A MODIFICATION OF THE CUMULATIVE WAVENUMBER METHOD APPLIED TO THE RADIATVE HEAT TRANSFER IN A CO_2 NON-UNIFORM MEDIA

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Abstract. *This work presents a modification of the cumulative wavenumber (CW) method to determine the radiative transfer in non-uniform participating gases to enforce the radiative energy balance to be satisfied. The modified method is applied together with the discrete ordinates method to solve the radiation heat transfer in a one-dimensional slab containing a non-isothermal, non-homogeneous layer of carbon dioxide. The walls are black and the distance from each other is 1 meter. The HITEMP database is used to extract the spectral lines information that is required by the method. The results of both the CW and the modified CW (MCW) methods are compared to the benchmark line-by-line (LBL) integration. The results show that the MCW leads to an accurate estimation of both the radiative heat flux and volumetric heat source, satisfying the radiative energy balance within the error of the numerical discretization of the radiative transfer equation.*

Keywords*: participating gas models, cumulative wavenumber, radiative heat transfer, absorption lines.*

1. INTRODUCTION

There is an increasing need for a better understanding and modeling of combustion process, which involves a number of coupled phenomena, such as chemical kinetics, fluid flow and heat transfer. In media compound by participating gases the thermal radiation is often the dominant heat transfer mechanism, especially in combustion where the formation of gaseous products at high temperatures commonly occurs. Modeling the spectral dependence of the radiative properties of participating gases plays a key role in the accurate prediction of radiation heat transfer in several problems in science and engineering. However, modeling participating gases imposes considerable difficulties due to the highly irregular dependence of their radiative properties of participating gases with the wavelength. The thermal radiation spectrum can present hundreds of thousands of absorption-emission lines, which are dependent on the thermodynamic state and composition of the medium. Integrating the radiative transfer equation (RTE) over the entire spectral lines is still excessively time demanding for most practical applications, so gas models are challenged to provide accurate answers in an acceptable time. An overview of some main models can be found in Siegel and Howell (2002).

The simplest model is the gray medium, which considers the absorption coefficient to be wavelength independent. Although the modeling presents a strong departure from the actual behavior of a real gas, the model can still be found in recent solutions of combustion problems, as presented in Al-Omari (2006) and, Narayanan and Trouvé (2009). 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 fractions of the blackbody energy in the spectrum region where the gray gases are located. In general, those coefficients are obtained from fitting experimental data, such as those presented in Smith *et alli* (1982) and Galarça *et alli* (2008), 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 and can lead to considerable deviations from more refined gas model solutions as presented by Maurente *et alli* (2008). The WSGG model was first proposed within the framework of the zone-method, proposed by Hottel and Cohen (1958). Modest (1991) applied the WSGG to the radiative transport equation (RTE), making it possible to use with any arbitrary solution method. Despite some important limitations of the WSGG model, this model is, together with the single gray gas model, the most largely employed method in the simulation of combustion processes, being available in most commercial CFDs codes.

In the past decades, databases such as HITEMP (Rothman *et alli*, 1995) and HITRAN (Rothman *et alli*, 2003) compile in detail the absorption lines of a variety of chemical species. The modern gas models are based on such data. With such information, thermal radiation heat transfer can be accurately solved with the line-by-line (LBL) integration, developed by Hartmann *et alli* (1983), which considers the emission and absorption of each individual spectral line. On the other hand, LBL integrations demand a very intense computational effort, and so their use has been limited to simple geometries, especially to obtain benchmark solutions.

Denison and Webb (1993a) presented the spectral-line weighted-sum-of-gray-gases (SLW) method. The modeling is based on a low resolution spectrum using the WSGG concept. Later, Denison and Webb (1993b) applied the absorption line blackbody distribution function (ALBDF) to calculate the absorption coefficients and the weights to be used with

