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A PROPOSED CORRECTION OF THE CUMULATIVE WAVENUMBER METHOD IN THE DETERMINATION OF THE RADIATIVE HEAT FLUX

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Abstract. *Spectral modeling of participating gases is a very important field of the thermal radiation in due to the relevance of accurately describing phenomena involving combustion processes. Previous works show that the cumulative wavenumber (CW) model yields accurate estimates of the radiative heat source, but presents considerable deviations in the radiative heat flux when compared with the line-by-line (LBL) benchmark solution. So, this paper proposes a modification of the original CW method in the radiative transfer equation (RTE). The modified method consists of including a term in the calculation of the RTE, which was incorrectly neglected in the original formulation, ensuring that the energy balance is satisfied. The proposed method is applied to a one-dimensional medium slab filled by a homogeneous concentration of carbon dioxide between the plates that delimit the domain, in which the spectral modeling is solved with the corrected CW model and the spatial integration is performed with the discrete ordinates method. Results obtained with the modified method are compared against those found by standard CW method and the LBL integration.*

Keywords: *thermal radiation, cumulative wavenumber model, line-by-line integration, radiative heat flux, energy balance*

1. INTRODUCTION

Thermal radiation is present in several problems in engineering, such as combustion chambers and steam generation. In these systems, the radiation is, frequently, one of the main mechanisms of heat transfer in due to the presence of soot and participating gases at high temperatures. As the radiative properties depend strongly with respect to the wavenumber, the radiation calculation in participating gases is a very complex task, so that a line-by-line (LBL) integration requires an elevated computational cost and, as a result, it can often become impracticable, since it is necessary, for example, the knowledge of spectral databases, such as HITEMP 2010 (Rothman *et al*., 2010)

Alternatively, the development of global spectral models provided the obtaining of reliable results faster. The cumulative wavenumber (CW) model, for example, is a method based on a distribution function, which is capable to provide good results in relation to the LBL benchmark solution for the radiative heat source (Solovjov and Webb, 2002; 2005). However, in due to a failure in the original formulation, the energy balance is not satisfied, so that, in some cases, the radiative heat flux presents discrepancies that cannot be neglected. Recent works have been developed in order to improve the method (Ismail and Salinas, 2005; Salinas, 2008; Solovjov and Webb, 2008; Solovjov and Webb, 2010; Solovjov *et al*., 2013) or to investigate the model behavior in the presence of soot (Solovjov and Webb, 2005; Mossi *et al*., 2012), in the sense of decreasing the computational time or of extending the formulation to non-gray surfaces or to correct problems in other gas models, such as the spectral line-based weighted-of-sum-of-gray-gases (SWL) model (Denison and Webb, 1993).

In Galarça *et al*., 2010, and Galarça *et al*., 2011, it is proposed the modified cumulative wavenumber (MCW) method in order to overcome the main deficiency of the CW model developed by Solovjov and Webb (2002), which imposes the radiative energy balance and keeps the radiative heat source calculated according to the original formulation. Although the inconsistency of the radiative heat flux has been resolved, the required computational time has become even greater, which may complicate its application in coupled combustion problems, in which the radiative transfer equation (RTE) must be solved several times within an iterative calculation process. So, the present work proposes a modification of the CW method in the RTE in which is included a term that was neglected in the first approach. Thus, the radiative heat flux and the radiative heat source are determined in the same way of the original formulation. It will be considered a one-dimensional medium slab bounded by black walls and filled by a homogeneous molar concentration of carbon dioxide of 0.1. The RTE is performed with the discrete ordinates method (DOM) adopting 8 directions and the domain is divided into 200 uniformly-sized cells. Line-by-line calculations are invoked to evaluate the accuracy of the proposed approach.

