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RADIATION CALCULATIONS ON FLUENT CFD: THREE APPROACHES FOR THE WEIGHTED-SUM-OF-GRAY-GASES MODEL

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Abstract. *Three approaches for the weighted-sum-of-gray-gases (WSGG) model were implemented with the software ANSYS/Fluent to predict radiation heat transfer for a laminar non-premixed methane/air flame: (i) Fluent standard WSGG model; (ii) WSGG for mixtures of CO_2 and H_2O with constant partial pressure ratio; and (iii) WSGG for arbitrary H_2O/CO_2 ratios. The fully coupled reactive flow/radiation transport equations problem was solved with the approach (ii) and the converged fields were used for the solution with the remaining methodologies. The fuel is diluted with N_2 in order to suppress soot formation, neglected in the solution. User-defined functions (UDF) were developed for the coupling of the WSGG (ii) and (iii) with ANSYS/Fluent. Results for the radiative heat flux were compared with experimental data and the methodologies (ii) and (iii) showed much better accuracy than approach (i). The methodology for non-constant ratio (iii) presented the most reliable results, followed by the WSGG for constant partial pressure ratio. As a way of understanding the Fluent WSGG calculation procedure, a UDF was written and some 1D isothermal/non-isothermal, homogeneous/non-homogeneous test cases were solved. Fluent WSGG is not recommended when good accuracy is required in the solution.*

Keywords: *radiative transfer, weighted-sum-of-gray-gases, combustion, ANSYS/Fluent.*

1. INTRODUCTION

Thermal radiation is the main heat transfer mechanism in combustion processes due to the high temperatures involved. The solution of radiation heat transfer covers the modelling of spectral properties of the medium such as the absorption coefficient that vary in a complex way with the wavenumber. In this way several spectral models were developed in order to emulate the behaviour of real gases and obtain reliable results with low computational costs.

The weighted-sum-of-gray-gases (WSGG) (Hottel and Sarofim, 1967) assume that the integration of the spectral properties over the spectrum can be replaced by a summation over a few gray gases with constant absorption coefficients plus the transparent window. Smith, *et al*., 1982, presented coefficients for the WSGG model for carbon dioxide and water vapour by fitting data generated from the exponential wide-band model, considering three gray gases. These coefficients are widely used in computational fluid dynamics codes such as in ANSYS/Fluent (Ansys, 2011a). Porter, *et al.*, 2010, performed a comparison between the full spectrum correlated-k (FSCK) and WSGG models under oxy-fuel combustion environments conditions. The absorption coefficient for the WSGG was obtained from the total emissivity of the medium by the Beer's Law and the mean beam length approach. The FSCK model proved to be more accurate than the WSGG model. Dorigon, *et al*., 2013, generated new coefficients for water vapour and carbon dioxide for partial pressure ratios equals to 1.0 and 2.0, using the up-to-date spectral database HITEMP2010 (Rothman et al., 2010). Cassol, *et al*., 2014, presented a new WSGG methodology for mixtures with arbitrary concentrations of the participating species.

In this study, three approaches for the WSGG model (Ansys 2011a, Dorigon, *et al*., 2013, and Cassol, *et al*., 2014) were coupled with ANSYS/Fluent to solve the radiative heat transfer in a non-premixed laminar flame of methane diluted with 50% of nitrogen, in volume, surrounded by a low-velocity air coflow for wich experimental measurements for the radiative heat flux are available (Machado, 2015).

User-defined-functions (UDF) (Ansys, 2011b), were developed for each WSGG approach. The fully coupled transport equations reacting flow/radiation problem was solved as in Rodrigues (2016), for the WSGG model presented by Dorigon, *et al.*, 2013. Calculations for the remaining approaches (Ansys, 2011a and Cassol, *et al.*, 2014) were

carried through the converged field of temperature, CO_2 and H_2O. The goal of the present study is then to compare different approaches accuracy on the solution of the radiative heat transfer problem in combustion process.

