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STUDY OF THE INFLUENCE OF SOOT ON THE THERMAL RADIATION ACROSS A UNIDIMENSIONAL FLAME PROFILE USING THE WSGG METHOD

Cesar Augusto Basso
Carlos Henrique Lauermann
Bruno de Luca Zimmer Gomes
Francis Henrique Ramos França
Universidade Federal do Rio Grande do Sul, Department of Mechanical Engineering - Rua Sarmento Leite, 425, Porto Alegre, Brazil
cesara.basso@gmail.com; carloslauermann@hotmail.com; bruno.luca@ufrgs.br; frfranca@mecanica.ufrgs.br

Abstract. *Heat transfer by thermal radiation is a complex phenomenon and takes a major role especially at high temperatures, such as in combustion chambers and furnaces. These applications add another level of complexity because of the presence of combustion products that are opaque to radiation and have a spectral dependence. The thermal radiative field is solved by the radiative transfer equation (RTE). In this framework, the method to solve the RTE on a participating medium is the line-by-line (LBL) integration, which provides the exact result, but at a high computational cost. Several methods were developed over the years aiming to provide accurate solutions, with smaller processing required. One of these methods, evaluated on this paper, is the weighted-sum-of-gray-gases (WSGG), which eliminates the spectral dependence of the RTE calculation. This paper evaluates the dependence of the number of gray gases employed on two different WSGG models for a medium consisting of* CO_2, H_2O *and soot. The analyzed medium consists of three unidimensional flame profiles, in which the molar fractions of the aforementioned products, as well as the temperature at different points, were evaluated experimentally. Results showed that for a total of four gray gases, the WSGG models provided a satisfactory agreement with the benchmark, where the average error reached a maximum of 4,35% and a minimum 0,16%.*

Keywords: *thermal radiation, weighted-sum-of-gray-gases model, numerical simulation, spectral models, combustion.*

1. INTRODUCTION

The heat transfer mechanism by radiation is of extreme importance and cannot be disregarded for most engineering applications from medium to high temperatures, such as combustion processes. In this field of study, the thermal radiation evaluation is dealt with a higher degree of complexity, due to the presence of combustion products, such as H_2O, CO_2 and soot, which are not transparent to electromagnetic waves, therefore can affect the intensity field on the domain of interest (Dorigon *et al.*, 2013).

The evaluation of radiation within participating media in a combustion environment might demand high computational efforts due to the spectral dependence and the strong variation in the thermodynamic state of the participating species (Da Fonseca *et al.*, 2018). Due to this behavior, to solve the radiative transfer equation (RTE) exactly, an integration over the spectrum is needed. This method is called the line-by-line integration method (LBL) and is considered the benchmark solution. It gives the exact solution to the RTE, since all of the spectral dependence for each species is available during the calculation, given the provided property database. As expected, the higher the complexity of the model, the computational time of the solution increases. As a way of avoiding this hurdle, many methodologies were developed over the years as a way of providing accurate results for the RTE, but with lower calculation times. The simplest of the methods is the Gray Gas (GG) model, which ignores the spectral dependence of the participating species and consider it a single gray gas. (Bordbar and Hyppänen, 2018). The WSGG model represents the spectrum as a combination of gray gases with uniform pressure absorption coefficients, which is still simple, but robust. (Da Fonseca *et al.*, 2018). Other models spanned from the WSGG, such as the spectral line WSGG (SLW), cumulative wave number (CW) and full spectrum correlated-k (FSCK). (Denison and Webb, 1993), (Solojov and Webb, 2002), (Modest and Singh, 2002).

Accurate and efficient numerical radiation models applied to participating media are still a task Gomes et al., (2020). Many previous studies provided good results when the WSGG model was compared to the LBL solution, for a wide range of applications. Dorigon *et al.*, (2013) provided a validated WSGG model for a mixture of H_2O and CO_2 at a range of temperatures between 400 and 2500K and to pressures up to 10 atm. Their results shown a good agreement with the benchmark model (LBL), achieving a maximum overall error of 5%.Cassol *et al.*, (2014) provided a correlation between the WSGG model and the LBL for a similar application to Dorigon, but applying a superposition model, which allowed for strong variations in molar concentration of the species, and also the evaluation of soot as one of the participants of the media. Coelho and França (2018) provided a correlation between the WSGG and LBL models for mixtures of CO2 and H2O at a wide range of pressures, from 1 to 40 atm with an average deviation of 5% for the heat flux and source term. Centeno et al., (2018), evaluated a superposition WSGG model over a non-gray sooting medium, representing an ethylene-air jet flame. Results showed good behavior, especially when soot was included as part of the participating medium.