2. PHYSICAL AND MATHEMATICAL MODELING

2.1 The standard CW model

Proposed by Solovjov and Webb (2002), the CW method is one of the most modern gas spectral models and is based on a distribution function. Distribution functions are usually defined on the basis of the high resolution molecular absorption cross-section. Molecular spectra of participating species present hundreds of thousands of lines and its direct and efficient application in radiative transfer analysis is very computationally costly, being, eventually, impracticable. As the scope of this study is not to discuss the formulation already well-established of the CW model, only the most fundamental equations will be presented here. More details about this method can be found in Solovjov and Webb, 2002.

For a participating medium where the scattering effects may be neglected, the spectral RTE is expressed by (Siegel and Howell, 2002; Modest, 2003):

$$\frac{dI_\eta}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{\eta b} \tag{1}$$

where I_η is the spectral radiative intensity, κ_η is the spectral absorption coefficient of the medium and $I_{\eta b}$ is the blackbody spectral intensity, described by the Planck's distribution function for a given radiation wavenumber η and for a given local medium temperature T.

Integrating the RTE over the fractional gray gas D_{ij}, according to the original proposition, leads to:

$$\underbrace{\int_{D_{ij}} \frac{dI_\eta}{ds} d\eta}_{(A)} = \underbrace{- \int_{D_{ij}} \kappa_\eta I_\eta d\eta}_{(B)} + \underbrace{\int_{D_{ij}} \kappa_\eta I_{\eta b} d\eta}_{(C)} \tag{2}$$

By integrating parts A, B and C of the previous expression, Eq. (2) yields:

$$\begin{aligned}
&(A) \int_{D_{ij}} \frac{dI_\eta}{ds} d\eta = u_{ij}(s) \int_{\Delta_i} \frac{dI_\eta}{ds} d\left[v_{ij}(\eta)\right] = u_{ij}(s) \frac{d}{ds} \int_{\Delta_i} I_\eta d\left[v_{ij}(\eta)\right] = u_{ij}(s) \frac{dJ_{ij}}{ds} \\
&(B) - \int_{D_{ij}} \kappa_\eta I_\eta d\eta = -\kappa_j u_{ij}(s) J_{ij}(s) \\
&(C) \int_{D_{ij}} \kappa_\eta I_{\eta b} d\eta = \kappa_j u_{ij}(s) J_{bij}
\end{aligned} \tag{3}$$

in which u_{ij} and v_{ij} are functions that describe, respectively, the thermodynamic state and the spectral behavior of the gas (the exact mathematical definition of these two functions is presented in Solovjov and Webb, 2002); Δ_i is a fixed interval of the spectrum; κ_j is the gray gas absorption coefficient; and J_{bij} is the fractional blackbody radiative intensity of the ij fractional gray gas. The summation of J_{bij} over all fractional gray gases leads to the total emission: $I_b = \sum_{i,j} J_{bij} = \sigma T^4 / \pi$, where σ is the Stefan-Boltzmann constant.

Lastly, by combining the terms of Eq. (3), the RTE for the CW model becomes:

$$\frac{dJ_{ij}}{ds} = -\kappa_j J_{ij} + \kappa_j J_{bij} \tag{4}$$

The solution of the total radiative heat flux in the medium requires two integrations of the RTE: one along the path and the other in all directions. In the framework of this paper, it will be considered a domain formed by a one-dimensional medium slab bounded by two infinite, parallel and black walls, as shown in Fig. 1, and the integration of the radiative transfer equation is carried out with the discrete ordinates method. For a given direction l, Eq. (4) can be written for the positive and negative intensities of the fractional gray gas, J_{ijl}^{+} and J_{ijl}^{-}, respectively, as (Solovjov and Webb, 2002):

$$\mu_l \frac{dJ_{ijl}^{+}}{ds} = -\kappa_j J_{ijl}^{+} + \kappa_j J_{bij} \tag{5}$$

$$-\mu_l \frac{dJ_{ijl}^{-}}{ds} = -\kappa_j J_{ijl}^{-} + \kappa_j J_{bij} \tag{6}$$

where μ_l is the directional cosine. Assuming black walls in x = 0 and x = X in Fig. 1, the boundary conditions for the equations above are J_{ijl}^{+} (x = 0) = J_{bij}(x = 0) and J_{ijl}^{-} (x = X) = J_{bij}(x = X).

