COMPUTATION OF THE RADIATIVE HEAT FLUX FROM A LAMINAR METHANE/AIR FLAME OBTAINED WITH THE GRAY GAS AND THE WEIGHTED-SUM-OF-GRAY-GASES MODELS

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Abstract. *In this study the weighted-sum-of-gray-gases (WSGG) and the gray gas (GG) models are coupled with the software ANSYS/Fluent to predict the radiation heat transfer of an open laminar coflowing methane/air flame. The problem is first solved only for the combustion process and after convergence the radiation modeling is included. Combustion is modeled by the laminar finite-rate model considering a detailed chemical mechanism (DRM19) and appropriate thermal and transport properties. Numerical results for both decoupled and coupled radiation/combustion are compared with experimental measurements. Both WSGG and GG models are implemented with correlations obtained with the HITEMP2010 spectral database. The absorption coefficient for the GG model is calculated as a function of local temperature and concentration of the participating species (carbon dioxide and water vapor). The coupling between Fluent and the spectral models is made by means of user-defined functions (UDF). Results point that the GG model is less expensive computationally than the WSGG model, but gives less accurate results. The WSGG model can predict both qualitatively and quantitatively the radiative heat flux with good accuracy and proved itself a viable alternative to predict radiation heat transfer in spite of its relative simplicity.*

Keywords*: radiative transfer, WSGG model, GG model, Combustion, CFD.*

1. INTRODUCTION

Radiation heat transfer process in participating media (which absorbs, emits and scatters radiant energy) has been studied since the past century due to its importance in many applications such as industrial furnaces, solar energy conversion, steel and glass industries, incinerators, flares in oil platforms and refineries, etc. Since the spectral behavior of radiative properties in gaseous media is highly irregular, its modeling is a challenging task. In the hydrocarbon fuels combustion process some gases are generated as products (as carbon dioxide and water vapor) which absorbs and emits of radiant energy. Acknowledging that the hydrocarbon fuels still represent the primary source of energy in a world basis, and that the energy demand tend to increase, the understanding of the coupled phenomena (such as radiation heat transfer, chemical kinetics, etc.) is needed in order to improve efficiency and reduce environmental harms.

Experimental/numerical studies with partially non-premixed methane/air flames with complex chemistry investigating the premixing level effect on flame structure coupled with the Optically Thin Approximation (OTA) considering CO_2, H_2O and CO as participating species, without a soot model coupled (Bennett et al., 2000) and considering CO_2, H_2O, CO and CH_4 as participating species with a soot model coupled (Claramunt et al., 2004) pointed to the importance of the premixing level and radiative heat loss on flame temperature. The radiation effect on soot formation for laminar non-premixed flames studies for flames of methane with the Statistical Narrow Band Correlated-κ model (Liu et al., 2004) and flames of ethylene with the Exponential Wide Band model (Smooke et al., 2005) showed that the radiation effect over soot have a major importance in flames of ethylene and acetylene where the concentration of soot is higher.

Diffusive turbulent flames studied with the Weighted-Sum-of-Gray-Gases (WSGG) model presented good agreement with experimental data for temperature and species concentrations (Bidi et al., 2008). Centeno et al., 2014, studied the turbulence-radiation interaction applying new correlations for the WSGG model obtained by Dorigon et al., 2013, based on HITEMP2010 spectral database showing that radiation modeling has major importance on global results such as flame peak temperature and radiant fraction. Cassol et al., 2014a, obtained new correlations for CO_2, H_2O and soot for the WSGG model and compared results with the Line-by-line (LBL) benchmark solution. A study evaluating the influence of the spectral database by Chu et al., using the LBL and the Statistical Narrow Band (SNB) models showed that the HITEMP2010 database can be used to generate benchmark solutions for the LBL integration.

In the present study, the WSGG model with correlations obtained by Dorigon et al., 2013, and a modified Gray Gas (GG) model with correlations obtained with the HITEMP2010 database presented by Cassol et al., 2014b, are applied in a Fluent simulation of a laminar non-premixed flame of CH_4 in air with the inert N_2 diluted. Detailed chemistry, thermal and transport properties are considered. The coupling of the gas models with Fluent is made with user-defined functions

(UDF). The objective of the present study is therefore to compare the accuracy of the WSGG and GG models on predicting the radiative heat flux along the flame axis comparing with experimental data.

