^2+2\left(\frac{v}{r}\right)^2\right)\right]\frac{\varepsilon}{k}-C_{2,\varepsilon}\frac{\varepsilon^2}{k}$
Energy	h	$\left(\frac{\mu}{\mathrm{Pr}}+\frac{\mu_t}{\mathrm{Pr}_t}\right)$	$S_{rad}+\sum_\alpha\left[h_\alpha^0+\int_{T_{ref,\alpha}}^{T}c_{p,\alpha}dT\right]R_\alpha$
CH_4, O_2, CO_2, CO and H_2O mass fraction	y_α	$\left(\frac{\mu}{Sc}+\frac{\mu_t}{Sc_t}\right)$	R_α

3.3 Radiation modeling

The radiative transfer equation (RTE) for non-scattering media, in cylindrical coordinates, with the discrete ordinates method (DOM), is given by:

$$\frac{\partial I_\eta}{\partial s}=\mu\frac{\partial I_\eta}{\partial r}+\xi\frac{\partial I_\eta}{\partial z}-\frac{\varsigma}{r}\frac{\partial I_\eta}{\partial\varphi}=-\kappa_\eta I_\eta+\kappa_\eta I_{b\eta} \tag{2}$$

which, for diffuse-gray surface boundaries, is subjected to:

$$I_{\eta w}=\varepsilon_{\eta w}I_{\eta b}(T_w)+\frac{(1-\varepsilon_{\eta w})}{\pi}\int_{\hat n\cdot\hat s}I_\eta\left|\hat n\cdot\hat s\right|d\Omega \tag{3}$$

where μ, ς, and ξ are the directions, η is the wavenumber, $I_{\eta b}$ is the blackbody intensity, I_η is the intensity, and κ_η is the spectral absorption coefficient. In the right side of Eq. (2), the first and the second terms represent, respectively, attenuation due to absorption and augmentation due to emission. Once the RTE is solved, the radiative heat source, presented in the energy equation as S_{rad}, is calculated as:

$$S_{rad}=-\nabla\cdot\vec q_r=\int_\Omega\int_\eta(\kappa_\eta I_\eta-\kappa_\eta I_{b\eta})d\eta d\Omega \tag{4}$$

The spectral absorption coefficient (κ_η) is strongly dependent on the wavenumber, which for participating gases can involve several thousands of spectral lines. Therefore, solving Eq. (2) for all spectral lines is in general excessively time consuming for coupled solutions of the conservation equations. As such, gas models have been developed to solve the RTE quickly. A brief description of the gas model selected for the present analysis (WSGG model) is described below.

ISSN 2176-5480

3.3.1 The weighted-sum-of-gray-gases (WSGG) model

The original formulation of the WSGG model (Hottel and Sarofim, 1967) consists of expressing the total gas emittance as a weighted-sum-of-gray-gas emissivities. The emission weighted factors, $a_j(T)$, and the absorption coefficients, k_j, for the j^{th} gray gas were determined from the best fit of the total emissivity with the constraint that the a_j must sum 1. From a more general point of view, the WSGG model can be applied as a non-gray gas model (Modest, 1991), solving the RTE for the N_G (number of gray gases) plus one (j = 0, representing spectral windows where H_2O and CO_2 are transparent to radiation) for a clear gas:

$$\frac{dI_j}{ds} = -k_j I_j + k_j a_j(T) I_{b,j}(T) \tag{5}$$

in which the emission weighted factor $a_j(T)$ is given by,

$$a_j(T) = \sum_{i=1}^{5} b_{j,i} T^{i-1} \tag{6}$$

with j varying from 0 to N_G, and $I = \sum_{j=0}^{N_G} I_j$ .The functional dependence of the weighted factors with temperature is generally fitted by polynomials, Eq. (6), where the polynomial coefficients as well as the absorption coefficients for each gray gas can be tabulated. For CO_2/H_2O mixtures, these coefficients are generally established for particular ratios of the partial pressure, p_{H2O}/p_{CO2}, which could limit the application of the method. In the present study the weighted factors polynomial coefficients and absorption coefficients were taken from Dorigon et al. (2013) for p_{H2O}/p_{CO2} = 2. Such WSGG correlations were fitted from HITEMP2010 (Rothman et al., 2010), which is the latest molecular spectroscopic database that is available nowadays. The same study (Dorigon et al., 2013), compared results obtained with the new coefficients against LBL benchmark calculations for one-dimensional non-isothermal and non-homogeneous problems, finding consistently satisfactory agreement with maximum and average errors of about 5% and 2% for different test cases. For convenience, Table 2 shows the $k_{p,j}$ and $b_{j,i}$ coefficients from Dorigon et al. (2013).

