AN ALYSIS OF THE EFFECT OF CHEMICAL SPECIES CONCENTRATIONS OF PARTICIPATING GASES IN THE RADIATION HEAT TRANSFER IN A CYLINDRICAL COMBUSTION CHAMBER USING THE MONTE CARLO-ALB DISTRIBUTION FUNCTION METHOD

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Abstract. *This paper presents results of radiation heat transfer obtained for three gas mixtures formed of water vapor, carbon dioxide and no participating species as the generated in the combustion of hydrocarbon fuels: (1) inhomogeneous medium, (2) homogeneous generated in the stoichiometric combustion of the methane and (3) homogeneous whose distribution concentrations equals the mean concentration of the inhomogeneous one. A typical cylindrical combustion chamber is considered. The distribution temperature for the three gas mixtures as well as the concentration of the inhomogeneous medium are the typically found in combustion chambers and were obtined with correlations presented here. The solution was performed by the Monte Carlo applied to the Absorption-Line-Blackbody (ALB) distribution function, a model that allows a detailed evaluation of the dependence of the absorption coefficient on the wavelength. Considerable departures are observed by comparing the results, showing that approximate the media generated in combustion process as homogeneous, that is usual, can lead to significant errors.*

Keywords*: Non-homogeneous participating media, typical cylindrical combustion chamber, Monte Carlo-ALB distribution function method*

1. INTRODUCTION

Radiation heat transfer is an important phenomenon in several processes in physics and engineering. In industrial combustion systems, such as furnaces and engine chambers, thermal radiation in participating media is often the dominant heat transfer mode due to the high temperature of the gases generated in the combustion process. Computing radiation exchange in participating media is in general a complex task, a reason for this being the highly irregular dependence of the radiative media properties with the wavelength.

To simplify the radiation heat transfer computations and so to reduce the computation time, many methods have been proposed. The simplest model is the gray gas medium, which considers the absorption coefficient to be wavelength independent. Despite its strong departure from the behavior of real gases, the model can still be found in the solution of combustion problems in the modern literature: Adams and Smith (1994), Magel *et al*. (1996), Xue and Cheng (2001) and Sijerčić *et al*.(2001). In the Weighted-Sum-of-Gray-Gases (WSGG) model, first proposed by Hottel and Sarofim (1967), the medium is treated as homogeneous and the entire spectrum is modeled by a few bands. Each band corresponds to a gray gas, in which the absorption coefficient is assumed uniform and temperature independent. The medium temperature dependence is incorporated through the weighted contribution of each gray gas, corresponding to the fraction of blackbody energy in the spectrum region where the absorption coefficient is correspondent to the gray gas. The absorption coefficients and the respective weighting functions are obtained from fitting tabulated data, as those presented by Smith *et al*. (1982) for two homogeneous media composed of water vapor, carbon and air. Perhaps the major limitation of the WSGG model is relying on only a few gray gases and its inability to treat non-homogeneous media, but due to its simplicity it has gained wide application in treatment of complex radiation heat transfer processes.

There is, nowadays, database compiling characteristics related to the emission and absorption behavior of molecules, as HITRAN and HITEMP. With the information provided by these databases, radiation heat transfer problems can be accurately solved by line-by-line (LBL) integration, which considers the emission and absorption of each individual spectral line. On the other hand, the LBL integration is difficult to implement and computationally expensive. To avoid the difficulties related to LBL integration, various band models have been developed in the later years. An extensive overview of these models can be found in the Siegel and Howell (2002).

The WSGG model can be applied to the general radiative transfer equation, as demonstrated by Modest (1991), allowing the solution of arbitrary radiation problems by any desired method replacing the spectral medium by a small number of gray gases with constant absorption coefficient. This important development led to the rise of new WSGG models, as the Spectral-Line-Based-Weighted-Sum-of-Gray-Gases (SLW) model, as proposed by Denison and Webb (1993a), which allows one to obtain the weights of the gray gases from detailed spectral database as HITRAN and

HITEMP. In later developments, the Absorption-Line Blackbody (ALB) distribution function was defined and applied to the SLW model, and numerical correlations to determine this function were presented for media composed of water vapor and air (1993b) and carbon dioxide and air (1995a). Appling the *K*-correlated assumption (Goody *et al*., 1989 and Goody and Yung, 1989), the method was extended to non-isothermal non-homogeneous media Denison and Webb (1995b). Finally, Denison and Webb (1995c) proposed an approximated equation for the ALB distribution function for a mixture of two chemical species, water vapor and carbon dioxide. More recently, Solovjov and Webb, (2000) presented models to improve the efficiency of the SLW in multicomponent gas mixtures, and (Solovjov and Webb, 2002, 2005) proposed the cumulative wavenumber model to allow the assumption of local-spectrum correlation, applying it to gas mixtures with soot. Modest and Zang (2002) proposed the full spectrum *K*-correlated distribution (FSK) method to extend the *K*-correlated and the *K*-distribution methods to the entire radiation spectrum. Wang and Modest (2005) and Modest and Singh (2005) presented database, obtained from the HITEMP and CDSD-1000 data that simplifies the implementation of the SLW and FSK models.