The objective of this study is to determine the effect of soot presence in the radiative heat transfer across a flame profile. The arrangement is based on the work of Gomes et al., (2020), where the Sandia flame D (Barlow and Frank, 1998) is employed. The mean temperature (T) and molar concentration profiles of CO_2 (X_c) and H_2O (X_w) are used as the simulation domain. Three flame radial cross sections were evaluated as the radiation optical paths under study, represented as a ratio of height above the jet nozzle to the nozzle diameter: x/d=30, x/d=45 and x/d=60. These sections were chosen in order to provide continuation of the investigation by Gomes, but with the implementation of soot as a participant species in the simulation domain. Moreover, the relative error is applied to evaluate the WSGG model in the simulations.

2. METHODOLOGY

2.1 Radiative Heat Transfer in Participating Media

In order to evaluate the heat transfer within a participating media, it is required to solve the radiative transfer equation (RTE), which demands the calculation of the spectral radiation intensity, I_η, along all optical paths in the domain. The present study evaluates only non-scattering media, therefore the RTE is given by (Modest, 2013)

$$\frac{dI_\eta}{ds} = \kappa_\eta (I_{b\eta} - I_\eta), \tag{1}$$

where I_b is the blackbody radiation intensity, κ is the spectral absorptivity coefficient of the medium and I is the radiation intensity. The subscript η for the aforementioned variables states their spectral dependence. Eq. (1) 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.

2.2 Line-by-Line (LBL) Integration

To evaluate the radiative transfer along a path, if the spectral data is available, one could solve the RTE, Eq. (1) for all segments of the spectrum. Then compute the integral of the results to obtain the total intensity (*I)* along the path *s*. This is the methodology known as the LBL method. With it, thermal radiation problems can be solved with a high degree of accuracy, however this method is expensive in computational resources. Also, it is reliant in high-resolution spectral databases, which are used to evaluate 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(a) shows a segment of the absorption coefficients for H_2O at 400 K and 1.0 atm, between 1500 anf 1700 cm^{-1}.

The present work employs the HITEMP database, in its latest release, 2010, as the means to calculate the absorption coefficient of the species. The only species evaluated are carbon dioxide (CO_2) and water vapor (H_2O), and the spectral database properties follow the ones from Gomes et al., 2020, where the absorption coefficients were obtained from wavenumbers η=0 cm^{-1} to η=10^4 cm^{-1} at a resolution of 0.067 cm^{-1}, this yielded an evaluation of a total of 150,000 spectral lines.

2.3 Weighted-sum-of-gray-gases (WSGG) Model

While the LBL method requires evaluating the RTE on each spectral line across the entire spectrum for each of the participating gases, the WSGG model provides the solution without the need to evaluate the spectral dependence. First developed by Hottel and Sarofim (1967), it is one of the most widely used models, due to its simplicity and robustness. (Cassol *et al.*, *2014)*, (Da Fonsec*a et al.*, 2018). This method consists of replacing the non-gray medium by a set of gray gases J, plus the transparent windows, J_0, which are optically transparent to radiation. With this method, the RTE is solved for each of the J gases along with J_0, where the Eq. (1) takes the form of

$$\frac{dI_j}{ds} = \kappa_j (a_j I_{bj} - I_j), \tag{2}$$

where the subscript j specifies the gray gas being computed, and the a_j is the weighing intensity factor of gas j. By solving Eq. (2) for all gray gases J and the transparent window J_0, the total intensity can be found by summing all of the partial intensities of each gray gas, by Eq. (3)

$$I = \sum_{j=0}^{J} I_j, \tag{3}$$

As mentioned before, this method decreases the computational time significantly, due to the fact that spectral manipulation of the absorption coefficients is not needed during the calculation. Instead, the WSGG model utilizes fitted pressure absorption coefficients obtained from the high-resolution spectral databases, mentioned in section 2.2. A representation of these coefficients can be observed on Figure 1(b).

