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A numerical study of the influence of radiation on turbulence in a 2D axisymmetric turbulent flame[1]

Um estudo numérico da influência da radiação sobre a turbulência em uma chama turbulenta 2D axissimétrica

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Abstract. This paper presents a study of the influence of thermal radiation on turbulence in the simulation of a turbulent, non-premixed methane-air flame. In such a problem, two aspects need to be considered for a precise evaluation of the thermal radiation: the turbulence-radiation interactions (TRI), and the radiative properties of the participating species, which are treated here with the weighted-sum-of-gray-gases (WSGG) model based on recently obtained correlations from HITEMP2010 database. The chemical reactions rates were considered as the minimum values between the Arrhenius and Eddy Break-Up rates. A two-step global reaction mechanism was employed, while the turbulence modeling was considered via

Resumo. Este artigo apresenta um estudo da influência da radiação térmica sobre a turbulência através da simulação de uma chama turbulenta, não pré-misturada, de metano-ar. Neste problema dois aspectos precisam ser considerados para uma avaliação precisa da radiação térmica: interações turbulência-radiação (TRI) e as propriedades radiativas das espécies participantes, as quais são tratadas aqui com o modelo da soma ponderada de gases cinza (WSGG) baseado em correlações recentemente obtidas a partir do banco de dados espectrais HITEMP2010. As taxas das reações químicas foram consideradas como os menores valores entre as taxas de Arrhenius e de Eddy Break-Up. Um mecanismo de reação global de duas etapas foi empregado, en-

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standard k–ε model. The source terms of the energy equation consisted of the heat generated in the chemical reaction rates as well as in the radiation exchanges. The discrete ordinates method (DOM) was employed to solve the radiative transfer equation (RTE), including the TRI. Comparisons of simulations with/without radiation demonstrated that radiation influenced turbulent-properties (root mean square of velocity and temperature fluctuations, and turbulent kinetic energy of the velocity fluctuations). Radiation smoothed turbulent-properties fields. The influence of radiation was more important on the temperature fluctuations than on the velocity fluctuations.

Keywords: thermal radiation, turbulence, TRI, CFD, non-premixed flame.

quanto a modelagem da turbulência foi considerada através do modelo k-ε padrão. Os termos fontes da equação da energia consistiram no calor gerado pelas reações químicas assim como pelas trocas radiantes. O método de ordenadas discretas (DOM) foi empregado para resolver a equação de transferência radiativa (RTE), incluindo as TRI. Comparações de resultados das simulações com e sem radiação térmica demonstraram que a radiação influenciou as propriedades turbulentas avaliadas (raiz média quadrática das flutuações de velocidade e de temperatura, e energia cinética turbulenta das flutuações de velocidade). A radiação suavizou os campos de propriedades turbulentas. A influência da radiação foi mais importante sobre as flutuações de temperatura do que nas flutuações de velocidade.

Palavras-chave: radiação térmica, turbulência, TRI, CFD, chama não pré-misturada.

Introduction

Combustion problems involve a number of coupled phenomena, such as fluid mechanics, heat transfer, and chemical kinetics of gaseous species and soot, in which thermal radiation can be the dominant heat transfer mode. Heat transfer directly affects the temperature field and, therefore, chemical kinetics and thermophysical properties (as density, heat capacity, and viscosity).

An important phenomenon to be considered 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 flow, it is not possible to deal with these phenomena in an independent way, but in a coupled form. In turbulent reactive flows, temperature and species concentration fields can undergo high levels of fluctuations, leading to variations on the radiative field. Since the radiative field is present in the energy conservation equation as a source term, and turbulent fluctuations influence radiative transfer, then turbulence also influences the temperature and density fields. Therefore, since the density field influences the velocity field and so the scalar fluctuations, it can be concluded that turbulence influences radiation and radiation influences turbulence. Few attention has been devoted to investigate the influence of radiation on turbulence. At the authors best knowledge, the only investigation dealing with such influence in high temperature flows is in Soufiani (1991), where it was found that radiation may smooth the intensity of temperature fluctuations. On the other hand, the influence of turbulence on radiation has been received much more attention.