the WSGG model. Correlations for the ALBDF were presented for H_2O and CO_2 (Denison and Webb, 1994). The SLW method leads to the appearance of Leibnitz terms in the RTE for the gray gases which makes the integration considerably more difficult. This scenario was treated by the assumption of ideal behavior of molecular spectra in temperature, assuming the correlated-*k*, or by simply neglecting the Leibnitz terms (Denison and Webb, 1995). The full-spectrum correlated-*k* distribution (Modest and Zhang, 2002) was introduced to extend the WSGG method to non-uniform media. Maurente *et alli* (2007) presented the application of the Monte Carlo method applied to the absorption line blackbody distribution function (MC-ALBDF) using participating media formed with water vapor and carbon dioxide. The stoichiometric ratios considered the combustion of methane and octane. Comparisons with the WSGG model were presented in Maurente *et alli* (2008). Recently, the 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 the 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. After, a gaseous medium using the multilayer approach by SLW and CW methods was modeled (Solovjov and Webb, 2008); the predictions showed high accuracy, even with few layers. Mossi *et alli* (2008) presented a study of the CW model application including an analysis of the molar concentration of CO_2 in a isothermal homogeneous medium. Salinas (2008) developed a fast approximate technique for the CW model. This approach reduced significantly the computational time in comparison with the standard method of solution for the CW model. More recently the RTE is solved for a non-isothermal medium by using the SLW modeling with local correction factors obtained from the CW modeling (Solovjov and Webb, 2010). In particular, the CW model led to results for the radiative volumetric heat source that proved accurate in comparison to the LBL integration for non uniform medium. However, tests carried out as part of the present research revealed that the CW model can lead to considerable errors in the estimation of the radiative heat flux, and as such violates the radiative energy balance. In fact, as will be demonstrated in this paper, the failure to satisfy the energy conservation arises from one of the main assumptions of the model.

This work proposes a modification of the CW method to enforce the radiative energy balance to be satisfied and, at the same time, to impose that the radiative volumetric heat source remains the same as computed by the CW method. The proposed method is still closely related to the CW method, but the modification to satisfy the energy balance seems sufficiently extensive to justify naming it as modified cumulative wavenumber (MCW) method. The method is presented in the framework of the discrete ordinates method; the example cases consider a one-dimensional, non-isothermal non homogeneous medium containing carbon-dioxide. The HITEMP database is used to extract the spectral lines information that is required by the method. The results show that the MCW leads to accurate estimation of both the radiative heat flux and volumetric heat source, satisfying the radiative energy balance within the error of the numerical discretization of the radiative transfer equation.

2. THE MODELING

The proposed methodology is presented in the framework of the discrete ordinates method, although it can be extended to other solution techniques. The example cases consider the one-dimensional slab, in which the participating medium is bounded by two parallel black surfaces. The spectral intensities in forward and backward directions, $I^+_{\eta l}(s)$ and $I^-_{\eta l}(s)$, are determined from the solutions of the radiative transfer equations below:

$$\mu_l \frac{\partial I^+_{\eta l}(s)}{\partial s} = -\kappa_\eta I^+_{\eta l}(s) + \kappa_\eta I_{\eta b}(s) \tag{1a}$$

$$-\mu_l \frac{\partial I^-_{\eta l}(s)}{\partial s} = -\kappa_\eta I^-_{\eta l}(s) + \kappa_\eta I_{\eta b}(s) \tag{1b}$$

In Eqs. (1a) and (1b), μ_l represents the cosine in *l* direction, κ_η is the spectral absorption coefficient, and $I_{\eta b}$ is the blackbody intensity at the temperature of the medium at position *s*. After solving Eqs. (1a) and (1b), the spectral radiative heat flux and volumetric heat source, $q''_{R\eta l}$ and $\dot{q}_{R\eta l}$, respectively, considering only the contribution of the ordinate direction *l*, can be determined by:

$$q''_{R\eta l}(s) = 2\pi\mu_l w_l \left[I^+_{\eta l}(s) - I^-_{\eta l}(s) \right] \tag{2a}$$

$$\dot{q}_{R\eta l}(s) = 2\pi\kappa_\eta w_l \left[I^+_{\eta l}(s) + I^-_{\eta l}(s) \right] - 4\pi\kappa_\eta w_l I_{\eta b}(s) \tag{2b}$$

The total heat flux and volumetric heat source are then computed by the summation of $q''_{R\eta l}$ and $\dot{q}_{R\eta l}$ in all ordinate directions l and by the integration over the wavelength spectrum η:

$$q''_R(s) = \sum_l \int_\eta q''_{R\eta l}(s) d\eta \tag{3a}$$

$$\dot{q}_R(s) = \sum_l \int_\eta \dot{q}_{R\eta l}(s) d\eta \tag{3b}$$

The global conservation of the radiative energy, $\dot{q}_R = -dq''_R / ds$, also turns to be a consequence of the exact solutions of Eqs. (1a) and (1b) for all directions and wavenumbers.