2. PROBLEM STATEMENT

The problem studied consists of a laminar non-premixed CH_4/air flame with 50% of N_2 dilution in fuel flow. This flame is from the constant power series identified as PC0050N50 as in (Machado, 2015 and Rodrigues, 2016). Experimental data for the radiative heat flux, radiant fraction and flame length were obtained by Machado (2015).The simulations were performed in the commercial software ANSYS Fluent v. 13.0. The convergence criteria for the computed variables were established for residuals lower than $1x10^{-6}$.

The problem geometry consists of a 2D axisymmetric domain based on the burner and flame dimensions (Machado, 2015). Details about dimensions, boundary and inlet conditions can be seen in Figure 1.

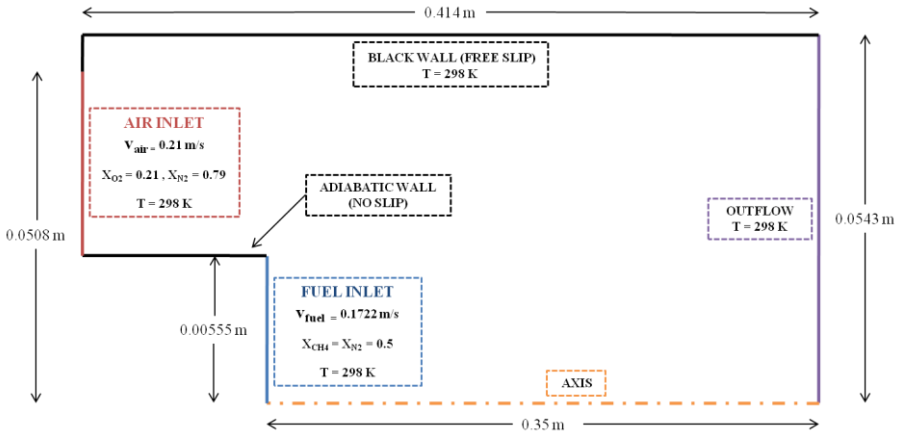

Figure 1. Schematic of domain dimensions, boundary and inlet conditions.

It was adopted a parabolic profile for the fuel velocity inlet given by

$$v(r) = 2\overline{v}\left[1-\left(\frac{r}{R}\right)^2\right] \tag{1}$$

in which R and $\overline{v}$ are the fuel inlet radius and velocity, respectively.

2.1 Reactive flow modeling

The steady state laminar reactive flow modeling is based on the solution of the transport equations for the mass, momentum, chemical species mass and energy, respectively:

$$\vec{\nabla}\cdot\left(\rho\vec{v}\right) = 0 \tag{2}$$

$$\vec{\nabla}\cdot\left(\rho\vec{v}\times\vec{v}\right) = \rho\vec{g} + \vec{\nabla}\cdot\hat{\tau} \tag{3}$$

$$\vec{\nabla}\cdot\left(\rho\vec{v}Y_i\right) = -\vec{\nabla}\cdot\vec{J}_i + \dot{\omega}_i, \quad \text{for } i = 1,\ N_s - 1 \tag{4}$$

$$\vec{\nabla}\cdot\left(\rho\vec{v}h\right) = -\vec{\nabla}\cdot\vec{J}_q + \dot{q}_R \tag{5}$$

The low Mach number assumption is valid and the specific mass ρ can be computed as a function of the temperature only. The shear stress tensor $\hat{\tau}$ is computed by Stokes' law for Newtonian fluids. The species fluxes $\vec{J}_i$

are computed by Fick's law. The heat flux $\vec{J}_q$ vector is composed of the Fourier's law and the mass diffusion flux (fickian like). To guarantee the mass conservation the mass fraction of the N_s specie is computed as $Y_{N_s} = 1 - \sum_{i=1}^{N_s-1} Y_i$

Transport and thermal properties of individual species are computed by CHEMKIN database. Transport coefficients for the mixture are computed as a mixture-averaged formulation. For chemical reactions modeling the skeleton DRM19 mechanism (Kazakov and Frenklach, 1994) with 21 species and 84 reactions was adopted. The chemical source term $\dot{\omega}_i$ on Eq. (4) is computed with the Arrhenius kinetic equations.