It is assumed here that the contribution from other radiating species, such as CO e CH_4, is negligible. The contribution from CO in the combustion gases is negligible, as long as its molar concentration does not exceed relatively high values of the order of 0.05%, while the contribution from CH_4 is even lower (Coelho et al., 2003).

Table 2. WSGG model coefficients (Dorigon et al., 2013), p_{H2O}/p_{CO2} = 2

j	$k_{p,j}$ [$m^{-1}atm^{-1}$]	$b_{j1}\times10^{1}$	$b_{j2}\times10^{4}$ [K^{-1}]	$b_{j3}\times10^{7}$ [K^{-2}]	$b_{j4}\times10^{10}$ [K^{-3}]	$b_{j5}\times10^{14}$ [K^{-4}]
1	0.192	0.5617	7.8440	-8.5630	4.2460	-7.4400
2	1.719	1.4260	1.7950	-0.1077	-0.6972	1.7740
3	11.370	1.3620	2.5740	-3.7110	1.5750	-2.2670
4	111.016	1.2220	-0.2327	-0.7492	0.4275	-0.6608

3.3.2 Turbulence-Radiation Interactions

The radiative transfer equation (RTE), Eq. (2), is only applicable to instant quantities, i.e., quantities that fluctuate in a turbulent flow, while the RANS turbulence model can only provide time-averaged (mean) quantities and possibly their mean square fluctuations. Considering the spectral integrated form of the RTE, and time averaging it, results in:

$$\frac{d\bar{I}}{ds} = -\overline{\kappa I} + \overline{\kappa I_b} \tag{7}$$

Decomposition of variables (temperature and species concentrations) into mean and fluctuating components followed by time-averaging reveals several terms which require modeling (Coelho, 2007):

- Temperature self-correlation, $\overline{T^4}$, or related mean values that depend only on the temperature, as $\overline{I_b}$ and $\overline{I_{b\eta}}$.
- Absorption coefficient self-correlation, $\overline{\kappa}$, or similar correlations that depend only on the radiative properties of the medium.
- Absorption coefficient-temperature correlation, $\overline{\kappa T^4}$, or analogous ones, such as $\overline{k_j a_j I_b}$.
- Absorption coefficient-radiation intensity correlation, $\overline{\kappa I}$, or analogous ones, such as $\overline{k_j I_j}$.

ISSN 2176-5480

The absorption coefficient-radiation intensity correlation, i.e., the first term in the right hand of Eq. (7), is expressed as $\overline{\kappa I} = \bar{\kappa}\bar{I} + \overline{\kappa' I'}$. Several studies have neglected the second term on the right of this expression ($\overline{\kappa' I'}$) based on arguments of Kabashnikov and Kmit (1979), known as the *optically thin fluctuation approximation* (OTFA), and relies on the assumption that absorption coefficient fluctuations are weakly correlated with the radiation intensity fluctuations, i.e., $\overline{\kappa' I'} \approx 0$, if the mean free path for radiation is much larger than turbulence integral length scale. According to literature data (Coelho, 2007) the OTFA is not generally valid over the entire spectrum, particularly at the center of strong spectral lines of absorbing gases. However, it is believed that the spectral regions where this approximation does not hold plays minor influence on the total radiation intensity, in this manner it is justifiable for the vast majority of engineering applications, with the possible exception of strongly sooty flames, and it has been employed in most works dealing with TRI and based on the time-averaged form of the RTE (Hall and Vranos, 1994; Coelho, 2004; Li and Modest, 2002a, 2002b; Poitou et al., 2012; Snegirev, 2004). Introducing this approximation into Eq. (7) results in