This method of solving the RTE is also based on two main assumptions: the first one is that the absorption coefficients, κ_j, are independent of the temperature and partial pressure of the medium; the second is that the spectral regions related to each gray gas J are also independent of the thermodynamic state of the mixture (Da Fonseca *et al.*, 2018). With these two assumptions, one can obtain the emittance data from the aforementioned spectral databases and compute the weighting coefficient a_j by solving Eq. (4) where $\kappa_\eta=\kappa_j$.

$$a_j(T) = \sum_{k=1}^{K} b_{j,k} T^{k-1}, \tag{4}$$

where K is the total number of spectral bands evaluated and k is the spectral band being solved for. The energy conservation of this model is obtained by the computation of the weighing coefficient a_0, that is, for the transparent windows, by Eq. (5), as following.

$$a_0(T) = 1 - \sum_{j=1}^{J} a_j(T), \tag{5}$$

Due to the requirement of calculating these weighting coefficients, WSGG models are not universal, requiring to fit the total emittance data from the spectral databases to obtain effective results for different applications, i.e., temperature, concentration and pressure ranges.

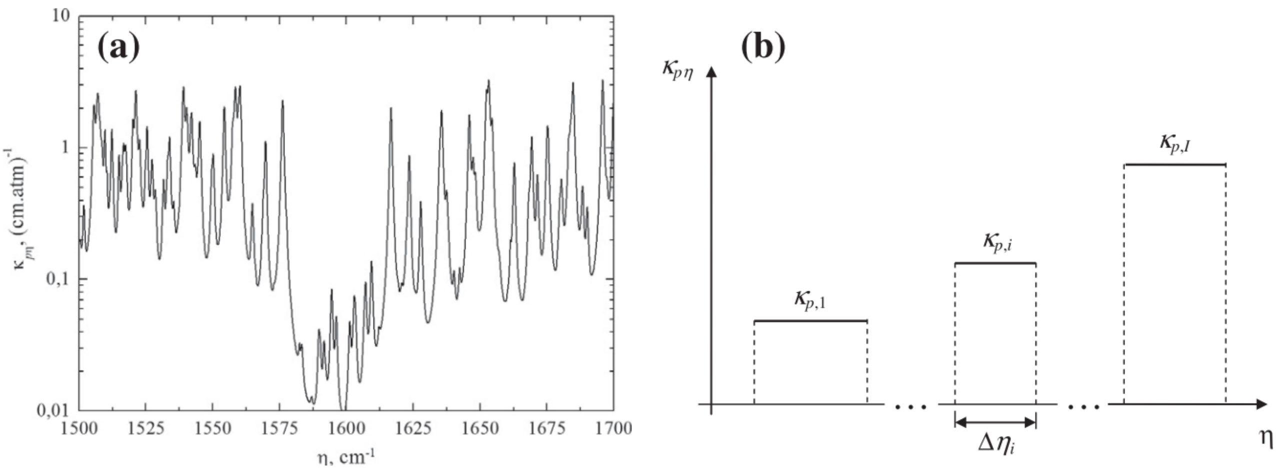

Figure 1. (a) Example of an absorption coefficient profile across the spectrum ranging from 1500 to 1700 cm^{-1} for H_2O at 400 K and 1 atm; (b) Illustration of an arbitrary representation of the absorption coefficients for J=I on the WSGG model.

In the present study, two WSGG models were evaluated. The first one, developed by Cassol *et al.*, (2014), which is within the range of applicability of the proposed domain. This model was validated by comparison to the LBL integration for a mixture of CO_2 and H_2O and soot, which are typical hydrocarbon combustion products, for a temperature range of 400 to 2500K and pressure ratios of 1.0 to 2.0. The second model evaluated was developed by Coelho and França (2018), which is validated for the same temperature and pressure ratios, but at a wider range of operating pressures. The latter did not evaluate the presence of soot, but being a superposition model, the soot molar concentration can be easily implemented in the WSGG calculation.

