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Application of the weighted-sum-of-gray-gases model in a simulation of a open flame with ANSYS/FLUENT

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Abstract. *In this study the weighted-sum-of-gray-gases model is applied to an ANSYS/Fluent simulation of an open flame. The flame is diffuse and laminar, and formed by the combustion of methane in air. The problem is first solved only for the combustion process, and after convergence the radiation model is included in the analysis. To solve the radiative transfer problem in the non-homogeneous, non-isothermal medium the discrete ordinates method combined with the weighted-sum-of-gray-gases model is adopted. The participating medium is divided into four gray gases plus one transparent window. The absorption coefficient of each gray gas was computed by taking into account the local concentration of each of the participating species (in this study carbon dioxide and water vapor in a ratio of partial pressures or molar concentrations of 2/1) making use of a user-defined function (UDF) written on a C programming language. The emissivity weighting factor of the participating medium, for each gray gas, is computed as a function of local temperature making use of the UDF as well. A test case is simulated and compared against a solution available in the literature. The gray gas model with one gray gas with constant absorption coefficient is considered as well to make a briefly comparison. The obtained result shows that the weighted-sum-of-gray-gases model is viable and accurate alternative to predict flame structure and thermal radiation in in spite of its simplicity.*
Keywords: *Radiative transfer, WSGG model, combustion, CFD*

1. INTRODUCTION

Fossil fuels still represent the main source of energy in a world basis. In Brazil, in spite of the abundance of hydric resources and the good potential of other renewable sources of energy, such as wind and solar, the fossil fuels still represent a significant portion in order to sustain the demand for energy. Considering its importance and that the burning of these fuels has environmental impacts, a better understanding of the involved phenomena becomes necessary. Recently, the United States and China, both of the main users of fossil fuels, signed an agreement where they compromised to reduce the emission of pollutant gases. As the demand for energy tends to improve and the fossil fuels are the main source of energy, higher efficiency and less pollution emission are important goals to meet.

Diffusive flames has an extensive use in the industry. Steel and glass production, incinerators and flares in platforms and oil refineries are typical processes in which diffusive flames play an important role. On the other hand, modeling these flames may not be an easy task if they are turbulent (the case of flares, for example) because of the complexity and the coupling of several phenomena, such as turbulence, chemical kinetics, thermal radiation, and others. However, several properties of turbulent flames can be better understood from the study of laminar flames.

Numerical and experimental studies with partially and non-premixed flames of methane/air (Bennett et al., 2000) and ethylene/air (Smooke et al., 2005) with the optically thin approximation (OTA) as the radiation submodel investigated the premixing effects on the flame structure. These studies reported the importance of the premixing level and the radiative heat loss on flame temperature.

A numerical study with methane/air flames with different levels of premixing and making use of several chemical mechanisms, implemented with OTA as radiation submodel, showed that radiation is an important factor on flame structure prediction with strong influence on temperature and pollutant formation (Claramunt et al., 2004). Other studies investigating the radiation importance on predicting the flame structure realized with microgravity (Zhang et al., 2014) and with normal and microgravity (Liu, Smallwood and Kong, 2011) pointed at the major importance of this phenomena principally on microgravity condition. Another study with detailed chemistry and a more sophisticated radiation modeling implementing the Statistical Narrow Band Correlated-K (SNBK) model showed the importance of the phenomena on soot formation and oxidation (Liu, Guo and Smallwood, 2004).

The Weighted-Sum-of-Gray-Gases (WSGG) model was implemented by Bidi, Hosseini and Nobari, 2008, with the objective to verify the radiation effect on temperature and species concentrations fields in turbulent diffusive flames, revealing its important influence. Moreover, the results with thermal radiation provided better agreement with experimental results when compared with the results without radiation.

Several recent studies have demonstrated the accuracy of the WSGG model with new correlations based on the HITEMP2010 database. Bordbar et al., 2014, compared the model with the Line-by-line (LBL) benchmark solution in 1D and 3D test cases with defined temperature and participating species profiles. Dorigon et al., 2013, generated the correlations for concentrations of water vapor and carbon dioxide in the ratios of 2/1 and 1/1, testing the WSGG solution against the LBL solution for 1D test cases.

