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NEW WAY FOR FITTING THE TOTAL EMITTANCE FOR THE WSGG METHOD USING TEMPERATURE AND PARTIAL PRESSURE IN THE WEIGHTING FUNCTION

Alexandre Huberto Balbino Selhorst
Francis Henrique Ramos França
Universidade Federal do Rio Grande do Sul - Avenida Sarmento Leite, 625
frfranca@mecanica.ufrgs.br

Abstract. *This study proposes a new method for fitting coefficients for the WSGG model. Traditionally, the WSGG models account only for the temperature on its weighting coefficients; however, the spectral behavior of combustion gases have a strong dependence on other parameters such as the partial pressure. It is proposed a method to account for the partial pressure of a mixture of CO_2 and H_2O at two fixed mole ratios. The chosen mole ratios are those present on methane and ethanol flames, which are of wide application. The results so far are showing an increase in the accuracy of the method.*

Keywords: *Radiation in participating media, WSGG model, Levenberg-Marquardt algorithm*

1. INTRODUCTION

To date, combustion processes are the main sources of global energy generation (IEA, 2017). This scenario leads to a vast emission of carbon dioxide and other greenhouse gases, which in turn contribute to the greenhouse effect. While new energy sources are under investigation, it is paramount to burn fuel most effectively. Burning fuels leads to the emission of participating gases at high temperatures, meaning that radiation is the main mechanism of energy transfer. Therefore, knowing how the emitted gases contribute to the radiation is an important instrument to optimize the burning of fuels in energy production.

There are a wide variety of methods to calculate the radiation in participating media. The most accurate is the Line-by-Line (LBL) integration and is generally used as a benchmark solution. However, the LBL is computationally costly and time demanding, which makes it unsuitable for most engineering applications. One of the alternatives to the LBL integrations is the weighted-sum-of-gray-gases (WSGG) model, which reduces the computational time significantly with the expense of some accuracy. Needless to say, there are other models with different accuracies and computational costs available in the literature.

Referring to the variety of models available, one model that is able to produce highly accurate results and could be used as a benchmark solution is the single narrow band (SNB) model, as pointed out by Chu *et al.* (2011). Conversely, the SNB model is still not suitable for daily engineering applications due to the number of spectral evaluations needed (Modest, 2013). Other models, such as the spectral line-based sum-of-gray-gases (SLW) (Denison and Webb, 1993) and the full spectrum correlated-k method (FSCK), are computationally less expensive than the SNB model.

Both SLW and FSCK models are based on redistributing the absorption lines on the wavenumber. As a consequence, these methods can avoid the abrupt variations presented by the absorption lines as a function of the wavenumber. Note, however, that reordering the absorption lines is also a weak point of both methods with respect to gas mixture applications, (Cai *et al.*, 2014), a characteristic not shared by the WSGG model.

Firstly introduced by Hottel Hottel (1954), the WSGG model assumes a few gray-gases representing the whole radiative spectrum. This way, there are one absorption coefficient and one weighting function for each gray-gas instead of thousands of absorption coefficients. Despite this utter simplicity, the WSGG model is capable of returning good results as shown by many works across the last decades. Also, the WSGG model can be computed with any method of spatial integration, (Modest, 1991).

One of the most used WSGG coefficients is those by Smith *et al.* (1982), which are embedded in some commercial CFD software. In this study, Smith et al. obtained coefficients for two different ratios between water vapor and carbon dioxide, p_{H_2O}/p_{CO_2}. The emittance was fitted to data obtained from the exponential wide band model (EWBM), (Edwards and Menard, 1964). However, with the development of new spectral databases, such as the HITEMP-2010, (Rothman *et al.*, 2010), new correlations that are more accurate than those proposed by Smith et al., were proposed.

