Paper CIT06-0366

ANALYSIS OF THE EFFECT OF THE CHEMICAL SPECIES CONCENTRATIONS ON THE RADIATION HEAT TRANSFER IN PARTICIPATING GASES USING A MONTE CARLO METHODOLOGY

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Abstract. This paper presents the application of the Monte Carlo method to solve the radiation heat transfer in an one-dimensional system formed by a gas mixture contained in a space between two infinite parallel plates. The proposed methodology consists of the application of the Monte Carlo method to the absorption line blackbody (ALB) distribution function, a gas model that allows a detailed evaluation of the dependence of the absorption coefficients of the absorbing species on the wavelength. The methodology allows solving for gaseous mixtures that are non-homogeneous and non-isothermal. In this work, the method is applied to the solution of heat transfer in a gas mixture formed with different concentrations of water vapor and carbon dioxide, two absorbing species, and non-participating species such as air or nitrogen. The results show that the concentration of the species have a strong effect on the heat transfer, and demonstrate the limitation of the conventional weighted-sum-of-gray-gases (WSGG) model, which relies on correlations that are valid for only a few concentrations of the absorbing species concentrations. The cases presented in the paper are related to gaseous mixtures resulting from the combustion of octane and methane.

Participating gases, wavelength dependence, Monte Carlo, absorption-line-blackbody distribution function, thermal radiation

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, several 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 et al., 2001and Sijercic 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 dioxide 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 achieved 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 is computationally expensive. To avoid the difficulties related to LBL integration, various band models have been developed in late 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 (SLWSGG) 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 SLWSGG model, and numerical correlations to determine this function were presented for media composed of water vapor and air (Denison and Webb, 1993b) and carbon dioxide and air (Denison and Webb, 1995b). 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, 1995a). 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. Further improvements in the use of the SLWSGG method may be possible with new information available in recent works (Wang and Modest, 2004, and Modest and Singh, 2004) on spectral band models.

The Monte Carlo method is a powerful technique for the solution of radiation problems Howell (1998), having the important advantage of easily dealing 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 Cherkaoui et al.,1996). In order to consider the effects of the non-uniformities of the media, Maurente et al. (2006) applied the Monte Carlo method to the ALB distribution function. The work demonstrated that the Monte Carlo method and the ALB distribution function can be combined in a relatively simple way, and taking the advantage of incorporating all the late advances of the SLWSGG model.

In this work the Monte Carlo combined to the ALB distribution function is used to solve the radiation heat transfer in a system formed by a homogeneous medium contained between two infinite parallel walls. The medium is a mixture of water vapor, carbon dioxide, two emitting absorbing chemical species, and nitrogen, a transparent medium. Since the conventional WSGG models are based on a few relations that are valid for only a limited number of chemical species concentrations, considering especially the stoichiometric chemical reaction, this work aims at demonstrating the errors that can incur from applying those models to compute radiation heat transfer for mixtures having different concentrations.

2. The used methodology: Monte Carlo-Absorption-Line-Blackbody distribution function

The Absorption-Line Blackbody (ALB) distribution function is defined (Denison and Webb, 1993b) as the fraction of the blackbody energy in the portions of the spectrum where the high-resolution spectral absorption cross-section of the medium, $K_{m,n}$, is less than a prescribed value K_m . For a single emitting absorbing species, it is given by:

$$F(K_m, T_b, T_g, P_T, Y_s) = \frac{1}{\sigma T_b^4} \sum_i \int_{\Delta \eta_i} E_{b,\eta}(\eta, T_b) \cdot d\eta$$
(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 the sub-index *i* refers to the *i*th spectral segment. The absorption cross-section coefficient, $K_{m,\eta}$, is related with the absorption coefficient by