$$\frac{d\bar{I}}{ds} = -\bar{\kappa}\bar{I} + \overline{\kappa I_b} \tag{8}$$

As for the second term in the right hand of Eq. (8), which is proportional to $\overline{\kappa T^4}$, instant values of κ and T correlate in a turbulent flow. In the present work it is applied the approximation proposed in Snegirev (2004), in which both absorption coefficient-temperature correlation and temperature self-correlation are considered. These two TRI correlations were found to be the most important in reactive flows (Li and Modest, 2002a, 2002b; Gupta et al., 2013, Habibi et al., 2007b). So, the absorption coefficient self-correlation was of minor importance and is neglected by the approximation in Snegirev (2004), despite this term could be treated if the composition PDF method (Mazumder and Modest, 1999) would be employed. Decomposition of temperature and absorption coefficient into average and fluctuating components, $T = \bar{T} + T'$ and $\kappa = \bar{\kappa} + \kappa'$, followed by time averaging yields (Snegirev, 2004):

$$\overline{\kappa T^4} = \overline{(\bar{\kappa}+\kappa')(\bar{T}+T')^4} = \bar{\kappa}\cdot\bar{T}^4\left(1 + \underbrace{6\frac{\overline{T'^2}}{\bar{T}^2} + 4\frac{\overline{T'^3}}{\bar{T}^3} + \frac{\overline{T'^4}}{\bar{T}^4}}_{\text{temperature self-correlation}} + \underbrace{4\frac{\overline{\kappa' T'}}{\bar{\kappa}\cdot\bar{T}} + 6\frac{\overline{\kappa' T'^2}}{\bar{\kappa}\cdot\bar{T}^2} + 4\frac{\overline{\kappa' T'^3}}{\bar{\kappa}\cdot\bar{T}^3} + \frac{\overline{\kappa' T'^4}}{\bar{\kappa}\cdot\bar{T}^4}}_{\text{absorption coefficient-temperature correlation}}\right) \tag{9}$$

where the expression in brackets on the right allows for turbulent fluctuations. Only the correlations of the lowest order, $\overline{T'^2}$ and $\overline{\kappa' T'}$, are taken into account in this work. The terms $\overline{T'^2}$ and $\overline{\kappa' T'}$ must be modeled by expressing them as functions of the averaged parameters of the flow. Species concentrations fluctuations play a minor role on TRI (Habibi et al., 2007a; Snegirev, 2004), although investigations have shown that their effects could not be negligible, particularly when advanced spectral methods are applied for determination of radiative heat fluxes (Coelho, 2004). Therefore, neglecting species concentrations fluctuations to compute $\overline{\kappa' T'}$ in Eq. (9), Snegirev (2004) replaces the dependence $\kappa(T) = \kappa(\bar{T} + T')$ by the Taylor series $\kappa \approx \kappa(\bar{T}) + T'\left.\frac{\partial\kappa}{\partial T}\right|_{\bar{T}} + \frac{T'^2}{2}\left.\frac{\partial^2\kappa}{\partial T^2}\right|_{\bar{T}} + \ldots$. Using the preceding Taylor series, the mean value, $\bar{\kappa}$, and the fluctuating component $\kappa' = \kappa - \bar{\kappa}$, the average of the product, $\overline{\kappa' T'}$, becomes $\overline{\kappa' T'} \approx \overline{T'^2}\left.\frac{\partial\kappa}{\partial T}\right|_{\bar{T}} + \frac{\overline{T'^3}}{2}\left.\frac{\partial^2\kappa}{\partial T^2}\right|_{\bar{T}} + \ldots \approx \overline{T'^2}\left.\frac{\partial\kappa}{\partial T}\right|_{\bar{T}}$. Neglecting higher order terms, Eq. (9) can be written as (Snegirev, 2004):

$$\overline{\kappa T^4} = \bar{\kappa}\cdot\bar{T}^4\left(1 + C_{TRI1}\,6\frac{\overline{T'^2}}{\bar{T}^2} + C_{TRI2}\,4\frac{\overline{T'^2}}{\bar{\kappa}\cdot\bar{T}}\left.\frac{\partial\kappa}{\partial T}\right|_{\bar{T}}\right) \tag{10}$$

Equation (10) is used in this work as an approximate estimate for $\overline{\kappa T^4}$ allowing for turbulent temperature fluctuations. The model constants C_{TRI1} and C_{TRI2} are assumed as 2.5 and 1.0, respectively. The value for C_{TRI1} was initially suggested by Snegirev (2004) from data fitting for $\overline{T^4}/\bar{T}^4$ and $\overline{T'^2}/\bar{T}^2$ as presented in Burns (1999), but an ad hoc adjustment performed in Snegirev (2004) led to a value of 2.5 for C_{TRI1}.