The Monte Carlo method is a powerful technique in the solution of radiation problems Modest (1992) and easily deals with geometrical complexities and/or directional radiation properties. The computational cost of the method is becoming less prohibitive with the rapid rising of the computer processing power. Thus, the Monte Carlo can be a competitive alternative for the solution of complex spectrally dependent radiation heat transfer problems. The method has already been applied to deal homogenous isothermals media in Modest (1992) and Cherkao (1996). In order to consider the effects of the non-uniformities of the media, in the later years the Monte Carlo has been applied in conjunction with spectral models: WSGG Snegirev (2004), narrow-band correlated-k model Tessé *et al*. (2002, 2004), Full-spectrum k-distribution method Wang *et al*. (2007) and ALB distribution function Maurente *et al*. (2007). In this later work was demonstrated that the Monte Carlo method and the ALB distribution function can be combined in a relatively simple way.

The standard WSGG model, based on correlating tabulated data as Smith *et al*. (1982), is a popular method to compute the radiation heat transfer in combustion cambers. It requires considerably less computational effort than more sophisticated models, since the real gas radiative properties is modeled by a set of a few gray gases. However, the model presents some significant limitations: the gas absorption coefficient of each gray-gas is supposed not to vary with the temperature and the chemical species concentrations have to be uniform. For instance, Smith *et al*. (1982), present correlations for typical gaseous products of combustion of methane (20% H_2O, 10% CO_2 and non absorbing species) and ethane (10% H_2O, 10% CO_2 and non absorbing species). While such correlations are adequate when chemical reaction is complete and the products are completely mixed in the specified set of concentrations, their validity is not expected for the non-homogeneous environment of the combustion chamber itself.

In order to evaluate the error that is related to the assumption of homogeneous gas mixture, the Monte Carlo applied to the ALB distribution function was used to obtain three results for the radiative heat exchange in a cylindrical enclosure containing participating gas with distribution temperature as typically found in combustion chambers. The three media are composed of water vapor, carbon dioxide and non absorbing species, differing only in the concentration distributions. The first medium is inhomogeneous and its distribution concentration is based in that resulting of the real combustion of methane. The second medium in homogenous and its concentration are the resulting of the stoichiometric combustion of methane, that is, 20% H_2O and 10% CO_2. For the last medium, the chemical species concentratiosn are the mean concentrations considered for the inhomogeneous medium.

2. TEXT FORMAT THE MONTE CARLO METHOD APPLIED TO THE ABSORPTION-LINE BLACKBODY DISTRIBUTION FUNCTION

The Absorption-Line Blackbody (ALB) distribution function is defined as the fraction of the blackbody energy in the portions of the spectrum where the high-resolution spectral absorption cross-section of the medium, $K_{m,\,\eta}$, is less than a prescribed value K_m. For a single emitting absorbing species, it is given by:

$$F\left(K_m, T_b, T_g, P_T, Y_s\right) = \frac{1}{\sigma T_b^4} \sum_i \int_{\Delta\eta_i} E_{b,\eta}\left(\eta, T_b\right) \cdot d\eta \tag{1}$$

where Y_s is the concentration of the single absorbing species s; T_b is the source radiation temperature at which the blackbody emissive power is evaluated; T_g is the medium local temperature at which the medium radiation properties are evaluated; P_T is the total pressure of the gaseous medium; η is the wavenumber; σ is the Stefen-Boltzmann constant; and sub-index i refers to the i^{th} spectral segment. The absorption cross-section coefficient, $K_{m,\,\eta}$, is related with the spectral absorption coefficient by

$$K_\eta = M_s K_{m,\eta} \tag{2}$$

where M_s is the molar concentration of the absorbing species s.

In most spectral models the fraction of blackbody energy needs to be calculated for each spectral interval where the medium absorbs and emits thermal radiation. The ALB distribution function has the advantage of computing at once the fraction of blackbody energy in all spectral intervals in which the absorption cross-section coefficient presents the specified value $K_{m,\eta}$. The fraction of the blackbody energy within spectral intervals corresponding to a cross-section interval $K_{m,j}$ and $K_{m,j+1}$ can be obtained from the ALB distribution function as

$$\Delta F_j = F\left[K_{m,j}(T_g, Y_s, P_T), T_b\right] - F\left[K_{m,j+1}(T_g, Y_s, P_T), T_b\right] \tag{3}$$

Different Monte Carlo implementations can be proposed to employ the ALB distribution function for the computation of radiative heat transfer in spectrally dependent media, depending for instance on how the number and the energy of the bundles are distributed along the spectrum. Each choice will lead to a different cumulative distribution function. The methodology used in this work was proposed in Maurent *et al.* (2007). According to this work, from the definition of the ALB function, the emission rate from a medium volume ΔV in the spectrum portions where the average absorption cross-section is K_m within an certain interval ΔK_m can be approximated by

$$q_{\Delta V,K_m} = 4\Delta V M_s K_m \Delta F(K_m)\sigma T_{\Delta V}^4 \tag{4}$$

where the $\Delta F(K_m)$ is the difference between the ALB distribution functions evaluated at $K_m + \Delta K_m/2$ and $K_m - \Delta K_m/2$ around a given value K_m. According to Eq. (2), the product $M_s K_m$ corresponds to the local absorption coefficient, where M_s is the molar concentration of the absorbing species s.