The first coupled calculation of radiative transfer in reactive flow to investigate TRI was reported in Song and Viskanta (1987), in which property functions were prescribed for the combustion gases. The most recent literature has been focused on analyzing the most important TRI correlations (temperature self-correlation, absorption coefficient-temperature correlation, absorption coefficient self-correlation, and absorption coefficient-radiation intensity correlation). Some examples of coupled investigations were reported in Li and Modest (2002a), Habibi *et al.* (2007a), Poitou *et al.* (2012) and Gupta *et al.* (2013). Results pointed that the absorption coefficient-temperature correlation and the 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 *optically thin fluctuation approximation* – OTFA) is important only for optically thick medium.

An accurate description of radiative heat transfer is of great importance for simulations of combustion systems. Modeling thermal radiation exchanges in combustion gases (such as water vapor and carbon dioxide) is a difficult task, due to the highly complex dependence of the absorption coefficient with the wavenumber, which is typically characterized by hundreds of thousands or millions of spectral lines. Thus, the integration of the radiative transfer equation (RTE) over the spectrum would be very expensive or even impossible without the use of spectral or global models. As a first simplification, the RTE is frequently solved with the gray gas (GG) model, where the dependence of the absorption coefficient over the wavenumber is simply neglected. In order to provide realistic results, more refined models are however needed. As one advance to the GG model, the weighted-sum-of-gray-gases (WSGG) (Hottel and Sarofim, 1967) makes perhaps the best compromise between accuracy and computation demand, 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 can be interpreted as the fractions of the blackbody energy in the spectrum region where the gray gases are located. In practice, those coefficients are obtained from fitting total emittances computed from experimental-gas-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, such as the narrow band, wide band, GG and global models, such as the WSGG and spectral-line-based WSGG (SLW). According to the authors, the WSGG is very efficient from a computational point of view, and can yield accurate predictions, although significant discrepancies can appear 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 excessively time consuming when fluid flow/combustion/radiative heat transfer are coupled.

This study presents a numerical RANS (Reynolds Average Navier-Stokes) simulation of a turbulent non-premixed methane-air flame in a cylindrical combustion chamber taking into account radiation effect of non-gray gases by means WSGG correlations (Dorigon *et al.*, 2013) generated from HITEMP 2010 database (Rothman *et al.*, 2010) and including TRI (Snegirev, 2004), with the objective of evaluating the influence of radiation on turbulence, since such influence has been received much less attention in the literature than the influence of turbulence on radiation.

Problem statement

The physical system consists of the natural gas combustion chamber described in Garréton and Simonin (1994), which presents several challenges for thermal modeling in the sense that the flame is turbulent, and with highly non-isothermal, non-homogeneous medium.

Keeping the same conditions as described 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, leading to a non-swirling flame. 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 about 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 that are provided by the burner. To complement the boundary conditions, Figure 1 depicts the thermal boundary conditions of the cylindrical chamber: symmetry in the centerline, and prescribed temperature on the walls, equal to 393.15 K. In addition, impermeability and no-slip conditions were assumed on the walls. In the symmetry line, it was assumed that both radial velocity and velocity gradient were null. The same procedure was adopted for the turbulent kinetic energy and its dissipation rate, enthalpy, and species concentrations in the symmetry line. In the outlet, null diffusive fluxes were assumed for all variables, the axial velocity component was corrected by a factor to satisfy mass conservation, and the radial velocity was imposed to be null. For radiation modeling, both chamber walls, inlet and outlet ducts were modeled as black surfaces. The temperature at the inlet duct was prescribed at the fuel and the oxidant temperatures, while the temperature at the outlet duct was equal to the outlet flow bulk temperature.

In addition, in the inlet, the velocity and concentration profiles were assumed uniform in the axial direction, while the turbulent kinetic energy was computed as $k = 3/2\ (u_{in} i)^2$, where i is the turbulence intensity (prescribed as 6% and 10% for the air and for the fuel streams, respectively) and u_{in} is the inlet axial mean velocity, and for the turbulent kinetic energy dissipation rate, the relation $\varepsilon = (C_\mu^{3/4}\, k^{3/2})/l$ was employed, where l is the turbulence characteristic length scale (taken as 0.04 m and 0.03 m for the air and the fuel streams, respectively). For both energy and momentum conservation equations, standard wall functions were applied for the combustor walls treatment, which take into account the viscous layer dominated by molecular diffusion close to the walls (Patankar, 1980).

