EVALUATION OF NEW WSGG MODEL CORRELATIONS ON RADIATIVE SOURCE TERM IN A 2D AXISYMMETRIC TURBULENT DIFFUSION FLAME

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Abstract. *In the present work, the radiation effect of non-gray gases were estimated by means of two different weighted-sum-of-gray-gases (WSGG) model correlations (classical ones of Smith et al. (1982) and new ones of Dorigon (2012) which were fitted from state-of-the-art gas spectroscopic database), in a turbulent diffusion methane–air cylindrical combustion chamber. The reaction rates were considered as minimum rates between Arrhenius and Eddy Breakup rates. A two step global reaction mechanism was used and turbulence modeling was considered via standard k-ε model, since the stress is on radiation calculations. The source terms of energy equation consisted of reaction rates and radiation effects. The discrete ordinates method (DOM) was employed to solve the radiative transfer equation (RTE). Comparing the results obtained with the different WSGG correlations it was possible to check that the temperature, wall heat flux and radiant fraction were affected by the different WSGG correlations, while the influence on species concentrations were negligible. The numerical results obtained considering the new WSGG correlations were closer to the experimental data (Garréton and Simonin, 1994) than the case with the classical model.*

Keywords*: Radiation heat transfer, weighted-sum-of-gray-gases, combustion, turbulent diffusion flames*

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, which is an important heat transfer mechanism in combustion, is necessary to achieve appropriate solutions for this complex phenomena. Heat transfer determination affect directly the computation of 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 can be characterized by several thousands of spectral lines. Thus, the solution of the radiative heat transfer equation 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 radiative transfer equation (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 models are commonly used. Among the spectral dependent models, the weighted-sum-of-gray-gases (WSGG) developed by 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, where 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 and global) and stated that the non-gray formulation of the WSGG is also very efficient from a computational point of 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 gray models, are often used in computational fluid dynamics (CFD) to simulate combustion problems (e.g. see Pierce and Moss, 2007), since more sophisticated models may become extremely time consuming when fluid flow/combustion/radiative transfer are coupled.

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 the partial pressures for CO_2 and H_2O mixtures, Krishnamoorthy (2010) obtained parameters for a new WSGG computed from total emissivity correlations encompassing the range of the H_2O/CO_2 ratios encountered within the Sandia Flame D. Predictions from the new model compared favorably against the spectral-line-based WSGG (SLW model) and existing benchmarks. With the same motivation, Johansson et al. (2011) modified the WSGG to account for various ratios of H_2O and CO_2 concentrations, covering from oxyfuel combustion of coal, with dry or wet flue gas recycling, as

well as combustion of natural gas. The modified WSGG model significantly improved the estimation of the radiative source term compared to the gray models, while the accuracy of wall fluxes was similar to the gray models or better. Galarça et al. (2008) also present new absorption coefficients and temperature dependent weighting functions for use with the WSGG model. Bidi et al. (2008) employed the DOM (discrete ordinate method) to solve RTE equation and the WSGG model to compute non-gray radiation effect of combustion gases in a cylindrical chamber, with the purpose of studying the radiation effect in the flame structure. The results indicated that the radiation can affect the temperature field and the species concentrations, and the numerical results including radiation were closer to the experimental data than the case in which radiation was neglected. Predictions of the radiative heat source with different gas models were analyzed in Mossi et al. (2010), where the authors simulated a laminar methane-air diffusion flame solving conservation equations (mass, momentum, species, soot, energy) through a finite volume code. In this work, the RTE was solved with DOM, and the authors compared the radiative effects obtained by a simple gray-gas model and the SLW model.

This work presents a numerical simulation of turbulent, non-premixed combustion of methane in air in a cylindrical chamber. For validation of the proposed solution the similar case described by Garréton and Simonin (1994) was studied, since detailed measurements are available of spatial distributions of major gas species concentrations and temperature, and also this flame was recently studied by our research group (Silva et al., 2007). On the previous work (Silva et al., 2007) the investigation emphasis was on general flame modeling, while in the present work the main objective is to verify the role of radiation heat transfer with the use of different correlations for the WSGG model.