Once the intensities J_{ijl}^{+} and J_{ijl}^{-} of the fractional gray gas are obtained, the radiative heat flux, q_R'', and the radiative heat source, S_R, can be determined by the following equations:

$$q_R''(x) = \sum_{l=1}^{L} \sum_{i,j=1}^{n_g} \left\{ 2\pi\mu_l \omega_l u_{ij}(x) \left[J_{ijl}^{+}(x) - J_{ijl}^{-}(x) \right] \right\} \tag{7}$$

$$S_R(x) = \left(-\frac{dq_R''}{dx} \right) = \sum_{l=1}^{L} \sum_{i,j=1}^{n_g} \left\{ 2\pi\omega_l \kappa_j u_{ij}(x) \left[J_{ijl}^{+}(x) + J_{ijl}^{-}(x) \right] - 4\pi\kappa_j u_{ij}(x) J_{bij}(x) \right\} \tag{8}$$

in which L is the number of discrete directions, n_g is the number of gray gases and ω_l is the weight of the Gauss-Legendre quadrature.

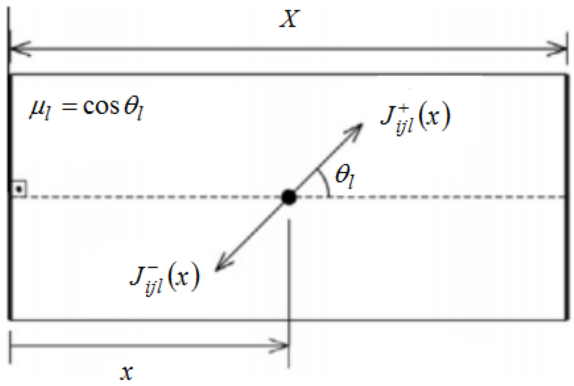


Figure 1. Schematic representation of the 1D-domain

2.2 The proposed approach

Besides reducing the computational time of a numerical simulation, it is expected that a spectral model, such as CW method, for instance, will reliably reproduce the behavior of the solution obtained by the LBL integration. The literature shows that the CW model can provide good results for the radiative heat source (Solovjov and Webb, 2002; 2005), but the radiative heat flux presents considerable deviations in relation to the LBL solution. Galarça *et al*., 2011, proposed a modification for the CW method in its original form, resulting in a change in the Eqs. (5) and (6) and ensuring that the radiative energy balance is satisfied. However, the modified cumulative wavenumber method requires an iterative procedure, which can significantly increase the computational time needed to solve radiative problems through the model.

In the standard CW model, was considered that $\sum_{i,j} J_{ij}^{+}\left(du_{ij}/ds\right) = 0$ and $\sum_{i,j} J_{ij}^{-}\left(du_{ij}/ds\right) = 0$, which is wrong and prevents the energy balance from being checked. Thus, the present paper proposes a correction in the RTE by inserting a term concerning the function u_{ij}, which is neglected in the original formulation. It follows that the energy balance is satisfied and it is not necessary an iterative calculation, as proposed previously by Galarça *et al*., 2011. In this approach, the radiative transfer equation in the forward and backward directions, Eqs. (5) and (6), respectively, becomes:

$$\mu_l \frac{dJ_{ijl}^{+}}{ds} = -\left[\kappa_j + \mu_l \left(\frac{\frac{du_{ij}}{ds}}{u_{ij}}\right)\right] J_{ijl}^{+} + \kappa_j J_{bij} \tag{9}$$

$$-\mu_l \frac{dJ_{ijl}^{-}}{ds} = -\left[\kappa_j - \mu_l \left(\frac{\frac{du_{ij}}{ds}}{u_{ij}}\right)\right] J_{ijl}^{-} + \kappa_j J_{bij} \tag{10}$$

In the original formulation of the CW method, the derivative term du_{ij}/ds is considered null, which is wrong and prevents the energy balance from being satisfied. With the insertion of the derivative term into the RTE correction, it is necessary to multiply it by the directional cosines μ_l and $-\mu_l$ included in the 1D-solution in the forward and backward directions, respectively. However, this term is the only modification in the original formulation, so no further alteration is required and the calculation of the radiative heat flux and the radiative heat source continues to be computed through Eqs. (7) and (8), without requiring an iterative procedure as previously proposed by Galarça *et al*., 2011.