The accurate results obtained with WSGG in problems even more complicated as in a 2D axysimmetric turbulent methane/air flame to investigate the turbulence-radiation interaction (Centeno et al., 2014) are encouraging to keep using this model in combustion applications.

In the present study the WSGG model is applied in a Fluent simulation of a laminar non-premixed flame (Bennett et al., 2000) with detailed chemistry, thermal and transport properties using up-to-date correlations obtained with HITEMP2010 (Dorigon ete al., 2013). To implement the model with Fluent, it was necessary to couple user-define-functions (UDF) to modify the treatment of radiation model. The objective of the present study is therefore to evaluate the accuracy of the WSGG on predicting the flame structure.

2. PROBLEM STATEMENT

The problem under investigation consists of a steady laminar coflowing non-premixed methane/air open flame at atmospheric pressure. The domain geometry is a 2D axisymmetric burner. For the computational purposes, only the region out of the jet inner tubes is simulated. Both domain and inner variables are the same of the Bennett et al., 2000, for the non-premixed flame case. The fuel enters at a velocity of $v_{fuel} = 0{,}0567\ m/s$ and mole fraction of $Y_{fuel} = 1{,}0$ and air enters at a velocity of $v_{air} = 0{,}1048\ m/s$ and mole fraction of $Y_{air} = 0{,}209$. Both fuel and air are at a temperature of $T = 298$ K. The fuel inner jet radius is $r_i = 0{,}00555$ m, while the coflow inner radius is $r_o = 0{,}476$ m. However, for the computational domain construction, the coflow radius was extended accounting the tube walls thickness (as shown in Figure 1). The length of the domain is $L = 0{,}2$ m. The boundary conditions are symmetry in the axis, outflow at the up exit and in the side is a wall with free slip condition and $T = 298$ K. The wall boundary condition at the side was adopted in order to make the convergence of the problem easier. Since the wall is sufficiently far from the flame, this modification is not expected to affect the open flame condition.

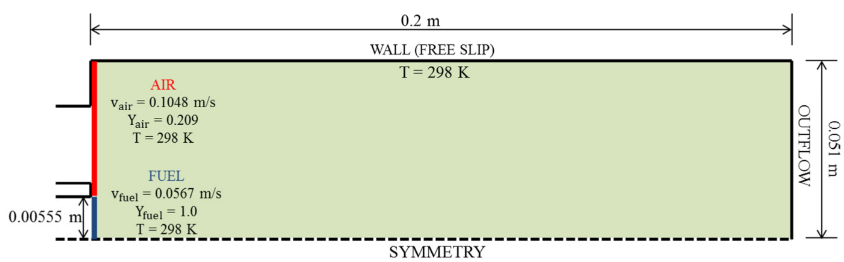

Figure 1. Schematic of the domain configuration, dimensions and conditions at boundaries.

3. MATHEMATICAL MODELS

The equations that govern the phenomena involved in the problem are presented in the subsections below.

3.1 Conservative governing equations

The mass conservation (continuity) is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \qquad (1)$$

where ρ is the mixture density and $\vec{v}$ the flow velocity. The momentum equation is

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot \hat{\tau} + \rho \vec{g} \qquad (2)$$

In the above equation, p is the pressure, $\vec{g}$ the field forces and $\hat{\tau}$ the stress tensor which assuming a Newtonian fluid is given by

$$\hat{\tau} = \mu[\nabla\vec{v} + (\nabla\vec{v})^T] - \frac{2}{3}\mu(\nabla \cdot \vec{v})\hat{I} \tag{3}$$

in which μ is the dynamic viscosity and $\hat{I}$ the identity matrix. The energy equation is

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho\vec{v}h) = -\nabla \cdot \vec{q} - \dot{Q}_R \tag{4}$$

where h is the mixture specific enthalpy, $\vec{q}$ is the heat flux vector and $\dot{Q}_R$ the radiative heat source term. And the mass species conservation equation is

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho\vec{v}Y_i) = -\nabla \cdot \vec{j}_i - R_i \tag{5}$$

In the above relation, Y_i is the species mole fraction, R_i the chemical source term and $\vec{j}_i$ the diffusive mass flux, which is given by Fick's Law

$$\vec{j}_i = -\rho D_{i,m}\nabla Y_i \tag{6}$$

where $D_{i,m}$ is the binary mass diffusion coefficient. The system is closed with the equation of state and with the boundary conditions at the computational domain.