2. MODELING LAMINAR DIFFUSIVE FLAMES

The mathematical modeling of laminar diffusion flames is made by means of the conservative equations for mass, momentum, species mass and energy presented and briefly discussed in the subsections below.

2.1 Mass conservation equation

The mass conservation equation, also known as continuity, is

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

where ρ is the mixture density and $\vec{v}$ the flow velocity. The approximation for low Mach numbers is valid and then the density is a function of the temperature only and can be calculated as

$$\rho = \frac{p_0 MW}{R_u T} \tag{2}$$

In the above equation, p_0 is the reference pressure (atmospheric), MW the molar weight of the mixture, R_u the ideal gases constant and T the temperature.

2.2 Momentum conservation equation

The momentum conservation can be expressed by the compressible form of the Navier-Stokes equation

$$\frac{\partial(\rho \vec{v})}{\partial t} + \vec{\nabla}.(\rho \vec{v} \times \vec{v}) = -\vec{\nabla} p + \rho \vec{g} + \vec{\nabla}.\hat{\tau} \tag{3}$$

where p is the pressure, $\vec{g}$ the field forces and $\hat{\tau}$ the stress tensor. The terms on the left hand side represent the material derivative of velocity (fluid particle acceleration) and the terms on the right hand side represent, respectively, the pressure forces, field forces and the viscous forces. For Newtonian fluids the stress tensor can be expressed as

$$\hat{\tau} = \mu\left[\vec{\nabla}\vec{v} + \left(\vec{\nabla}\vec{v}\right)^T\right] - \frac{2}{3}\mu\left(\vec{\nabla}.\vec{v}\right)\hat{I} \tag{4}$$

in which μ is the dynamic viscosity and $\hat{I}$ the identity tensor.

2.3 Species mass conservation equation

The species mass conservation can be expressed in terms of the individual mass fractions for the N_s involved species as it follows

$$\frac{\partial(\rho Y_i)}{\partial t} + \vec{\nabla}.(\rho \vec{v} Y_i) = -\vec{\nabla}.\vec{J_i} + \dot{\omega}_i, \qquad \text{for } i = 1 \text{ to } N_s - 1 \tag{5}$$

where $\vec{J_i}$ is the mass flux diffusion vector and $\dot{\omega}_i$ the source term due to chemical reactions modeled as finite-rate with Arrhenius equations (Ansys, 2011a). In order to guarantee the mass conservation, the mass fraction of the specie N_s (the inert N_2) is calculated as

$$Y_{N_s} = 1 - \sum_{i=1}^{N_s - 1} Y_i \tag{6}$$

The mass flux diffusion is due three effects, where the diffusion fluxes due to the pressure gradients and due to the thermal diffusion (Soret effect) can be neglected (Coelho and Costa, 2007) and the concentration gradients effect is accounted by the Fick's law approximation for binary diffusion as

$$\overrightarrow{J_i^d} = -\rho D_i^M \vec{\nabla} Y_i \tag{7}$$

in which D_i^M is the mean mass diffusion coefficient of the species i and can be calculated as proposed by the Hirschfelder et al., 1954, as

$$D_i^M = \frac{1-Y_i}{\sum_{i=1,i\neq j}^{N_S} \frac{X_j}{D_{i,j}}} \tag{8}$$

where $D_{i,j}$ is the binary diffusion coefficient of the species i into the j species.

2.4 Energy conservation equation

The energy conservation equation can be expressed in terms of the total energy, internal energy, temperature or enthalpy. For CFD calculations, usually, the energy conservation is accounted by the total specific enthalpy of the mixture as

$$\frac{\partial(\rho h)}{\partial t} + \vec{\nabla}.(\rho\vec{v}h) = \frac{Dp}{Dt} + \hat{\tau}:\vec{\nabla}\vec{v} - \vec{\nabla}.\overrightarrow{J_q} + \dot{Q}_R \tag{9}$$