To evaluate $\overline{T'^2}$, required for Eq. (10), the transport equation for temperature variance is solved:

$$\frac{\partial}{\partial x}\left(\rho\bar{u}\overline{T'^2}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\bar{v}\overline{T'^2}\right) = \frac{\partial}{\partial x}\left(\left(\mu + \frac{\mu_t}{\text{Pr}_t}\right)\frac{\partial\overline{T'^2}}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\mu + \frac{\mu_t}{\text{Pr}_t}\right)\frac{\partial\overline{T'^2}}{\partial r}\right) + 2\frac{\mu_t}{\sigma_t}\left(\frac{\partial\bar{T}}{\partial x} + \frac{\partial\bar{T}}{\partial r}\right)^2 - C_T\rho\overline{T'^2}\frac{\varepsilon}{k} \tag{11}$$

ISSN 2176-5480

where C_T = 2.0 is the model constant. Equation (10) must be solved together with the set of equations presented in Table 1, considering $\phi = \overline{T'^2}$, $\Gamma_\phi = \mu + \mu_t / \mathrm{Pr}_t$ and S^ϕ the two last terms in the right hand of Eq. (11). Also, in solving Eq. (11), $\overline{T'^2}$ was set as zero in the boundaries as in Snegirev (2004).

4. RESULTS AND DISCUSSIONS

Figure 1 depicts the thermal boundary conditions of the cylindrical chamber: symmetry in the centerline, and prescribed temperature on the wall, equal to 393.15 K. The set of equations were solved using the finite volume method by means of a Fortran code. The power-law was applied as the diffusive-advective interpolation function on the faces of the control volumes. The pressure-velocity coupling was made by the SIMPLE method. The resulting system of algebraic equations was solved by the TDMA algorithm, with block correction in all equations but the k and ε. A grid with 90 volumes in the axial direction and 50 volumes in the radial direction was used. The numerical accuracy was checked by comparing predicted results calculated using this grid with results obtained using coarser and thinner grids, as reported in Centeno et al. (2013). As found, the 90×50 grid provided grid independent results, and required reasonable computational effort. This grid is non-uniformly spaced in the radial direction and is uniformly spaced in the axial direction. The radiative transfer calculations were performed using the same spatial grid, and S_6 quadrature, while both chamber walls, inlet and outlet ducts were modeled as black surfaces. The radiative transfer in molecular gases depends on the number of (radiative) participant molecules per unit volume. In the present work, the pressure absorption coefficient for the j-th gray gas for the WSGG model, $k_{p,j}$ (in $m^{-1}atm^{-1}$), presented in Table 2, was multiplied by the sum of the partial pressures of H_2O and of CO_2 for each computational volume cell, obtaining the absorption coefficient for the j-th gray gas, k_j (in m^{-1}), necessary to compute Eq. (5). In this manner, inhomogeneity of H_2O and CO_2 concentrations inside the combustion chamber were also taken into account to compute the radiative transfer. The simulations were performed in a desktop computer with AMD FX-8150 Eight-Core 3.6 GHz processor and 16.0 GB of memory. Running the code with the WSGG model required about 16 hours of simulation, while the simulations without radiation heat transfer required less than 1 hour. The radiative transfer calculations were performed only after a reasonably converged solution had been achieved, and then at each iterative step. The time required to run the code considering or neglecting the TRI was essentially the same (about 16 hours), demonstrating the efficiency of the TRI methodology applied in the present work.

In order to study the importance of the above mentioned TRI correlations on the radiation modeling of the current combustion chamber simulation, four different scenarios were considered. In the first scenario, radiation was completely ignored; in the second scenario, radiation was considered but without TRI; in the third scenario, radiation was considered with TRI computed according to Eq. (10), and is identified as “TRI-full” in the following results; finally in the fourth scenario, radiation was considered with TRI computed according to a partial version of Eq. (10), in which the last term in brackets on that equation was neglected, leading to:

$$\overline{\kappa T^4} = \overline{\kappa} \cdot \overline{T}^4 \left(1 + C_{TRI1} 6 \frac{\overline{T'^2}}{\overline{T}^2} \right) \tag{12}$$

This fourth scenario is identified as “TRI-partial” in the following results, and the major advantage of this scenario would be that the derivative of the absorption-coefficient in relation to the temperature is not computed, while that derivative can be difficult to compute depending on the absorption-coefficient model employed. A similar partial TRI approximation was employed in Krishnamoorthy (2010a, 2010b). Comparisons were made to verify how the different TRI scenarios affect the radiative heat source and temperature fields.