Since main goal of this work is the modeling of the energy equation source term $\dot{q}_R$, it will be discussed in a separate chapter.

3. RADIATION MODELING

The radiative transfer equation (RTE) for an absorbing/emitting and non-scattering medium along a path S is written as

$$\frac{dI_\eta}{dS} = -\kappa_\eta I_\eta + \kappa_\eta I_{\eta,b} \tag{6}$$

The directional dependence of the above equation is computed by the discrete ordinates method (DOM) with a total number of 160 directions. The spectral modeling of the absorption coefficient κ_η is made by three different approaches for the WSGG model: (i) the Fluent standard WSGG; (ii) the constant ratio WSGG; and (iii) the non-constant ratio WSGG briefly presented in the following subsections.

3.1 Fluent standard WSGG (Fluent-WSGG)

In this formulation the RTE is written as for the gray gas model, in which the spectral dependence of the absorption coefficient is neglected. However the spectral dependence is taken into account by the absorption coefficient (ANSYS, 2011a), then

$$\frac{dI}{dS} = -\kappa I + \kappa I_b \tag{7}$$

$$\kappa = -\frac{\ln(1-\varepsilon)}{s} \tag{8}$$

where s is the mean beam length written as

$$s = 3.6\frac{V}{A} \tag{9}$$

in which V is the fluid volume and A is the total surface area of the fluid boundaries (ANSYS, 2011a). The total emissivity ε for the N_g gray gases computed as

$$\varepsilon = \sum_{j=0}^{N_g} a_j(T)\left(1 - e^{-\kappa_{p,j} pS}\right) \tag{10}$$

The weighting factor a_j is the blackbody energy fraction that is emitted by the gray gas and is given by a polynomial function of the temperature according to

$$a_j = \sum_{k=1}^{N_g+1} b_{j,k} T^{k-1} \tag{11}$$

The pressure-based absorption coefficient $\kappa_{p,j}$ and the polynomial coefficients $b_{j,k}$ implemented by the Fluent solver are the ones presented by Smith, *et al.*, 1982 (Table 1). For the spectral window the absorption coefficient is zero and the weighting factor is computed as

$$a_0 = 1 - \sum_{j=1}^{N_g} a_j \tag{12}$$

The link between the RTE and the energy conservation is made by the radiative heat flux that is given by the negative of the heat flux divergence

$$\dot{q}_R = -\vec{\nabla} \cdot \vec{q}''_R = \kappa \left[\left(\int_{4\pi} I d\Omega \right) - 4\pi I_b \right] \tag{13}$$

Table 1. Fluent-WSGG coefficients by Smith, et al., 1982, for $p_{H_2O} / p_{CO_2} = 2$.

j	$\kappa_{p,j}$ $(atm\ m)^{-1}$	$b_{j,0}$	$b_{j,1}$ (K^{-1})	$b_{j,2}$ (K^{-2})	$b_{j,3}$ (K^{-3})
1	0.402	6.508×10^{-1}	-5.551×10^{-4}	3.029×10^{-7}	-5.353×10^{-11}
2	6.516	-0.2504×10^{-1}	6.112×10^{-4}	-3.882×10^{-7}	6.528×10^{-11}
3	131.9	2.718×10^{-1}	-3.118×10^{-4}	1.221×10^{-7}	-1.612×10^{-11}

3.2 Constant ratio WSGG (CR-WSGG)

The RTE for the CR-WSGG model can be written as

$$\frac{dI_j}{dS} = -\kappa_j I_j + \kappa_j a_j I_b \tag{14}$$

The absorption coefficient for the gaseous mixture is computed as a function of the species partial pressures (or mole fraction X) as

$$\kappa_j = \kappa_{p,j}\, p \left(X_{CO_2} + X_{H_2O} \right) \tag{15}$$

The weighting factor for the gray gases and the transparent windows are computed by Eqs (11) and (12). The $\kappa_{p,j}$ and the polynomial coefficients $b_{j,k}$ implemented via UDF for the CR-WSGG model are the ones obtained by fitting the total emittance data computed by the LBL integration of the absorption lines generated with the HITEMP2010 spectral database presented by Dorigon, *et al.*, 2013 (Table 2).