In Eq. (4) the ALB distribution function is computed at the local conditions of the medium volume ΔV, so the dependence of ΔF on the local temperature, absorbing species concentration and total pressure was dropped.

Considering that the total number of bundles released from the volume ΔV is $N_{\Delta V}$, it was proposed in Maurent *et al.* (2007) that the number of bundles that are released from the spectral portion where the average absorption cross-section is K_m within an interval ΔK_m be proportional to the amount of blackbody energy, at the medium volume temperature, that is contained in that portion:

$$N_{\Delta V,K_m} = \Delta F_{K_m} N_{\Delta V} \tag{5}$$

It follows that the energy of a bundle emitted from the portions where the absorption cross-section is K_m is given by:

$$q_{\Delta V,K_m}^{(b)} = \frac{q_{\Delta V,K_m}}{N_{\Delta V,K_m}} = \frac{4\Delta V M_s K_m \sigma T_{\Delta V}^4}{N_{\Delta V}} \tag{6}$$

which shows that the amount of energy of the bundle depends on the value of the absorption cross-section of the spectral portions from where it is released.

Following the procedure outlined in Siegel and Howell (2002), the cumulative distribution which governs the number of bundles that are released from all the portions where the absorption cross-section is less than K_m is equivalent to the ALB distribution function:

$$R(K_m) = F(K_m) \tag{7}$$

Turning to the bundles emitted from the wall boundaries, the energy that is emitted by a gray wall element having area ΔA and total emissivity ε_w can be approximated by:

$$q_{\Delta A,K_m} = \varepsilon_w \Delta A \Delta F_{K_m} \sigma T_{\Delta V}^4 \tag{8}$$

As done with medium emission, it can be proposed that the number of wall element bundles that are released from the portions where the medium absorption cross-section is K_m, within the interval ΔK_m, be proportional to the fraction of blackbody energy (at the wall element temperature, $T_{\Delta A}$) of those portions, that is:

$$N_{\Delta A,K_m} = \Delta F_{K_m} N_{\Delta A} \tag{9}$$

where $N_{\Delta A}$ is the total number of bundles released from the wall element. It follows that the energy of each bundle is given by:

$$q_{\Delta A,K_m}^{(b)} = \frac{\varepsilon_w \Delta A e_b(T_{\Delta A})}{N_{\Delta A}} \tag{10}$$

Thus, the bundles released from the wall elements have all the same amount of energy, and do not depend on the selected portions of spectrum. Following the same procedure that was presented for the medium, it can be shown that Eq. (7), which relates the cumulative distribution to the ALB distribution, can also be applied for the emission from the wall elements.

The above Monte Carlo equations were obtained for a medium whose temperature and properties are uniform. However, those equations can be employed for non-isothermal non-homogeneous media by the application of the following relation presented by Denison and Webb (1995b), based on a *K*-correlated hypotheses:

$$F\left\lfloor K_m(T_g, Y_s, P_T), T_b \right\rfloor = F\left\lfloor K_m(T_{g,ref}, Y_{s,ref}, P_{T,ref}), T_b \right\rfloor \tag{11}$$

which states that the ALB distribution function for a given value K_m, evaluated at given local conditions, is equal to the ALB distribution function evaluated at any other reference local conditions. In other words, for the same temperature T_b (at which the blackbody emissive power is evaluated) and different T_g, Y_s and P_T, for the same spectral intervals, the medium absorbing emitting property, K_m, changes but the fraction of blackbody energy less than these K_m's (evaluated at the different local conditions) remains the same.

As demonstrated by Denison and Webb(1995c) the ALB distribution function for a medium composed of two emitting absorbing species can be obtained by the following approximation:

$$F_{s_1,s_2}\left(K_{m,s_1}, K_{m,s_2}\right) \cong F_{s_1}\left(K_{m,s_1}\right) \cdot F_{s_2}\left(K_{m,s_2}\right) \tag{12}$$

where the indices s_1 and s_2 refer to the two emitting absorbing species in the medium. The absorption coefficient of the medium composed of these two emitting absorbing species is

$$K = M_{s_1} K_{m,s_1} + M_{s_2} K_{m,s_2} \tag{13}$$

To determine the energy transported by the bundles emitted from a volume element, ΔV, from Eq. (6), it is necessary to prescribe the number of emitted bundles, $N_{\Delta V}$, and to set a value of the absorption cross-section, K_m, related to the spectral interval of the bundle energy. Using the Monte Carlo method, K_m is obtained from the cumulative distribution function. Equation (7) is then rewritten to allow determining K_m from the Monte Carlo cumulative distribution function. The final procedure in determining K_m is to generate a random number for the ALB distribution function, *F*, once it is equivalent to the cumulative distribution function, *R*, so that

$$K_m = K_m(R) = K_m(F) \tag{14}$$

According to Siegel and Howell (2002), once an energy bundle is released, the length traveled, *l*, before its absorption in a medium of constant absorption coefficient, $K = M_s K_m$, is

$$l = -\ln(R_l)/(M_s K_m) \tag{15}$$

where R_l, is a random number.

