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APPROACH FOR THE ABSORPTIVITY ESTIMATION OF A NON-GRAY SURFACE BOUNDING PARTICIPATING MEDIA

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Abstract: *The thermal radiation is a complex phenomenon, and of great importance for processes that involve high temperatures, such as combustion. Therefore, to evaluate these usual engineering problems, such as the design of combustion chambers, furnaces and ovens, it is essential to estimate the heat transfer by radiation. However, these problems attain an even higher degree of complexity, due to the possible presence of participating medium, such as carbon dioxide and water vapor, common combustion products. These chemical species, are called participating media due to their influence on the thermal radiation that permeates them, by absorbing a portion of the incoming radiation, or also by emission. This occurs at different portions of the spectrum, depending on local thermodynamic factors and the species of interest, increasing the complexity to model these systems. In order to solve these problems, it can be employed the line-by-line integration of the radiation intensity over the entire spectrum, which is the benchmark solution, providing the exact result, but at a high computational cost. To overcome this computational limitation, several models were developed over the years, such as the gray-gas (GG) and the weighted-sum-of-gray-gases (WSGG), which are excellent models to represent the thermal radiation transfer across participating media. However, they are limited to be used with black and gray boundaries, while most of engineering problems have the presence of non-gray bounding walls. In recent years, researchers were able to employ the WSGG model in test cases involving non-gray bounding walls, with good accuracy when compared to the LBL solution. But it comes with a certain limitation, where a temperature had to be arbitrated in order to perform the total absorptivity calculation for the non-gray wall, form its respective spectral emissivity profile. The objective of this study is to perform an in-depth analysis of the total absorptivity of a non-gray surface, subjected to incoming radiation from a black surface that has travelled across a participating medium with a non-uniform temperature distribution. This media is composed of carbon dioxide and water vapor. Multiple reference temperatures were evaluated, based on the temperature profile studied. From the results obtained, it is possible to estimate a reference temperature that provides accurate results, and a good estimation of the total absorptivity of a non-gray surface.*

Keywords: *thermal radiation, numerical heat transfer, non-gray, absorptivity*

1. INTRODUCTION

Over the years, the increase of computational power has been significant, making it possible the usage of numerical simulation in various steps of engineering design. However, even with these technological advancements, it is still very difficult to simulate the effects of thermal radiation in larger scales within participating media, without compromising the accuracy of the results. These applications match common engineering problems, such as the design of burners, ovens, furnaces and its flues. These devices operate at high temperatures and handle gases that are not transparent to radiation.

For the correct design of these devices, the thermal radiation must be correctly accounted for. Nevertheless, due to the directional and spectral dependence of thermal radiation, the solution of the radiative intensity field, if done by the line-by-line integration, is excessively time consuming. To obtain the most accurate result, hundreds of thousands of spectral lines must be evaluated, for every direction that the thermal radiation is transported. For larger three-dimensional models, the computational power required for the iterative development of some designs, can deem this approach non-feasible.

To overcome this, a number of models have been developed over the years, providing good accuracy at moderate computational times. The drawback of some of these models are their strict applicability, where not many can handle the behavior of participating media bound by non-gray walls, hampering the correct estimation of the intensity field and causing deviations from the exact solution. However, in recent years, some models were developed aiming to improve the solution of the intensity field on domains bounded by non-gray walls, with greater accuracy and less computational resources.

Da Fonseca et al. 2018 assessed the usage of the WSGG methodology for use on heat transfer over a participating medium comprised of a mixture of CO_2 and H_2O bound by non-gray walls. The methodology consisted in the assumption that the absorption coefficient of the medium is assumed to be randomly spread over the entire spectrum, with an equal probability. The encountered heat flux deviation from the LBL solution was reduced in one of the studied scenarios from 9% with the assumption of a gray wall, to 4.6% when the wall was assumed non-gray. The researchers noted that the estimation of the absorptivity equal to the emissivity at the wall temperature is not an adequate assumption for most scenarios, and that could provide larger deviations in some situations.