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

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

When desiring to account for spectral behavior in radiation heat flux calculations the blackbody energy distribution function is used to assist in determining the distribution of emitting absorbing energy along of the spectrum. In the most spectral models the blackbody energy fraction within each considered spectral interval is calculated. However, as demonstrated by Denison and Webb (1993b, 1995b), the ALB distribution function can be used to obtain significant computer time savings by computing at the same time the fraction of blackbody energy in several spectral intervals in which the absorption cross-section coefficient, $K_{m, \eta}$, presents the same value. The fraction of the blackbody energy within spectral intervals corresponding to a high-resolution absorption cross-section interval $K_{m, j}$ and $K_{m, j+1}$ can be obtained by ALB distribution function as

$$\Delta F_{j} = F \left[K_{m,j}(T_{g}, Y_{s}, P_{T}), T_{b} \right] - F \left[K_{m,j+1}(T_{g}, Y_{s}, P_{T}), T_{b} \right]$$
(3)

Different Monte Carlo implementation can be proposed to employ the ALB distribution function for 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 having as guiding factors simplicity of implementation and computational efficiency. According (Maurente et al, 2006), 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 of a given K_m value and, according Eq. (2), the product $M_s K_m$ corresponds to the local absorption coefficient, where M_s is the molar concentration of the absorption species s.

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

Considering that the total number of bundles released from volume ΔV is $N_{\Delta V}$. It was proposed that the number of bundles that are released from a 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:

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

As demonstrated in (Maurente eat al, 2006) following the procedure outlined in (Siegel and Howell, 2002), the frequency of the bundles released from the portions where the absorption cross-section is K_m is obtained by:

$$f(K_m) = \lim_{\Delta K_m \to 0} \frac{N_{\Delta V, K_m}}{\Delta K_m} = \lim_{\Delta K_m \to 0} \frac{\Delta F_{K_m} N_{\Delta V}}{\Delta K_m} = F'(K_m) N_{\Delta V}$$
(7)

The probability density function is defined as:

$$P(K_m) = \frac{f(K_m)}{\int_{K_m=0}^{K_m,\max} f(\xi)d\xi} = \frac{F'(K_m)N_{\Delta V}}{[F(K_{m,\max}) - F(K_m=0)]N_{\Delta V}} = F'(K_m)$$
(8)

The above result follows from the definition of the ALB distribution functions, in which $F(K_{m,max}) = 1$ and $F(K_m = 0) = 0$. Finally, the cumulative function becomes:

$$R(K_m) = \int_{-\infty}^{K_m} P(\xi) d\xi = \int_0^{K_m} F'(\xi) d\xi = F(K_m)$$
(9)

Equation (9) shows that for the Monte Carlo implementation based on Eq. (5), the cumulative distribution function $R(K_m)$, 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.

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:

$$q_{\Delta A,K_m} = \varepsilon_w \Delta A \Delta F_{K_m} \sigma T_{\Delta V}^4 \tag{10}$$

Although there are no medium involved in the wall emission, the fraction of the emitted blackbody energy is given by ALB distribution function which is a function of arbitrary values of K_m . It assists in computing the media absorption of the bundles provided from walls.

As done for the medium emission, it was proposed that the number of wall element bundles that are released from the portions where the 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_{AA}) of these portions, that is:

$$N_{\Delta A,K_m} = \Delta F_{K_m} N_{\Delta A} \tag{11}$$

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:

$$q_{\Delta A,K_m}^{(b)} = \frac{\varepsilon_w \Delta A e_b(T_{\Delta A})}{N_{\Delta A}}$$
(12)

Thus, the bundles released from the wall elements have all the same amount energy, and does not depend on the selected portions of spectrum.

As well as for emission from the medium, Eq. (9) can also be applied to the wall elements.

As demonstrated by Denison and Webb (1995c) the ALB distribution function for media composed for tow emitting absorbing species can be obtained by the following adequate approximation:

$$F_{s_1,s_2}(K_{m,s_1}, K_{m,s_2}) \cong F_{s_1}(K_{m,s_1}) \cdot F_{s_2}(K_{m,s_2})$$
(13)

where the sub-index s_1 and s_2 refer to the both emitting absorbing species present in the medium. The absorption coefficient to the medium composed by these both emitting absorbing species is

$$K = M_{s_1} K_{m,s_1} + M_{s_2} K_{m,s_2} \tag{14}$$

For to determine the energy carried out for the bundles emitted from an uniform volume element, ΔV , by Eq. (6), it is necessary to prescribe the number of emitted bundles, $N_{\Delta V}$, and to know the value of absorption cross-section, K_m , related to the spectral interval of bundle energy. Using the Monte Carlo method the K_m is obtained from the cumulative distribution function. For so much, the Eq. (9) is rewritten as

$$K_m = K_m(R) = K_m(F) \tag{15}$$

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, in this case.