Mathematical formulation

The proposed work is stated as: considering a steady turbulent non-premixed methane-air flame in a cylindrical chamber, compute the temperature, species concentrations and velocity fields, and verify the influence of radiation on turbulence main parameters, taking into account the WSGG model based on HITEMP 2010 data (Dorigon *et al.*, 2013) and TRI effects (Snegirev, 2004).

Governing equations

Conservation equations for mass, momentum in the axial and radial directions, k-ε turbulence model, energy, and chemical species (CH_4, O_2, CO_2, CO, H_2O) for steady low-Mach flow in 2D axisymmetric coordinates are solved. Detailed information about governing equations can be found in Centeno *et al.* (2014a).

Combustion kinetics

As a basic assumption, it is considered that the combustion process occurs at finite rates with methane oxidation taking two global steps:

$$2CH_4^{(16)} + 3(O_2^{(32)} + 3.76N_2^{(28)}) \rightarrow 2CO^{(28)} + 4H_2O^{(18)} + 11.28N_2^{(28)}$$

$$2CO^{(28)} + 1(O_2^{(32)} + 3.76N2^{(28)}) \rightarrow 2CO_2^{(44)} + 3.76N_2^{(28)}$$

The rate of formation or consumption, $R_{\alpha,c}$, of each α-th species in each c-th reaction (there are two reactions in the present study, so $c = 2$) is obtained by the Arrhenius-Magnussen's model (Eaton *et al.*, 1999; Turns, 2000; Fluent, 2009), in which the rate of formation or consumption of the chemical species are taken as the smallest one between the values obtained from Arrhenius kinetics or from Magnussen's equations (Eddy Break-Up) (Magnussen and Hjertager, 1977). The investigation in Silva *et al.* (2007), which considered the same combustion chamber, provided the relative importance of the combustion kinetics by computing the Damköhler number, and found that the combustion process is governed by Arrhenius rates in the flame core and by Magnussen's rates in all the other regions. This formulation was also successfully employed in Silva *et al.* (2007), Nieckele *et al.* (2001) and Centeno *et al.* (2013, 2014a).

The average volumetric rates of formation or consumption of the α-th chemical species, R_α, which appears in both energy and species

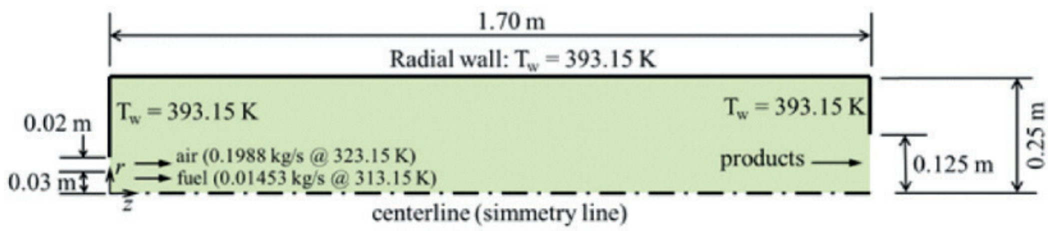

Figure 1. Combustion chamber geometry.

conservation equations, are then computed from the summation of the volumetric rates of formation or consumption in all the c-th reactions where the α-th species is present, i.e., $R_a = \sum_c R_{a,c}$.

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 by weighted-sum-of-gray-gas emittances. The emission weighted factors, $a_j(T)$, and the absorption coefficients, k_j, for the j^{th} gray gas are in general determined from the best fit of the total emittance with the constraint that the a_j must sum to 1. From a more general point of view, the WSGG model can be applied as a non-gray gas model (Modest, 1991), solving the radiative transfer equation (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:

$$\frac{dI_j}{ds} = -\kappa_j I_j + \kappa_j a_j(T) I_{b,j}(T) \quad (1)$$

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

$$a_j(T) = \sum_{i=1}^{5} b_{j,i} T^{i-1} \quad (2)$$

with j varying from 0 to N_G, and $I = \sum_{j=0}^{NG} I_j$.The functional dependence of the weighted factors with temperature is generally fitted by polynomials, Eq. (2), where the polynomial coefficients ($b_{j,i}$) as well as the absorption coefficients for each gray gas can be tabulated. For H_2O/CO_2 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 HITEMP 2010 (Rothman *et al.*, 2010), which is the most recent molecular spectroscopic database for high temperatures. In the same study, Dorigon *et al.* (2013) compared results obtained with the new coefficients against line-by-line (LBL) benchmark calculations for one-dimensional non-isothermal and non-homogeneous problems, finding consistently satisfactory agreement between the LBL and WSGG solutions, with maximum and average errors of about 5% and 2% for different test cases. Centeno *et al.* (2013) tested the coefficients presented in Dorigon *et al.* (2013) against old ones presented in Smith *et al.* (1982) for an axisymmetric cylindrical combustion chamber, and found that the new coefficients provided better agreement with experimental data. 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, since its molar concentration is not expected to exceed 0.1%, while the contribution from CH_4 is even lower (Coelho *et al.*, 2003).

Turbulence-radiation interactions

The radiative transfer equation (RTE) is applicable to instant 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 spectrally integrated form of the RTE, and time averaging it, it results in:

$$\frac{d\bar{I}}{ds} = -\overline{\kappa I} + \overline{\kappa I_b} \quad (3)$$

The absorption coefficient-radiation intensity correlation, i.e., the first term in the right hand of Eq. (3), is expressed as $\overline{\kappa I} = \bar{\kappa}\bar{I} + \overline{\kappa' I'}$. Several studies have neglected the second term on the right hand side of this expression ($\overline{\kappa' I'}$) based on arguments of Kabashnikov and Kmit (1979), known as the optically thin fluctuation approximation (OTFA), which relies on the assumption that the 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.

In the second term in the right hand of Eq. (3), which is proportional to $\overline{\kappa T^4}$, the instant values of κ and T correlate in a turbulent flow. In the present study, it is applied the approximation proposed in Snegirev (2004), in which both the absorption coefficient-temperature correlation and the temperature self-correlation are considered. These two TRI correlations were found to be the most important in reactive flows (Li and Modest, 2002a, 2002b; Habibi *et al.*, 2007b; Gupta *et al.*, 2013). Decomposition of temperature and absorption coefficient into average and fluctuating components,

$T = \overline{T} + T'$ and $\kappa = \overline{\kappa} + \kappa'$, followed by time averaging, and neglecting higher order terms, $\overline{\kappa T^4}$ can be written as (Snegirev, 2004):

$$\overline{\kappa T^4} = \overline{\kappa} \cdot \overline{T}^4 \left(1 + C_{TRI}\, 6\, \frac{\overline{T'^2}}{\overline{T}^2} + 4\, \frac{\overline{T'^2}}{\overline{\kappa} \cdot \overline{T}} \left. \frac{\partial \kappa}{\partial T} \right|_{\overline{T}} \right) \quad (4)$$

which allows the consideration of the absorption coefficient-temperature correlation and the temperature self-correlation. The value for C_{TRI} was initially suggested by Snegirev (2004) from data fitting for $\overline{T^4} / \overline{T}^4$ and $\overline{T'^2} / \overline{T}^2$, as presented in Burns (1999), followed by an adjustment leading to a value of 2.5 for C_{TRI}.

To evaluate $\overline{T'^2}$, required for Eq. (4), an additional transport equation for temperature fluctuation variance is solved.

Results and discussions

The set of equations were solved using the finite volume method (Patankar, 1980) 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 except the equations for k and ε. A grid with 140 volumes in the axial direction and 48 volumes in the radial direction was used. The numerical accuracy was checked through the grid convergence index (GCI) method (Roache, 1994; Celik *et al.*, 2008) comparing predicted results calculated using this grid with results obtained using coarser grids. As found, the 140×48 grid provided grid independent results, and required reasonable computational effort. The grid is uniformly spaced in both radial and axial directions. The radiative transfer calculations were performed with the discrete ordinates method using the same spatial grid and S_6 quadrature. Convergence criteria were based on the imposition that the normalized residual mass in the SIMPLE method was 10^{-8}. For the other equations, the maximum relative variation between iterations was 10^{-6}.

In order to study the effect of the gas radiation heat transfer inside the combustion chamber, allowing to analyze its influence on turbulence, two different scenarios were considered. In the first scenario, radiation was completely ignored, while, in the second scenario, radiation was completely considered, including TRI. Comparisons were made to verify how the different radiative scenarios affect some turbulence-related parameters, as the root mean square (RMS) of the temperature fluctuations and the turbulent kinetic energy of the velocity fluctuations.

