MODELING OF RADIATIVE HEAT TRANSFER IN PARTICIPATING GASES WITH THE CUMULATIVE WAVENUMBER MODEL

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Abstract. *This work presents in detail the application of the cumulative wavenumber (CW) model using the discrete ordinate method to solve the radiative heat exchange in isothermal, homogeneous participating gases taking into account the strong dependence of the properties with the wavenumber. A spectral integration of the radiative transfer equation is performed with the CW model, which is capable of considering the highly complex spectral nature of real participating gases. The radiative properties were obtained from HITRAN database. The methodology is applied to a one-dimensional geometry with black walls with a mixture of water vapor and carbon dioxide in between. The results were compared with the line-by-line integration and MC-ALBDF model.*

Keywords*: Radiative transfer, participating gas, cumulative wavenumber, discrete ordinates*

1. INTRODUCTION

Radiative heat transfer in gases has important applications in combustion systems, such as furnaces and engine chambers operating at high temperature. Thermal radiation in participating media is often the dominant heat transfer mode in such systems due to the presence of gaseous products at high temperatures. On the other hand, the modeling is made even more difficult due to the highly irregular dependence of the radiative properties with the wavelength. In most engineering applications, gases emit and absorb radiation only in frequencies where the corresponding photon energies match the transitions between fixed energy states in the gas molecules. This results in hundreds of thousands narrow lines in the absorption spectra of gases. With such complexity, the solution of the radiative heat transfer equation requires special methods to tackle the spectral integration of the intensity field.

The weighted-sum-of-gray-gases (WSGG), first proposed by Hottel and Sarofim (1967), models the entire spectrum by a few bands having uniform absorption coefficients, each band corresponding to a gray gas. The weighting coefficients that account the contribution of each gray gas correspond to the fraction of the blackbody energy in the spectrum region where the gray gas is located. In general, those coefficients are obtained from fitting of experimental data, such as those presented in Smith *et al*. (1982), for a mixture of water vapor and carbon dioxide in nitrogen. Such data are limited, however, to a few mixtures that in addition are required to be homogeneous.

There are nowadays databases compiling characteristics related to the emission and absorption behavior of molecules, as the HITRAN and HITEMP, which have been used to obtain spectral properties of gases in much greater detail than a few decades ago. With such information, thermal radiation heat transfer can be accurately solved by line-by-line (LBL) integration, which considers the emission and absorption of each individual spectral line. LBL integrations are on the other hand difficult to implement and computationally expensive, and so they are only used in special cases, for instance, to obtain benchmark solutions. To avoid the difficulties related to LBL integration, various gas models have been proposed (SLW, ADF, ADFFG). Spectral integration of the Radiative Transfer Equation (RTE) in the Spectral-Line Weighted-Sum-of-gray-gases (SLW) method leads to the appearance of Leibnitz terms in the equation for the gray gases which complicates the integration. This scenario was treated by the assumption of ideal behavior of molecular spectra in temperature, or by a simple neglect of the Leibnitz terms (Denison and Webb, 1995). The full-spectrum correlated-*k* distribution (Modest, 2002) was introduced to extend the WSGG method to non-uniform media. An extensive overview of these models can be found in Siegel and Howell (2002).

Maurente et al. (2007) proposed the application of the Monte Carlo method applied to the absorption-line blackbody distribution function (MC-ALBDF) using participating media constituted by water vapor and carbon dioxide. The stoichimetric ratios considered the combustion of methane and octhane. Comparisons with the WSGG model was presented in Maurente et al. (2006a, 2008).

Cumulative wavenumber model was proposed by Solovjov and Webb (2002) for the solution of the RTE in non-uniform gas media at high temperature. This approach allows accommodation of non-isothermal and non-homogeneous gases, with non-gray boundaries. Solovjov and Webb (2005) applied the CW model for modeling radiative transfer in gas mixtures with soot, and compared the results with LBL approach. Solovjov and Webb (2008) modeled gaseous medium using the multilayer approach by SLW and CW methods, the predictions showed high accuracy, even with few layers. Salinas (2008) developed a fast approximate technique for the CW model. This approach significantly reduced the computational time in comparison with the standard method of solution using the CW model.