The radiative heat source for this approach is the sum of the source term of the individual gray gases as follows

$$\dot{q}_R = \sum_{j=1}^{N_g} -\vec{\nabla} \cdot \vec{q}''_{R,j} = \sum_{j=1}^{N_g} \kappa_j \left[\left(\int_{4\pi} I_j d\Omega \right) - 4\pi a_j I_b \right] \tag{16}$$

Table 2. CR-WSGG coefficients by Dorigon, *et al.*, 2013, for $p_{H_2O} / p_{CO_2} = 2$.

j	$\kappa_{p,j}$ $(atm\ m)^{-1}$	$b_{j,0}$	$b_{j,1}$ (K^{-1})	$b_{j,2}$ (K^{-2})	$b_{j,3}$ (K^{-3})	$b_{j,4}$ (K^{-4})
1	0.192	5.617×10^{-2}	7.844×10^{-4}	-8.563×10^{-7}	4.246×10^{-10}	-7.440×10^{-14}
2	1.719	1.426×10^{-1}	1.795×10^{-4}	-1.077×10^{-8}	-6.971×10^{-11}	1.774×10^{-14}
3	11.370	1.362×10^{-1}	2.574×10^{-4}	-3.711×10^{-7}	1.575×10^{-10}	-2.267×10^{-14}
4	11.016	1.222×10^{-1}	-2.327×10^{-5}	-7.492×10^{-8}	4.275×10^{-11}	-6.608×10^{-15}

3.3 Non-constant ratio WSGG (NCR-WSGG)

The RTE for the NCR-WSGG model can be written as

$$\frac{dI_{j_m}}{dS} = -\kappa_{m,j_m} I_{j_m} + \kappa_{m,j_m} a_{m,j_m} I_b \tag{17}$$

where the absorption coefficient and the weighting factor are computed for the participating species individually and then they are superposed to generate the coefficients for the mixture according to

$$\kappa_{m,j_m} = \kappa_{H_2O,j_{H_2O}} + \kappa_{CO_2,j_{CO_2}} = \left(X_{H_2O}\kappa_{p,H_2O,j_{H_2O}} + X_{CO_2}\kappa_{p,CO_2,j_{CO_2}} \right) p \tag{18}$$

$$a_{m,j_m} = a_{H_2O,j_{H_2O}} \times a_{CO_2,j_{CO_2}} = \sum_{k=1}^{J_{H_2O}+1} b_{H_2O,j_{H_2O},k} T^{k-1} \times \sum_{k=1}^{J_{CO_2}+1} b_{CO_2,j_{CO_2},k} T^{k-1} \tag{19}$$

The $\kappa_{p,j}$ and $b_{j,k}$ coefficients for the individual species were coupled with the Fluent solver via UDF were obtained by Cassol, *et al.*, 2014, by fitting the total emittance data computed by the LBL integration of the absorption lines generated with the HITEMP2010 spectral database (Tables 3 and 4). In this methodology the weighting factor $a_{\chi j}$ represents the probability that the blackbody energy is emitted in the spectrum region for which the absorption coefficient is $\kappa_{p,\chi j}$ (with $\chi = CO_2, H_2O$).