Figure 2 shows the results for the radiative heat source (S_{rad}) field, while Fig. 3 shows the results for the temperature fields, for all radiative scenarios. In both figures, it is also shown the relative deviation between results computed with TRI-full and TRI-partial approximations (subscripts *TRI-full* and *TRI-partial* indicate which scenario was used to compute S_{rad} or T, both represented as V in the equation):

$$\%Dev = 100 \frac{V_{TRI-full} - V_{TRI-partial}}{V_{TRI-full}} \tag{13}$$

As shown in Fig. 2, radiation fields changed significantly as a result of the different radiative scenarios (neglecting and considering TRI). TRI can contribute to increase the mean radiation intensities in turbulent diffusion flames by 10% to above 50% in methane or natural gas flames (Coelho, 2007), which was verified in the present simulations when comparing results from Fig. 2(a) with results from Figs. 2(b) or 2(c). The flame region with the highest temperatures emits more radiation than absorbs, leading to a negative heat source as expected, while the flame region with the

ISSN 2176-5480

smallest temperatures absorbs more radiation than emits, leading to a positive heat source. Also, Fig. 2(d) shows the relative deviation of the radiative heat source obtained with the different TRI scenarios (TRI-full and TRI-partial). Despite the relative deviation can reach values of about 40%, it must be recognized that the highest deviations between TRI-full and TRI-partial results are located in small regions of the chamber domain where the radiative heat source term is relatively small; additionally, those deviations are typically small in the most part of the chamber domain, including the highly radiative emission region.

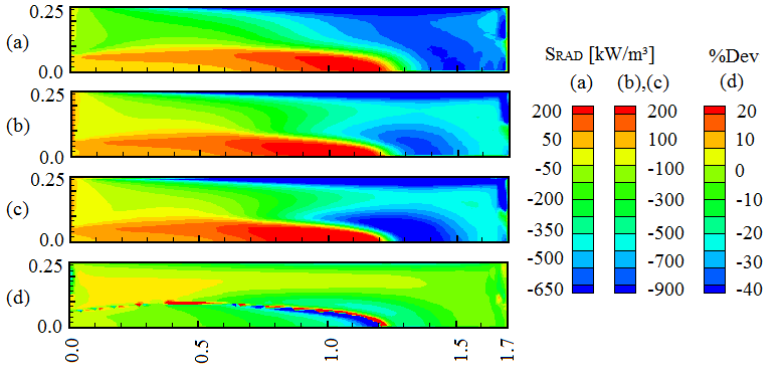

Figure 2. Radiative heat source fields: (a) radiation computed without TRI; (b) radiation computed with TRI-full; (c) radiation computed with TRI-partial; (d) relative deviation between (b) and (c)

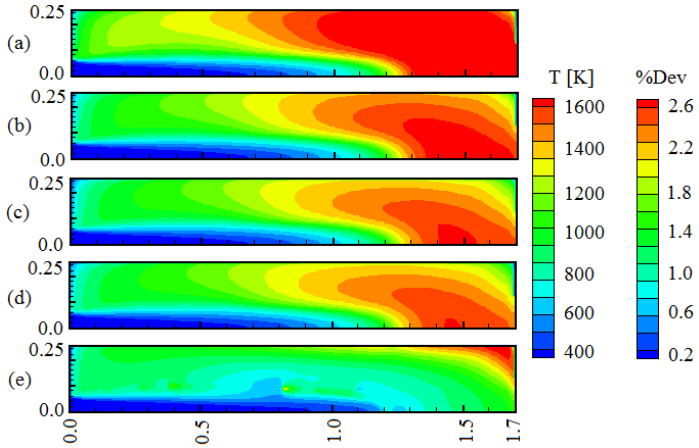

Figure 3. Temperature fields: (a) radiation neglected; (b) radiation computed without TRI; (c) radiation computed with TRI-full; (d) radiation computed with TRI-partial; (e) relative deviation between (c) and (d)