The main purpose of the present work is presenting in detail how the CW model can be implemented for an isothermal homogeneous gas mixture filling the space between two parallel infinite plates (one-dimensional geometry). The participating gas mixture is composed of water vapor and carbon dioxide and the concentrations are evaluated

according to the stoichiometric combustion of methane and octane. The results also include an analysis of the effect of varying the concentration of water vapor, mixed with air, on the radiative heat transfer. Comparisons of the CW model with the LBL integration and MC-ALBDF model are also made.

2. SOLUTION METHODOLOGY

2.1. The Cumulative Wavenumber Model

The absorption cross-section, C_η (cm^2/molecule), is described by the Lorentz profile due to molecular collision or pressure broadening. Including the overlap contribution of neighboring lines, it can be written as:

$$C_\eta = \sum_i \frac{S_i}{\pi} \frac{\gamma_i}{(\eta - \eta_i)^2 + \gamma_i^2} \tag{1}$$

where S_i is the integrated line intensity (cm^{-1}/molecule·cm^{-2}), γ_i is the half-width (cm^{-1}/atm) and η_i is the location (cm^{-1}). The value γ_i is calculated by the following relation (Ribeiro, 2007):

$$\gamma_i = \gamma_{self,i} \times \left(\frac{296}{T} \right)^{n_i} \tag{2}$$

where T is the temperature (K), γ_{self} and γ_{air} are the half-widths (cm^{-1}/atm) and n is the coefficient of temperature dependence. The values of η_i, S_i, γ_{self}, γ_{air} and n can be taken form the HITRAN 2004 molecular spectroscopic database.

For any fixed value of absorption cross-section C and the wavenumber η, the cumulative wavenumber function, which is based on the molecular absorption spectra of gases given by Eq.(1), is defined by the following relation:

$$w(C,\eta) = \begin{cases} \sum_{i=1}^{L} (\beta_i - \alpha_i) + (\eta - \eta^*) & \text{if } C_\eta < C \\ \sum_{i=1}^{L} (\beta_i - \alpha_i) & \text{if } C_\eta \geq C \end{cases} \tag{3}$$

where the wavenumbers α_i and β_i are obtained from the intersection of the absorption cross-sections, C_η, with the line $C_\eta = C$, and η^* is the largest wavenumber of the intersection for the case when the absorption cross-section C_η is less than the value C (Solovjov and Webb, 2002), as depicted in Fig.1.

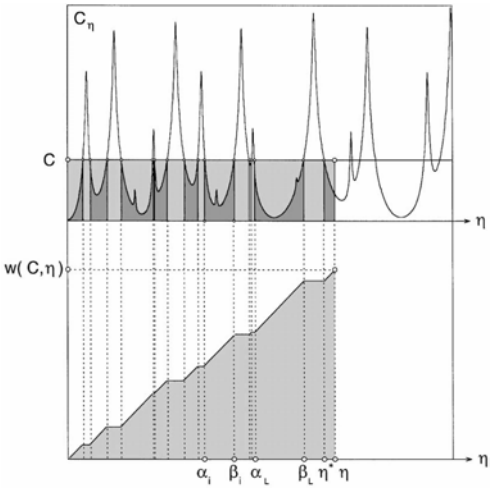

Figure 1 – Cumulative wavenumber function (Solovjov and Webb, 2002).

More formally, the cumulative wavenumber can be defined by the equation below:

$$w(C,\eta) = \int_0^\eta H(C - C_\eta) d\eta \tag{4}$$

For gases mixture with m species, in the assumption of non-overlapping spectral lines for the absorption cross-section, $C_\eta = Y_1C_1 + Y_2C_2 + ... + Y_mC_m$, the cumulative wavenumber for the mixture may be expressed as

$$w_{C_\eta}(C,\eta) = w_1\left(\frac{C}{Y_1},\eta\right) + w_2\left(\frac{C}{Y_2},\eta\right) + \ldots + w_m\left(\frac{C}{Y_m},\eta\right) - (m-1)\eta \tag{5}$$

where $H(C-C_\eta)$ is the Heaviside step-function. Differentiation of Eq. (4) with respect to η yields:

$$\frac{\partial w(C,\eta)}{\partial \eta} = H(C-C_\eta) = \begin{cases} 1 \text{ for } C > C_\eta \\ 0 \text{ for } C \le C_\eta \end{cases} \tag{6}$$