The proposed procedure to compute radiation heat transfer in a medium having non-uniform absorption coefficient is to divide the path length into small segments where the properties can be assumed uniform. For each segment, the absorption cross-section coefficient K_m (and, therefore, the absorption coefficient of the medium *K*) is found for the spectral region correspondent to the emitted energy. This spectral interval is related to the random number generated, in the interval between 0 and 1, to represent *F* in the computation of the bundle energy. From the *K*-correlated hypothesis, the local value of K_m in the segment, corresponding to the spectral region of the energy bundle, can be found from Eq. (14) using the same random number generated for the emission process, but taking the local medium properties for the evaluation of the ALB distribution function with Eq. (11). This procedure is the same no matter the energy bundle is emitted from a medium volume or from a surface element.

Finally, the total radiation heat exchange in the system results from accounting all the bundles (with their respective energy) emitted and absorbed by the medium and the walls.

More information about Monte Carlo applied to the ALB distribution function as well as results that demonstrate the method validity may be found in Maurente *et al*. (2006a, 2006b, 2007).

3. PROBLEM DESCRIPTION

Thermal radiation in participating gases is in general the dominant heat transfer mode in combustion systems such as furnaces, steam generators and engines. However, modeling of this complex process is not limited to thermal radiation, for it also involves combustion chemical reactions, turbulent fluid flow and convective heat transfer. The application of the more advanced gas radiation models in this problem is one of the most challenging on-going researches in the field.

Due to its simplicity, the conventional weighted-sum-of-gray-gases (WSGG) model is probably the most commonly applied model for such problems. The price of the simplicity is that the WSGG is unable to incorporate inhomogeneous media and the entire wavelength is covered by only a few gray gases, usually three. On the other hand, real gases absorption and emission results from the contribution of a much larger number of lines and bands. In addition, the effect of the gas temperature is limited to the weighting factors of each gray gas, while its absorption coefficient is assumed temperature independent and uniform in the entire gas.

The goal of this work is to investigate the deviations that can occur due to approximate inhomogeneous media as homogeneous resulting from stoichiometric combustions in order to use the WSGG model. The Monte Carlo method combined to the ALB distribution function was used to solve the problems, once it is a detailed spectral model that hands well with the inhomogeneous and homogenous media, allowing at limit the analysis to the homogeneous medium approximation. The heat exchanges are performed for a cylindrical combustion chamber shown in Fig. 1, having a length of 1.7 m and a diameter of 0.25 m. The walls are black and are at 600 K. The figure also shows the temperature. Figure 2 shows the concentration distribution of the inhomogeneous medium. Temperature and distribution profiles are typical of such combustion chambers and were bases on the results obtained by Silva *et al* (2004), which solved the combustion, convection and radiation coupled problem, being that to obtain the radiation heat exchanges it was employed the WSGG model. Correlations for these temperature and concentration distributions are presented in Annex A.

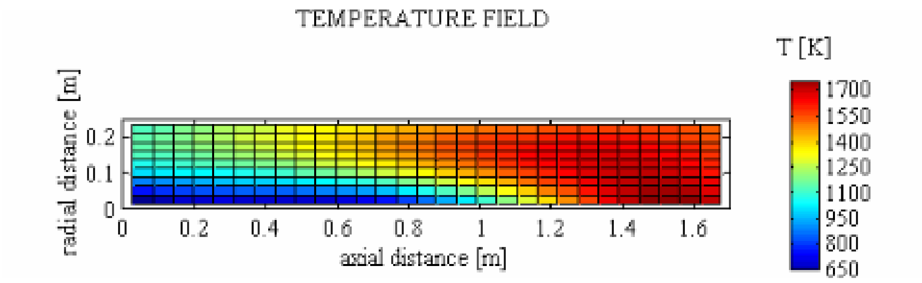
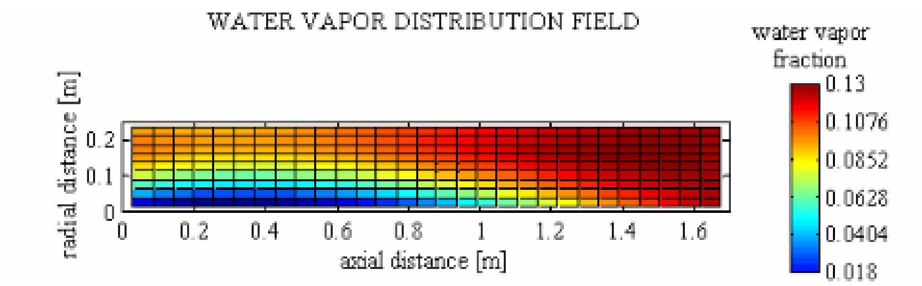
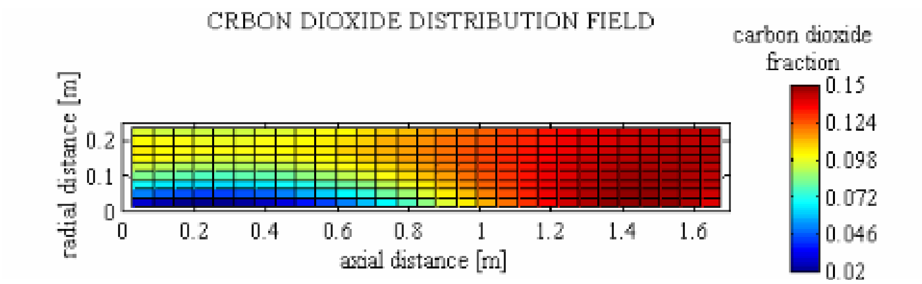