According Siegel and Howell (2002), the length traveled, l, before absorption of a bundle in a medium of constant absorption coefficient, $K = M_s K_m$, is

$$l = -\ln(R_l)/(M_s K_m) \tag{16}$$

where R_l , is a random number.

The Monte Carlo equations above presented were obtained to local conditions of medium and wall elements whose temperature and properties are uniform, however, these equations can be used to non-isothermal non-homogeneous media. The numerical procedure to compute radiation heat transfer in a medium of non constant absorption coefficient consist basically in to discrete the path length in small segments of uniform properties. For each segment of different properties must be found the respective absorption cross section, K_m , and subsequent absorption coefficient of the medium, K, relative to the spectral interval of the emitted energy. The K_m of the medium in each traveling path segment can be related with spectral interval of emitted energy applying a K-correlated hypothesis, as demonstrated by Denison and Webb (1995a).

Although there are no K_m involved in the gray walls emission, for each bundle emitted from a wall it is necessary to generate a random number for F to relate the spectral interval of the bundle energy with the medium properties and so proceed as well as to compute the medium absorption of the bundles emitted for volume elements.

Finally, the radiation heat exchange in the domain of a given approached problem can be evaluated accounting all the bundles (and its respective carried energy) emitted and absorbed by the medium and the walls.

3. Results and discusion

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 chemical reactions of combustion, 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 to such problems. However a few approximations are necessary to apply this method. It is postulated that the total emittance and absorptance of the gas can be represented by a weighted average of gray gases emittances and absorptances, where the absorption coefficients are constant and the weights are solely dependent on the temperature. In addition, the gas is assumed homogeneous. The data presented in Smith et al. (1982) for the gray gases absorption coefficients and the polynomials weighting functions has been widely employed, but they are valid for only two different gas mixtures having water vapor and carbon dioxide as the emitting absorbing chemical species. Those gas mixtures correspond to the products of the stoichiometric combustion of methane and fuel oil, and they differ only in the water vapor fractions: 20% against 10% for the combustions of the methane and of fuel oil, respectively. In both cases, the concentration of the carbon dioxide is 10 %. The remaining species in the mixtures can be either nitrogen or air, which are non-participating species.

In contrast to the homogeneous stoichiometric products of methane and oil combustion, the gaseous products that are present in combustion systems are often non-homogenous and the compositions can differ from those related to stoichiometric chemical reaction. In actual combustion process, it is common practice to use more air than the stoichiometric amount to enhance the possibility of complete combustion or to control the temperature of the combustion chamber. For complete combustion of the hydrocarbon fuels, the gaseous products contain only water vapor, carbon dioxide, which are absorbing species, and inert (non-participating) gases such as nitrogen and oxygen, this last one occurring in the case of combustion with excess of air.

Aiming at investigating the departure of the WSGG model when using the data limited to stoichiometric combustion reactions, as the one presented in Smith et al. (1982), the Monte Carlo combined to the ALB distribution function is used to solve for thermal radiation in gases with different concentrations. As a simple example case, it is considered the radiation heat transfer in a gas mixture contained between two infinite parallel black walls. Gas mixtures originated from the combustion of two different fuels, octane and methane, are considered. The geometry of all the solved cases consists of two parallel black walls that are 1.0 m departed from each other. The system is shown in Fig. 1. The numerical solutions involved the division of the domain into 30 (thirty) equal-sized elements in the *x*-direction.



Figure 1. Gas layer between infinite parallel walls.