In 2019, Da Silva and colleagues implemented a modification to the SLW methodology, where it was assumed a reference state, for the computation of properties, such as the absorption cross-section. This reference state is also used to compute the total hemispherical absorptivity, by the assumption of a diffuse surface. The group evaluated the radiative heat flux and radiative source terms over an 1D slab containing a mixture of CO_2 and H_2O, at 1 atm, subjected to non-uniform temperature distributions. The group found similar results that of Da Fonseca et al. 2018, where the methodology provided a better representation of the radiative transfer, when comparing to the black and gray wall handling.

Da Fonseca et al. in 2019 provided a deeper evaluation of the usage of reference temperatures for the estimation of the heat transfer over participating media, accounting for non-gray bounding walls. The main problem was solved assuming the reference temperature being a spatial average of the media temperature, following the work of Da Silva et al. 2019, for the calculation of the total hemispherical absorptivity. The method provided good agreement with the LBL integration method, providing a reduction in computational time proportional to the number of the wall spectral bands, when compared to similar methods that evaluate the spectral bands separately. The group also evaluated the influence on the heat flux and source term deviations for a range of reference temperatures, which proved to impact greatly the final result, ranging from 2% deviation, up to 20%.

With the good accuracy of the results obtained in the aforementioned study and the relative efficiency in computational time, the present study proposes to evaluate the usage of the reference temperature, identifying possible methodologies for its calculation for different scenarios, comprising different temperature profiles, species concentrations for a specific non-gray wall, evaluated by previous studies in the literature.

2. METHODOLOGY

2.1. Spectral Properties of Surfaces

Surfaces can be represented as an idealized model, called blackbody, which is a perfect emitter and absorber. Surfaces considered black, absorb all of the incoming radiation incident to them, independent of the wavelength, therefore are called gray. Also, regardless the temperature or wavelength being evaluated, no other surface can emit more energy than the blackbody. Finally, the blackbody is diffuse, therefore the emitted energy is independent of the outgoing angle (Bergman and Lavine, 2017).

Real surfaces, do not follow the same principles as the ones mentioned for the blackbody, instead they are compared to it. The emission of a real surface is compared to the one of a blackbody using the property emissivity, which in its spectral directional form is given by:

$$\varepsilon_{\lambda,\theta}(\lambda,\theta,\phi,T)=\frac{I_{\lambda,e}(\lambda,\theta,\phi,T)}{I_{\lambda,b}(\lambda,T)} \quad (1)$$

where ε is the emissivity, λ is the wavelength, T is the temperature, I is the radiative intensity, θ is the polar direction, φ is the azimuthal direction, and the subscripts e and b correspond to the emitted portion and the blackbody energy, respectively.

$$\alpha_{\lambda,\theta}(\lambda,\theta,\ \phi)=\frac{I_{\lambda,i,abs}(\lambda,\theta,\phi)}{I_{\lambda,i}(\lambda,\theta,\ \phi)} \quad (2)$$

where α is the absorptivity and the subscripts i and abs correspond to the incident and absorbed radiation portions, respectively. In respect of the absorbed portion of a real surface, the property called absorptivity is employed, shown in Eq. (2), in its spectral directional form. It should be noted that this is not a surface property, due to its relation to the incoming radiation (Modest, 2013). Therefore, with the modification of the incoming radiation, a common occurrence in problems with changes in composition of participating media, the total absorptivity value can suffer changes.

2.2. Radiative Heat Transfer in Participating Media

The thermal radiation incident to a molecule or particle of the media can alter the amount of radiation of the particular path the rays were travelling along. This is caused by the distinct energy levels of the atoms in the molecules, where at specific levels, the atom can receive the impact of a incident photon and absorb its energy, therefore attenuating the intensity along the radiation path. Or, at a specific level, release a photon, which would consist in the augmentation of the incident ray (Modest, 2013).