Dorigon *et al.* (2013) presented coefficients for open-atmosphere combustion of methane, and fuel-oil. In this study, Dorigon *et al.* (2013), obtained the coefficients by fitting emittances generated from the HITEMP-2010 database, (Rothman *et al.*, 2010). Later, (Cassol *et al.*, 2014) developed a method to use together coefficients initially obtained for individual species. It was presented correlations for CO_2, H_2O, and soot obtained from fitting emittance obtained with the HITEMP-2010 database. Then, using the proposed method, the coefficients were combined according to the medium concentration. Coelho and França (2018) presented different WSGG correlations for methane combustion, therefore at a fixed mixture partial pressure, that are to be used at total pressures ranging from 1 atm to 40 atm.

Recently, Wang and Xuan (2019) proposed a modification in the traditional WSGG method to account for the variation of the total pressure within a medium. Instead of generating different absorption coefficients, the authors proposed a single set of absorption coefficients, and modified the weighting function, so that it depends on the temperature and total pressure.

As can be inferred, throughout the years different WSGG models have been proposed for different applications. However, none of the existing WSGG models account for a variation of the partial pressure within the medium. This study proposes to use the method presented by Wang and Xuan (2019) to fit WSGG correlations that account for the variation of the partial pressure within the medium.

2. METHODOLOGY

The complete determination of radiative heat transfer in participating media involves the solution of the Radiative Transfer Equation (RTE). This work, however, intends to focus on generating WSGG coefficients, which is the fitting to the total emittances of a given species or mixture.

First, the total emittances are generated according to the LBL integration, then the WSGG coefficients are fitted to the set of total emittances obtained from the LBL integration.

2.1 The Absorption Coefficient

One of the difficulties present in problems involving radiation in participation media is the high dependence of the absorption coefficient on the wavenumber, η. As a simplification, the WSGG model represents the whole spectrum with a few gray gases, as shown in Fig. 1.

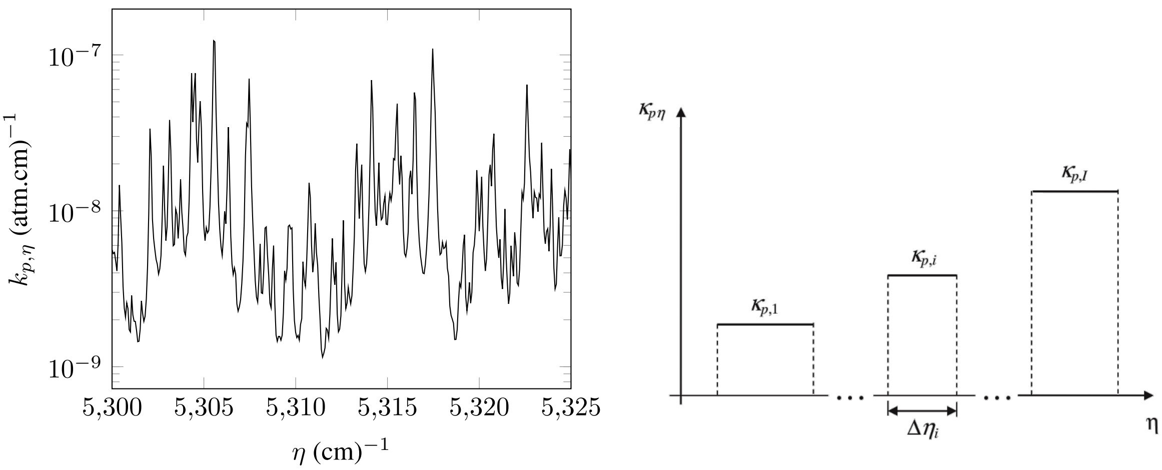

Figure 1: Comparison between the spectral pressure absorption coefficient for LBL integration and the WSGG model.

Note that the pressure absorption coefficient is expressed by:

$$k_{p,\eta} = k_\eta / p_a \tag{1}$$

where p_a is the partial pressure of the mixture or species.

The absorption coefficient can be obtained for each wavenumber by, (Howell *et al.*, 2015):

$$k_\eta(\eta, T, p, Y) = N(T,p) Y C_\eta(\eta, T, p, Y) \tag{2}$$

in which Y is the molar fraction of the species, T is the temperature, C_η is the absorption cross-section, and N is the molecular density given in $molecule/cm^2m$, that is expressed by:

$$N(p,T) = \frac{pN_a}{R_{ug}T} \tag{3}$$

where N_a is the Avogradro's number, and R_{ug} is the universal gas constant.