3.1. Octane fuel

Most familiar fuels consist primarily of hydrogen and carbon. They are called hydrocarbon fuels. For a complete stoichiometric combustion of hydrocarbon fuels, the gaseous product is composed of water vapor, carbon dioxide and nitrogen, and their concentrations are fixed by the chemical reaction balance. The concentrations however are dependent on the many different types hydrocarbon fuels. The available data for the conventional WSGG model is limited to a few hydrocarbon fuels. In the widely cited work of Smith et al., 1982, data is only presented for gas mixtures having 10% H₂O and 10% CO₂ (fuel oil combustion) and 20% H₂O and 10% CO₂ (methane oil combustion), so using this model for different concentrations will probably lead to significant errors.

The octane is the main hydrocarbon found in the gasoline. The stoichiometric combustion of octane leads to a gas mixture that is composed of 14% H₂O and 12.5% CO₂, the remaining species being non-participating. To evaluate the effect of the absorbing species concentration, it is also considered a gas mixture having 10% H₂O and 10% CO₂, the closest concentration that is found in Smith et al., 1982. For the two gas mixtures, the radiative heat transfer in the above referred geometry was computed using the methodology presented in Section 2. The gas temperature was taken as the adiabatic of flame, obtained according the procedure outlined in Çengel and Boles (2002), which is 2304 K. The walls, assumed black, are at the a temperature of 300 K. Figure 2 presents the volumetric radiative heat rate, in kW/m³, in the gas for the two mixtures.



Figure 2. Volumetric radiative heat rate and heat flux on the walls for two different gaseous mixtures. In both cases, the gas temperature is 2304 K, and the remaining species in the mixture is non-participating.

As can be observed in Fig. 2, there is a significant difference between the volumetric radiative heat rate results, which was even greater near the walls. The radiative heat fluxes on the walls are shown on the top of the figure. As indicated in the figure, the heat flux on the wall for the for the gaseous mixture composed of 10% H₂O and 10% CO₂ is 16.6% lower than for the mixture composed of 14% H₂O and 12.5% CO₂, that is 170.5 kW/m² against 204.5 5 kW/m². This result is in agreement with the volumetric radiative heat rate being larger for the later mixture, a straightforward consequence of the energy conservation. Accordingly, the integral of the volumetric radiative heat rate is about 16.6% greater for the second gas mixture than for the first one. According to the adopted convention, negative volumetric radiative heat rate indicates that the zone emits more than absorbs. As seen in the figure, the amount of energy lost by the gas increases with the proximity of the wall. The oscillations that appear in the Fig. 2 are expected from the statistical nature of the Monte Carlo method and can become less important if the number of bundles be increased. A total of eight million (8×10⁶) energy bundles were released from each wall and gas zones for the gaseous mixture composed of 10% H₂O and 12.5% CO₂, a total of five million (5×10⁶) energy bundles were released from the wall and gas zones.

3.2. Methane fuel

Different from the octane, there are correlations in Smith at al., 1982, for the weighting factors related to a gaseous mixture resulting from the stoichiometric combustion of methane (20% H₂O and 10% CO₂). However in real combustion systems, the combustion processes usually do not occur following the stoichiometric balance, but with excess of air, leading to different products concentrations. To evaluate its effect on the radiative heat transfer, two combustion reactions differing in the excess of air were considered.

The combustion reaction with 50% of excess of air generates a medium whose emitting absorbing species are 13.1% H₂O and 6.55% CO₂. The radiative heat transfer was computed for this medium at the adiabatic flame temperature, which is 1780 K. The walls, assumed black, are again kept at a temperature of 300 K. The volumetric radiation heat rate and the wall radiative heat fluxes are shown in Fig. 3. For comparison, this figure also shows the results for a gas mixture at the same temperature generated in the stoichiometric combustion of the methane, composed of 20% H₂O and 10% CO₂. For an excess of air of 100%, the gas resulting from the combustion process is composed of

10% H_2O and 5% CO_2 . Figure 4 shows the volumetric radiative heat rate for this gas mixture at the adiabatic flame temperature of 1476 K. The figure shows also the result when the concentrations of H_2O and CO_2 are taken at the stoichiometric values of 20% and 10%, respectively.