3.2 Radiation modeling

For an absorbing, non-scattering medium the spectral radiative transfer equation (RTE) is written with the discrete ordinates method as

$$\frac{\partial I_\eta}{\partial s} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta} \tag{7}$$

where I_η is the spectral intensity, $I_{b\eta}$ the blackbody spectral intensity and κ_η is the spectral absorption coefficient. The negative term on the right side of Eq. (7) is the attenuation on the intensity by the medium absorption, while the positive term accounts for the increase in the intensity by the medium emission. Since the spectral absorption coefficient has a major dependence with the wavenumber, which can involve thousands of spectral lines for participating gases (such as carbon dioxide and water vapor), the integration of the RTE may become unviable because of the computational demand. In order to outline this issue, some gas models were developed to make the time to integrate the RTE faster. One of the gas models is the weighted-sum-of-gray-gases, which is described in the next subsection.

3.3 The wighted-sum-of-gray gases (WSGG) model

The WSGG model was first proposed by Hottel and Sarofim, 1967. The basic assumption is that the entire spectrum can be divided into a few gray gases with constant absorption coefficient plus one transparent window. Each gray gas covers a defined region of the spectrum that is not necessary continuous. An important assumption of this model is that the total emittance of a gas along a path S can be approximated by

$$\varepsilon(s) = \sum_{j=0}^{J} a_j(T)\left[1 - e^{-\kappa_{p,j}pS}\right] \tag{8}$$

where $\kappa_{p,j}$ is the pressure absorption coefficient, $a_j(T)$ the weighting factor and j is the number of gray gases (usually 3 or 4). The weighting factor represents, physically, the blackbody energy fraction that is emitted for each gray gas (Figure 2), and can be expressed as a polynomial function of temperature as (Smith et al., 1982)

$$a_j(T) = \sum_{k=1}^{J+1} b_{j,k}T^{k-1} \tag{9}$$

where $b_{j,k}$ are the polynomial coefficients.

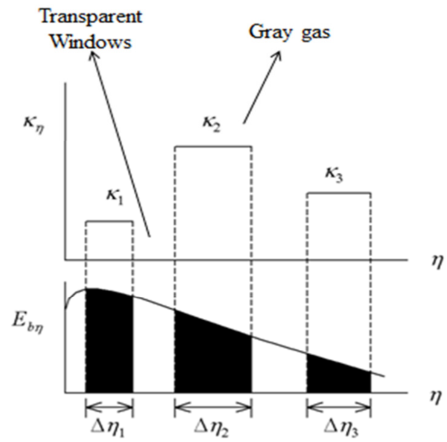

Figure 2. Physical meaning of the weighting factor.

Dorigon et al., 2013, obtained $\kappa_{p,j}$ and $b_{j,k}$ coefficients for WSGG model evaluated using the HITEMP2010 database for mixtures of carbon dioxide and water vapor. Table 1 presents the coefficients for a gas mixture of H_2O and CO_2 with a pressure ratio of 2/1, respectively.