Thus,

$$\int_{\{\eta:C>C_\eta\}} d\eta = \int_{\eta=0}^{\infty} H(C-C_\eta)\,d\eta = \int_{\eta=0}^{\infty} \frac{\partial w(C,\eta)}{\partial \eta}\,d\eta = \int_{\eta=0}^{\infty} dw(C,\eta) \tag{7}$$

Next, the full spectral C_η can be subdivided in gray gases C_j and in wavenumber subintervals so that:

$$H_j = \{\eta \ : \ C_{j-1} \le C_\eta \le C_j,\ j = 1,2,\ldots,n\} \tag{8}$$

$$\Delta_i = [\eta_{i-1},\eta_i],\ i = 1,2,\ldots,p \tag{9}$$

At this point, it can be defined the set D_{ij}, named fractional gray gas, which are formed by the intersection of the sets Δ_i and H_j:

$$D_{ij} = \Delta_i \cap H_j \tag{10}$$

The consideration of local-spectrum correlation establishes that:

$$w(C_j,s,\eta) - w(C_{j-1},s,\eta) = u_{ij}(s)\,v_{ij}(\eta) \text{ for } \eta \in \Delta_i \tag{11}$$

Setting $u_{ij}(s^*) = 1$, in which s^* is chosen as a reference point from where the values of temperature and species concentrations are taken, the function $u_{ij}(s)$ can be calculated by:

$$u_{ij}(s) = \frac{w(C_j,s,\eta) - w(C_{j-1},s,\eta)}{w(C_j,s^*,\eta) - w(C_{j-1},s^*,\eta)} \tag{12}$$

Integrating the spectral intensity of radiation I_η over the fractional gray gases D_{ij}, using the concept of cumulative wavenumber, yields:

$$\int_{D_{ij}} I_\eta\,d\eta = u_{ij}(s)\int_{\Delta i} I_\eta\,d\left[v_{ij}(\eta)\right] = u_{ij}(s)\,J_{ij}(s) \tag{13}$$

where J_{ij} is viewed as a fractional gray gas intensity, and u_{ij} as a local correction factor. The total intensity of radiation can be found by:

$$I(s) = \int_{\eta=0}^{\infty} I_\eta(s)\,d\eta = \sum_{i,j} u_{ij}(s)\,J_{ij}(s) \tag{14}$$

The variation of the spectral intensity along a path length in the medium is given by the radiative transfer equation:

$$\frac{\partial I_\eta}{\partial s} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta} \tag{15}$$

Applying the cumulative wavenumber approach, the integration of Eq. (15) over D_{ij} :

$$\frac{\partial J_{ij}}{\partial s} = -\kappa_j J_{ij} + \kappa_j J_{bij} \tag{16}$$

where κ_j is the gray gas absorption coefficient, determined by a function of absorption cross-section, C_j , and the molar density N (molecule/cm^3), by the following relation:

$$\kappa_j = YN\sqrt{C_j C_{j-1}} \text{ or for a mixture } \kappa_j = (Y_1 + Y_2 + ... + Y_n)N\sqrt{C_j C_{j-1}} \tag{17}$$

where Y is the species concentration. The term J_{bij} is the fractional blackbody radiative energy source, defined by:

$$J_{bij}(s) = \int_{\Delta i} I_{b\eta}\left[T(s), \eta\right] d\left[v_{ij}(\eta)\right] \tag{18}$$

Finally, the summation of the $J_{bij}(s)$ gives the total emission:

$$\sum_{i,j} J_{bij} = \sigma T^4 / \pi \tag{19}$$

2.2. Procedure

Applying the CW model to a homogeneous medium using the equations above requires a few steps, as follow:

Step 1: Obtain the data from HITRAN database using the JavaHAWKS software. The software is designed for easy manipulation of the HITRAN (High Resolution Transmission) molecular spectroscopic database and associated molecular databases by proper utilization of the JavaHAWKS software package. The range of temperatures is from 70 K to 3000 K. The parameters in a HITRAN transition that depend on temperature, namely the intensity of the line, S_i, the air half-widths, γ_{air}, and the dependence temperature coefficient, n, which are presented in Eqs.(1) and (2) are given at the desired temperature, while the self half-widths, γ_{self}, are given at a standard reference of 296K. HITRAN has been distributed via an ftp-site at the Harvard-Smithsonian Center for Astrophysics. Information for accessing the ftp-site is provided by completing the request form located in the HITRAN web-site.