2.1 The Cumulative Wavenumber Method

The cumulative wavenumber (CW) is a distribution function used on modeling of the spectral properties of gases. The model is well detailed by Solovjov and Webb (2002). Previous works make use of the model successfully (Galarça *et alli*, 2009). As demonstrated in literature, integrating the directional spectral intensities over the fractional gray gas D_{ij} (defined by the CW modeling), using the concept of cumulative wavenumber, yields:

$$\int_{D_{ij}(s)} I^+_{\eta,l}(s) d\eta = u_{ij}(s) J^+_{ijl}(s) \tag{4a}$$

$$\int_{D_{ij}(s)} I^-_{\eta,l}(s) d\eta = u_{ij}(s) J^-_{ijl}(s) \tag{4b}$$

$$\int_{D_{ij}(s)} I_{\eta b}(s) d\eta = u_{ij}(s) J_{bij}(s) \tag{4c}$$

where J^+_{ijl}, J^-_{ijl} and J_{bij} are the fractional gray gas intensities and $u_{ij}(s)$ is the local correction coefficient as proposed by Solovjov and Webb (2002). It follows that the integrations of the spectral radiative heat flux and volumetric heat source over the fractional gray gas D_{ij} lead to:

$$q''_{Rijl}(s) = \int_{D_{ij}(s)} q''_{R\eta l}(s) d\eta = 2\pi \mu_l w_l u_{ij}(s) \left[J^+_{ijl}(s) - J^-_{ijl}(s) \right] \tag{5a}$$

$$\dot{q}_{Rijl}(s) = \int_{D_{ij}(s)} \dot{q}_{R\eta l}(s) d\eta = 2\pi \kappa_j w_l u_{ij}(s) \left[J^+_{ijl}(s) + J^-_{ijl}(s) \right] - 4\pi \kappa_j w_l u_{ij}(s) J_{bij}(s) \tag{5b}$$

where κ_j, in units of m^{-1}, is the corresponding gray gas absorption coefficient, which can be computed as $\kappa_j = N\sqrt{C_j C_{j+1}}$ (Denison and Webb, 1993b), where N is the molecular density of the absorbing species, in molecule/m^3. Finally, the total radiative heat flux and volumetric heat source are given by:

$$q''_R(s) = \sum_l \sum_{i,j} q''_{Rijl}(s) \tag{6a}$$

$$\dot{q}_R(s) = \sum_l \sum_{i,j} \dot{q}_{Rijl}(s) \tag{6b}$$

As shown above, the application of the cumulative wavenumber renders an effective way to integrate the radiative heat flux and the volumetric heat source over the spectrum. However, for the computations of Eqs. (5a) and (5b), it is required the determination of the fractional gray gas intensities J^+_{ijl} and J^-_{ijl}. This can be accomplished by the integration of the radiative transfer Eqs. (1a) and (1b) over the fractional gray gas wavenumbers D_{ij}. The integration leads to (Solovjov and Webb, 2002):

$$\mu_l \frac{\partial J^+_{ijl}(s)}{\partial s} = -\kappa_j J^+_{ijl}(s) + \kappa_j J_{bij}(s) \tag{7a}$$

$$-\mu_l \frac{\partial J^-_{ijl}(s)}{\partial s} = -\kappa_j J^-_{ijl}(s) + \kappa_j J_{bij}(s) \tag{7b}$$

A close analysis of the above equations reveals one approximation in the derivation of the derivative terms on the right-hand sides. In respect to the Eq. (7a), for instance, the integration of the first term of Eq. (1a) over D_{ij} can be computed from:

$$\begin{aligned}\int_{D_{ij}(s)} \frac{\partial I^+_{\eta l}(s)}{\partial s} d\eta &= \int_{D_{ij}(s)} \frac{I^+_{\eta l}(s+ds/2) - I^+_{\eta l}(s-ds/2)}{ds} d\eta \\ &= \frac{\int_{D_{ij}(s)} I^+_{\eta l}(s+ds/2) d\eta - \int_{D_{ij}(s)} I^+_{\eta l}(s-ds/2) d\eta}{ds}\end{aligned} \tag{8}$$

In the above integrals, the points of evaluation of D_{ij} and of the two $I^+_{\eta l}$ (which are s, $s+ds/2$ and $s-ds/2$) are not the same, so it is not possible to apply the relation (4a) with exactitude. Making use of some mathematical handling, the integration of Eq. (1a) over the entire spectrum becomes:

$$\mu_l \sum_{i,j} \left[u_{ij}(s) \frac{\partial J^+_{ijl}(s)}{\partial s} + J^+_{ijl}(s) \frac{\partial u_{ij}(s)}{\partial s} \right] = -\sum_{i,j} \kappa_j u_{ij}(s) J^+_{ijl}(s) + \sum_{i,j} \kappa_j u_{ij}(s) J^+_{bij}(s) \tag{9}$$

On the other hand, multiplying Eq. (7a) by $u_{ij}(s)$ and summing up for all fractional gray gases i, j results:

$$\mu_l \sum_{ij} u_{ij}(s) \frac{\partial J^+_{ijl}(s)}{\partial s} = -\sum_{ij} \kappa_j u_{ij}(s) J^+_{ijl}(s) + \sum_{ij} \kappa_j u_{ij}(s) J^+_{bij}(s) \tag{10}$$