The absorption cross-section, can be obtained to the LBL integration, according to Howell *et al.* (2015), by:

$$C_\eta = \sum_{i=\eta-\Delta\eta}^{I=\eta+\Delta\eta} \frac{S_i(T)}{\pi} \frac{\gamma_i}{\gamma_i^2 + (\eta - \eta_i)^2} \tag{4}$$

where $\Delta\eta$ cm^{-1} is the spectral span around η, S_i is the line intensity, and γ_i is the band half-width at half-maximum induced by the spectral line broadening phenomenom. In this work, $\Delta\eta_{CO_2}$ was kept at 400 cm^{-1}, and $\Delta\eta_{H_2O}$ was kept at 40 cm^{-1}, as pointed by Ziemniczak (2014).

Using the HITEMP-2010 database, (Rothman *et al.*, 2010), it is possible to obtain γ_i using:

$$\gamma_i(p,T) = \left(\frac{T_{ref}}{T}\right)^{n_c} \left[\gamma_{air,i}\left(p_{ref}, T_{ref}\right)(p - p_a) + \gamma_{self,i}\left(p_{ref}, T_{ref}\right) p_a\right] \tag{5}$$

in which the pressure reference p_{ref} is kept at 1 atm, n_c is the temperature dependence coefficient, and the temperature reference T_{ref} equals 296 K.

Also, using the HITEMP-2010 database, it is possible to obtain the line intensity by:

$$S_i(T) = S_i(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\mathrm{e}^{(-C_2 E_i T)}}{\mathrm{e}^{(-C_2 E_i T_{ref})}} \frac{\left[1 - \mathrm{e}^{(-C_2 \nu_i T)}\right]}{\left[1 - \mathrm{e}^{(-C_2 \nu_i T_{ref})}\right]} \tag{6}$$

where C_2 is the second Planck's constant, E_i is the energy of the lower state, ν_i is the energy difference between the initial and final state, and the total internal partition sums Q depends on molecule characteristics and is the sum of all energy states, such as vibrational, and rotational.

Note that from all the quantities presented at Eq. (6), only Q is obtained through a FORTRAN routine provided within the database, (Fischer *et al.*, 2003), whereas the other quantities are readily available to be read from the database.

2.2 The Total Emittance

In participating gases, although not limited to, the total emittance is regarded as a fraction of energy emitted by a medium over the energy emitted by a blackbody at same thermodynamic conditions. The total emittance is described by, (Howell *et al.*, 2015):

$$\varepsilon(T) = \frac{\int_{\eta=0}^{\infty} I_{b,\eta}(\eta,T)\varepsilon_\eta(T)\mathrm{d}\eta}{\int_{\eta=0}^{\infty} I_{b,\eta}(\eta,T)} \tag{7}$$

in which $\varepsilon_\eta(T)$ is the spectral emittance, and $\int_{\eta=0}^{\infty} I_{b,\eta}(\eta,T)$ is the blackbody intensity equals $\sigma T^4/\pi$. Note that σ is the Stefan-Boltzmann constant.

Kirchhoff's Law states that the spectral emittance ε_η is equal to the spectral absorptance α_η, which is defined by, (Howell *et al.*, 2015):

$$\alpha_\eta = 1 - \mathrm{e}^{(-k_{p,\eta} p_a S)} \tag{8}$$

where S is the path-length of the medium, and $k_{p,\eta}$ is the spectral pressure absorption coefficient.

Thus, substituting Eq. (8) into Eq. (7), gives:

$$\varepsilon(T, p_a S) = \frac{\int_{\eta=0}^{\infty} I_{b,\eta}(\eta,T)[1 - exp(-k_{p,\eta} p_a S)]\mathrm{d}\eta}{\sigma T^4/\pi} \tag{9}$$

in which $p_a S$ is the pressure path-length of the medium. This work considered 23 different temperatures in the range of 300-2500 K, 9 different partial pressures in the range of 0.05-1 atm for the mixtures, and 24 pressure-path-lengths ranging from 0.0001 to 10 atm.m.