Step 2: The next step after acquiring the data is to correct the self half-widths, e.g. water half-widths γ_{water}. This can be made using the Eq.(2).

Step 3: Once all the data has been obtained, the spectrum can be constructed by the application of the Lorentz profile, Eq.(1). This equation evaluate the effects of the collision broadening, which is the most important for most engineering conditions involving infrared radiation (Siegel and Howell, 2002).

Step 4: Calculate the $w(C,\eta)$ functions for each fractional gray gas using the complete equations as presented previously.

Note that, if a single gas is used the $w(C,\eta)$ function is evaluated from Eq.(4). However, if a gas mixture is applied the $w(C,\eta)$ function is obtained from Eq.(5).

3. SOLUTION FOR A ONE-DIMENSIONAL SLAB

For a one dimensional slab, Eq. (16) can be written as:

$$\frac{\partial J_{ij}}{\partial x} = -\kappa_j J_{ij} + \kappa_j J_{bij} \tag{20}$$

This equation can be solved by the discrete ordinate method, by the following relations:

$$\mu_l \frac{\partial J^+_{ij}}{\partial x} = -\kappa_j J^+_{ij} + \kappa_j J_{bij} \tag{21}$$

$$-\mu_l \frac{\partial J_{ij}^-}{\partial x} = -\kappa_j J_{ij}^- + \kappa_j J_{bij} \tag{22}$$

In this method, the angular variable μ is discretized into a finite number of ordinates μ_l, taken at the zeros of the Gaussian quadrature formula of the numerical integration.

The boundary conditions for this case, with black walls, have the form:

$$J_{ij}^+(0,\mu_l) = J_{bij}(0) \tag{23}$$

$$J_{ij}^-(L,\mu_l) = J_{bij}(L) \tag{24}$$

Using the calculated fractional gray gas intensities, the net radiative flux, $q''(x)$, and the radiative dissipation source, $Q(x)$, can be calculated by:

$$q''(x) = \sum_{i,j} q''_{ij}(x), \text{ where } q''_{ij}(x) = 2\pi \sum_l \mu_l w_l \left[J_{ij}^+(x,l) - J_{ij}^-(x,l) \right] \tag{25}$$

$$Q(x) = \sum_{i,j} Q_{ij}(x), \text{ where } Q_{ij}(x) = 2\pi\kappa_j(x) \sum_l \left[w_l \left(J_{ij}^+(x,l) + J_{ij}^-(x,l) \right) \right] - 4\pi\kappa_j(x) J_{bij}(x) \tag{26}$$

4. RESULTS

To test the code developed from the method described above, some different problems in one dimensional heat transfer are analyzed. For all cases, the medium occupies the space between two infinite, parallel black walls. In the first problem, both walls are held at 0 K. The medium is filled with water vapor at 1000 K and the wall spacing is 1.0 m. Figure 2 shows the divergence of the radiative flux predicted by CW model and compared with the solution of the line-by-line integration obtained by Denison and Webb (1993a). The predictions show a very satisfactory agreement with the *benchmark* solution. The same trends are noted in the values of net wall flux (-28.7 against -29.0 kW/m^2), with a relative deviation of about 1.0%.

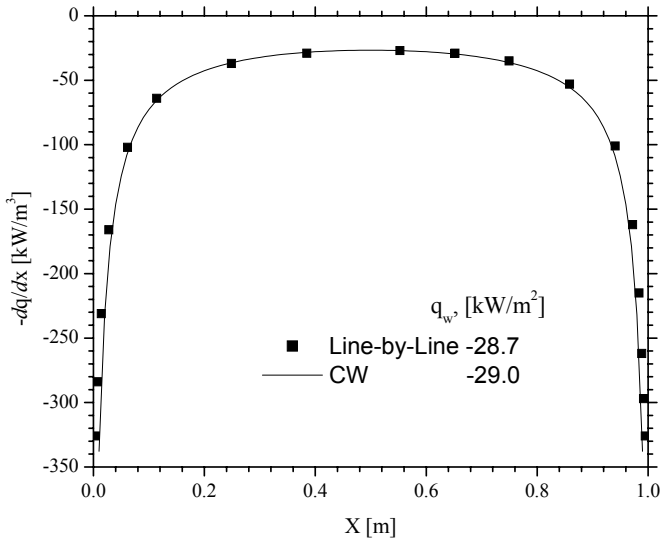

Figure 2 - Radiative source and net wall flux for water vapor medium at 1000 K.