2. PROBLEM STATEMENT

The physical system consists of the same natural gas combustion chamber that was analyzed in Magel et al. (1996) and Silva et al. (2007), which were test cases proposed in Garréton and Simonin (1994). The cylindrical chamber has a length and a diameter of 170 cm and 50 cm, respectively, as shown in Fig. 1. Natural gas is injected into the chamber by a duct aligned with the chamber centerline. The burner is capable of providing 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 0.0125 kg/s at a temperature of 313.15 K, this requires an air mass flow rate of 0.186 kg/s, at a temperature of 323.15 K. The fuel enters the chamber through a cylindrical duct having diameter of 6 cm, while air enters the chamber through a centered annular duct having a spacing of 2 cm. For such mass flow rates, the fuel and air velocities are 7.76 and 36.29 m/s, respectively. The Reynolds number at the entrance, approximately 18000, 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.

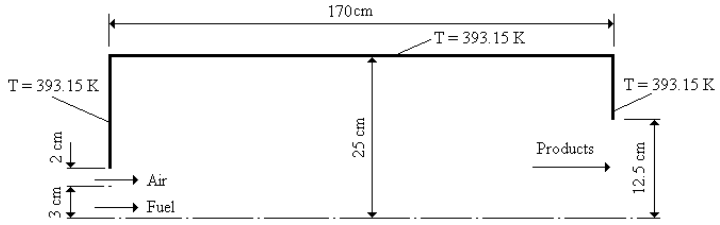

Figure 1. Combustion chamber geometry.

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.

3. MATHEMATICAL FORMULATION

The proposed work can be stated as follows: considering a steady turbulent diffusion flame of methane in air, for a cylindrical chamber, compute temperature, chemical species concentrations and velocity fields, and verify the influence of the thermal radiation on the process, taking into account Smith et al. (1982) and Dorigon (2012) WSGG correlations.

3.1 Governing equations and combustion kinetic

The conservation equations for mass, momentum in the axial and radial directions, k-ε turbulence model, energy and chemical species conservation are solved for steady incompressible flow in 2D axisymmetric coordinates. A detailed description of those equations and their solution methods can be found in Silva et al. (2007). Since the main objective of the present work is to evaluate the radiative heat source term ($\overline{S}_{rad}$), calculated as the divergence of the radiative heat flux, special attention is given for it and a discussion on radiation modeling and radiative proprerties used in the present work is provided Section 3.2 below.

In relation to combustion kinetics, as a basic assumption it is considered that the combustion process occurs at finite rates with methane oxidation taking two global steps according to Eq. (1), given by:

$$\begin{aligned} &2CH_4^{(16)} + 3\left(O_2^{(32)} + 3.76N_2^{(28)}\right) \rightarrow 2CO^{(28)} + 4H_2O^{(18)} + 11.28N_2^{(28)} \\ &2CO^{(28)} + 1\left(O_2^{(32)} + 3.76N_2^{(28)}\right) \rightarrow 2CO_2^{(44)} + 3.76N_2^{(28)} \end{aligned} \tag{1}$$

The rate of formation or destruction, $\overline{R}_{\alpha,k}$, of each α-th species in each k-th reaction (in this formulation there are 2 reactions as shown in Eq. (1), so $k = 2$) is obtained by the Arrhenius-Magnussen's model (Eaton et al., 1999; Fluent Inc., 1997), 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, 1976). This formulation is employed in Silva et al. (2007) and Nieckele et al. (2001), where all parameters (applicable for each model) are described in detail. The average volumetric rate of formation or destruction of the α-th chemical species $\overline{R}_{\alpha}$, which appears in both energy and species mass fraction conservation equations is then computed from the summation of the volumetric rates of formation or destruction in all the k-th reactions where the α-th species is present, i.e. $\overline{R}_{\alpha} = \sum_k \overline{R}_{\alpha,k}$.

The above mentioned two-equation chemistry assumption was employed in the current study to conserve 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 many 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, the chemistry presented in Eq. (1) does not involve soot formation/oxidation, while it was an assumption in the present work that the flame is low sooting.