Figures 2 and 3 present fields of the turbulent kinetic energy of the velocity fluctuations and the root mean square of the temperature fluctuations (computed from the temperature fluctuation variance square root: $T'_{rms} = \sqrt{\overline{T'^2}}$), respectively, computed in both scenarios – neglecting radiation calculations and considering them. These two turbulence-related properties were selected to verify the influence of radiation on turbulence. As observed, the different radiative scenarios investigated in the present work did not affect importantly those turbulent properties. However, the turbulent fields were smoothed when comparing results obtained without radiation (fields “a” in Figures 2 and 3) against those results obtained with radiation (fields “b” in Figures 2 and 3), in agreement with the findings in Soufiani (1991).

Additionally, Figures 4 and 5 present profiles of the root mean square of the temperature fluctuations and of the root mean square

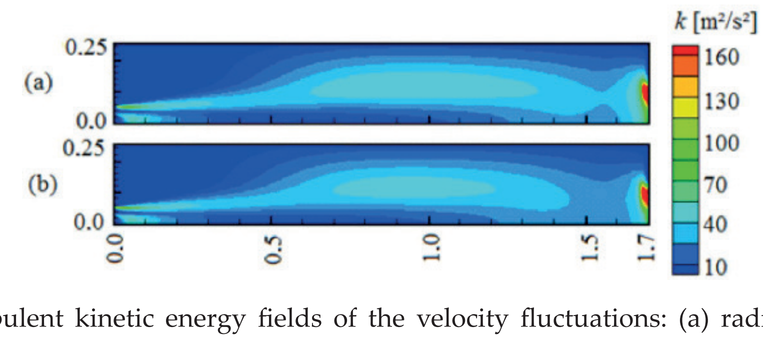

Figure 2. Turbulent kinetic energy fields of the velocity fluctuations: (a) radiation neglected; (b) radiation computed.

Source: Figure extracted from Centeno *et al.* (2014b), as a courtesy of ABCM - Rio de Janeiro, Brasil.

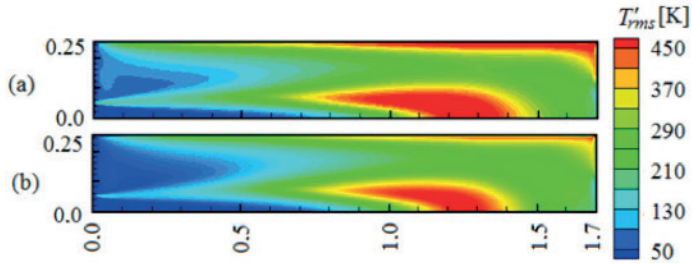

Figure 3. RMS of the temperature fluctuation fields: (a) radiation neglected; (b) radiation computed.

Source: Figure extracted from Centeno *et al.* (2014b), as a courtesy of ABCM – Rio de Janeiro, Brasil.

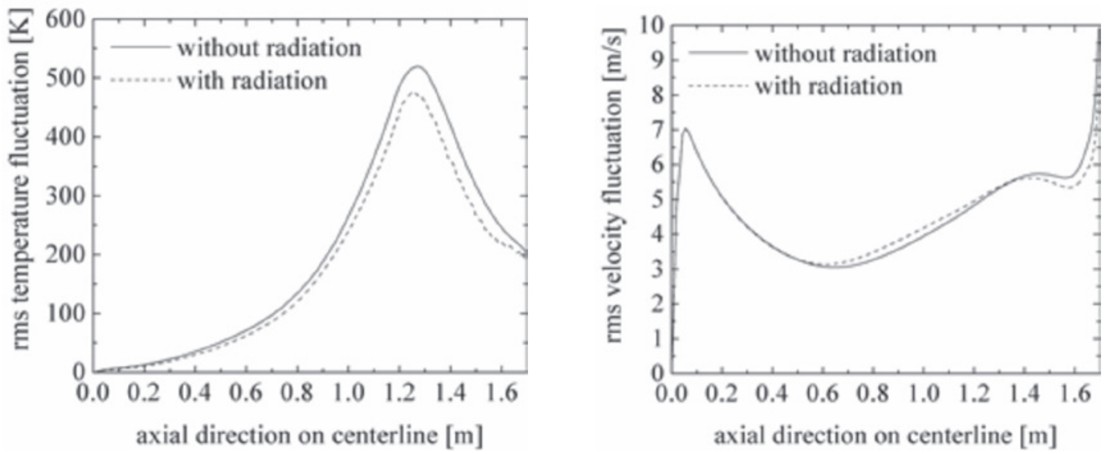

Figure 4. RMS of the temperature fluctuations and of the velocity fluctuations: profiles at chamber symmetry-line (axial direction).