Another comparison between the results from the CW model and the line-by-line solution is shown in Fig.3. In this case the walls are spaced by 2.0 m and held at 0 K. The medium is composed of 20% of water vapor and 80% of air at 1500 K. As seen in the figure, the divergence of the flux obtained by the CW approach agrees very well with the one showed by Denison and Webb (1993b). The relative deviation in the computation of the heat flux on the walls was about 1.5%.

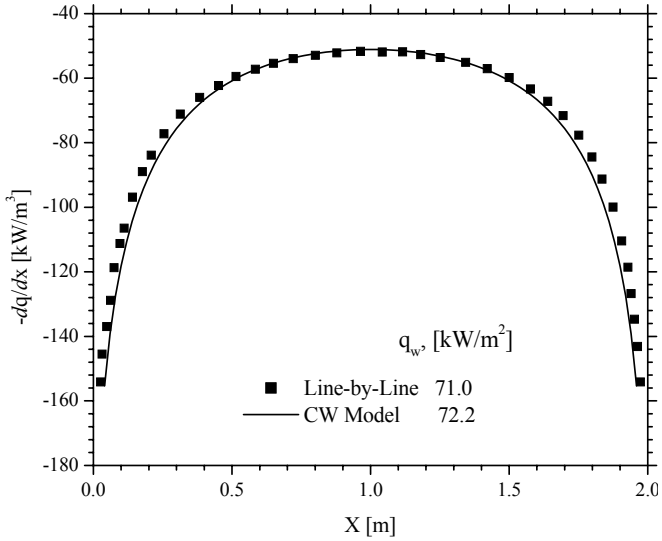

Figure 3 - Radiative source and net wall flux for a gas medium with 20 % water vapor at 1500 K.

The most used fuels are composed mainly by hydrogen and carbon, the so called hydrocarbon fuels. The complete combustion process of hydrocarbon fuels yields gas constituted by water vapor and carbon dioxide. Its concentration depends on the type of fuel and the ratio air/fuel in the chemical combustion reaction. For the three following cases, the methane stoichiometric combustion products are considered as the gas mixture. The results for the radiative exchanges are compared with those obtained from the methane combustion in reactions that occur with air excess. Stoichimetric air excess ratios of 50 and 100% are considered. A comparison to the MC-ALBDF model obtained by Maurente *et al.* (2006b) is made.

Three cases are compared. *Case* 1: in a reaction with 50% of air excess, the water vapor and carbon dioxide ratios are 13.1 and 6.55%, respectively. *Case 2*: assuming a reaction with 100% of air excess, the medium is constituted by 10% of water vapor and 5% of carbon dioxide. *Case 3*: the octhane combustion, for which is considered the stoichiometric ratios, the gas generated is constituted by 14% of H_2O and 12.5% of CO_2 besides the non-participating species. The adiabatic flame temperatures are 1780 K for the first case, 1476 K for the second one and 2304 K for the last one. The walls are assumed as black and kept at 300 K with a gap of L = 1.0 m. Figure 4 shows the results for the radiative flux divergence and the heat flux on the walls.