The total amount of radiation absorbed through the medium at a specific optical path is proportional to the magnitude of the energy and the length travelled by the radiation beam (Modest, 2013). By this definition, it is possible to describe the variation of intensity due to absorption by:

$$dI_{\lambda,abs}=-\kappa_\lambda I_\lambda ds \tag{3}$$

where κ is the absorption coefficient of the participating media and s is the radiation path.

The radiation can also be emitted by the media, therefore the radiation travelling along the path can be augmented by emission. This is expressed by:

$$dI_{\lambda,em}=\kappa_\lambda I_{b,\lambda} ds \tag{4}$$

where the subscript *em* represents the emission portion of the intensity.

When neglecting the effects of scattering, one can combine Eq. (3) and Eq. (4), which results in the radiative transfer equation, (RTE).

$$\frac{dI_\lambda}{ds}=\kappa_\lambda(I_{b,\lambda}-I_\lambda) \tag{5}$$

Eq. (5) represents the variation of intensity along an optical path *s*, which can occur as augmentation due to emission or attenuation due to absorption. These effects are represented by the first and second terms inside the parentheses of the right-hand side of the equation.

2.3. Line-by-Line (LBL) Integration

To evaluate the radiative transfer along a path, if the spectral data is available, one could solve the radiative transfer equation, Eq. (5) for all portions of the spectrum. Then the integral of the results is computed to obtain the total intensity (*I*) along the path *s*. This is the methodology known as the line-by-line integration (LBL) method. With it, thermal radiation problems can be solved with a high degree of accuracy. However, due to the fact that thousands of spectral lines are evaluated to compute the spectral integration over a single direction, this method is deemed computationally expensive. Also, this method requires the knowledge of the spectral properties of the participating medium over the entire spectrum. This is usually done by using spectral databases, which are used to provide the absorption coefficients of each of the participating species. The most commonly used databases are the HITRAN (Gordon *et al.*, 2017) and HITEMP (Rothman *et al.*, 2010). To illustrate, Figure 1 shows a segment of the absorption coefficients for CO_2 at 1000 K and 1.0 atm, between 3400 and 3850 cm^{-1}. It can be seen the strong spectral dependence of the absorption coefficient, which could affect the resultant absorptivity values of non-gray walls bounding such media.

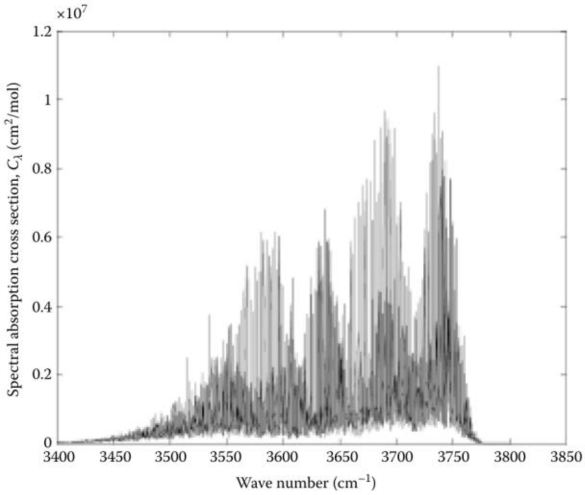

Figure 1. Spectral absorption cross-section for CO_2 at 1000K and 1atm for a portion of the spectrum [Howell *et al.* 2012].

2.4. Total Surface Absorptivity and Benchmark Reference Temperature

One of the main aspects of this work is to determine the total absorptivity of a non-gray surface bounding a non-gray media, by utilizing the blackbody distribution and a certain reference temperature (Howell *et al.*, 2012).

$$\alpha_\theta=\varepsilon_1 F_{0\rightarrow\lambda_1 T}+\varepsilon_2 F_{\lambda_1 T\rightarrow\lambda_2 T}+... \quad (6)$$

where F corresponds to the blackbody emission fraction and its subscripts represent the spectral bands at constant spectral emissivity of the non-gray surface.