As can be seen in Fig. 3(a) to 3(d), consideration of the radiative transfer and TRI play an important role in the temperature field, while the effect of the different TRI correlations (TRI-full and TRI-partial) is very small, as observed in Fig. 3(e) and comparing Figs. 3(c) and 3(d). It is observed that the temperature values and temperature gradients are decreased when radiation heat transfer is considered since in that case there is an additional heat transfer mode inside the computational domain. The same behavior is observed comparing results obtained with and without TRI, i.e., since computation of radiation with TRI provides higher radiative heat source in comparison to the computation without TRI, the temperature and gradients levels are smaller when TRI is considered. Computed flame peak temperatures for the current simulations are presented in Tab. 3. While these peaks are local, they can be taken as a measure to characterize the entire temperature field. The decrease in the peak temperature as a result of considering or neglecting radiative transfer (ΔT_{RAD}) and considering or neglecting TRI (ΔT_{TRI}) are then analyzed. The peak temperature drops ΔT_{RAD} = 166 K, $\Delta T_{TRI\text{-}full}$ = 62 K, and $\Delta T_{TRI\text{-}partial}$ = 79 K, when comparing results for the scenario without radiation against the scenario with radiation but without TRI, results for the scenario with radiation without TRI against the scenario with radiation but with TRI-full and with TRI-partial, respectively. In similar investigations, Li and Modest (2002a) reported a decrease on peak temperature of ΔT_{TRI} = 110 K when comparing results with and without TRI, while Li and Modest (2002b) found decreases of ΔT_{RAD} = 145 K and ΔT_{TRI} = 64 K for a flame with an optical thickness similar to that of the flame studied here. Coelho (2007) reported that the radiative transfer led to cooler flames, especially when considering TRI, which accounted for about one-third of the total drop in the flame peak temperature of a turbulent non-premixed flame of methane-air. Also, Poitou et al. (2012) found drops of ΔT_{RAD} = 150 K on peak temperature for a propane-air turbulent non-premixed flame. So, the results in Tab. 3 are in agreement with literature data.

ISSN 2176-5480

Table 3. Computed flame peak temperature

	without radiation	without TRI	With TRI-full	with TRI-partial	ΔT_{RAD} [K]	$\Delta T_{TRI-full}$ [K]	$\Delta T_{TRI-partial}$ [K]
Peak temperature [K]	1851	1685	1623	1606	166	62	79

An important quantity that describes the overall radiation field of a flame is the net radiative heat loss from the flame and its normalized variable, the radiant fraction (f_{rad}). The net radiative heat loss corresponds to the integral of S_{rad} over the computational domain; the radiant fraction is the ratio of this value to the heat released in combustion. In all simulation scenarios, these quantities were calculated and the results are shown in Table 4. The radiation loss and the corresponding radiant fraction from the present flame have significant values. It is observed on Table 4 that radiant fraction increases about 30% when TRI-full is considered on the calculations and 39% when TRI-partial; both results are in agreement with data from literature for methane-air flames (Li and Modest, 2002a, 2002b; Snegirev, 2004).

Table 4. Predicted net radiative heat loss and fraction of radiative heat loss

	Net radiative heat loss [kW]	Radiant fraction (f_{rad}) [%]
without TRI	125.5	20.8
with TRI-full	163.0	26.9
with TRI-partial	174.3	28.8

5. CONCLUSIONS

This study presented an analysis of the thermal radiation in a turbulent non-premixed methane–air flame in a cylindrical combustion chamber. The radiation field was computed with the WSGG model using updated correlations (Dorigon et al., 2013) and considering TRI effects (Snegirev, 2004; Krishnamoorthy, 2010a, 2010b). A two-step global reaction mechanism was used and turbulence modeling was considered via standard k-ε model. The RTE was solved employing the discrete ordinates method. The TRI approximation employed for the current investigation was able to accounting for both absorption coefficient-temperature correlation and temperature self-correlation, so this work evaluated the importance of these two TRI correlations on the radiation modeling and, consequently, on the thermal behavior of the combustion chamber. That evaluation was performed by comparing results for four different scenarios: radiation neglected from calculations, radiation computed without TRI, radiation computed with TRI (identified as TRI-full) as proposed in Snegirev (2004), and radiation computed with TRI (identified as TRI-partial) as employed in Krishnamoorthy (2010a, 2010b). The comparison of the results obtained from the different scenarios showed that the temperature (especially at high temperature regions), radiative heat source and radiant fraction were mainly affected by the radiation transfer in general, independently of the TRI correlation employed. Therefore, the major finding of this investigation is that it is important to consider thermal radiation in the calculations and that the TRI effect can be approximated by the short version of the TRI correlation.