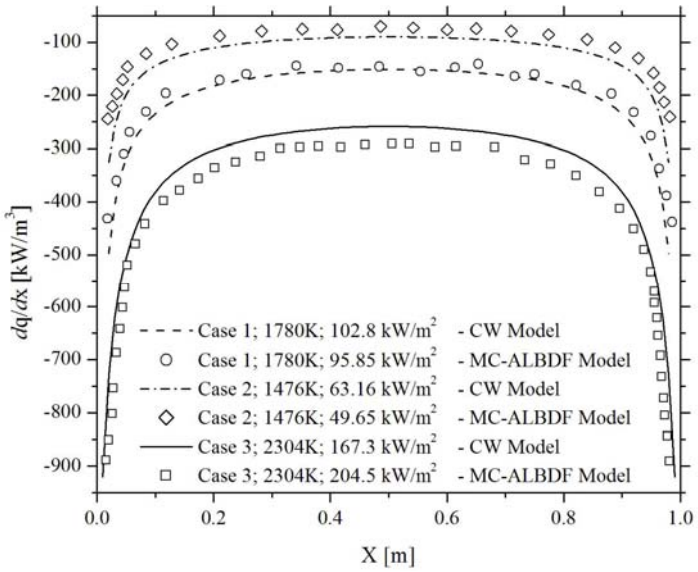

Figure 4 – Comparison to the results obtained from CW model
in the present work and MC-ALDF model (Maurente, 2006b).

The results show an acceptable agreement between the CW and MC-ALBDF models. Although the curves have the same trend and are failry close, the heat flux on the walls presents significant deviation for all the cases, which are 7.3%, 27.2% and 18.2% for cases 1, 2 and 3, respectively. Since the CW is the model that presents the best agreement

with the LBL solution when compared with the ALB and SLW according to Solovjov and Webb (2002), the difference between the models can be explained by errors in the correlations for the absorption-line blackbody distribution functions that were used in the MC-ALBDF model.

Figure 5 shows the medium concentration effect for the case when the walls are spaced by 1.0 m and held at 500 K. The medium is filled with water vapor and air at 1000 K with the H_2O concentration varying in a stepwise way from 10% up to 100%. As seen, in the region close to the halfway between the two walls, *i.e.*, around x = 0.5 m, the effect of the gas concentration is negligible, because the medium is isothermal, then the effects of the walls do not contribute much for the divergence of the flux. The closer is the medium of the walls, the more important is the effect of the walls and, therefore, the higher is the radiative heat source. Increasing the water vapor concentration from 10% to 100%, the heat flux on the wall more than duplicated, increasing from -12.7 to -26.6 kW/m^2.

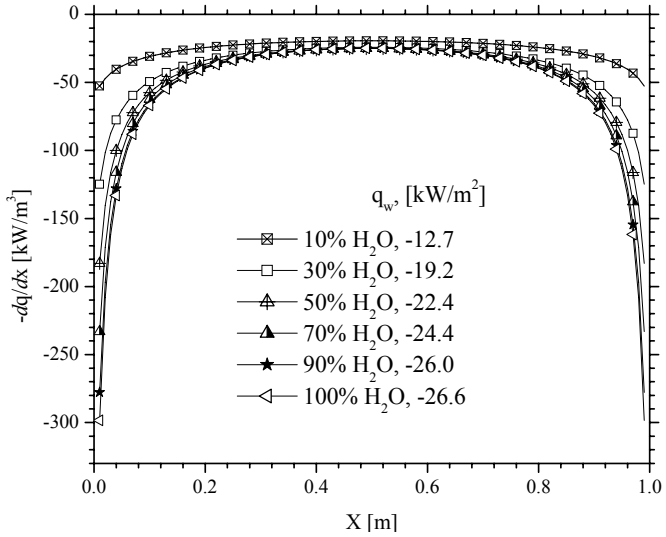

Figure 5 – Comparison of the results obtained from CW model for different concentrations of the gas.

5. CONCLUSIONS

In this work, the cumulative wavenumber model, developed by Solovjov and Webb (2002), was applied to the radiative transfer equation to solve the radiative exchanges in isothermal, homogeneous participating media. The method was applied to one-dimension slabs for the prediction of the radiative volumetric heat source in the medium and of the heat fluxes on the walls. The results obtained for a single gas were compared with the line-by-line integration, and the ones obtained for gas mixtures were compared with the MC-ALBDF method. The predictions obtained from the CW model were very close to the ones obtained by the line-by-line integration. For the gas mixtures, the results for the walls heat fluxes were considerably different from those obtained from the MC-ALBDF model.

It was also discussed the influence of the gas concentration on the radiative heat source and on the wall heat flux. As verified, the effect of the gas concentration was higher in the regions closer to the walls. As suggested next steps, the CW model can be applied to non-isothermal, non-homogeneous medium for further comparisons with the line-by-line integration and other gas models that are capable of dealing with non-uniformity in participating media.

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