3.2 Radiation modeling and the weighted-sum-of-gray-gases (WSGG) model

The radiative transfer equation for non-scattering media, in cylindrical coordinates, with the discrete ordinates method, is given by Eq. (2), which is subject to the boundary condition in Eq. (3).

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

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

where μ, ς, and ξ are the directions, η is the wavenumber, $I_{b\eta}$ is the blackbody intensity, I_η is the intensity, and κ_η is the absorption coefficient, given by:

$$\kappa_\eta = N\sum_i \frac{S_i}{\pi}\frac{\gamma_i}{(\eta-\eta_i)^2+\gamma_i^2} \tag{4}$$

where S_i (in cm^{-1}/(molecule.cm^{-2})) is the integrated line intensity, η_i (in cm^{-1}) is the line location, and γ_i (in cm^{-1}/atm) is the half-width, which is a function of the mole fraction X_s, described by:

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n X_s \gamma_{self,i} + \left(\frac{T_{ref}}{T}\right)^{0.5}(1-X_s)\gamma_{air,i} \tag{5}$$

where T is the temperature, γ_{self} and γ_{air} are the self broadening half-width and air broadening half-width, respectively, and n is the temperature dependent coefficient. The values of η_i, S_i, γ_{self}, γ_{air} and n can be obtained from HITRAN (Rothman et al., 2005) or HITEMP (Rothman et al., 2010), among other databases.

On the right hand side of Eq. (2) the first term represents attenuation due to absorption and the second term augmentation due to emission. Once the RTE is solved, the radiative heat source ($\overline{S}_{rad}$) is calculated as:

$$\nabla\cdot q_r = \int_\Omega\int_\eta \left(-\kappa_\eta I_\eta + \kappa_\eta I_{b\eta}\right) d\eta d\Omega \tag{6}$$

The absorption coefficient represented by Eq. (4) is strongly dependent on the wavenumber, being represented by several thousands of spectral lines. Therefore, solving Eq. (2) for all spectral lines value is excessively time consuming for coupled solutions of the conservation equations. Due to this fact, gas models have been used to solve the RTE quickly. A brief description of the gas model selected for the present analysis, the WSGG model, is described below.

Considering Reynolds averaging, the mean radiative source term and the mean RTE a priori are unclosed due to instantaneous fluctuating terms related to the absorption coefficient and the blackbody emissive power, a problem known as turbulence-radiation interaction (or TRI). In the current work these interactions were not accounted for, so all fundamental equations, relations, results and analysis were related to mean quantities. This is a good assumption for optically thin flames, but should be addressed for in optically thick flames, as implied from Li and Modest (2002). Flame optical thickness for the flame studied here is 0.43, which is considered of medium optical thickness. In this manner, despite TRI was not considered, it was expected that the analysis obtained were not pronounced affected by this simplification, since the objective here was comparing radiative calculations using two different WSGG correlations, while both analysis were taken without TRI.

The original formulation of the WSGG model consists of expressing the total gas emissivity 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 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):

$$\frac{dI_j}{ds} + k_j I_j = k_j a_j(T) I_{b,j}(T) \tag{7}$$

with j 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, 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 limits the application of the method (Porter et al., 2010).

In the present study both formulations of Smith et al. (1982) and Dorigon (2012) are considered for $p_{H2O}/p_{CO2} = 2$, which then have their results compared. Dorigon (2012) obtained WSGG coefficients fitted from HITEMP2010 molecular spectroscopic database (Rothman et al., 2010), which are the most accurate database nowadays available. In that work, Dorigon (2012) compared results obtained with these new coefficients against line-by-line calculations in one-dimensional problems and found good agreement (average errors of less than 1.6 %). For convenience, Tab. 1 shows the coefficients obtained by Dorigon (2012).

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 concentration does not exceed relatively high values of the order of 2%, while the contribution from CH_4 is even lower than that of CO (Coelho et al., 2003).