In the present study, the cumulative wavenumber method will be applied to a 1D-configuration, as depicted in Fig. 1, for a homogeneous molar concentration of carbon dioxide for two different temperature profiles. The plates are considered black and infinite and are separated by the distance of 1 m, the total pressure of the system is 1 atm, and the molar concentration of CO_2 is 0.1 and is uniform throughout the domain. The radiative transfer equation is performed with 8 directions, adopting the discrete ordinates method, and the mesh is discretized in 200 cells. Results obtained with the proposed methodology are presented, in the next section, for both temperature profiles in terms of the radiative heat flux, the radiative heat source and the normalized percentage deviations compared with those found by the LBL solution.

3. RESULTS AND DISCUSSION

In order to evaluate the performance of the CW method, the solutions are compared against the LBL integration. The following temperature profiles (given in K) are considered:

$$T(x) = 400 + 1400\sin^2(\pi x) \tag{11}$$

$$T(x) = \begin{cases} 880 + 920\sin^2(2\pi x), \text{ if } x \le 0.25\,\text{m} \\ 400 + 1400\left\{1 - \sin^{3/2}\left[\frac{2}{3}\pi(x - 0.25)\right]\right\}, \text{ if } x > 0.25\,\text{m} \end{cases} \tag{12}$$

In the next subsections, the equations above will be referenced as Profile 1 and Profile 2, respectively. Figure 2 illustrates the behavior of these temperature profiles. Equation (11), i.e., Profile 1, presents simple symmetry, with the average temperature of the medium at 1100 K, the maximum temperature of 1800 K and both walls at 400 K. Equation (12), i.e., Profile 2, has different temperatures on each of the walls, more specifically 880 K on the left and 400 K on the right, the average medium temperature of 1100 K and maximum temperature of 1800 K.

In this paper, the results presented were generated based on a 1D-domain bounded by two infinite, parallel and black walls in which carbon dioxide is confined with a molar concentration of $Y_{CO2} = 0.1$, which is constant throughout the medium. The domain is spatially discretized in 200 uniformly-sized cells, the radiation wavenumber is divided into 100 equal segments, and the directional integration of the radiative transfer equations is performed with the DOM adopting 8 total directions and 20 gray gases.

The accuracy of the proposed method is computed through comparisons of the normalized deviations between the radiative heat flux and the radiative heat source obtained with the CW model and the LBL solution, according to the equations below:

$$\delta = \left|\frac{q''_{R,CW} - q''_{R,LBL}}{\max\left(q''_{R,LBL}\right)}\right| \times 100\% \tag{13}$$

$$\zeta = \left| \frac{S_{R,CW} - S_{R,LBL}}{\max\left(S_{R,LBL}\right)} \right| \times 100\% \tag{14}$$

where δ and ζ are the local deviations of q''_R and S_R, respectively; and max($q''_{R,LBL}$) and max ($S_{R,LBL}$) are the maximum absolute values of q''_R and S_R, respectively. Further, more specifically in Table 2, the percentage differences that will be interesting for the analysis of this work are the maximum and average deviations, denoted by the terms "max" and "avg", respectively.