Table 1. WSGG coefficients for four gray gases for an H_2O /CO_2 mixture with partial pressures ratio of $\frac{H_2O}{CO_2} = 2$.

j	$\kappa_{p,j}(m^{-1}atm^{-1})$	$b_{j,1}$ x 10^{-1}	$b_{j,2}$ x 10^{-1} (K^{-1})	$b_{j,3}$ x 10^{-2} (K^{-2})	$b_{j,4}$ x 10^{-3} (K^{-3})	$b_{j,2}$ x 10^{-4} (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

Modest, 1991, demonstrated that the WSGG can be applied with any solution method of the RTE, which can be rewritten as

$$\frac{\partial I_j}{\partial s} = -\kappa_j I_j + \kappa_j a_j I_b \tag{10}$$

where κ_j is the absorption coefficient and I_j the radiation intensity of the gray gas j. For a mixture of carbon dioxide (CO_2) and water vapor (H_2O), the absorption coefficient is given by

$$\kappa_j = \kappa_{p,j}\left(Y_{CO_2} + Y_{H_2O}\right)p \tag{11}$$

in which Y_{CO_2} and Y_{H_2O} are the mole fractions and p the total pressure. With this expression the absorption coefficient is computed locally as a function of the mole fractions of the participating species, providing more accuracy in the solution,

4. COMPUTATIONAL APPROACH

The set of equations was implemented on the software ANSYS/Fluent 14.0. The pressure-velocity coupling was given by the SIMPLE algorithm (Patankar, 1980). For the chemical species, energy, momentum and discrete ordinates equations, a second order upwind discretization scheme was adopted.

A uniform and structured mesh with 18423 control volumes was used. An adaptive grid algorithm was also adopted to refine the mesh during the solution of the reactive flow based on the temperature gradient. This algorithm refines the mesh in the region of larger gradients providing an accurate solution without excessively increasing the computational time. The refinement is controlled by levels following the rule of 4^n subdivisions of the original volume where n represents the refinement level (Figure 3.). For this work a level 3 refinement was adopted.

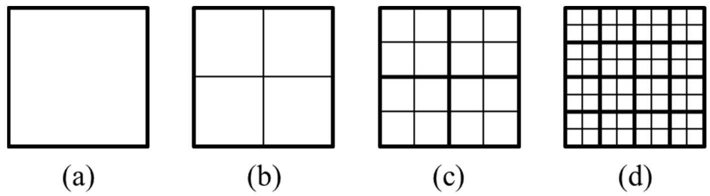

Figure 3. Schematic of the grid refinement with the adaptive grid algorithm. In (a) the original volume, (b) the first level of refinement or $n = 1$, (c) second level of refinement or $n = 2$ and (d) the third level of refinement or $n = 3$.

As a solution strategy, first the cold transport of the fuel and the oxidizer was solved. In other words, only methane and air entered the domain without any chemical reactions. Next, a region near the inlets was selected and a temperature gradient capable of starting the combustion process was imposed. A reduced version of GRI-MECH 1.2 mechanism with 84 reactions and 21 species with appropriate thermal and transport properties was considered. The chemical source term was set as finite rate and uses the Arrhenius equations (Ansys, 2011a).

Once the convergence criteria were reached for the reactive flow, the radiation problem was set to be solved. For the implementation of the WSGG model in the code, two user-defined-functions (UDF's) were developed. UDF's are small routines written on C programming language that can be coupled with Fluent in order to modify the models or change variables treatments. In the specific case of the WSGG two UDF's were necessary (Ansys, 2011b): one for the absorption coefficient and one for the medium emissivity weighting factor.

5. RESULTS AND DISCUSSIONS

The results of the simulations are presented in the subsections bellow. First, the validation of the user-defined-functions is discussed, then the results for the flame are shown.

5.1 User-defined-functions validation

Before solving a coupled radiation/combustion problem, the UDF's were tested to reproduce the solution presented by Dorigon et al., 2013, in which the WSGG was compared against the Line-by-line (LBL) solution, to verify if the UDF's work correctly when implemented with Fluent. The problem consists on a non-isothermal, non-homogeneous gas mixture composed of carbon dioxide and water vapor that fills the medium between two parallel and infinite black walls separated by a distance S. The temperature and species mole fractions profiles are

$$T(s^*) = 400\ \mathrm{K} + (1400\ \mathrm{K})\sin^2(\pi s^*) \tag{12}$$

$$Y_{CO_2}(s^*) = 0.2\sin^2(\pi s^*) \tag{13}$$

where $s^* = s/S$, $S = 0.5, 1.0$ and 2.0 and $Y_{H_2O} = 2Y_{CO_2}$. The implementation in Fluent platform was carried through a 2D geometry (due to minimum supported dimensions) of $L \times S$ sides, where $L = (50,100,1000)S$. The obtained results are in Table 2. The error is calculated as

$$\chi = \frac{|q'_{R,WSGG} - q'_{R,LBL}|}{\max|q'_{R,LBL}|}(100\%) \tag{14}$$

where q'_R is the radiative heat flux.