Finally, subtracting Eq. (10) from (9) leads to the following relations, considering both intensity directions:

$$\sum_{ij} \left(J^+_{ijl}(s) \frac{\partial u_{ij}(s)}{\partial s} \right) = 0 \tag{11a}$$

$$\sum_{ij} \left(J^-_{ijl}(s) \frac{\partial u_{ij}(s)}{\partial s} \right) = 0 \tag{11b}$$

Therefore, the consistency of the method requires that Eqs. (11a) and (11b) be satisfied, but in general they do not hold true. Applying the same reasoning to all directions, it can be proved that the radiative energy balance, $\dot{q}_R = -dq''_R / ds$, will be verified only if Eqs. (11a) and (11b) are valid for all directions, which again is not true in general.

In spite of the aforementioned approximation of the CW method it has been demonstrated, including in the present research, that the method is consistently precise to determine the radiative volumetric heat source $\dot{q}_R$ (Solovjov and Webb, 2002; 2005; 2008 and 2010). However, tests carried out in this study have shown that the radiative heat flux q''_R can present considerable deviations from the correct solution, an expected consequence of the radiative energy balance not being satisfied by the CW method. It is presented next a modification of the CW method to enforce the radiative energy balance in every point of the domain, without modifying the radiative volumetric heat source that is provided by the method.

2.2 The Modified Cumulative Wavenumber Method

The use of Eqs. (7a) and (7b) leads to an error in the computation of the fractional gray gases defined by Eqs. (4a) and (4b). It is proposed here a modification of Eqs. (7a) and (7b). The modified fractional gray gases are denoted by

K_{ijl}^{+} and K_{ijl}^{-} to distinguish of J_{ijl}^{+} and J_{ijl}^{-}, which will continue to be used in the proposed correction. The modified fractional gray gases are defined in the same way as J_{ijl}^{+} and J_{ijl}^{-}:

$$\int_{D_{ij}(s)} I_{\eta,l}^{+}(s)d\eta = u_{ij}(s)K_{ijl}^{+}(s) \tag{12a}$$

$$\int_{D_{ij}(s)} I_{\eta,l}^{-}(s)d\eta = u_{ij}(s)K_{ijl}^{-}(s) \tag{12b}$$

The integration of the spectral radiative heat flux and volumetric heat source over the fractional gray gas D_{ij} leads to:

$$q''_{Rijl}(s) = \int_{D_{ij}(s)} q''_{R\eta l}(s)d\eta = 2\pi\mu_l w_l u_{ij}(s)\left[K_{ijl}^{+}(s) - K_{ijl}^{-}(s)\right] \tag{13a}$$

$$\dot{q}_{Rijl}(s) = \int_{D_{ij}(s)} \dot{q}_{R\eta l}(s)d\eta = 2\pi\kappa_j w_l u_{ij}(s)\left[K_{ijl}^{+}(s) + K_{ijl}^{-}(s)\right] - 4\pi\kappa_j w_l u_{ij}(s)J_{bij}(s) \tag{13b}$$

It is convenient to keep the symbol J_{bij} to represent the integration of $I_{\eta b}$ over D_{ij}, since this parameter remains unaltered in the correction. Finally, the total radiative heat flux and volumetric heat source, q''_R and can $\dot{q}_R$, be determined by the application of Eqs. (6a) and (6b).

In the proposed method, the integrations of Eqs. (1a) and (1b) over D_{ij} are represented by the following relations:

$$\mu_l \frac{\partial K_{ijl}^{+}(s)}{\partial s} = -\kappa_j K_{ijl}^{+}(s) + \kappa_j J_{bij}(s) + f_{ijl}^{+}(s) \tag{14a}$$

$$-\mu_l \frac{\partial K_{ijl}^{-}(s)}{\partial s} = -\kappa_j K_{ijl}^{-}(s) + \kappa_j J_{bij}(s) + f_{ijl}^{-}(s) \tag{14b}$$

where the terms f_{ijl}^{+} and f_{ijl}^{-} are added to the equations to correct the approximations that are involved in the integration of the derivative terms over D_{ij}. A priori, these terms are left to depend on the position s, the ordinate direction l, and the fractional gray gas D_{ij}.