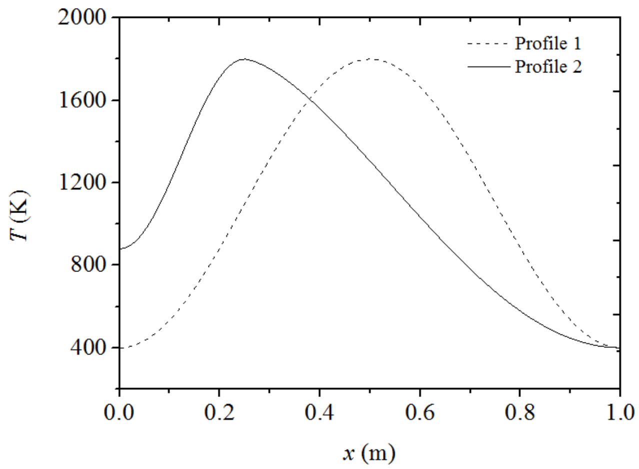


Figure 2. Temperature profiles.

3.1 Verification of the energy balance

As the scope of this study is to present a methodology in which the radiative energy balance is conserved, the first step of the analysis is to verify that this condition is satisfied. Then, by applying the correction of Eqs. (9) and (10) of the RTE in the forward and backward directions, the radiative heat flux and the radiative heat source were calculated for Profiles 1 and 2. From the definition of the radiative heat source, presented in Eq. (8), it follows that:

$$\int_{x=0}^{x=X} S_R dx = \int_{x=0}^{x=X} dq''_R \tag{15}$$

Once the problem is solved numerically in a discretized form, Eq. (15) becomes:

$$\sum_i \left(S_R \Delta x\right)_i = q''_R\left(x = X\right) - q''_R\left(x = 0\right) \tag{16}$$

in which Δx is the increment of the mesh and the index i represents the i-th segment of the discretized domain. In this paper, $\Delta x = X / (N - 1)$, where X is the distance that separates the walls and N is the number of regions in which the domain was discretized (X = 1 m and N = 200 in this study).

Table 1 shows the calculation of the radiative energy balance through the original formulation of the CW model and with the proposed correction in the RTE presented in this paper by means of two approaches for the temperature profiles of the Eqs. (11) and (12), based on the approximation of the Eq. (16). The first approach is based on the summation of the radiative heat source obtained in each domain element; the second one consists in evaluating the difference between the heat fluxes calculated at each of the boundaries. By the table, it can be observed that the values of q''_R found with the application of the proposed methodology are closer to the two approaches employed, both for Profile 1 and Profile 2, when compared with the results obtained through the standard CW model. With respect to the original formulation, the energy balance of the modified CW model is satisfied with a deviation of 0.48% for Profile 1 and 4.38% for Profile 2. Nevertheless, it is easy to verify that the correction performed in the RTE was not enough for the energy balance to be fully satisfied, as shown in the result obtained for Profile 2. Thus, it can be concluded that only the inclusion of the derivative term du_{ij}/ds, which was neglected in a wrong way by Solovjov and Webb, 2002, did not lead to the energy conservation. Probably, it would have been necessary to include some more hypotheses in the correction of the CW model to ensure that the energy balance was met.

Table 1. Energy balance calculated with the original formulation of the CW model and the proposed methodology.

Approach	Profile 1		Profile 2	
	CW standard (kW/m²)	**CW modified** (kW/m²)	**CW standard** (kW/m²)	**CW modified** (kW/m²)
$\sum_i (S_R \Delta x)_i$	27.0532	15.0324	24.4717	16.6235
$q''_R(x=X) - q''_R(x=0)$	6.2004	14.9610	10.2413	17.3852