Table 1. WSGG model coefficients (Dorigon, 2012). $p_{H2O}/p_{CO2} = 2$.

j	$k_{g,j}$ [$m^{-1}atm^{-1}$]	$b_{g,j1}\times10^{1}$	$b_{g,j2}\times10^{4}$ [K^{-1}]	$b_{g,j3}\times10^{7}$ [K^{-2}]	$b_{g,j4}\times10^{10}$ [K^{-3}]	$b_{g,j5}\times10^{14}$ [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

4. RESULTS AND DISCUSSIONS

A symmetry boundary condition was applied in the center line and prescribed temperature boundary conditions in the side wall, as shown in Fig. 1. The set of equations were solved using the finite volume method by means of a dedicated Fortran code. A grid with 70 volumes in the axial direction and 35 volumes in the radial direction was used. The numerical accuracy was checked by comparing the predicted results calculated using the grid mentioned above with those obtained using coarser and thinner grids, and the 70 × 35 grid showed to provide grid independent results, as well as reasonable computational effort. This grid is non-uniform spaced in the radial direction with 24 volumes between 0 and 12.5 cm (the centerline and the chamber outside radius), and is uniformly spaced in the axial direction. The radiative transfer calculations were performed using the same spatial grid, and S_6 quadrature. The simulations were performed in a desktop computer with Intel Core 2 DUO 3.0 GHz processor and 2.0 GB of memory. Running the code with the WSGG model, it takes about 12 hours of simulation, while a simulation without radiation heat transfer the time is less than 1 hour. It must be noticed that radiative transfer calculations are performed only after a reasonably converged solution has been achieved, and then at each iteration of CFD code.

In order to study the influence of radiative transfer and radiative properties modeling, three different scenarios were considered. In the first scenario, radiation is completely ignored in order to analyze the importance of radiation in the flame simulations in general. In the second and third scenarios, radiation is considered and the gas absorption coefficient is modeled using two different WSGG models. Comparisons were made to verify how the radiative heat transfer affects the temperature field, the H_2O and CO_2 for the three scenarios.

Figure 2 shows the results for the temperature and for the divergence of the radiative heat flux ($\overline{S}_{rad}$). On the left hand side of that figure, the temperature plots were obtained for three cases: radiation neglected, radiation computed using Smith et al. (1982) correlations, and radiation computed using Dorigon (2012) correlations. The right hand side is showing the radiative heat source obtained with both WSGG correlations, as well as the relative error between them, according to the following relation (where subscripts *Smith* and *Dorigon* indicate which WSGG correlation was used in the calculation of $\overline{S}_{rad}$):

$$\%Error = 100\frac{\overline{S}_{rad,Smith} - \overline{S}_{rad,Dorigon}}{\overline{S}_{rad,Smith}} \tag{8}$$

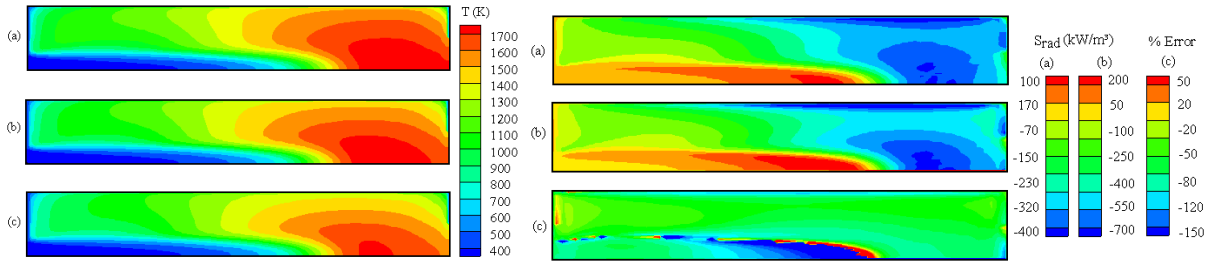

Figure 2. LEFT: temperature fields for (a) radiation neglected; (b) radiation computed with Smith et al. (1982) correlations; (c) radiation computed with Dorigon (2012) correlations. RIGHT: Radiative heat source computed with (a) Smith et al. (1982) correlations; (b) Dorigon (2012) correlations; (c) relative error between (a) and (b).