To solve Eqs. (14a) and (14b), additional information are required to determine f_{ijl}^{+} and f_{ijl}^{-}. Following the discussion in the previous section, it is first required that the radiative energy balance is conserved. As with the derivation of Eq. (9), the integration of Eq. (1a) over the entire spectrum η leads to:

$$\mu_l \sum_{i,j}\left[u_{ij}(s)\frac{\partial K_{ijl}^{+}(s)}{\partial s} + K_{ijl}^{+}(s)\frac{\partial u_{ij}(s)}{\partial s}\right] = -\sum_{i,j}\kappa_j u_{ij}(s)K_{ijl}^{+}(s) + \sum_{i,j}\kappa_j u_{ij}(s)J_{bij}(s) \tag{15}$$

Multiplying Eq. (14a) by $u_{ij}(s)$ and summing up for all i, j leads to:

$$\mu_l \sum_{i,j} u_{ij}(s)\frac{\partial K_{ijl}^{+}(s)}{\partial s} = -\sum_{i,j}\kappa_j u_{ij}(s)K_{ijl}^{+}(s) + \sum_{i,j}\kappa_j u_{ij}(s)J_{bij}(s) + \sum_{i,j} u_{ij}(s)f_{ijl}^{+}(s) \tag{16}$$

Subtracting Eq. (15) from (16) results, for both modified intensities:

$$\mu_l \sum_{i,j}\left[K_{ijl}^{+}(s)\frac{\partial u_{ij}(s)}{\partial s}\right] = -\sum_{i,j}\left[u_{ij}(s)f_{ijl}^{+}(s)\right] \tag{17a}$$

$$\mu_l \sum_{i,j}\left[K_{ijl}^{-}(s)\frac{\partial u_{ij}(s)}{\partial s}\right] = -\sum_{i,j}\left[u_{ij}(s)f_{ijl}^{-}(s)\right] \tag{17b}$$

In the MCW method, the correcting terms f_{ijl}^{+} and f_{ijl}^{-} are required to make Eqs. (17a) and (17b) correct, and thus assuring the radiative energy balance.

Next, it is imposed that the volumetric heat sources computed from Eqs. (5b) and (13b) be the same. As discussed previously, this requirement is based on observations that the CW method leads to accurate computation of the radiative volumetric heat source. It follows that:

$$J_{ijl}^{+}(s)+J_{ijl}^{-}(s)=K_{ijl}^{+}(s)+K_{ijl}^{-}(s) \tag{18}$$

The Eqs. (5a) and (5b) and of Eqs. (13a) and (13b) can be combined and, after a few mathematical steps, using the information in (18), results:

$$f_{ijl}^{+}(s)+f_{ijl}^{-}(s)=\mu_l\left[\frac{\partial K_{ijl}^{+}(s)}{\partial s}-\frac{\partial K_{ijl}^{-}(s)}{\partial s}\right]-\mu_l\left[\frac{\partial J_{ijl}^{+}(s)}{\partial s}-\frac{\partial J_{ijl}^{-}(s)}{\partial s}\right] \tag{19}$$

Equations (17a), (17b) and (19) enforce the radiative energy balance to be satisfied and the volumetric heat source to retain the same value of the CW method. However, there are an infinite number of solutions for f_{ijl}^{+} and f_{ijl}^{-} that can satisfy Eqs. (17a), (17b) and (19), so more relations are needed. It is proposed that:

$$f_{ijl}^{+}(s)=g_{ijl}(s)+f_{l}^{+}(s) \tag{20a}$$

$$f_{ijl}^{-}(s)=g_{ijl}(s)+f_{l}^{-}(s) \tag{20b}$$

The relations (20a) and (20b) are not based on physical considerations; they are proposed to allow the determination of the correcting terms f_{ijl}^{+} and f_{ijl}^{-}. A priori, other relations can be attempted, although the above relations have been proved to be the most stable among a set of other propositions attempted in this study. Combining Eqs. (20) to (19) and (17) leads to:

$$g_{ijl}(s)=\mu_l\left[\frac{\partial K_{ijl}^{+}(s)}{\partial s}-\frac{\partial K_{ijl}^{-}(s)}{\partial s}\right]-\mu_l\left[\frac{\partial J_{ijl}^{+}(s)}{\partial s}-\frac{\partial J_{ijl}^{-}(s)}{\partial s}\right]-\left[f_{l}^{+}(s)+f_{l}^{-}(s)\right] \tag{21a}$$

$$f_{l}^{+}(s)=\frac{\mu_l\sum_{ij}\left[K_{ijl}^{+}(s)\dfrac{\partial u_{ij}(s)}{\partial s}\right]-\sum_{ij}\left[u_{ij}(s)g_{ijl}(s)\right]}{\sum_{ij}u_{ij}(s)} \tag{21b}$$

$$f_{l}^{-}(s)=\frac{\mu_l\sum_{ij}\left[K_{ijl}^{-}(s)\dfrac{\partial u_{ij}(s)}{\partial s}\right]-\sum_{ij}\left[u_{ij}(s)g_{ijl}(s)\right]}{\sum_{ij}u_{ij}(s)} \tag{21c}$$

2.3 Solution Methodology

The implementation of the MCW method can be accomplished by the following steps:

1. Solve for the fractional gray gas intensities $J_{ijl}^{+}(s)$ and $J_{ijl}^{-}(s)$ from Eqs. (7a) and (7b);
2. Set $K_{ijl}^{+}(s)=J_{ijl}^{+}(s)$ and $K_{ijl}^{-}(s)=J_{ijl}^{-}(s)$;
3. Set $g_{ijl}(s)=0$;
4. Solve for $f_{l}^{+}(s)$ and $f_{l}^{-}(s)$ from Eqs. (21a) and (21b), and then determine $f_{ijl}^{+}(s)$ and $f_{ijl}^{-}(s)$ from Eqs. (20a) and (20b);
5. Solve for the corrected fractional gray gas intensities $K_{ijl}^{+}(s)$ and $K_{ijl}^{-}(s)$ from Eqs. (14a) and (14b);
6. Return to step (4) to compute $f_{l}^{+}(s)$ and $f_{l}^{-}(s)$ from Eqs. (21a) and (21b) using the new values of $K_{ijl}^{+}(s)$ and $K_{ijl}^{-}(s)$, and repeat until convergence of $f_{l}^{+}(s)$ and $f_{l}^{-}(s)$;

7. Compute $g_{ijl}(s)$ from Eq. (21a);
8. Return to step (4), and repeat until convergence of $g_{ijl}(s)$.

2.4 Numerical solution and verification

For both the CW and the MCW methods, the solutions will be verified by comparison of the radiative volumetric heat source and heat flux with the solution provided by the LBL integration. All the solutions were based on the same numerical discretization of the space, so the difference between the solutions will result solely of the spectral integration of the radiative transfer equation.

The global deviation of the energy balance is determined by:

$$\gamma_G = \left| \frac{\left[q_R''(s=0) - q_R''(s=L) \right] - \dot{E}_G}{\dot{E}_G} \right| \times 100 \tag{22a}$$

where $\dot{E}_G$ is the total energy generated in the domain per unit of area, giving by:

$$\dot{E}_G = \dot{q}_R(s=0) \times \frac{\Delta s}{2} + \sum_{m=1}^{M-1} \left[\dot{q}_R(s = \frac{\Delta s}{2} + (m-1) \times \Delta s) \right] + \dot{q}_R(s=S) \times \frac{\Delta s}{2} \tag{22b}$$

For an exact solution of the RTE, the global deviation of the energy balance should be null, so it is an effective measure of the internal consistency of the solution. In the next section, a few examples will be presented to show the performance of the MCW method against the benchmark line-by-line results and the CW method.

3. RESULTS

3.1 One-dimensional slab

The CW method was applied to problems involving a layer of CO_2 mixed in an inert gas (air or nitrogen, for instance) as participating gas. The geometry that was considered corresponds to a one-dimensional slab, with parallel black walls placed at a distance of L=1 m. The physical mesh between the two black surfaces was divided in one hundred equal-sized elements, M = 100. A spectral mesh of 20 logarithmically spaced absorption cross-sections in the range 10^{-25} m^2/molecule ≤ C_j ≤ 10^{-17} m^2/molecule (Solovjov and Webb, 2002) and $\Delta\eta$ = 100 cm^{-1} were used for the wavenumber range of 0 to 10000 cm^{-1}. The HITEMP database was applied since it provides more accurate spectral data when considering high temperatures, such as in the proposed cases. The discrete ordinates method was applied to 30 directions. The slab is filled with a non-isothermal, non homogeneous gas, according to the following cases: *Case 1* – Parabolic temperature (Eq.23) and concentration (Eq.25) profiles; *Case 2* – Exponential temperature (Eq.24) and linear concentration (Eq.26) profiles; *Case 3* – Parabolic temperature and sinusoidal concentration (Eq.27) profiles.

$$T(s) = 1000 - 500\left[(2s/L) - 1 \right]^2 \tag{23}$$

$$\begin{aligned} T(s) &= 500 e^{(\pi s/L)} \qquad 0 \le s \le L/2 \\ T(s) &= 11570 e^{(-\pi s/L)} \qquad L/2 < s \le L \end{aligned} \tag{24}$$

$$Y_{CO_2}(s) = 0.2 - 0.15\left[(2s/L) - 1 \right]^2 \tag{25}$$

$$Y_{CO_2}(s) = 0.15\left(s/L \right) + 0.05 \tag{26}$$

$$Y_{CO_2}(s) = 0.05 + 0.15\left[\sin\left(\pi s/L \right) \right] \tag{27}$$

The RTE solutions are performed with the discrete ordinates method, while the gas properties are modeled with the LBL, CW and MCW models, according to the Eqs.(1a) and (1b), (7a) and (7b), (14a) and (14b), respectively. The walls are assumed black in all cases, so the boundary conditions are:

$$J_{ij}^{+}\left(0,\mu_l\right)=J_{bij}\left(0\right) \tag{28a}$$

$$J_{ij}^{-}\left(L,\mu_l\right)=J_{bij}\left(L\right) \tag{28b}$$

The integration of the spectral volumetric heat source and radiative heat flux over the fractional gray gases are calculated from Eqs. (5a) and (13a), and (5b) and (13b), respectively.