As for the Fluent-WSGG and the CR-WSGG, the sum of the weighting factor for all gray gases is

$$\sum_{j_m=0}^{J_m} a_{m,j_m}(T) = 1 \tag{20}$$

Where the mixture gray gases number J_m considering the clear gases ($\kappa_{H_2O,0}$ and $\kappa_{CO_2,0}$) is

$$J_m = \left(J_{H_2O} + 1 \right) \times \left(J_{CO_2} + 1 \right) = 25 \tag{21}$$

Table 3. NCR-WSGG coefficients by Cassol, *et al.*, 2014, for H_2O.

j	$\kappa_{p,H_2O,j}$ $(atm\ m)^{-1}$	$b_{H_2O,j,0}$	$b_{H_2O,j,1}$ (K^{-1})	$b_{H_2O,j,2}$ (K^{-2})	$b_{H_2O,j,3}$ (K^{-3})	$b_{H_2O,j,4}$ (K^{-4})
1	0.171	6.617×10^{-2}	55.48×10^{-5}	-48.41×10^{-8}	22.27×10^{-11}	-40.17×10^{-15}
2	1.551	11.045×10^{-2}	0.576×10^{-5}	24.00×10^{-8}	-17.01×10^{-11}	30.96×10^{-15}
3	5.562	-4.915×10^{-2}	70.63×10^{-5}	-70.12×10^{-8}	26.07×10^{-11}	-34.94×10^{-15}
4	49.159	23.675×10^{-2}	-18.91×10^{-5}	-0.907×10^{-8}	4.082×10^{-11}	-8.778×10^{-15}

Table 4. NCR-WSGG coefficients by Cassol, *et al.*, 2014, for CO_2.

j	$\kappa_{p,H_2O,j}$ $(atm\ m)^{-1}$	$b_{H_2O,j,0}$	$b_{H_2O,j,1}$ (K^{-1})	$b_{H_2O,j,2}$ (K^{-2})	$b_{H_2O,j,3}$ (K^{-3})	$b_{H_2O,j,4}$ (K^{-4})
1	0.138	9.990×10^{-2}	64.41×10^{-5}	-86.94×10^{-8}	41.27×10^{-11}	-67.74×10^{-15}
2	1.895	0.942×10^{-2}	10.36×10^{-5}	-2.277×10^{-8}	-2.134×10^{-11}	6.497×10^{-15}
3	13.301	14.511×10^{-2}	-30.73×10^{-5}	37.65×10^{-8}	-18.41×10^{-11}	30.16×10^{-15}
4	340.811	-2.915×10^{-2}	25.23×10^{-5}	-26.10×10^{-8}	9.965×10^{-11}	-13.26×10^{-15}

The radiative heat source term for this methodology is given by the sum of the source term for the J_m gray gases according to

$$\dot{q}_R = \sum_{j_m=1}^{J_m} -\vec{\nabla}\cdot\vec{q}''_{R,j_m} = \sum_{j_m=1}^{J_m} \kappa_{m,j_m}\left[\left(\int_{4\pi} I_{j_m} d\Omega\right) - 4\pi a_{m,j_m} I_b\right] \tag{22}$$

4. RESULTS AND DISCUSSIONS

Before solving the coupled reactive flow/radiation problem, a UDF was written to calculate de WSGG model as it is implemented on ANSYS/Fluent solver to make sure that the methodology is fully comprised. Tests were carried through the infinite parallel black walls separated by a distance *S* filled with participating gases problem (Dorigon, *et al.*, 2013). Since Fluent doesn't work with 1D problems, a 2D domain was constructed with dimensions *LxS* where *L = 1000S* and *S = 0.5, 1.0 and 2.0 m*. Four test cases were studied: (i) isothermal (medium at *1100 K*, walls at *400 K*) and homogeneous (X_{CO2} *= 0.1,* X_{H2O} *= 0.2*); (ii) isothermal, non-homogeneous Eq. (22); (iii) non-isothermal Eq. (23), homogeneous; and (iv) non-isothermal, non-homogeneous.

$$X_{CO_2}(s^*) = 0.2\sin^2(\pi s^*) \tag{22}$$

$$T(s^*) = 400K + (1400K)\sin^2(\pi s^*) \tag{23}$$

where, $s^* = s/S$. Figure 2 shows the results obtained for the radiative heat source given by Eq. (13).