In the above equation, $\overrightarrow{J_q}$ is the heat flux vector and $\dot{Q}_R$ the radiative heat source (as the modeling of this term is the main objective of this work, it will be discussed with more details in the Chapter 3). The terms on the left hand side of the equation represent the enthalpy transport due to advection. The pressure material derivative and the viscous dissipation term on the right hand side are usually neglected for low Mach number approximation and open non-premixed flames. The heat flux vector is composed by three effects, where the flux due to species concentration gradient (Duffour effect) is neglected and the heat flux vector is expressed in terms of the heat conduction (Fourier's law) and the mass diffusion effect as

$$\overrightarrow{J_q} = -\lambda\vec{\nabla}T + \sum_{i=1}^{N_s} h_i\overrightarrow{J_i} \tag{10}$$

where λ is the mixture thermal conductivity, h_i the specific enthalpy of species i and $\overrightarrow{J_i}$ the mass diffusion vector which can be approximated by the Fick's law. The chemical reactions effect is accounted in the specific enthalpy according to

$$h = \sum_{i=1}^{N_S} Y_i h_i \tag{11}$$

$$h_i = h_i^0 + \int_{T_{REF}}^{T} C_{p_i}(T)dT \tag{12}$$

in which h_i^0 is the formation specific enthalpy of the species i in the reference temperature, $T_{REF} = 298\ K$ and C_{p_i} the constant pressure specific heat.

3. RADIATION MODELING

For an absorbing/emitting and non-scattering medium, the spectral form of the radiative transfer equation (RTE) is expressed as

$$\frac{\partial I_\eta}{\partial S} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta} \tag{13}$$

In the above equation, 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 hand side represents the attenuation on the intensity due to medium absorption while the positive term represents the increase due to medium emission. Since the spectral absorption coefficient has a major dependence on 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 shorter the integration time of the RTE. The Gray gas (GG) model and the Weighted-sum-of-gray-gases (WSGG) model, adopted in this work are discussed in the subsections below.

3.1 The gray gas (GG) model

Usually the Gray gas model considers the entire medium as a gray gas with constant absorption coefficient and the spectral behavior is neglected. One way to improve the accuracy of this model is to consider the absorption coefficient as a function of the temperature and the concentration of the participating species (CO_2 and H_2O).

Cassol et al., 2014, presented correlations based on the spectral database HITEMP2010 to compute the absorption coefficient for carbon dioxide, water vapor and soot (Table 1). Since the soot modeling is neglected in this study, the absorption coefficient for the GG model can be expressed as

$$\kappa_i = p_i(c_0 + c_1 T + c_2 T^2 + c_3 T^3 + c_4 T^4 + c_5 T^5) \tag{14}$$

where p_i is the partial pressure of the participating species i and can be calculated as

$$p_i = p_0 X_i \tag{15}$$

in which p_0 is the total pressure (1 atm) and X_i the mole fraction of the participating species.

Table 1. Correlations for the absorption coefficient computing.

	$i = CO_2$	$i = H_2O$
c_0 [cm^{-1} atm^{-1}]	-6.4750.10^{-1}	7.5702.10^{-1}
c_1 [cm^{-1} atm^{-1} K^{-1}]	4.2895.10^{-3}	-1.9716.10^{-3}
c_2 [cm^{-1} atm^{-1} K^{-2}]	-6.6089.10^{-6}	2.1998.10^{-6}
c_3 [cm^{-1} atm^{-1} K^{-3}]	4.4190.10^{-9}	-1.2492.10^{-9}
c_4 [cm^{-1} atm^{-1} K^{-4}]	-1.3796.10^{-12}	3.5385.10^{-13}
c_5 [cm^{-1} atm^{-1} K^{-5}]	1.6484.10^{-16}	-3.9663.10^{-17}

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

The WSGG model considers that the integration of the spectral properties can be replaced by a summation over a few number of gray gases plus a transparent window as first proposed by Hottel and Sarofim, 1967. Each gray gas covers a defined region of the spectrum which is not necessarily continuous. One important assumption is that the total emittance of a gas along a path S can be approximated by

$$\varepsilon(s) = \sum_{j=0}^{J} a_j(T)\left[1 - e^{-\kappa_{p,j} pS}\right] \tag{16}$$

where $\kappa_{p,j}$ is the pressure based absorption coefficient, $a_j(T)$ the weighting factor and J is the number of gray gases (usually three or four). The weighting factor represents physically the blackbody energy fraction that is emitted for each gray gas (Figure 1), and can be expressed as a polynomial function of temperature as proposed by Smith et al., 1982:

$$a_j(T) = \sum_{k=1}^{J+1} b_{j,k} T^{k-1} \tag{17}$$

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

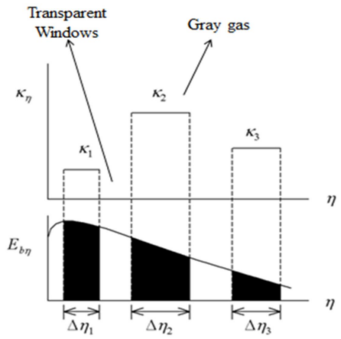

Figure 1. Physical meaning of the weighting factor.