6. ACKNOWLEDGEMENTS

FHRF thanks CNPq (Brazil) for research grants 304728/2010-1 and 473899/2011-6.

7. REFERENCES

Bidi, M., Hosseini, R., Nobari, M.R.H., 2008. “Numerical analysis of methane-air combustion considering radiation effect”, *Energy Conversion and Management*, 49, pp. 3634-3647.

Burns, S.P., 1999. “Turbulence radiation interaction modeling in hydrocarbon pool fire simulations”, *Sandia Report SAND 99-3190*.

Centeno, F.R., Cassol, F., Silva, C.V., França, F.H.R., 2013. “Comparison of different WSGG correlations in the computation of thermal radiation in a 2D axisymmetric turbulent non-premixed methae-air flame”, submitted to *JBSMSE* in March of 2013.

Coelho P.J., 2002. “Evaluation of a model for turbulence/radiation interaction in flames using a differential solution method of the radiative transfer equation”, *12th international heat transfer conference*, Grenoble, France, 705 - 710.

Coelho P.J., 2004. “Detailed numerical simulation of radiative transfer in a non-luminous turbulent jet diffusion flame”, *Combustion and Flame*, 136, pp. 481 - 492.

Coelho, P.J., 2007. “Numerical simulation of the interaction between turbulence and radiation in reactive flows”, *Progress in Energy and Combustion Science*, 33, pp. 311 - 383.

ISSN 2176-5480

Coelho, P.J., Teerling, O.J., Roekaerts, D., 2003. "Spectral radiative effects and turbulence/radiation interaction in a non-luminous turbulent jet diffusion flame", *Combustion and Flame*, 133, pp. 75 - 91.

Demarco, R., Consalvi, J. L., Fuentes, A., Melis, S., 2011. "Assessment of radiative property models in non-gray sooting media", *Int. J. of Thermal Sciences*, 50, pp. 1672-1684.

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 H_2O/CO_2 mixtures", submitted to *IJHMT* in February of 2013.

Eaton, A.M., Smoot, L.D., Hill, S.C., Eatough, C.N., 1999. "Components, formulations, solutions, evaluations and applications of comprehensive combustion models", *Progress in Energy and Combustion Sciences*, 25, 387-436.

Foster, P.J., 1969. "The relation of time–mean transmission of turbulent flames to optical depth", *Journal of the Institute of Fuel*, 42, pp. 179 - 82.

Garréton, D., Simonin, O., 1994. "Final results", *Proc. of the 1th Workshop of Aerodynamics of Steady State Combustion Chambers and Furnaces*, 25, EDF-ERCOFTAC, 29-35.

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*, 34, pp. 1281-1288.

Habibi, A., Merci, B., Roekaerts, D., 2007a. "Turbulence radiation interaction in Reynolds-averaged Navier-Stokes simulations of nonpremixed piloted turbulent laboratory-scale flames", *Combustion and Flame*, 151, pp. 303 - 320.

Habibi, A., Merci, B., Roekaerts, D., 2007b. "The importance of Turbulence-Radiation Interaction in RANS simulations of a turbulent non-premixed laboratory-scale bluff-body flame", *3rd European Combustion Meeting*, Crete, Grécia.

Hall, R.J., Vranos, A., 1994. "Efficient Calculations of Gas Radiation from Turbulent Flames", *IJHMT*, 37, n. 17, pp. 2745 - 2750.

Hottel, H. C., Sarofim, A. F., 1967. "Radiative Transfer", *McGraw-Hill Book Company*.

Johansson, R., Leckner, B., Andersson, K., Johnsson, F., 2011. "Account for variations in the H_2O to CO_2 molar ratio when modeling gaseous radiative heat transfer with the weighted-sum-of-grey-gases model", *Combustion and Flame*, 158, pp. 893-901.

Kabashnikov, V.P., Kmit, G.I., 1979. "Influence of turbulent fluctuations on thermal radiation", *Journal of Applied Spectroscopy*, 31, pp. 963 - 967.

Krebs, W., Koch, R., Bauer, H.J., Kneer, R., Wittig, S., 1994. "Effect of turbulence on radiative heat transfer inside a model combustor", *Eurotherm seminar no. 37 - heat transfer in radiating and combusting systems 2*, pp. 349 - 362, Saluggia, Italy.