Figure 1 – Typical temperature distribution in a cylindrical combustion chamber.



(a)



(b)

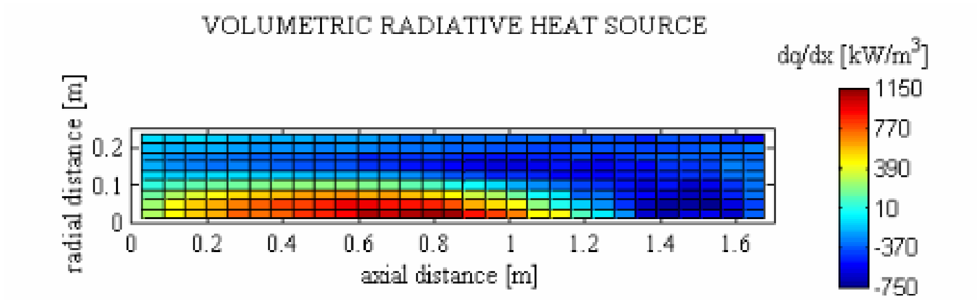
Figure 2 – Typical concentrations distributions of water vapor (a) and carbon dioxide (b) in a cylindrical combustion chamber.

The fuel considered for obtaining the temperature and concentration fields were the methane. Therefore, the first homogeneous gas mixture represents a typical product of the stoichiometric combustion of methane, composed of 20% of water vapor and 10% of carbon dioxide.

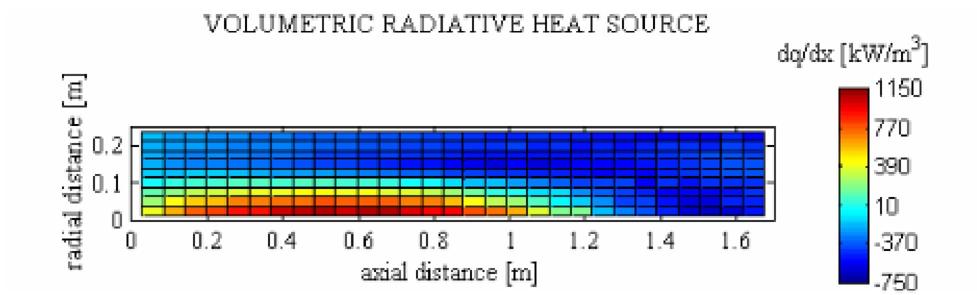
Although it is usual to approximate the media generated in combustion process as the resulting from the stoichiometric combustion related to the respective fuel, the concentration of the combustion products can be rather different from that for stoichiometric combustion. The reason for this is that real combustion processes generally occur with excess of air, instead stoichiometric fractions. Therefore, to employ the WSGG with correlations for another medium that not the generated in stoichiometric combustion could improve the accuracy of the result. However it is still required that media be approximated as homogeneous. A homogeneous medium that somewhat reproduces a certain inhomogeneous medium is that whose concentration equals to the mean concentration of it. To analyze the errors that can arise from this homogenous medium assumption, the chemical species concentration for the second homogeneous medium is 9,45% water vapor and 11,13% carbon dioxide, that is the mean concentration of the inhomogeneous medium, shown in the Fig. 2.

4. RESULTS AND DISCUSSION

The Monte Carlo solution for the radiation exchanges in the enclosure were computed with the zonal analysis. It involved the division of the domain into 30 (thirty) and 10 (ten) equal-sized elements in the axial and radial directions. Figures 3a, 3b and 3c present, respectively, the solutions for the inhomogeneous gas mixture, for the generated in the stoichiometric combustion of the methane and for a gas with chemical species concentration equal the mean concentrations of the inhomogeneous gas. Figure 3 shows the volumetric radiative heat rate in the gas, in kW/m^3, with the adopted convention that negative volumetric radiative heat rate indicates that the zone emits more than absorbs thermal radiation, so that it is losing energy to the surroundings. The opposite applies when the value is positive.