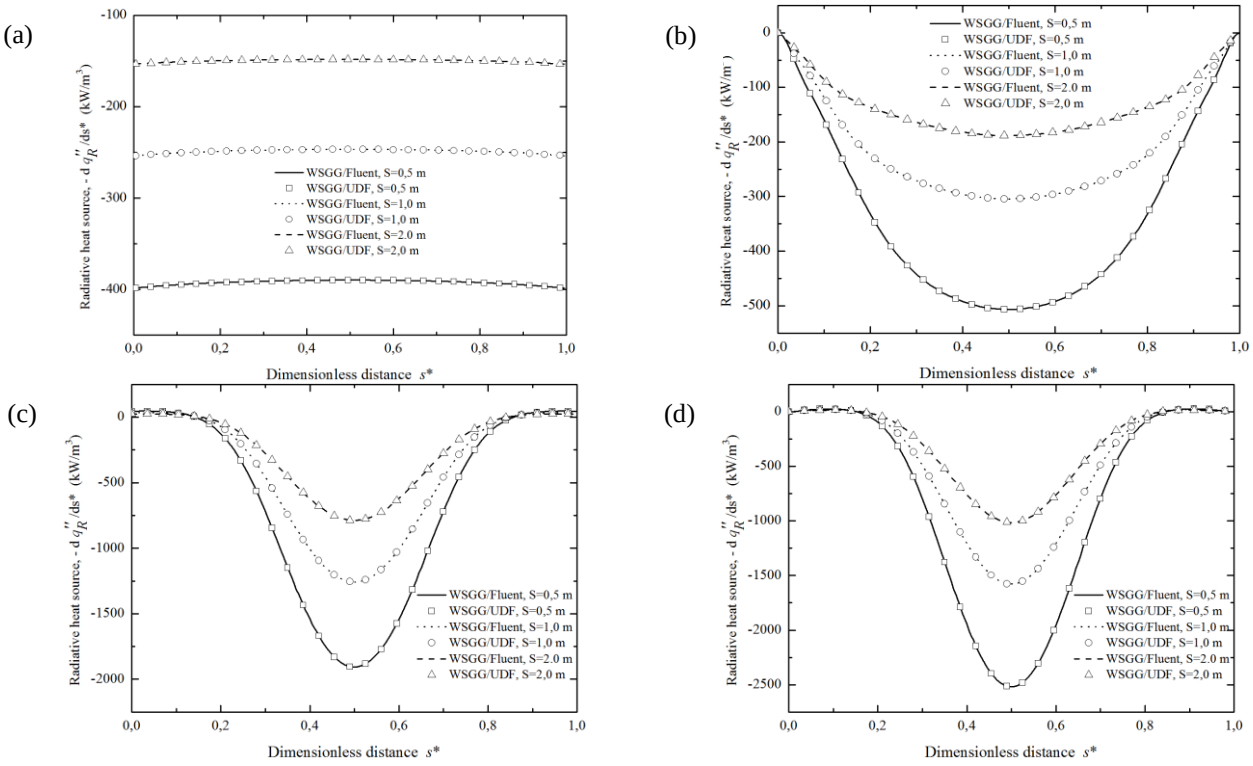

Figure 2. Comparison for Fluent-WSGG with the Fluent-WSGG (UDF): (a) isothermal and homogeneous, (b) isothermal and non-homogeneous, (c) non-isothermal and homogeneous and (d) non-isothermal and non-homogeneous.

Table 5 presents the average error according to Eq. (24) (calculated as the average of the errors calculated as Eq. 4) for all cases. As it can be seen, the curves for both Fluent WSGG and the WSGG implemented as UDF are practically coincident and the error are in order of 0.05%, indicating that the written UDF reproduce well the Fluent standard WSGG methodology.

$$err(\%) = \frac{\left|\dot{q}_{R,FLUENT} - \dot{q}_{R,UDF}\right|}{\max\left|\dot{q}_{R,FLUENT}\right|} \tag{24}$$

Table 5. Average error for all test cases.