It is important to point out that solving Eq. (9) for a given number of wavenumbers will return the total emittance by the LBL integration for a given temperature and $p_a S$. In this work, it was considered a total of 150000 wavenumbers spaning from 0 to 10000 cm^{-1}, (Ziemniczak, 2014).

Figure 2 shows total emittances obtained for a pressure-path-length equals 10 atm.m. Note that, despite the same $p_a S$, there is a difference between the plots. It happens due to the dependence of Eq. (5) on p_a.

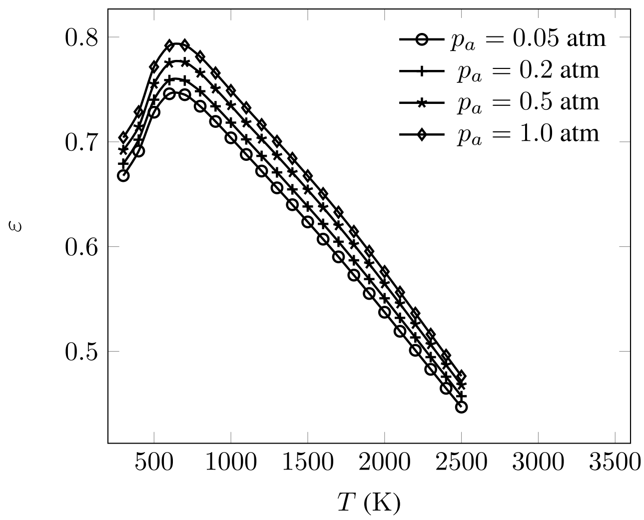

Figure 2: Differences in total emittances due to partial pressure variation at a pressure-path-length of 10 atm.m.

2.3 Total Emittance for the WSGG Method

In the new WSGG method, (Wang and Xuan, 2019), Eq. (9) is rewritten as:

$$\varepsilon(T, p_aS, p_a) = \sum_{i=1}^{I} w_i(T, p_a)[1 - exp(-k_{p,i}p_aS)] \tag{10}$$

where, $w_i(T)$ is a weighting function based not only in the temperature, but also in the p_a, as in:

$$w_i(T) = \sum_{j=0}^{J} a_{i,j}\left(\frac{T}{T_{ref}}\right)^j b_{i,j}\left(\frac{p_a}{p_{a,ref}}\right)^j \tag{11}$$

where T_{ref}, fixed at 1000 K, and $p_{a,ref}$, fixed at 1 atm, are respectively the temperature, and partial pressure of reference. Mathematically, there is no need to use a $p_{a,ref} = 1$; however, to keep the term adimensional, this work decided to do so.

The transparent window is given by:

$$w_0(T, p_a) = 1 - \sum_{i=1}^{I} a_i(T)b_i(p_a) \tag{12}$$

To obtain the WSGG coefficients, Eq. (10) is rewritten utilizing sub-idexes, as in:

$$\varepsilon_{n,u,v} = \sum_{i=1}^{I} a_i(T_n)b_i(p_{a,v})\left\{1 - exp\left[-k_{p,i}(p_aS)_u\right]\right\} \tag{13}$$

where for the present study, $n = 23$, $u = 24$, and $v = 9$. Note that the sub-indexes n, u, and v represent the 23 temperatures, the 24 pressure-path-length, and the 9 partial pressures. Therefore, the amount of total emittances used on this study is 4968.

Next, the emittances that were obtained by the LBL integrations of Eq. (9) are summed up. First, they are summed up for each p_a, as in:

$$\varepsilon_{n,u,V} = \sum_{v=1}^{V} \varepsilon_{n,u,v} \tag{14}$$

where $\varepsilon_{n,u,V}$ is, according to Eq. (13):

$$\varepsilon_{n,u,V} = \sum_{i=1}^{I} a_i(T_n)B_i\left\{1 - exp\left[-k_{p,i}(p_aS)_u\right]\right\} \tag{15}$$

in which B_i is described by:

$$B_i = \sum_{v=1}^{V} b_i(p_{a,v}) \tag{16}$$

Next, the 552 $\varepsilon_{n,u,V}$ emittances with different temperatures are added together as in:

$$\varepsilon_{N,u,V} = \sum_{n=1}^{N} \varepsilon_{n,u,V} \tag{17}$$

which gives 24 $\varepsilon_{N,u,V}$ emittances represented by:

$$\varepsilon_{N,u,V} = \sum_{i=1}^{I} A_i B_i \left\{1 - exp\left[-k_{p,i}(p_a S)_u\right]\right\} \tag{18}$$

where A_i is composed by:

$$A_i = \sum_{n=1}^{N} a_i(T_n) \tag{19}$$

Now, with all the 24 $\varepsilon_{N,u,V}$ emittances, the set of $A_i B_i$, and $k_{p,i}$ can be determined. This work performed analyses with 3, 4, 5, and 6 i-gray gases before choosing the one with better performance, finding results that concur with those presented by Ziemniczak (2014). The correlations with 5, and 6 gray gases returned better results, yet not significantly. The increase in the number of gray gases greatly impacts the computation time in complex problems. Considering this increasing, this study optioned to report a correlation with only 4 gray gases. Having 4 gray gases gives an amount of 8 uncertainties, 4 $A_i B_i$, and 4 $k_{p,i}$ that are fitted against Eq. (18) using a non-linear regression by the Levenberg-Marquardt method, (Marquardt, 1963).

In possession of the pressure absorption coefficients, $k_{p,i}$, and the summation of the weighting function, it is possible to obtain each coefficient a_i, and b_i. The Levenberg–Marquardt method, (Marquardt, 1963), is used over Eq.(15) to fit the coefficients a_i.

Note that since $A_i B_i$ is a product from a multiplication, any value could be assumed for each one, insofar the other one respect the limit imposed by the obtained $A_i B_i$. Wang and Xuan (2019) let their summation B_i to be equal to 1. Although the choice of these values does not compromise the final results when using the correlations, leaving B_i equals 1 returned coefficients with different magnitude. Therefore, this work correlates A_i, and B_i by:

$$\frac{A_i}{N} = \frac{B_i}{V} \tag{20}$$

Note that Eq. (20) does not guarantee that the coefficients will have the same magnitude; however, it increases the likelihood.

The next step is to obtain the coefficients b_i. To do so, all of 23 emittances with different temperature are summed up, which gives:

$$\varepsilon_{N,u,v} = \sum_{i=1}^{I} A_i b_i(p_{a,v}) \left\{1 - exp\left[-k_{p,i}(p_a X)_u\right]\right\} \tag{21}$$

The Levenberg-Marquardt method, (Marquardt, 1963), is now used over Eq. (21) to fit the coefficients b_i, which results in a set of 36 coefficients, 9 for each gray gas.

At last, a multiple linear regression is performed over the coefficients a_i, and b_i, according to:

$$a_i = \sum_{j=0}^{J} c_{i,j} \left(\frac{T}{T_{ref}}\right)^j \tag{22}$$

$$b_i = \sum_{k=0}^{K} d_{i,k} \left(\frac{p_a}{p_{a,ref}}\right)^k \tag{23}$$

This work decided to let J=4, and K=3. Note that other values could be used, returning different results. The correlations obtained are presented on Tab. 1, and 2.

Table 1: WSGG Correlations for $p_{H_2O}/p_{CO_2} = 1$.

i	1	2	3	4
$k_{p,i}(atm^{-1}m^{-1})$	1.80778E-1	1.56481E0	1.03154E+1	1.14971E+2
$c_{i,0}$	9.94207E-2	1.84705E-1	5.17026E-1	7.99000E-1
$c_{i,1}$	1.44866E0	9.49831E-1	3.20342E-1	-1.06194E0
$c_{i,2}$	-1.58565E0	-7.50629E-1	-6.96793E-1	8.75350E-1
$c_{i,3}$	7.57256E-1	1.88966E-1	3.29837E-1	-4.01898E-1
$c_{i,4}$	-1.28754E-1	-1.50186E-2	-5.14702E-2	6.95324E-2
$d_{i,0}$	6.00213E-1	4.01871E-1	2.87807E-1	2.12692E-1
$d_{i,1}$	-1.11589E-2	1.59837E-1	1.19742E-1	2.41787E-2
$d_{i,2}$	-1.44426E-2	-1.61749E-1	-6.64824E-2	-2.21451E-2
$d_{i,3}$	1.14260E-2	6.41249E-2	2.00948E-2	7.68255E-3