The results for the first case are presented in Fig.1. As can be noted, the values for the volumetric heat source obtained from the CW and MCW solutions around the center region of the slab are not the exact behavior as the LBL integration (Fig.1a). Despite the assumption of Eq.(18) it is possible to observe that the MCW volumetric heat source seems to be closer to the benchmark solution than the CW modeling. However, the radiant energy balance is satisfied as well. The global deviation, Eq.(22a), is about 2,25% for the MCW and 55,91% for the CW. Thus, the radiative heat flux presents a better agreement to the LBL solution (Fig.1b).

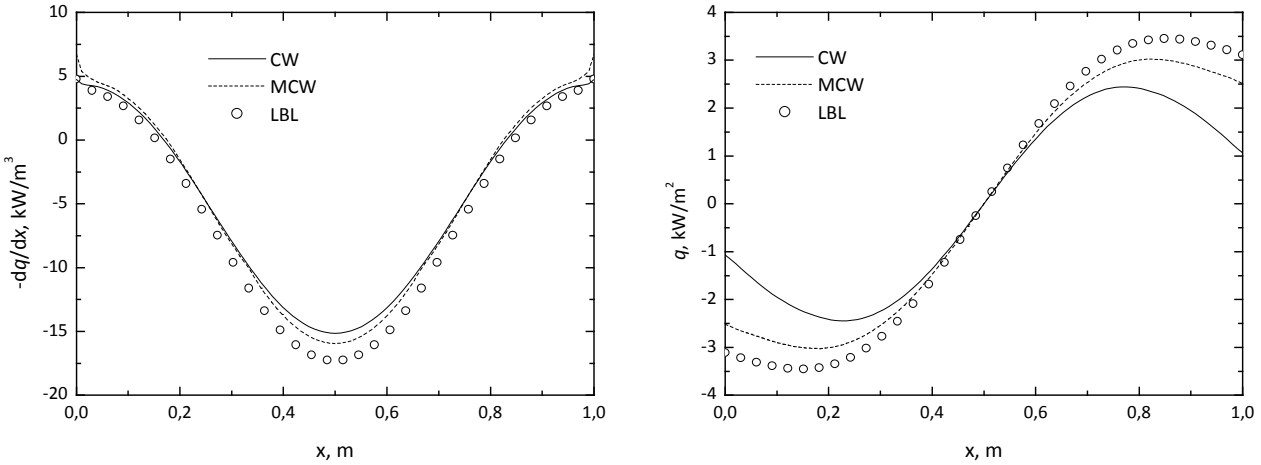
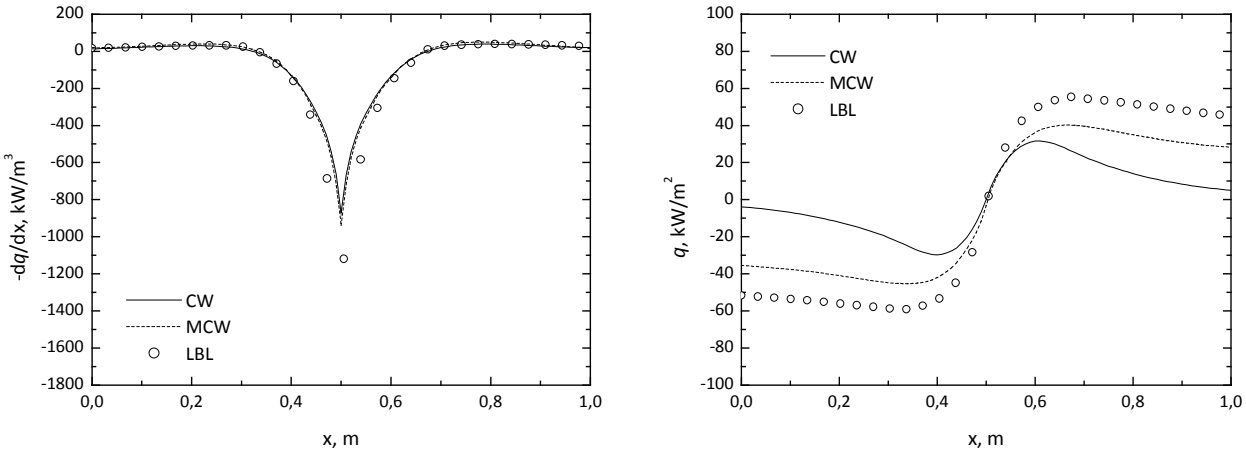


Figure 1. (a) Radiative volumetric heat source; (b) Radiative heat flux. Temperature profile: parabolic. Concentration profile: parabolic.