As can be seen in Fig. 2(left), the different radiation models affect directly the temperature field. Computed flame peak temperatures are 1856.30 K, 1772.93 K and 1726.91 K for cases neglecting radiation, computing radiation with Smith et al. (1982) correlations and with Dorigon (2012) correlations, respectively. The peak temperature drops 83 K and 129 K when comparing results without radiation and considering results with radiation computed with Smith et al. (1982) and with Dorigon (2012) correlations, respectively. While peak temperature apply only to a single point, it usually characterizes the entire temperature field. When the temperature changes, the reaction rate coefficient also changes, so it could affect directly in the formation and destruction of the species involved in the process. Despite that, the mean variations of H_2O and CO_2 concentrations using the different correlations are only about 2%. For this particular test problem, the difference of those species concentration fields for the two different WSGG models is not as large as that of the temperature field. This is caused by the use of the reduced-chemistry assumption, in which chemical reaction rate is primarily controlled by turbulent mixing and, therefore, is less sensitive to temperature change.

Besides the temperature field change, radiation fields also change significantly as a result of the different WSGG models, which is expected since the radiation field is present in energy equation. Figure 2(right) shows the radiative heat source, which is estimated as the divergence of the radiative heat flux. It is observed that the flame region with the highest temperatures emits more radiation than absorbs, leading to a negative heat source as expected per Eqs. (2) or (6). On the other hand, the flame region with the smallest temperatures absorbs more radiation than emits, leading to a positive heat source. Also, on the right side of Fig. 2 it is shown the radiative heat source difference obtained with the different WSGG correlations, obtained using Eq. (8). The radiative heat source calculated with Dorigon (2012) correlations are higher than the one calculated with Smith et al. (1982). The higher differences are located at the flame core, where the temperature is relatively low and the net radiative source is positive (absorbing region).

Figure 3 shows the temperature, H_2O molar fraction and CO_2 molar fraction profiles along the chamber centerline, while Fig. 4 shows the same quantities along the radial direction at axial position 0.912 m from the chamber entrance, considering four different scenarios: experimental data from Garréton and Simonin (1994) (data not available for H_2O), simulation neglecting radiation heat transfer, simulations with radiation heat source computed by WSGG with Smith et al. (1982) and WSGG with Dorigon (2012) correlations. 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 source inside the computational chamber domain. In addition, the same behavior is observed comparing results obtained with the different WSGG correlations, i.e., since the use of Dorigon (2012) correlations provides higher radiative heat source than Smith et al. (1982) correlations, temperature peak, values and gradients are smaller for the former correlations. The

same analysis can be implied from Fig. 2. H_2O and CO_2 molar fraction profiles are less affected by the radiative heat source modeling, as discussed previously.

Figures 3 and 4 show that for all the radiation models the mean temperature and the mean molar fraction of CO_2 follow the experimental data tendency, but differences are found. Basically, those differences have nothing to do with the choice of the radiation model, but show a limitation of the other models, namely the turbulence and combustion models. On the other hand, it was found that the radiative calculations, namely the radiative heat source, heat transfer rate through chamber side wall, net radiative heat loss and radiant fraction, strongly depends on the radiation model, as revealed in Figs. 2 and 5, and Tabs. 2 and 3.

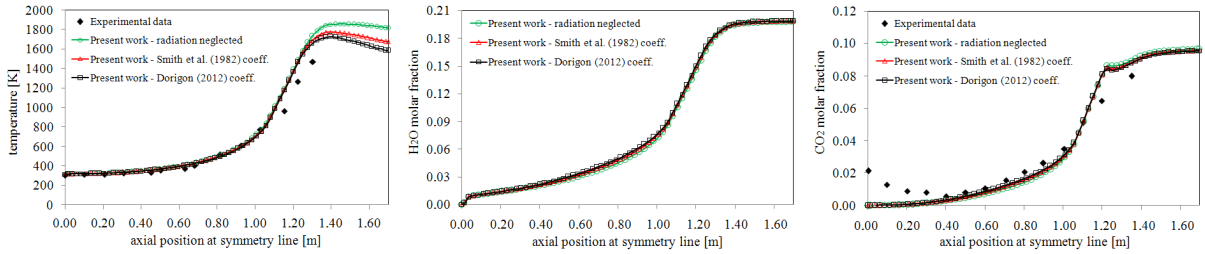

Figure 3. Centerline temperature, H_2O molar fraction and CO_2 molar fraction profiles.