(a)



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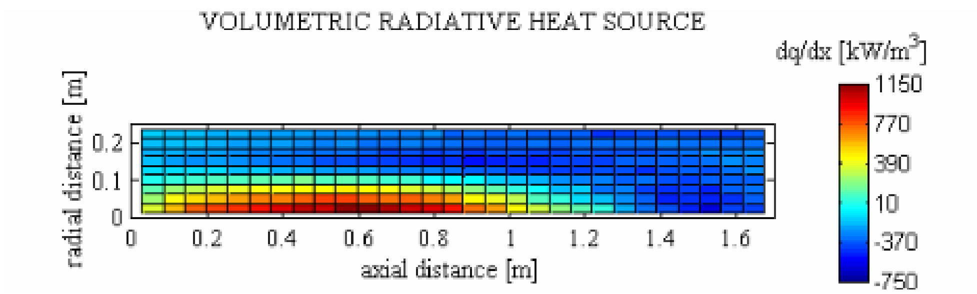

(c)

Figure 3 – Volumetric radiative heat source: (a) inhomogeneous medium,(b) homogenous stoichiometric medium and (c) homogeneous medium with concentration equal to the mean concentration of the inhomogeneous.

A total of one million (5.10^5) energy bundles were released from each gas and wall zones. As can be observed the volumetric radiative heat rates are similar. However, there is a significant difference in the magnitude of the results for the inhomogeneous and stoichiometric media. The absolute value of the integral of the volumetric heat source over entire the medium is 32.87% higher for the medium resulting from stoichiometric combustion. For the second homogeneous mixture, composed of 9.45% H_2O, 11.13% CO_2 and non absorbing species, discrepancies between the two solution can also be observed, although they are less significant than for the first gas mixture. The integral of the volumetric heat source over entire the medium is 15.41% lower (in absolute value) for the homogeneous medium from the combustion inhomogeneous.

The discrepancy between the solutions can be further explored in Fig. 4, which shows the results for the radiation heat flux, in W/m^2, along the cylindrical chamber wall. The general trends for the thee solution are similar, however the difference between the solutions become more relevant in the high gas temperature region, which is characterized by the peak in the heat flux. In this point, the relative difference between the inhomogeneous and stoichiometric media solutions reaches the value of 12.24 %. As shown in Fig. 4, the radiative heat flux in the cylindrical chamber wall from the homogeneous media composed of the mean concentration of the inhomogeneous media is close of it for most regions of the cylindrical wall, although a error great from the stoichiometric medium can be,1314%, for the maximum heat fluxes. Besides, the peak occur at different location for the medium composed of the mean concentration, at 1.33 m instead 1,388 as for the other two cases.

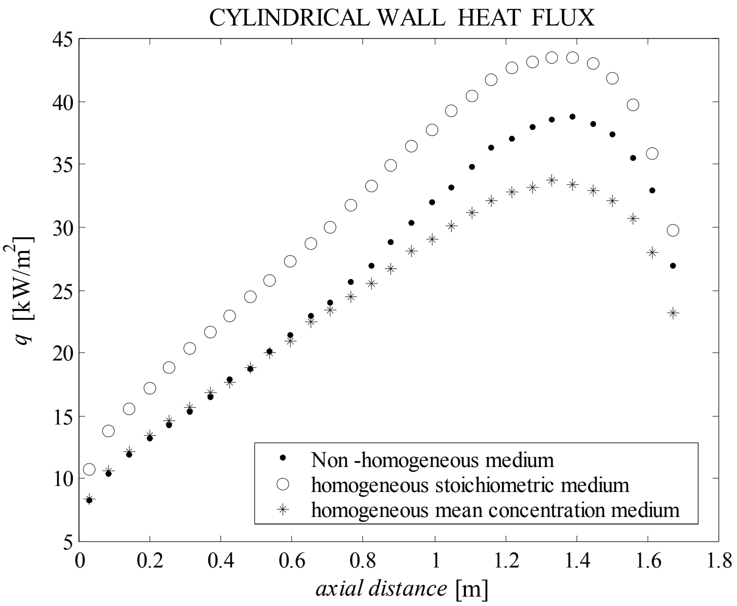

Figure 4 – Wall radiative heat fluxes for the three considered medium.

Oscillations that appear in results of volumetric radiative heat source in the medium due to the number of emitted bundles be low, regarding the Monte Carlo implementation used here, five hundred thousand ($5\cdot10^5$) from each gas and wall zones. However, there is no significant oscillation in the results used to accomplish the analysis. The standard deviation was lower than 1% for the integrals of the volumetric heat source over the media and for the wall radiative heat flux it remained lower then, in the three cases.

5. CONCLUSION

This paper presented a comparison between results for the radiative heat transfer in a cylindrical combustion chamber. Three different mixtures of water vapor, carbon dioxide and non absorbing species are considered: one inhomogeneous and two homogeneous. The inhomogeneous has a distribution concentration profile as typically found in combustion system. The first homogenous medium considered is the resulting of the stoichiometric combustion of methane fuel for with Smith *et al* (2002) presented correlations for use with the WSGG model. The second homogeneous considered medium has chemical species concentration that equals the mean concentration of the inhomogeneous medium. The comparison involved both the volumetric radiative heat rate in the medium and the heat flux on the cylindrical chamber wall. The maximum relative difference between the two solutions for the homogeneous media compared with the solution for the inhomogeneous were about 33% and 15%.