Table 2. Calculated errors at the walls for the radiative heat flux.

WSGG		χ (%)			χ (%)			χ (%)		
	S	0.5	1.0	2.0	0.5	1.0	2.0	0.5	1.0	2.0
Eq. (12) (13)	$S^* = 0$	2.03	0.43	2.34	2.03	0.43	2.34	2.03	0.42	2.34
	$S^* = 1$	2.03	0.43	2.34	2.03	0.43	2.34	2.03	0.42	2.34
		L = 50S			L = 100S			L = 1000S		

The results presented in Table 2 shows that the deviations between the results were in the order of 2% or less. This indicates that the WSGG model coupled with Fluent works correctly, and gives reliable results. The next step was the application of the UDF's in a coupled combustion/radiation problem.

5.2 Open flame numerical results

The problem was first solved without radiation and then with the WSGG coupled with UDF's and with the gray gas model with constant absorption coefficient of $\kappa = 0.1\ m^{-1}$. The first results to be compared are the height where the maximum temperature occurs (H_t) and the maximum temperature (T_{max}) showed in Table 3.

Table 3. Height where the maximum temperature occurs (H_t) and the maximum temperature (T_{max}) obtained for the different models.

	H_t (cm)	T_{max} (K)
Bennett et al. Exp.	5.70	1960
Bennett et al. Comp.	8.00	1868
Fluent no radiation	5.86	2114.04
Gray gas	5.85	2084.94
Fluent WSGG	5.90	2037.09

As shown in Table 3, the results for the height where the maximum temperature occurs have a satisfactory agreement with the numerical results with differences of 2.6% for the gray gas model and 3.5% for the WSGG model. In the case of the maximum temperature, the WSGG model shows a percentage difference of 3.9%, while the gray gas model has the difference of 6.4%. Plots of temperature and species mole fractions are presented in Figures 4 and 5 respectively.

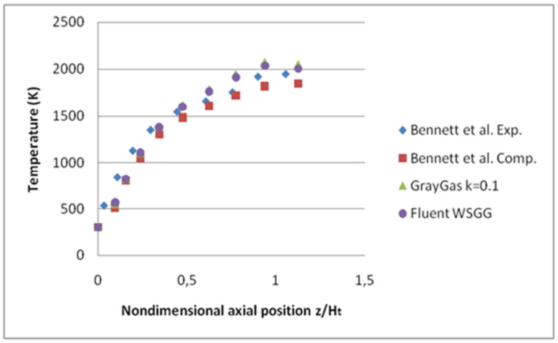

Figure 4. Temperature at centerline (symmetry line) plotted against the nondimensional axial position z/H_t.

As it is shown in Figure 4, the numerical temperatures are in general lower than the experimental measurements (Bennett et al., 2000). In the lower temperatures region, the gray gas and the WSGG models give similar results, but when the higher temperature region are considered the results for the WSGG shows a better agreement with experimental data. The differences between the numerical results and between the present work and the selected paper are affected in a significant way by the radiation model and by the choice of the chemical mechanisms (this factor has a huge influence on species concentrations as well).

In Figure 5, the mole fractions of methane and air show a good agreement except for the region closer to the inlets. The concentration of methane decreases after entrance by dilution and chemical reactions. The numerical results can predict well the disappearing of the fuel and the oxidant.

The participating species (carbon dioxide and water vapor) behavior along the centerline is well described by the numerical models. For carbon dioxide the agreement of the WSGG is very good with the experimental data whereas for water vapor a difference can be observed in the region of higher concentrations. The average mole fraction of $H_2O/CO_2 \cong 2$, therefore the adopted correlations for the WSGG models are able to be applied.