Figure 3. Volumetric radiative heat rate and heat flux on the walls for gas mixtures having concentrations of 20% H₂O and 10% CO₂ and of 13.1% H₂O and 6.55% CO₂. Gas mixtures temperatures of 1780 K.



Figure 4. Volumetric radiative heat rate and heat flux on the walls for gas mixtures having concentrations of 10% H₂O and 10% CO₂ and of 10% H₂O and 5% CO₂. Gas mixtures temperatures of 1476 K.

For both cases in Figs. 3 and 4, a total of three million (3×10^6) energy bundles were released from each wall and gas zones. To reduce the statistical oscillations, it was taken an arithmetic average between the values obtained for both sides of symmetry line of the problems.

In real combustion systems, the medium is non-isothermal. To illustrate this situation, the Monte Carlo combined to the ALB distribution function was applied to solve the radiative heat transfer in two non-isothermal gaseous mixtures, differing in the fractions of the emitting absorbing species. For both gases, the temperature varies, according to the below relation, from 1476 K on the walls to 2327 K in the center position between the plates:

(17)

$$T(x) = -3404 x^2 + 3404 x + 1476$$

These minimum and maximum temperatures are the adiabatic flame temperature in the stoichiometric methane combustion with 100% of excess of air. One of the gas mixtures has the concentration of the methane stoichiometric combustion (20% H₂O and 10% CO₂), while the other has the concentration of a gas mixture resulting from the combustion process with 100% of excess of air: 10% H₂O and 5% CO₂.

Figure 5 presents the volumetric radiative heat rate for the two gaseous mixtures. As seen, the discrepancy in the two cases was the greatest in the middle of the enclosure (x = 0.5 m), where temperatures are higher, and near the walls (x = 0 m). The heat fluxes on the walls are presented on the top of the figure, showing a considerable difference between the results. The stoichiometric gaseous mixture loses 52% more energy (70.3 kW/m²) to the walls than the gas mixture composed of 10% H₂O and 5% CO₂ (46.2 kW/m²). For this case, the Monte Carlo solution was obtained for a total of four million (4×10⁶) bundles being released from each gas and wall zone.



Figure 5. Volumetric radiative heat rate and heat flux on the walls for gas mixture having concentrations of 20% H₂O and 10% CO₂ and of 10% H₂O and 5% CO₂. The gas mixtures temperatures are given by Eq. (17).

4. Conclusions

This work presented the application of the Monte Carlo method to the absorption line blackbody (ALB) distribution function to solve the radiation heat transfer in gas mixtures composed of different concentrations of carbon dioxide and water vapor. The absorption line blackbody (ALB) distribution function is a gas model that allows a detailed evaluation of the dependence of the absorption coefficients of the absorbing species on the wavelength. In addition, it enables the consideration of different concentrations of the absorbing species, an important advance with respect to the WSGG model, which relies on limited data for a few specific concentrations. As shown in the work, the Monte Carlo can be implemented so that its cumulative distribution function becomes equal to the ALB distribution function, which leads to a direct coupling between the methods.

The methodology was applied to a few example cases aiming at demonstrating the effect of the concentrations of water vapor and carbon dioxide on the radiation heat transfer. The system was an one-dimensional gas layer contained between two infinite parallel black walls. The medium composition was chosen to relate to the gas mixtures that can be formed in the combustion of octane and methane. 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, indicating the need of more advanced gas models than the conventional WSGG model.

5. Acknowledgement

The authors thank the financial support from CAPES-Brazil through a doctorate scholarship grant to the first author.