Table 2: WSGG Correlations for $p_{H_2O}/p_{CO_2} = 2$.

i	1	2	3	4
$k_{p,i}(atm^{-1}m^{-1})$	1.83614E-1	1.54146E0	9.56465E0	9.24920E+1
$c_{i,0}$	1.01293E-1	2.57484E-1	3.03511E-1	9.25284E-1
$c_{i,1}$	1.28673E0	5.29665E-1	1.06073E0	-1.23808E0
$c_{i,2}$	-1.38933E0	-1.90672E-1	-1.44047E-1	9.26738E-1
$c_{i,3}$	6.82007E-1	-7.25550E-2	6.34401E-1	-3.91610E-1
$c_{i,4}$	-1.18770E-1	2.61063E-2	-9.62227E-2	6.50164E-2
$d_{i,0}$	5.99654E-1	4.18685E-1	2.90936E-1	2.16870E-1
$d_{i,1}$	-4.03518E-2	1.74123E-1	1.91240E-1	3.93602E-2
$d_{i,2}$	2.32950E-2	-2.17455E-1	-1.36858E-1	-3.61964E-2
$d_{i,3}$	-5.45832E-3	9.58939E-2	4.72085E-2	1.50435E-2

3. RESULTS

Figure 3 presents results obtained with the set of coefficients from Tab. 1. Each plot presents the effect of the temperature and pathlength on the total emittance of the mixture of H_2O and CO_2, with the two gases having a given combined partial pressure, and mole fraction equals 1. The total pressure is 1.0 atm, with the remaining gas being no participating in the radiation transfer. The figure compares the total emittance obtained through LBL integration (reference solution), and the WSGG model with the present coefficients and with the coefficients presented in Dorigon *et al.* (2013) for four different partial pressures, 0.05, 0.2, 0.5, and 1.0 atm. As seen, the WSGG model presented by this paper makes a good prediction of the emittance for the three pressure-path-lengths for all different partial pressures, while Dorigon's coefficients lead to considerable deviations. The reason for this is that the latter coefficients were obtained at a fixed partial pressure, whereas the coefficients from this paper are fitted to data for nine different partial pressures.

Figure 4 presents results obtained with the set of coefficients from Tab. 2, which means the mole fraction equals 2. Again, each plot presents the effect of the temperature and pathlength on the total emittance of the mixture of H_2O and CO_2, with the two gases having a given combined partial pressure. The total pressure is also 1.0 atm, with the remaining gas being no participating in the radiation transfer. The figure compares the total emittance obtained through LBL integration, and the WSGG model with the present coefficients and with the coefficients presented in Dorigon *et al.* (2013) for four different partial pressures, 0.075, 0.3, 0.6, and 1.0 atm. The same pattern shown in Fig. 3 is noticed on Fig. 4, where the WSGG model presented by this paper makes a good prediction of the emittance for the three pressure-path-lengths for all different partial pressures, while Dorigon's coefficients lead to considerable deviations.

4. FINAL DISCUSSION

This paper used the method proposed by Wang and Xuan (2019). The results obtained by this paper have shown that a fitting to data for different partial pressures led to better results of total emittances. The next step is to calculate and compare different WSGG models when calculations for the radiative heat source and flux are performed. One may argue about the extra computational time that will be demanded by adopting such an approach when calculating the radiative heat source and flux. However, it is unlikely that the model proposed by this paper will significantly impact the computational cost. The reason for that lies in the fact that this paper keeps the same amount of gray-gases; therefore, the number of spectral calculations for a given problem will remain the same.