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

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

$$\frac{\partial I_j}{\partial s} = -\kappa_j I_j + \kappa_j a_j I_b \tag{18}$$

Table 2. 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	$\kappa_{p,i}$ (m^{-1} atm^{-1})	$b_{i,1}$ x 10^{-1}	$b_{i,2}$ x 10^{-1} (K^{-1})	$b_{i,3}$ x 10^{-2} (K^{-2})	$b_{i,4}$ x 10^{-3} (K^{-3})	$b_{i,5}$ 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

where κ_j is the absorption coefficient and I_j the intensity of the j^{th} gray gas. For the mixture, the absorption coefficient can be calculated as

$$\kappa_j = \kappa_{p,j}\left(X_{CO_2} + X_{H_2O}\right)p \tag{19}$$

in which X_{CO_2} and X_{H_2O} are the mole fractions of the participating species and p the total pressure. With this expression the absorption coefficient is given as a function of the local concentration of the participating species, giving more accuracy in this parameter evaluation.

4. PROBLEM STATEMENT

The problem under investigation consists of a laminar non-premixed open flame composed by the combustion of methane (with 50% of N_2 dilution) in air for which experimental data for the radiative heat flux is available. The flame is from constant power flame series identified as PC0050N50 as in Machado, 2015. Domain geometry is a modified Santoro burner (Ibid). Only the region out the burner is modeled. The schematic of the domain, dimensions and inlet and boundary conditions are presented in Figure 2.

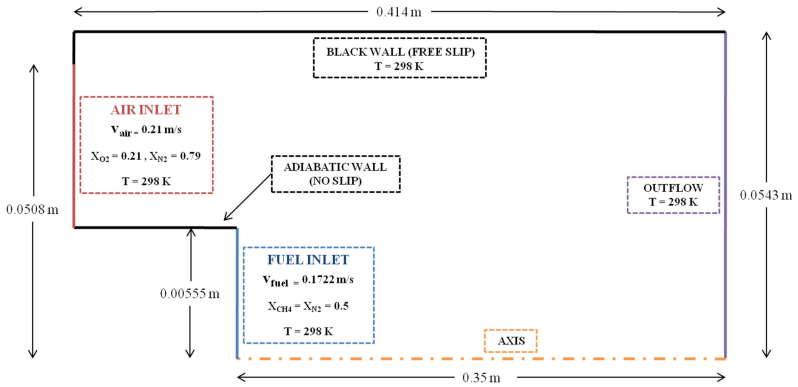

Figure 2. Schematic of domain dimensions, inlet and boundary conditions.

5. COMPUTATIONAL APPROACH

The set of equations is solved with the software ANSYS/Fluent13.0. The pressure-velocity coupling is made by the SIMPLE algorithm (Patankar, 1980). For continuity, energy, species and momentum equations a second order discretization scheme is adopted. A structured mesh with 70875 control volumes is adopted with an adaptive grid algorithm for refinement based on temperature gradient. The adaption is made following the rule of 4^n subdivisions of the original volume where n represents the levels of refinement (2 for this work) as showed in Figure 3.

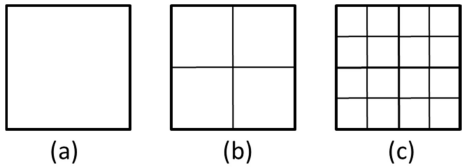

Figure 3. Subdivisions of the control volumes for a 2 levels refinement, where in (a) is the original volume, (b) the first level of refinement and (c) the second level of refinement.

For chemical reactions modeling the DRM19 mechanism is imported with 19 species and 84 reactions with appropriate thermal and transport properties.

Before solving the reactive flow the cold transport of reactants into the domain is calculated and this field is used to start the combustion applying a temperature gradient in the region near the inlets (where fuel and oxidant are mixed). The flame is first converged only for the combustion process and after the radiation modeling is included.