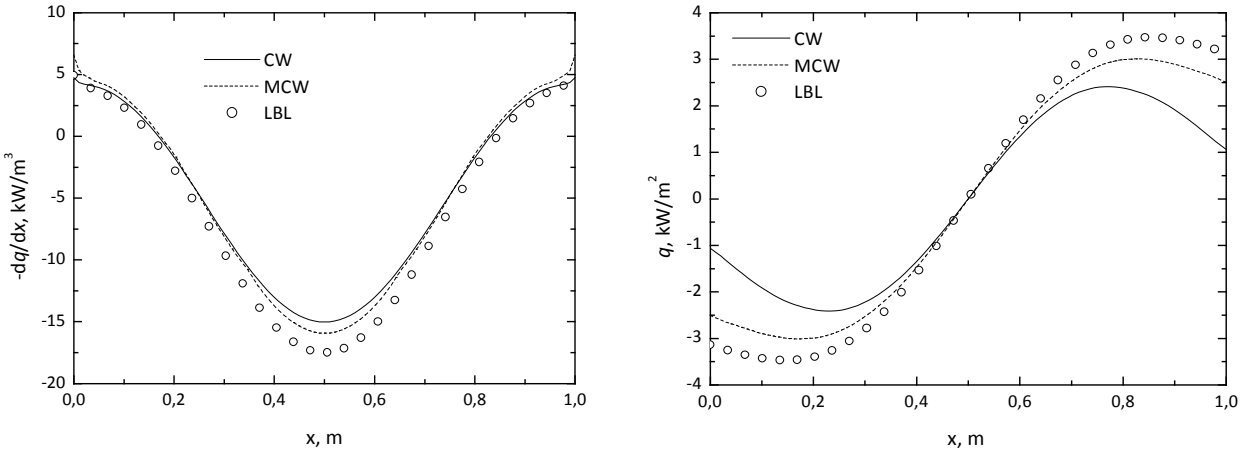
The results for the second case in respect to the volumetric heat source are very close when comparing the CW to MCW model (Fig.2). In fact, this is an expected answer. Based on the Fig.2a it can be noted that the benchmark solution next to the middle of the slab differs from the CW and MCW models. As the aim of this work is to enforce the energy balance, keeping the same volumetric heat source, it is an expected behavior. Since the original model (CW) does not provide results closer to the LBL integration, the MCW model does not so. On the other hand, the proposed modification here ensures the energy conservation for the problem (γ_G = 2,2% for the MCW model; γ_G = 85,42% for the CW model). This way, the radiative heat flux curve for the modified model (MCW) presents a better agreement to the LBL (Fig. 2b).

Finally, the results regarding to the *Case 3* are presented in Fig.3. It can be observed that the curves for both the radiative volumetric heat source and the heat flux are very similar to those presented for the *Case 1*. It is suggested that the variations on the concentration are less perceived than the temperature change into the medium. Since the concentration range is based on the products from the stoichiometric combustion of methane or fuel oil, in fact, the range is not large, contrary to the temperature range. Therefore, a better agreement is found for the MCW in respect to the heat flux when comparing to the LBL integrations. The global deviation for the energy balance is 4,4% and 56,1% for the MCW and CW, respectively.



(a) (b)

Figure 2. (a) Radiative volumetric heat source; (b) Radiative heat flux. Temperature profile: exponential. Concentration profile: linear.



(a) (b)

Figure 3. (a) Radiative volumetric heat source; (b) Radiative heat flux. Temperature profile: parabolic. Concentration profile: sinusoidal.

3. CONCLUSIONS

This work presented a modification of the cumulative wavenumber (CW) method to improve the estimation of the radiative heat flux in participating gases. The method is formulated to retain the radiative volumetric heat source that is obtained from the CW, which has been shown to be consistently accurate in comparison to the line-by-line (LBL) integration. At the same time, it requires that the radiative energy balance be satisfied in every point of the domain, one aspect that the CW method cannot satisfy in general. The proposed method was applied to a one-dimensional layer of non-isothermal non homogeneous participating gas bounded by two black surfaces. For the two temperature profiles combined to the three concentration profiles, the proposed method led to satisfactory solutions for the radiative heat flux and volumetric heat source when compared to the LBL solution. The method led to additional terms, which in turn required additional relations for the closure of the system equations. While the additional relations proposed in this work were purely mathematical, it is open for future studies the attempt to use more physically based relations.

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