New possibilities of application for the WSGG model may arise from the model reproduced by this paper. A further

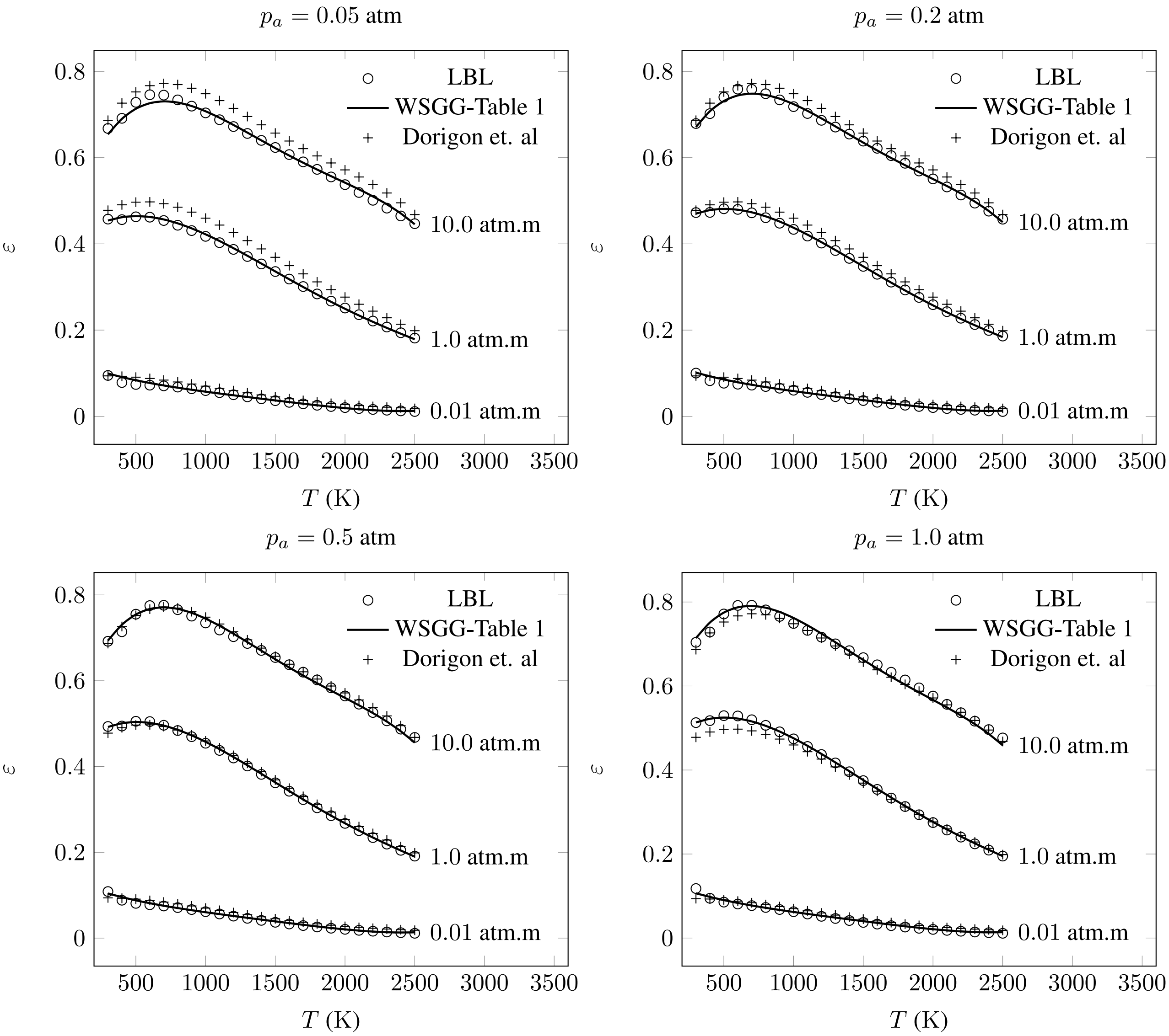

Figure 3: Comparison between emittances for $p_{H_2O}/p_{CO_2} = 1$.

study could lead to a new set of coefficients for different partial pressures and mole ratios, for instance.