Krebs, W., Koch, R., Ganz, B., Eigenmann, L., Wittig, S., 1996. "Effect of temperature and concentration fluctuations on radiative heat transfer in turbulent flames", *26th symposium (internat.) on combustion*, Pittsburgh, 2763 - 2770.

Krishnamoorthy, G., 2010a. "A new weighted-sum-of-gray-gases model for CO_2-H_2O gas mixtures", *Int. Comm. Heat and Mass Transfer*, 37, pp. 1182-1186.

Krishnamoorthy, G., 2010b. "A comparison of gray and non-gray modeling approaches to radiative transfer in pool fires simulations", *Journal of Hazardous Materials*, 182, pp. 570-580.

Li, G., Modest, M.F., 2002a. "Application of composition PDF methods in the investigation of turbulence-radiation interactions", *JQS&RT*, 73, pp. 461 - 472.

Li, G., Modest, M.F., 2002b. "Importance of Turbulence-Radiation Interactions in turbulent reacting flows", *Proceedings of 2002 ASME IMECE*, Louisina, USA.

Magel, H.C., Schnell, U., Hein, K.R.G., 1996. "Modeling of hydrocarbon and nitrogen chemistry in turbulent combustor flows using detailed reaction mechanisms", *Proceedings of the 3rd Workshop on Modeling of Chemical Reaction Systems*, Heidelberg.

Magnussen, B.F., Hjertager, B.H., 1977. "On mathematical models of turbulent combustion with special emphasis on soot formation and combustion", *Proceedings of the 16th Symposium (International) on Combustion – The Combustion Institute*, pp. 719-729. Cambridge, MA.

Mazumder, S., Modest, M.F., 1999. "A probability density function approach to modeling turbulence-radiation interactions in nonluminous flames", *IJHMT*, 42, pp. 971-991.

Modest, M.F., 1991. "The weighted-sum-of-gray-gases model for arbitrary solution methods in radiative transfer", *ASME J. Heat Transf.*, 113, pp. 650-656.

Modest, M.F., Mehta, R.S., 2006. "Modeling absorption TRI in optically thick eddies", *Eurotherm 78 – Computational Thermal Radiation in Participating Media II*, Poitiers, France.

Nieckele, A.O., Naccache, M.F., Gomes, M.S.P., Carneiro, J.E., Serfaty, R., 2001. "Models evaluations of combustion process in a cylindrical furnace", *Proceedings of 2001 ASME IMECE*, New York, NY.

Poitou, D., Amaya, J., El Hafi, M., Cuénot, B., 2012. "Analysis of the interaction between turbulent combustion and thermal radiation using unsteady coupled LES/DOM simulations", *Combustion and Flame*, 159, pp. 1605 - 1618.

Rothman, L.S., Gordon, I.E., Barber, R.J., Dothe, H., Gamache, R.R., Goldman, A., Perevalov, V.I., Tashkun, S.A., Tennyson, J., 2010. "HITEMP, the high-temperature molecular spectroscopic database", *JQS&RT*, 111, p. 2130-2150.

Silva, C.V., França, F.H.R., Vielmo, H.A., 2007. "Analysis of the turbulent, non-premixed combustion of natural gas in

ISSN 2176-5480

a cylindrical chamber with and without thermal radiation", *Combustion Sci. and Tech*., 179, pp. 1605-1630.
Smith, T. F., Al-Turki, A. M., Byun, K. H., Kim, T. K., 1987. "Radiative and Conductive Transfer for a Gas/Soot Mixture Between Diffuse Parallel Plates", *J. Thermophys. Heat Transfer*, vol. 1, pp.50-55.
Smith, T. F., Shen, Z. F., Friedman, J. N., 1982. "Evaluation of Coefficients for the Weighted Sum of Gray Gases Model", *J. Heat Transfer*, 104, pp.602-608.
Snegirev, A.Y., 2004. "Statistical modeling of thermal radiation transfer in buoyant turbulent diffusion flames", *Combustion and Flame*, 136, pp. 51 - 71.
Song, T.H., Viskanta, R., 1987. "Interaction of radiation with turbulence: application to a combustion system", *Journal of Thermophysics*, vol. 1, n. 1, pp. 56 - 62.
Spalding, D.B., 1979. "Combustion and mass transfer", *Pergamon Press*, Inc., New York.
Turns, S.R., 2000. "An introduction to combustion: concepts and applications", 2nd ed., *McGraw-Hill*.

8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.