5. References

- Adams BR, Smith PJ., 1994, "Modeling effects of soot and turbulence-radiation coupling on radiative transfer in an industrial furnace", ASME Radiative Heat Transfer: Current Research, HTD-Vol. 276, pp. 177-190.
- Cengel Y. A., Boles M. A., 2002, "Thermodyamics: An Engineering Approach", Fourth Edition, McGraw-Hill, New York.
- Cherkaoui M., Dufresne J. L, Fournier R, Grandpeix JY, Lahellec, 1996, "A. Monte Carlo simulation of radiation is gases with a narrow-band model and a net-exchange formulation", Journal of Heat Transfer, Vol. 118,pp. 401-407.
- Denison M. K., Webb B. W., 1993, "A spectral line-based weighted sum-of-gray-gases model for arbitrary RTE solvers", Journal of Heat Transfer, 1993, Vol. 115, pp. 1004-1011.
- Denison M. K., Webb B. W., 1993, "An absorption-line blackbody distribution function for efficient calculation of total gas radiative transfer", Journal of Quantitative Spectroscopy and Radiative Transfer, Vol. 50, pp. 499-510.
- Denison M. K., Webb B. W., 1995, "Development and application of an absorption-line blackbody distribution function for CO₂", International Journal of Heat and Mass Transfer, Vol. 38, pp. 1813-1821.
- Denison M. K., Webb B. W., 1995, "The spectral line-based weighted sum-of-gray-gases model in nonisothermal nonhomogeneous media", Journal of Heat Transfer, Vol. 117, pp. 359-365.
- Denison M. K., Webb B. W., 1995, "The spectral line-based weighted sum-of-gray-gases model for H₂O/CO₂ mixtures", Journal of Heat Transfer, Vol. 117, pp. 788-792.
- Goody R, West R, Chen L, Crisp D., 1989, "The correlated-K method for radiation calculations in nonhomogeneous atmospheres", Journal of Quantitative Spectroscopy and Radiative Transfer, Vol. 42, pp. 539-550.
- Goody R. M., Yung Y. L., 1989, "Atmospheric Radiation", New York: Oxford University Press.
- Hottel H. C., Sarofim A. F., 1976, "Radiative Transfer", New York: McGraw-Hill Book Company.
- Howell, J. R. The Monte Carlo in Radiative Heat Transfer. Journal of Heat Transfer, 1998; 120: 547-560.
- Magel HC, Schnell U, Hein KR., 1996, "Simulation of detailed chemistry in a turbulent combustor flow", Twenty-Sixth Symposium (International) on Combustion/The Combustion Institute, pp. 67-74.
- Maurente A., Vielmo H. A., França F. H. R., 2006, "A Monte Carlo Implementation to Solve Radiation Heat Transfer in Non-uniform Media with Spectrally Dependent Properties", Submitted for JQSHT.
- Modest M. F., 1991, "The weighted-Sum-of-Gray-Gases Model for Arbitrary Solution Methods in Radiative Transfer", Journal of Heat Transfer, Vol. 113, pp. 650-656.
- Modest M. F., 1992, "The Monte Carlo method applied to gases with spectral line structure", Numerical Heat Transfer, Part B, Vol. 22, pp. 273-284.
- Modest M. F., Zhang H., 2002, "The full-spectrum correlated-K distribution for thermal radiation for molecular gasparticulate mixtures", Journal of Heat Transfer, Vol. 124, pp. 30-38.
- Modest M. F., Singh V., 2004, "Engineering correlations for full spectrum K-distribution of H₂O from the HITEMP spectroscopic databank". In Radiation Transfer: Gas Mixtures. Fourth International Symposium on Radiative Transfer, Istanbul Turkey, 2004.
- Siegel R., Howell, J. R., 2002, "Thermal Radiation Heat Transfer", New York: Taylor & Francis.
- Sijerčić M, Stevanović Z, Belošević S., "Modeling of non-confined turbulent flow of two coaxial streams under combustion conditions", Mechanical Engineering, 1, pp. 981-988.
- Smith T. F., Shen Z., F., Friedman, J. N., 1982, "Evaluation of coefficients for the weighted sum of gray gases model", Journal of Heat Transfer, Vol. 104, pp. 602-608.
- Xue H, Ho JC, Cheng YM, 2001 "Comparison of different combustion models in enclosure fire simulation", Fire Safety Journal, 36, pp. 37-54.
- Wang A., Modest M. F., 2004, "High-accuracy compact database of narrow-band K-distributions for water vapor and carbon dioxide", In: Radiation Transfer: Gas Mixtures. Fourth International Symposium on Radiative Transfer, Istanbul Turkey, 2004.

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