3.2 Comparison between the CW model and the LBL solution

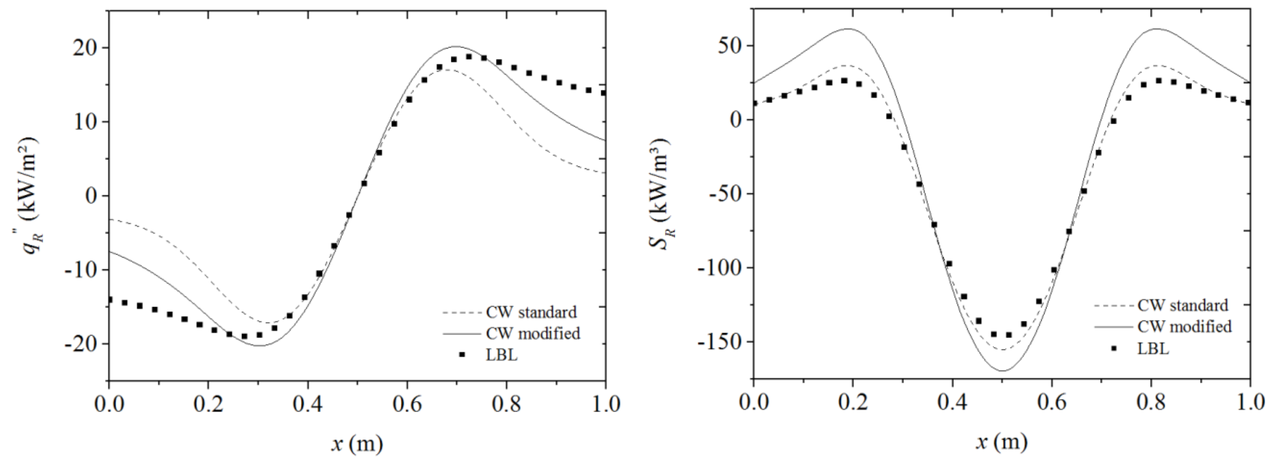
To measure the improvement that the proposed implementation in this study provided for the calculation of q''_R and S_R, Figs. 3(a) and 3(b) respectively, illustrate the behavior of these two quantities. As can be seen in Fig. 3(a), the curve of the radiative heat flux obtained by the proposed cumulative wavenumber model agrees better with the line-by-line integration than the result found by the CW method in its original formulation, especially near boundaries, which are regions where the largest discrepancies between the solutions are observed. According to Table 2, which shows the maximum and average percentage discrepancies between the CW models and the LBL method, the maximum deviation of q''_R drops from 57.33% with the original model to 34.15% with the proposed approach considering Profile 1, which represents an improvement in the result, but is still not capable to reliably reproduce the benchmark solution. Figure 3(b) presents the radiative heat source for the same temperature profile and shows that, as reported in the literature (Solovjov and Webb, 2002; 2005), the CW model represents very well the behavior of the solution when compared to the LBL integration, since the maximum deviation found is 7%. Regarding the modification of the CW method proposed in this work, the deviation from the LBL method became greater than that obtained by the original formulation, reaching 24.12%, so that, unfortunately, the RTE correction was not favorable for the accuracy of the solution.

Figures 4(a) and 4(b) show the behavior of the radiative heat flux and the radiative heat source, respectively, for Profile 2. Similar to the previous case and as it may be noted in Fig. 4(a), an enhancement in the determination of q''_R is perceived, since the maximum deviation in relation to the LBL integration reduces from 16.22% (with the standard model) to 9.51% (with the modified model), as stated in Table 2. On the other hand, in the radiative heat source, i.e., Fig. 4(b), the observed effect of the proposed correction is the opposite: a worsening in the performance of the solution appears, so that the results generated by the modeling of Solovjov and Webb, 2002, more accurately represent the behavior described by the line-by-line integration, since the maximum deviation increased from 6.76% to 22.72%. Once more, the simple adjustment that was proposed did not affect the solution of the problem adequately, which indicates that the applied methodology should be reformulated in order to overcome this issue.

Table 2. Normalized percentage deviations for the radiative heat flux and the radiative heat source comparing the CW methods and the LBL solution.