Source: Figure extracted from Centeno *et al.* (2014b), as a courtesy of ABCM – Rio de Janeiro, Brasil.

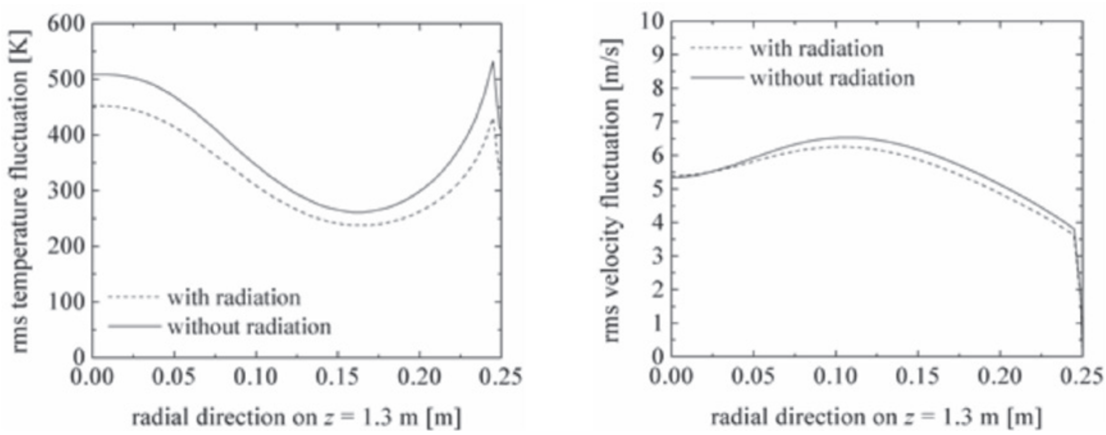

Figure 5. RMS of the temperature fluctuations and of the velocity fluctuations: profiles at z = 1.3 m (radial direction).

Source: Figure extracted from Centeno *et al.* (2014b), as a courtesy of ABCM – Rio de Janeiro, Brasil.

of the velocity fluctuations (considering fully developed isotropic turbulence, RMS of the velocity fluctuations can be computed as the square root of the turbulent kinetic energy of the velocity fluctuations: $v'_{rms} = \sqrt{k}$). In such figures, profiles are shown for the axial direction at the chamber symmetry-line and for the radial direction at axial position z = 1.3 m. It can be observed that the influence of radiation on those turbulence-related properties was small, but not negligible (for example, a difference of nearly 70 K for the rms temperature fluctuation was noticed for r = 0.0 m at z = 1.3 m). Radiation tended to smooth turbulent fluctuations of temperature and velocity. Besides, the influence of radiation was more pronounced on the temperature fluctuations than on the velocity fluctuations; such behavior can be especially important for consideration in problems involving transition from laminar to turbulent flows, which in general are determined considering isothermal flows.

Conclusions

This study presented an analysis of the influence of thermal radiation on the turbulence in a turbulent non-premixed methane–air flame in a cylindrical combustion chamber. The radiation field was computed with the WSGG model using recently obtained correlations (Dorigon *et al.*, 2013) based on the up-to-date HITEMP2010 and considering TRI effects (Snegirev, 2004). 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. This work showed the influence of radiation on turbulence in a combustion problem by means of two scenarios: radiation neglected from calculations, and radiation included into calculations. Comparison of the results obtained from the different radiative scenarios showed that radiation did not importantly influence the turbulence-related properties (root mean square of the temperature fluctuations and of the velocity fluctuations, and the turbulent kinetic energy of the velocity fluctuations), but such influence, despite small, was not negligible. Radiation tended to smooth turbulent fields, in agreement with results reported in the literature for high temperature flows. The influence of radiation on temperature fluctuations was more important than its influence on velocity fluctuations. Some possible future advances in the radiation-turbulence analysis are testing different turbulence models (other than standard k-ε) and performing simulations with different turbulence methodology (other than RANS).

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