Equation (6) is used in this study alongside a set of reference temperatures to estimate the total absorptivity of the surface. These references are, the average temperature of the mediam, T_{avg}, the wall temperature, T_{wall} and the arithmetic average between both of them, $T_{w,avg}$. The benchmark reference temperature, T_{reb} is a concept introduced in this work. This quantity represents the required temperature in which the total directional absorptivity calculated by means of a blackbody distribution would equate the one by the LBL solution. Using this new reference temperature, it is possible to compare its value to the respective references detailed on the previous section, then evaluating how they fare against the LBL solution for either the temperature and total absorptivity.

3. PROBLEM DESCRIPTION

The study comprises the evaluation of the heat transfer through radiation of hemispherical domain of radius r=1m, permeated by participating medium at the pressure of 1atm. Due to the conditions of symmetry proposed, where there is no variation of properties in the polar and azimuthal coordinates, only on the radial one, this domain is considered unidimensional, as seen in **Figure 2**(a). In this study, two mixtures of CO_2 and H_2O were evaluated. These mixtures represent a molar ratio of H_2O of 1.0 and 2.0, where the CO_2 molar fraction was kept constant, at 0.1.

At the center of the hemisphere, r=0, is located a non-gray surface, called the control surface in this study. Two different spectral properties were evaluated for this control surface, shown as ε-Profile 1 and 2 on **Figure 2**(b). The hemisphere border, coordinate $r=R$ shown in **Figure 2**(a), is modelled as a blackbody, where its temperature follows the participating media temperature distribution.

$$T(r)=(400\ K)*\left[1+\left(\frac{10}{0,9}\right)\frac{r}{R}-\frac{5}{0,9^2}\left(\frac{r}{R}\right)^2\right] \quad (7)$$

$$T(r)=(400\ K)*\left[1+\left(\frac{10}{0,9}\right)\left(\frac{R-r}{R}\right)-\frac{5}{0,9^2}\left(\frac{R-r}{R}\right)^2\right] \quad (8)$$

Two non-symmetrical temperature profiles were evaluated, called Profile 1 and Profile 2. These temperature profiles follow a temperature distribution given by Eq. (7) and Eq. (8). The difference between these temperature profiles is the position at which the maximum temperature is located on the radial coordinate. Profile 1 represents a temperature distribution where T_{max} occurs at r^*=0.9 and Profile 2, at r^*=0.1. The variable r^* is the non-dimensional radial length of the hemisphere. Both profiles possess a temperature of 400K at r=0 and achieve a maximum temperature of 2400K. T_{wall} is 2032.65K and 2375.31K for Profiles 1 and 2, respectively.

For the spectral integration of the RTE, the LBL method was employed, where the HITEMP 2010 database was used as the means to obtain the absorption coefficient of the species. The HITEMP files were generated within the spectral range from 0 to 25000 cm^{-1} at a resolution of approximately 0.067 cm^{-1}. With this configuration, a total of 375.000 spectral lines were evaluated for each case. The spatial integration of the RTE was performed using the finite-volume-method (FVM). The domain was divided into equally spaced elements in the radial direction of the hemisphere, and the polar and azimuthal coordinates were neglected due to the symmetry condition of the domain. A mesh sensitivity analysis was performed and showed that 100 elements is sufficient disregard any significant errors due to the spatial discretization.