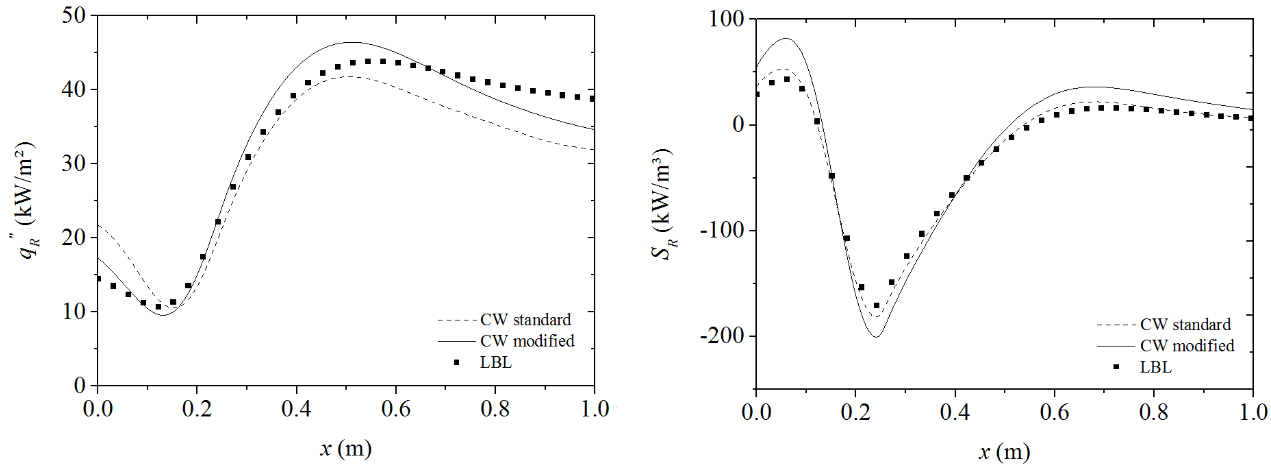
Profile	CW standard				CW modified			
	q''_R		S_R		q''_R		S_R	
	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)
1	57.33	25.88	7.00	3.68	34.15	13.34	24.12	14.84
2	16.22	8.22	6.76	2.85	9.51	4.48	22.72	10.12

For the two cases studied, the proposed correction for the radiative transfer equation did not provide as good results as expected. The initial prediction was that only such a modification in the CW model would be sufficient for the radiative energy balance to be met and the method becomes conservative. However, it was found that, in the best of perspectives, the energy balance was checked with a deviation of 0.48% and that, in the second test case, the discrepancy found was greater than 4%. As a consequence, although the result of the radiative heat flux has been improved, it was not possible to observe and improvement in the performance of the radiative heat source, which means that it would be necessary to investigate the model with greater depth to propose some way to perfect the solutions.



(a) (b)

Figure 3. Results for the radiative heat transfer obtained with the CW models and the LBL solution considering Profile 1: (a) Radiative heat flux; (b) Radiative heat source.



(a) (b)

Figure 4. Results for the radiative heat transfer obtained with the CW models and the LBL solution considering Profile 2: (a) Radiative heat flux; (b) Radiative heat source.

4. CONCLUSIONS

In the present paper, it was proposed a simple manner to correct the cumulative wavenumber method in order to the radiative energy balance was checked, a fact that was treated in the wrong way in the original formulation of the model developed by Solovjov and Webb, 2002. The modification consisted in including a term in the solution of the RTE, which corresponds to the derivative of the function u_{ij} with respect to the position and is neglected in the standard modeling. As this term is not, in fact, null, it cannot be ignored. So, the proposed methodology was applied to solve the radiative transfer in a one-dimensional medium slab with carbon dioxide in a homogeneous concentration between the plates. Although the presented correction has promoted an improvement in the result of the radiative heat flux, the energy balance was not completely met, so that the found results still show considerable deviations concerning the LBL integration. Moreover, for the two test cases analyzed, the radiative heat source had a lower performance than that obtained by the CW model in its original formulation, since the deviations in relation to the benchmark solution increased. Anyhow, it is important to emphasize that this work is only an introductory study on the CW model in the search for energy conservation and, therefore, it is recommended that an in-depth study of the standard formulation to understand why the correction of the method was not sufficient for check the energy balance completely and obtain greater accuracy of the solution in relation to the LBL integration.

5. ACKNOWLEDGEMENTS

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