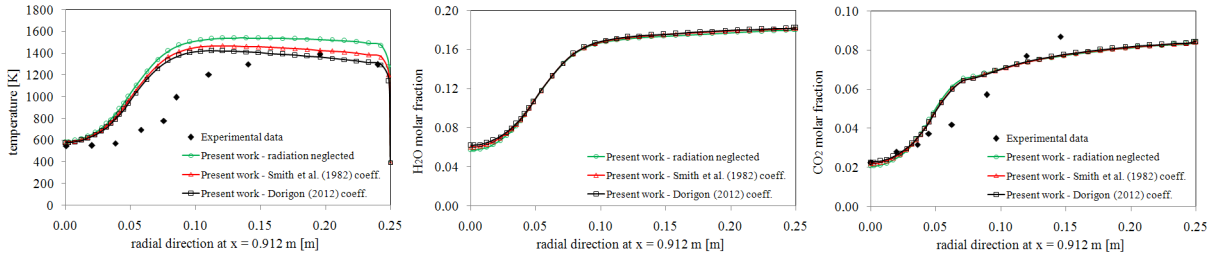

Figure 4. Temperature, H_2O molar fraction and CO_2 molar fraction profiles along radial direction at $x = 0.912$ m.

An additional view of the effect of thermal radiation is presented in Tab. 2, which shows the heat transfer through the chamber side wall. The inclusion of thermal radiation has a major effect in the heat transfer, which is given by the sum of heat transfer by radiation and convection, leading to an increase in the total heat transfer from 77.48 kW (only convection, without radiation heat transfer) to a maximum of 154.86 kW (sum of convection and radiation heat transfer). The pattern of these results are in agreement with Silva et al. (2007), where it was shown that the predicted heat transfer through the chamber sidewall is approximately doubled when radiation was taken into account. It is interesting to note that when thermal radiation is included, the convective heat transfer decreases in comparison to when thermal radiation is neglected, since the temperature gradients in the chamber are reduced (as a consequence of an additional volumetric heat source). Also, the results show that radiation heat transfer is increased when the new WSGG correlations are used, as expected since the radiative heat source (Fig. 2) is higher with these new correlations.

The role of using different WSGG correlations on radiative heat transfer can be better shown by isolating their effects on the radiation calculations alone. This can be done by freezing the species concentrations and temperature fields and then calculating radiation fields using WSGG correlations from Smith et al. (1982) and Dorigon (2012). These calculations are decoupled from CFD, therefore errors arising from turbulence and combustion models do not influence these radiative calculations. This procedure was applied using the same converged temperature, H_2O and CO_2 fields obtained from a specific simulation. The results of this analysis are presented as "decoupled CFD/Radiation calculations" in Tab. 3 and Fig. 5.

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 (Q_{net}) corresponds to the integral of $\nabla \cdot q_r$ over the computational domain, and the radiant fraction is the ratio of this value to the power released in combustion. In every simulation scenario, these quantities were calculated and the results are shown in Tab. 3. The radiation loss from the present flame has a significant value, making the present analysis worthwhile since the radiant fraction has doubled using the new WSGG model correlations, which were fitted from state-of-the-art radiant spectral properties data. Also, it is observed in Tab. 3 that the radiant fraction follows the same tendency for both coupled and decoupled CFD/Radiation calculations, i.e., it has the same order of magnitude and it increases (about double) due different WSGG correlations.

Figure 5 presents profiles of radiative heat source at chamber centerline for coupled and decoupled CFD/Radiation calculations cases. It is shown that the radiative heat source is essentially the same in the two cases, with a multiplication factor between them in some regions, supporting the results of Tab. 3.