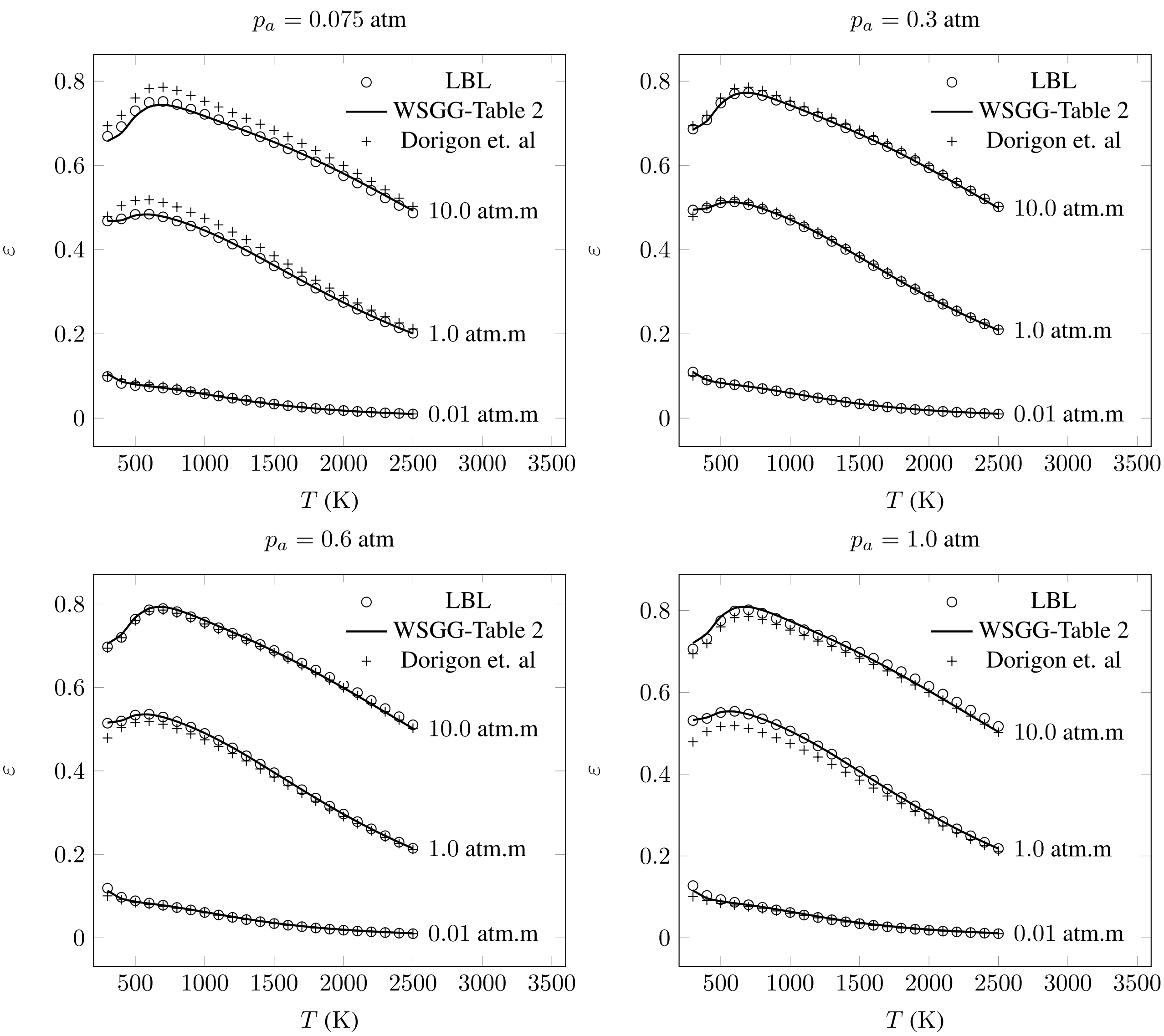

Figure 4: Comparison between emittances for $p_{H_2O}/p_{CO_2} = 2$.

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