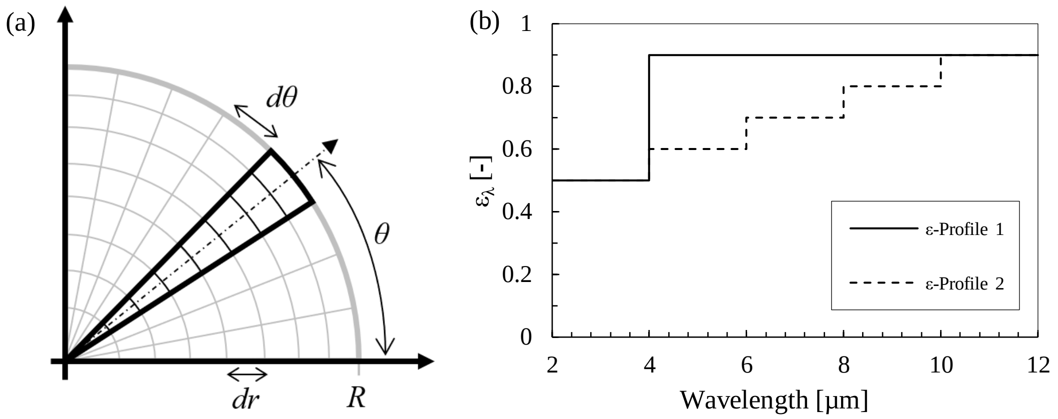

Figure 2. (a) Domain representation. (b) Spectral properties of the control surface.

4. RESULTS AND DISCUSSION

4.1. Total Absorptivity for Temperature Profile 1

The first set of cases is presented in this section, where the focus is on the temperature profile 1, represented by Eq. (7). The results are organized in function of the molar fraction of H_2O of the mixture, for each of the spectral emissivity profiles, or ε-Profiles, of the control surface.

Figure 3(a) present the obtained results of the total absorptivity of the control surface corresponding to the ε-Profile 1. It can be seen that from the two mixtures of participating medium, there was little variation in the absorptivity value for the control surface, where the absorptivity values obtained by the LBL integration ranged from 0.53 to 0.528. These values are shown in markers When comparing these values to the reference temperature methodology, traced as lines in the figure, the reference temperature that provided the better agreement to the LBL results was the hemisphere wall temperature, T_{wall}. With this reference, the total absorptivity error achieved values of 1.7% and 2.1% for the cases with a molar ratio of H_2O of 1.0 and 2.0, respectively.

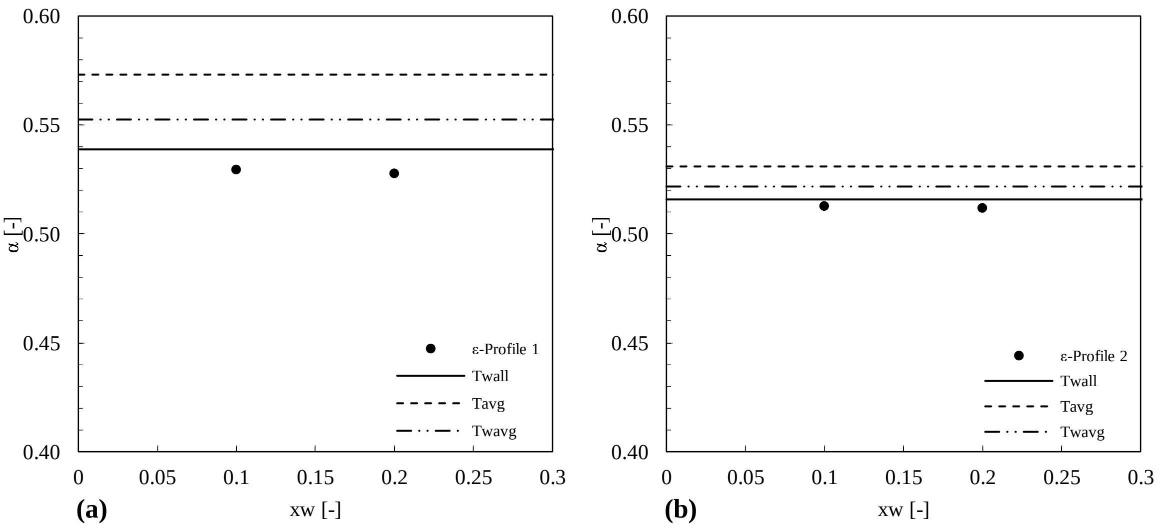

Figure 3. (a) Total absorptivity for the spectral emissivity profile (ε-Profile) 1 and (b) for ε-Profile 2.