Taking into account the previous analysis from Tab. 3 and Fig. 5, the radiation calculations results can be evaluated and analyzed considering that the influence of the other models (combustion, turbulence, CFD solver, etc) on them are small and known.

Table 2. Heat transfer rate on the combustion chamber side wall.

	Without radiation	With radiation[(a)]	With radiation[(b)]
Convection heat transfer rate (kW)	77.48	68.72	63.10
Radiative heat transfer rate (kW)	0.00	51.29	91.76
Total rate (radiation + convection) (kW)	77.48	120.01	154.86

(a) using WSGG correlations of Smith et al. (1982). (b) using WSGG correlations of Dorigon (2012).

Table 3. Predicted net radiative heat loss (Q_{net}) and fraction of radiative heat loss (f_{rad}).

	Coupled CFD / Radiation		Decoupled CFD / Radiation	
	Q_{net} [kW]	f_{rad} [%]	Q_{net} [kW]	f_{rad} [%]
Smith et al. (1982) correlations	74.31	12.38	90.56	15.09
Dorigon (2012) correlations	120.14	20.02	175.01	29.16

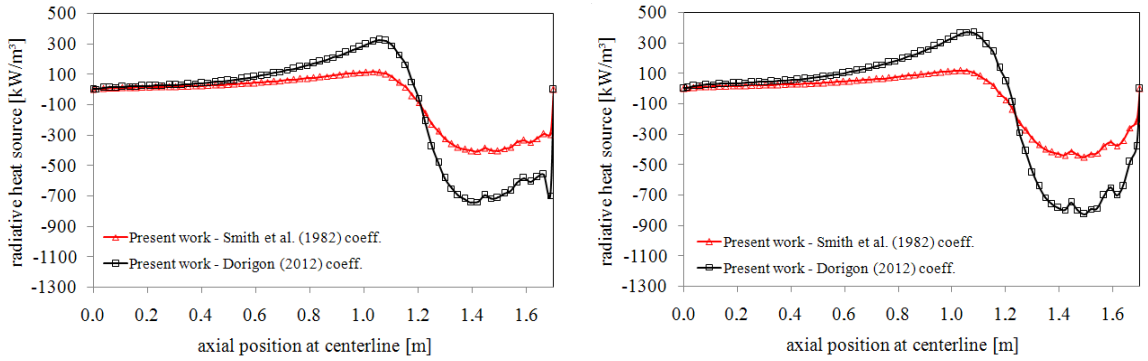

Figure 5. Profiles of radiative heat source at chamber centerline (LEFT: coupled CFD/Radiation. RIGHT: decoupled.)

5. CONCLUSIONS

A turbulent diffusion methane–air combustion in a cylindrical chamber was numerically simulated considering radiation effect of non-gray gases by means of two different weighted-sum-of-gray-gases (WSGG) models: the well-known of Smith et al. (1982) and the new one of Dorigon (2012) in which correlations were fitted from state-of-the-art gas spectroscopic database. A two step global reaction mechanism was used and turbulence modeling was considered via standard k-ε model, since the stress was on radiation calculations. The discrete ordinate method (DOM) was employed to solve the radiative transfer equation (RTE). This work showed the importance of a good prediction in the radiative heat transfer for combustion problems. The comparison of the results obtained with the two WSGG correlations showed that temperature, radiative heat source, heat transfer through chamber wall and radiant fraction were sensible and affected by the different WSGG correlations applied as radiation model, while its effect on species concentrations was of minor relevance. Since the radiative heat source changed significantly with the two correlations, it is conclusive that to get correct approaches for the chamber temperature and wall chamber heat transfer is mandatory to use a good radiation model in the simulations. Also, the numerical results obtained considering the new WSGG correlations were closer to the experimental data (Garréton and Simonin, 1994) than the case with the classical model. In this manner, it is clear that radiation heat transfer and radiative properties modeling are very important issues and cannot be undertreated in combustion predictions. The sequence of the current research is related to radiative properties modeling using line-by-line calculations, study of turbulence-radiation interactions on the studied flame, and analyze soot formation/oxidation and its role in radiation heat transfer inside the chamber.

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