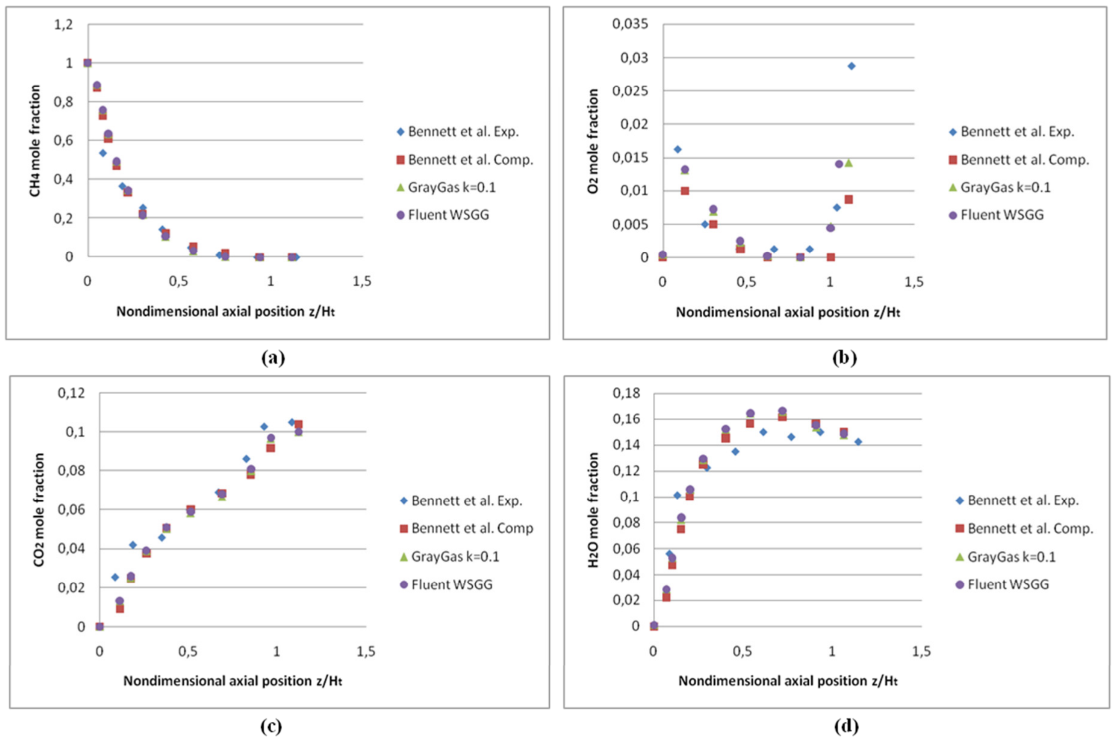

Figure 5. (a) CH_4 mole fraction; (b) O_2 mole fraction; (c) CO_2 mole fraction, and (d) H_2O mole fraction versus the nondimensional axial position z/H_t. All values reefers to the centerline (symmetry line).

6. CONCLUSIONS

In the present study, a laminar non-premixed methane/air flame was implemented numerically in the Fluent platform with detailed chemical mechanism (with 84 reactions and 21 species) and user-defined-functions (for the absorption coefficient as function of local concentration of participating species and the weighting factor of the medium emissivity as function of local temperature) coupled to modeling the nongray radiation problem with the weighted-sum-of-gray-gases model. The gray gas model with one gray gas with constant absorption coefficient was considered as well for additional comparison. Numerical results were compared with a numerical/experimental study (Bennett et al., 2000) available in literature. The UDF's were first tested against a 1D problem for validation, giving accurate results when compared to a solution available in the literature. To solve the coupled combustion/radiation problem an adaptive grid mesh refinement based on the temperature gradients was adopted. The results showed that the WSGG model is capable of describing the flame structure (as temperature and species concentrations) with good accuracy.

7. ACKNOWLEDGEMENTS

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