Figure 3(b) shows the results for the second spectral emissivity profiles of the control surface, called ε-Profile 2. With this emissivity profile, the total absorptivity results calculated via LBL integration of the RTE achieved values between 0.513 and 0.512. When comparing these values to the ones obtained by assuming a blackbody distribution and the reference temperatures, the closest match to the benchmark values was still T_{wall}. The deviation to the LBL solution using this reference temperature achieved impressive values, ranging between 0.6% and 0.8%, proving to be an excellent estimation of the total absorptivity of a non-gray surface bounding non-gray medium. It should be noted that with the ε-Profile 2, the range of total absorptivities obtained was much narrower than the ones obtained from ε-Profile 1. Therefore the deviations from the LBL solution was significantly lower for all reference temperatures, in this case.

4.2. Total Absorptivity for Temperature Profile 2

The following four test cases present the total absorptivity results for the second temperature profile in this study, Profile 2, represented by Eq. (8). Again the results are presented as a function of the molar concentration of H_2O of the mixture.

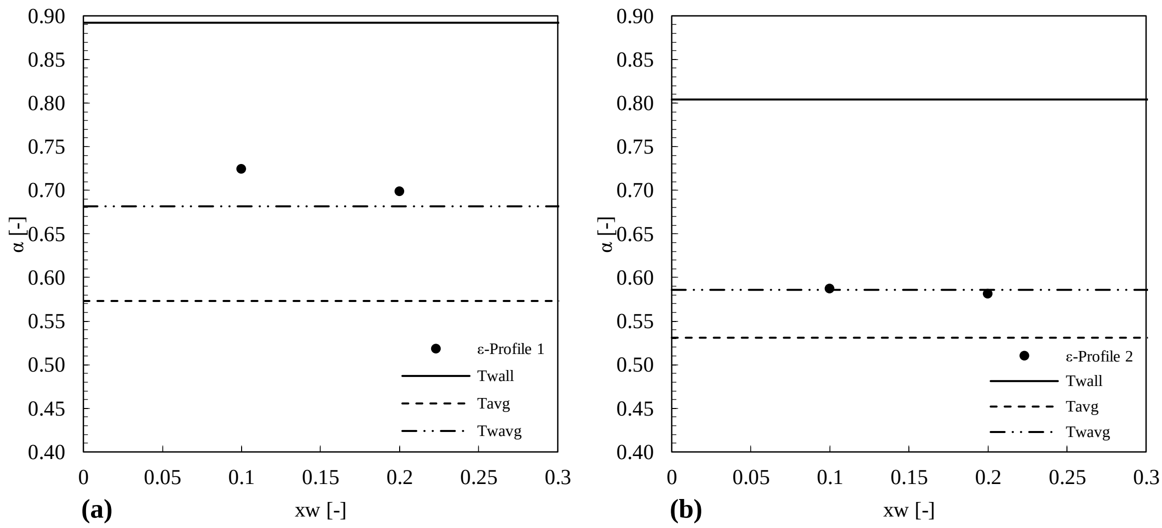

Figure 4. (a) Total absorptivity for the spectral emissivity profile (ε-Profile) 1 and (b) for ε-Profile 2.

Figure 4(a) presents the total absorptivity of the control surface modeled with the spectral properties given by ε-Profile 1.The markers represent the benchmark absorptivity values calculated by the LBL integration and achieved values of 0.724 and 0.699 for an H_2O molar ratio of 1.0 and 2.0, respectively. From these values, the reference temperature that provided the least deviation to the benchmark results was the mean between the average temperature of the mixture and the temperature of the hemisphere wall, $T_{w,avg}$. Comparing to the previous test cases, this temperature provided a larger variation of the absorptivity value with respect of the optical thickness of the medium, but not large enough justify the selection of a different reference temperature for the total absorptivity estimation. This reference temperature is of importance due to the strong influence to the absorptivity value of the hemisphere wall, represented as a blackbody.