The radiative heat exchange was solved by the Monte Carlo with the ALB distribution function, which accounts for the detailed spectral behavior and can be applied with good accuracy for homogenous and inhomogeneous media, so that the difference between results can be solely attributed to the approximate the inhomogeneous medium produced in the combustion process as being homogenous.

The results for both the volumetric radiative rate in the gas and for the heat flux on the wall demonstrated the importance of the concentrations of the absorbing species on the radiative heat transfer. However, it is verified that the errors associated with to approximate gases products of combustion as homogeneous can be reduced by selecting an appropriated homogeneous medium to approximate the medium generated in the real combustion process. .

6. ACKNOWLEDGMENTS

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7. REFERENCES

Adams BR, Smith PJ. Modeling effects of soot and turbulence-radiation coupling on radiative transfer in an industrial furnace. ASME Radiative Heat Transfer: Current Research, HTD-Vol. 276, 1994. p. 177-190.

Cherkaoui M., Dufresne JL, Fournier R, Grandpeix JY, Lahellec A. Monte Carlo simulation of radiation is gases with a narrow-band model and a net-exchange formulation. Journal of Heat Transfer, 1996; 118: 401-407.

Denison MK, Webb BW. A spectral line-based weighted sum-of-gray-gases model for arbitrary RTE solvers. Journal of Heat Transfer, 1993; 115: 1004-1011.

Denison MK, Webb BW. An absorption-line blackbody distribution function for efficient calculation of total gas radiative transfer. Journal of Quantitative Spectroscopy and Radiative Transfer, 1993; 50: 499-510.

Denison MK, Webb BW. Development and application of an absorption-line blackbody distribution function for CO_2. International Journal of Heat and Mass Transfer, 1995; 38: 1813-1821.

Denison MK, Webb BW. The spectral line-based weighted sum-of-gray-gases model in nonisothermal nonhomogeneous media. Journal of Heat Transfer, 1995; 117: 359-365.

Denison MK, Webb BW. The spectral line-based weighted sum-of-gray-gases model for H_2O/CO_2 mixtures. Journal of Heat Transfer, 1995; 117: 788-792.

Goody R, West R, Chen L, Crisp D. The correlated-*K* method for radiation calculations in nonhomogeneous atmospheres. Journal of Quantitative Spectroscopy and Radiative Transfer, 1989; 42: 539-550.

Goody RM, Yung YL. Atmospheric Radiation. New York: Oxford University Press, 1989.

Solovjov V. P. and Webb B.W. SLW modeling of radiative transfer in multicomponent gas mixtures. Journal of Quantitative Spectroscopy and Radiative Transfer, 2000; 65: 655-672.

Hottel HC, Sarofim AF. Radiative Transfer. New York: McGraw-Hill Book Company, 1967.

Smith TF, Shen ZF, Friedman, JN. Evaluation of coefficients for the weighted sum of gray gases model. Journal of Heat Transfer, 1982; 104: 602-608.

Magel HC, Schnell U, Hein KR. Simulation of detailed chemistry in a turbulent combustor flow. Twenty-Sixth Symposium (International) on Combustion/The Combustion Institute, 1996. p. 67-74.

Maurente A., Vielmo H. A., França F. H. R. A Monte Carlo Implementation to Solve Radiation Heat Transfer in Non-uniform Media with Spectrally Dependent Properties. Accepted to publication in the JQSHT., 2007

Maurente A., Vielmo H. A., França F. H. R. Analysis of The Chemical Species Concentrations on The Radiative Heat Transfer in Participating Gases Using a Monte Carlo Methodology. Encit, Brazilian Congress of Thermal Engineering and Science, 2006, Curitiba, PR, Brasil.

Maurente A., Vielmo H. A., França F. H. R. Comparison of The Monte Carlo Method Applied to The Absorption-Line-Blackbody Distribution Function with a Conventional WSGG model. IMECE, International Mechanical Engineering Congress and Exposition, 2006, Chicago, IL, United States of America.

Modest M F, Singh V. Engineering correlations for full spectrum *k*-distribution of H_2O from the HITEMP spectroscopic databank. Journal of Quantitative Spectroscopy and Radiative Transfer, 2005; 93: 263-271.

Modest MF, Zhang H. The full-spectrum correlated-*K* distribution for thermal radiation for molecular gas-particulate mixtures. Journal of Heat Transfer, 2002; 124: 30-38.

Modest MF. The Monte Carlo method applied to gases with spectral line structure. Numerical Heat Transfer, Part B, 1992; 22: 273-284.

Siegel R, Howell, JR. Thermal Radiation Heat Transfer. New York: Taylor & Francis, 2002.

Sijerčić M, Stevanović Z, Belošević S. Modeling of non-confined turbulent flow of two coaxial streams under combustion conditions. Mechanical Engineering, 2001; 1: 981-988.