Both WSGG and GG models are coupled with Fluent by user-defined functions (UDF). The UDF's are small routines written in C programming language and allows the user to modify models, parameters treatment, boundary conditions, etc. (Ansys, 2011b). For the purposes of this work two UDF's are coupled with fluent: one for the absorption coefficient and another for the emissivity weighting factor (which is set as 1 for the GG model). For the WSGG model 4 gray gases plus the transparent window are accounted. A UDF to prescribe a parabolic profile at fuel inlet is also adopted according to

$$v(r) = v_{max}\left[1 - \left(\frac{r}{R}\right)^2\right] \tag{20}$$

where $v_{max} = 2v_{fuel}$ and R is the fuel inner tube radius.

6. RESULTS AND DISCUSSIONS

The results for the peak temperature at centerline for the solution without radiation and with the WSGG and GG models are presented in Table 3. As it can be seen, when the radiation modeling is included the peak temperature decreases and the height increases because of the heat release and the lift caused by the dilution level effects appear.

Table 3. Peak temperature and position for both WSGG and GG models along the centerline.

Modeling	T_{peak} (K)	Position (m)
No Radiation	2020.66	0.102
WSGG	1857.24	0.103
GG	1840.39	0.103

The comparisons between numerical results for the radiative heat flux are presented in Figure 4. As it can be seen the solution with WSGG lead to more accurate results when compared with the GG model, since the distribution for the first fits better the experimental data.

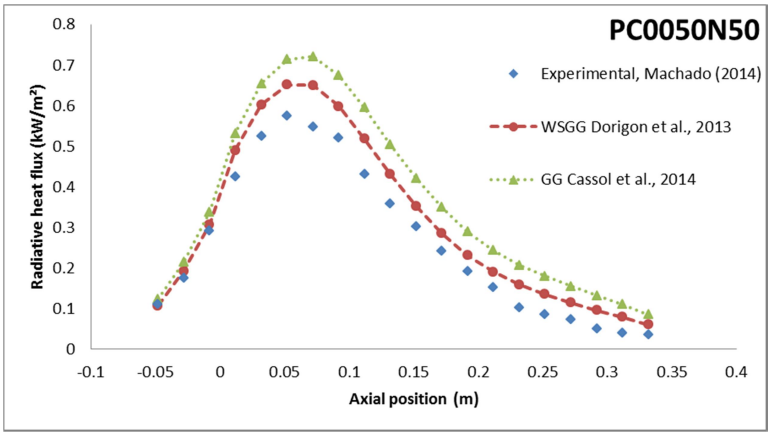

Figure 4. Radiative heat flux distributions along axial position for experimental data, WSGG and GG models.

In order to quantify the accuracy of the models, the average error is calculated as the arithmetic mean of the error calculated point to point according to

$$error(\%) = \left(\frac{|q''_{exp} - q''_{num}|}{q''_{exp,max}}\right) x100 \tag{21}$$

where q''_{exp} is the measured radiative heat flux, q''_{num} is the radiative heat flux obtained with the numerical solution and $q''_{exp,max}$ is the measured maximum radiative heat flux. For the WSGG model the calculated average error is 8.9% while for GG model 17.4%, showing that the WSGG can predict the radiative heat flux with more precision. Although the WSGG lead to better results, the computing time is considerably higher when compared with the GG model. Table 4 presents the calculation time (in days) for the solutions without radiation and with WSGG and GG models. All calculations were made in serial in a Intel (R) Core (TM) i5-4200U CPU @1.60 GHz machine with 4 GB (RAM).

Table 4. Computing time, in days, for the simulation without radiation, WSGG and GG models.

	Time (days)
No Radiation	10
WSGG	15
GG	9

7. CONCLUSIONS

Both WSGG and GG models are coupled with the software ANSYS/Fluent to evaluate the accuracy of the models against experimental data. The absorption coefficient for the GG model is calculated as a function of temperature and concentration of the participant species and new correlations for both models based on HITEMP2010 spectral database are accounted. The coupling between the spectral models with the software is made by UDF. A detailed chemical mechanism with appropriate thermal and transport properties is considered. Results showed that the WSGG model can predict better the radiative heat flux (average error of 8.9%) when compared with the GG model (average error of 17.4%), but the time to perform the computing is considerably higher for the WSGG model (15 days against 9 days for the GG model). The WSGG model showed itself, in spite of its simplicity, capable to give reliable results for computing the radiative properties of a flame.

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