In **Figure 4**(b) the ε-Profile 2 is evaluated. With this surface emissivity profile, there was little modification to the total absorptivity value for the two mixtures studied, going from 0.587 for the mixture of CO_2 and H_2O molar fraction of 0.1 and 0.1 respectively, to 0.582 when the molar fraction of H_2O was increased to 0.2. When compared to the values obtained by the reference temperature, shown as lines in the figure, it is noted that again $T_{w,avg}$ provides the best agreement to the benchmark values, reaching a deviation of only 0.2% for a molar ratio of 1.0 and 0.7% for a molar ratio of 2.0 of the mixture.

4.3. Benchmark Reference Temperature

The benchmark reference temperature, T_{reb}, calculated by the procedure described in section 2.4 is evaluated against the reference temperatures obtained by the two temperature profiles studied. The objective of the evaluation of this variable, is to determine the applicability of this reference temperature methodology, for the different surface emissivity profiles. This is done due to the fact that the reference temperature is independent of the ε-Profiles, hence they can be more easily compared.

In **Figure 5**, the values for T_{reb} are shown as markers, for the two different ε-Profiles evaluated. On the abscissa one can observe the influence of the increase of molar fraction of water vapor. The reference temperatures, being unaltered by the mixture, are represented as lines in the graph.

Figure 5(a) presents the results obtained for the temperature Profile 1, where the maximum temperature occurs close to the hemisphere wall, at the non-dimensional radial position $r^*=0.9$. From the results of T_{reb}, one can observe that for the four test cases, the benchmark temperature achieved values higher than the wall temperature, being even higher than the maximum temperature of the domain, 2400K. This could be linked to the approximation that is being executed for the calculation of the total absorptivity of the surface, where it is being assumed a blackbody energy distribution over the spectrum for the representation of a non-gray-surface bounding non-gray medium. This non-gray medium posses a spectral signature, where it can emit or absorb energy at widely different levels over the spectrum. This in turn can weigh the total absorptivity value toward a specific value of the profile. In this case, since the total absorptivity resulted in a small value through the LBL integration, this correspond to higher temperatures when dealing with a blackbody energy distribution. Nonetheless, even with a significant deviation of the value of T_{wall} against T_{reb}, this reference methodology still provided an excellent estimation of the total absorptivity value for the control surface, as seen on the previous section.

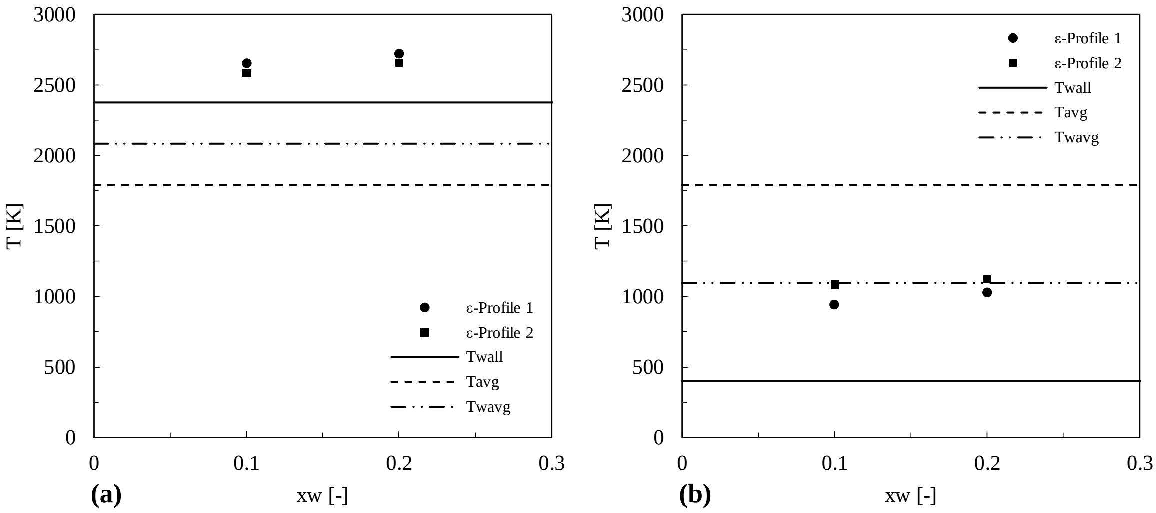

Figure 5. (a) Benchmark reference temperature for the temperature profile 1 (a) and profile 2 (b).