Silva C. V., Vielmo, H. A.,0 França F. H. R. Simulação Numérica de Processos de Combustão em Câmaras Cilíndricas Usando o Modelo SCRS. Encit, Brazilian Congress of Thermal Engineering and Science, 2004, Rio de Janeiro, Brasil.

Snegirev, A. Y., Statistical modeling of thermal radiation transfer in bouyant turbulent diffusion flames, Combustion and Flame, 136 (1 – 2), 51 – 71, 2004.

Solovjov V. P. and Webb B.W. A local-spectrum correlated model for radiative transfer in non-uniform gas media. Journal of Quantitative Spectroscopy and Radiative Transfer, 2002; 73: 361-373.

Solovjov V. P. and Webb B.W. The cumulative wavenumber method for modeling radiative transfer in transfer in gas mixtures with soot. Journal of Quantitative Spectroscopy and Radiative Transfer, 2005; 93: 273-287.

Tessé, L., Dupoirieux, F., Zamuner, B., and Taine, J., Radiative transfer in real gases using reciprocal and forward Monte Carlo methods and a correlated-k approach. Int. J. Heat Mass Transfer, 45, 2797 – 2814, 2002.

Tessé, L., Dupoirieux, and Taine, J., Monte Carlo modeling of radiative transfer in a turbulent soot flame. Int. J. Heat Mass Transfer, 47, 555 – 572, 2004.

Xue H, Ho JC, Cheng YM. Comparison of different combustion models in enclosure fire simulation. Fire Safety Journal, 2001; 36: 37-54.

Wang A, Modest M F. High-accuracy compact database of narrow-band *K*-distributions for water vapor and carbon dioxide. Journal of Quantitative Spectroscopy and Radiative Transfer, 2005; 93: 245-261.

Wang L., Yang, J. Modest, M. F., and Howorth, D. C. Application of the full-spectrum k-distribution method to photon Monte Carlo solvers. Journal of Quantitative Spectroscopy and Radiative Transfer, 2007; 104: 297-304.

8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.

ANNEX A

This section presents the polynomials correlations that allow one to obtain the distributions of the temperature and the water vapor and carbon dioxide in the cylindrical combustion chamber shown in Figures 2 and 3, having length of 1.7 m and a diameter of 0.5 m.

The gas distribution temperature relates with the radial distance, r, and an axial position dependent term, PT_i, according to

$$T(z,r) = 540\sum_{i=1}^{3} PT_i \cdot r^{(3-i)} + 144 \tag{A.1}$$

The term PT_i relates to the axial distance, z, with the following equation:

$$P_i(z_D) = \sum_{j=1}^{5} CT_j \cdot z^{(5-j)} \tag{A. 2}$$

The CT_j coefficients for each PT_i are presented in Table A. 1

Table A. 1. Coefficients for the temperature distribution in a typical cylindrical combustion chamber with a length of 1.7 m and a diameter of 0.5 m

	PT_1	PT_2	PT_3
CT_1	-131,4504	46.2986	-4.1176
CT_2	455.2128	-152.4484	12.3165
CT_3	-452.0936	140.6828	-10.0183
CT_4	125.1324	-35.0872	2.8384
CT_5	-41.8856	14.3664	0.6096

The water vapor distribution concentrations relates with the radial distance, r, and an axial position dependent term, PH_i, according to

$$Y_{H_2O}(z,r) = \sum_{i=1}^{4} PH_i \cdot z^{(4-i)} \tag{A.3}$$

The PH_i relates to the axial distance, z, with the following equation:

$$PH_i(z_D) = \sum_{j=1}^{3} CH_j \cdot r^{(3-j)} \tag{A. 4}$$

The coefficients for each PH_i are presented in Table A. 2.

Table A. 2. Coefficients for the water vapor concentration distribution in a typical cylindrical combustion chamber with a length of 1.7 m and a diameter of 0.5 m

	PH_1	PH_2	PH_3	PH_4
CH_1	1.5636	-2.6345	2.1509	-3.3564
CH_2	-0.1823	-0.0777	-0.0857	1.1550
CH_3	-0.0627	0.2155	-0.1090	0.0032

The carbon dioxide distribution concentrations relates with the radial distance, r, and an axial position dependent term, PC_i, according to

$$Y_{CO_2}(z,r) = \sum_{i=1}^{4} PC_i \cdot z^{(4-i)} \tag{A. 5}$$

The term PC_i relates to the axial distance, z, with the following equation:

$$PC_i(z_D) = \sum_{j=1}^{3} CC_j \cdot r^{(3-j)} \tag{A. 6}$$

The CC_j coefficients for each PC_i are presented in Table A. 3

Table A. 3. Coefficients for the carbon dioxide distribution in a typical cylindrical combustion chamber with a length of 1.7 m and a diameter of 0.5 m

	PC_1	PC_2	PC_3	PC_4
CC_1	-3.4339	7.8648	-1.9982	-3.1588
CC_2	1.3104	-3.0295	0.8932	1.0357
CC_3	-0.1628	0.3941	-0.1395	0.0206