Case	*S = 0.5 m*	*S = 1.0 m*	*S = 2.0 m*
(i)	0.04146%	0.03800%	0.03768%
(ii)	0.03039%	0.02980%	0.00219%
(iii)	0.02754%	0.02325%	0.03022%
(iv)	0.04130%	0.03862%	0.03286%

The results for the radiative heat flux are presented in Figure 3 for the three WSGG approaches and are compared with experimental measurements by Machado (2015). The average deviation is calculated as the mean deviation computed by Eq. (25). The solution for both Fluent WSGG (implemented via UDF) and NCR-WSGG was obtained with the converged fields of temperature, H_2O and CO_2 mole fractions of the fully coupled CR-WSGG simulation.

$$\text{dev}(\%) = \frac{\left|q''_{R,EXP} - q''_{R,WSGG}\right|}{\max\left|q''_{R,EXP}\right|} \tag{25}$$

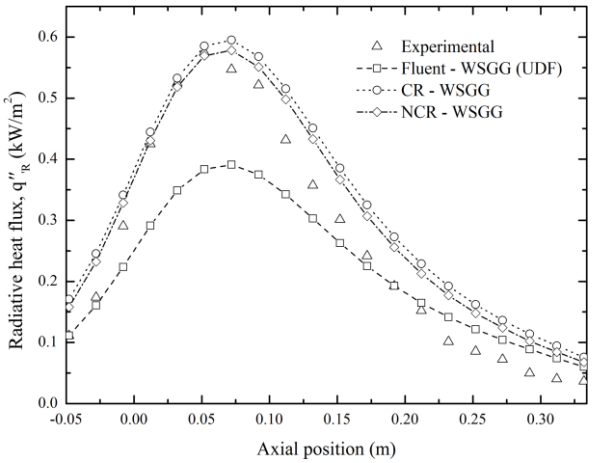

Figure 3: Radiative heat flux for all three WSGG approaches in comparison with experimental data.

As it can be seen, Fluent-WSGG provides the less accurate results mainly in the region of the maximum fluxes (approximately the flame length region). The underestimated flux values can be related to the gray formulation of the methodology as it can be seen by the model RTE Eq. (7). The average error and the error at the maximum flux point for all WSGG models are presented in Table 6.

Table 6. Average and maximum errors for all WSGG approaches.

Model	Average error (%)	Error at maximum flux (%)
CR-WSGG	10.52	1.82
NCR-WSGG	8.15	0.92
Fluent-WSGG	11.31	33.25

As showed in Table 6, the NCR-WSGG presented by Cassol, *et al.*, 2014, gave the most accurate results. It is related to the formulation of the methodology which takes into account that the ratio between the participant gases is not constant. For the CR-WSGG formulation presented by Dorigon, *et al.*, 2013, showed good results with a considerably lower computational effort. The Fluent-WSGG methodology (ANSYS, 2011a) presented the less accurate results and the largest error in the region of the maximum fluxes.

Since the fully coupled combustion/radiation problem is computationally demanding, the relation accuracy/computational effort must be carefully taken. In this way even though the Fluent-WSGG being the most computationally efficient and the NCR-WSGG being the most accurate approach, the CR-WSGG is the methodology that has the better precision in relation to computational cost, being recommended as an approach for the radiation solution in the coupled reactive flow/radiation problem.

5. CONCLUSIONS

The Fluent WSGG was implemented via UDF to make sure that the calculation process of the software was fully comprised. After the coupled reactive flow/radiation problem was solved with the CR-WSGG, the converged fields were used for the decoupled calculations for the remaining approaches. The NCR-WSGG gave the most accurate results for the radiative heat flux while the Fluent-WSGG gave the less accurate ones reaching to deviations in order of 33% in the maximum flux region (flame length reagion). The CR-WSGG showed the better relation between accuracy/computational effort being recommended for coupled reactive flow/radiation calculations. The Fluent gray WSGG approach gave the less accutate results mainly for the region of flame length (maximum fluxes zone).

6. ACKNOWLEDGEMENTS

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