Figure 5(b) presents the same evaluation of T_{reb} against the references. It is observed a small difference in the value for the benchmark reference temperature with respect of variation in molar concentration of the species, with a small tendency of increase for thicker medium. Also, between the two surface emissivity profiles, the value of $T_{w,avg}$ closely matched the LBL calculated ones. This corroborates with the results obtained in the previous section and shows the excellent applicability of this reference temperature for the estimation of the total absorptivity of the control surface.

Table 1 presents the summary of the results obtained in this study, comprising T_{reb}, the total LBL absorptivities and the deviations encountered for each of the references. Overall, the reference temperature methodology promised good agreement with the results, with the selected references that better correlate with LBL data were T_{wall} for the temperature Profile 1 and $T_{w,avg}$ for the Profile 2.

Table 1. Summary of results obtained.

Temp. Profile	ε-Profile	X_c [-]	X_w [-]	T_{reb} [K]	α_{LBL} [-]	δT_{avg} [-]	δT_{wall} [-]	$\delta T_{w,avg}$ [-]
Profile 1	ε-1	0.1	0.1	2657.2	0.530	8.2%	1.7%	4.3%
		0.1	0.2	2722.5	0.528	8.6%	2.1%	4.6%
	ε-2	0.1	0.1	2590.8	0.513	3.5%	0.6%	1.8%
		0.1	0.2	2656.7	0.512	3.7%	0.8%	1.9%
Profile 2	ε-1	0.1	0.1	944.2	0.724	20.9%	23.1%	5.9%
		0.1	0.2	1030.0	0.699	18.0%	27.6%	2.5%
	ε-2	0.1	0.1	1086.9	0.587	9.6%	37.0%	0.2%
		0.1	0.2	1126.7	0.582	8.7%	38.3%	0.7%

5. CONCLUSIONS

The present study consisted in the evaluation of the thermal radiation heat transfer over a participating media bound by a non-gray wall, called control surface, and a black hemisphere. A total of 8 test cases were evaluated, being two different participating media compositions, two surface emissivity profiles for the control surface and two non-uniform temperature profiles over the domain.

The total absorptivity of the control surface was calculated by the LBL integration method, and its results were compared by the ones obtained through a blackbody distribution and different reference temperatures given by the temperature profiles. The benchmark reference temperature, that is, the reference temperature that would achieve the total absorptivity obtained by the LBL integration method was also investigated.

The results showed excellent results for the estimation of the total absorptivity using the reference temperatures, where deviations from the LBL solution achieved values as low as 0.2% for the preferred references. For the temperature profile 1, which is described by a parabolic temperature distribution with its maximum value of 2400K close to the black hemisphere, at a non-dimensional distance of r^{*}=0.9. For this profile, the preferred reference temperature was the temperature of the hemisphere wall, T_{wall}. This showed a strong influence of the black surface over the results.

For the temperature distribution represented by the temperature profile 2, which is a mirrored version of the aforementioned profile, with the maximum temperature occurring at r^{*}=0.1. The total absorptivity value calculated via $T_{w,avg}$ provided the closest match to the LBL solution. Using this reference temperature, the error ranged from 0.2% to 5.9% for the total absorptivity values.

The benchmark reference temperatures provided an interesting insight on the evaluation of the results, showing higher values than the maximum temperature of the domain. These results can be explained by the cire development of the methodology, where a blackbody distribution is used for the determination of total properties of non-gray walls bounding non-gray media. The results obtained in this study can provide a better understanding of the applicability of the reference temperature approach, and guide the selection of the optimal reference temperature for the application on global models, such as WSGG and SLW methodologies.

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7. RESPONSIBILITY NOTICE