2.4 Diffusion Flames

Diffusion flames are widely employed in industry processes and power plants. Diffusive flame burners use two different streams, where fuel and oxidizer enter in the chamber separately. In this study a piloted CH_4/air jet flame is chosen to evaluate the WSGG model. The jet composition was 25% of methane and 75% of air in volume, which operates with an equivalence ratio of 0.77. The nozzle diameter is 7.2 mm and the pilot has a diameter of 18.2 mm. The composition profile of species along the flame is available from a preview work available. The flame presents a Reynolds number of 22400 (BARLOW *et al.*, 2005).

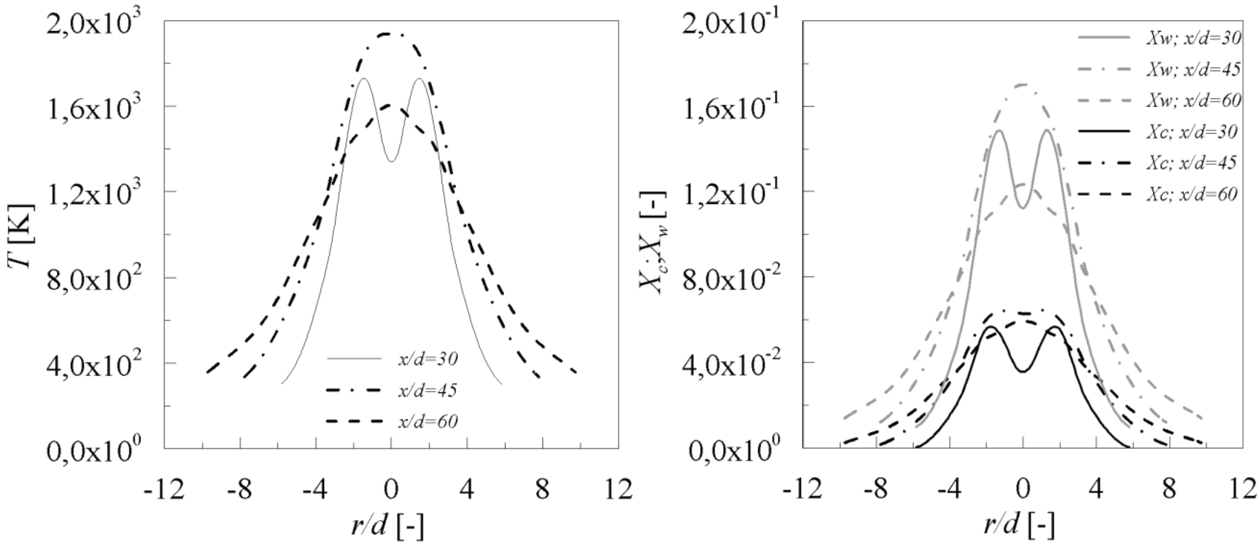

Figure 2. Temperature (left) and mole fractions of CO_2 and H_2O in black and gray respectively (right).

3. RESULTS AND DISCUSSION

In this section, the results obtained from all the cases simulated are presented, divided by three subsections. First the influence of the number of gray gases J used to perform the WSGG calculation are discussed, then the comparison between both models studied, Cassol *et al.*, (2014) and Coelho and França, (2018) is made. Finally, the difference between the flame sections simulated are assessed. The accuracy of the WSGG results, or mentioned also as the relative error, are calculated for the radiative heat fluxes (Eq. (6)) and radiative heat source (Eq. (7)).

$$\Delta q" = \left|\frac{q"_{WSGG} - q"_{LBL}}{max\ (q"_{LBL})}\right| * 100\%, \tag{6}$$

$$\Delta S_r = \left|\frac{S_{r_{WSGG}} - S_{r_{LBL}}}{max\ (S_{r_{LBL}})}\right| * 100\%, \tag{7}$$

where $q"$ is the heat flux and and S_r is the radiative heat source, while max (q'') and max (S_r) are the maximum absolute values of the heat flux and radiative heat source of the simulation domain, obtained from the LBL solution.

3.1 Influence of the number of soot gray gases

When performing the calculation of the RTE by the WSGG method, is important to select an appropriate number of gray gases J used in the mathematical model, in order to maximize the correlation against the benchmark solution but also taking into account the processing time for the solution, especially with two- and three-dimensional domains. In order to test the influence of this parameter in a sooting medium, the test cases evaluated in this work were simulated for J=2, 3 and 4 and Figure 3 presents the heat flux and source term results across the studied domain.

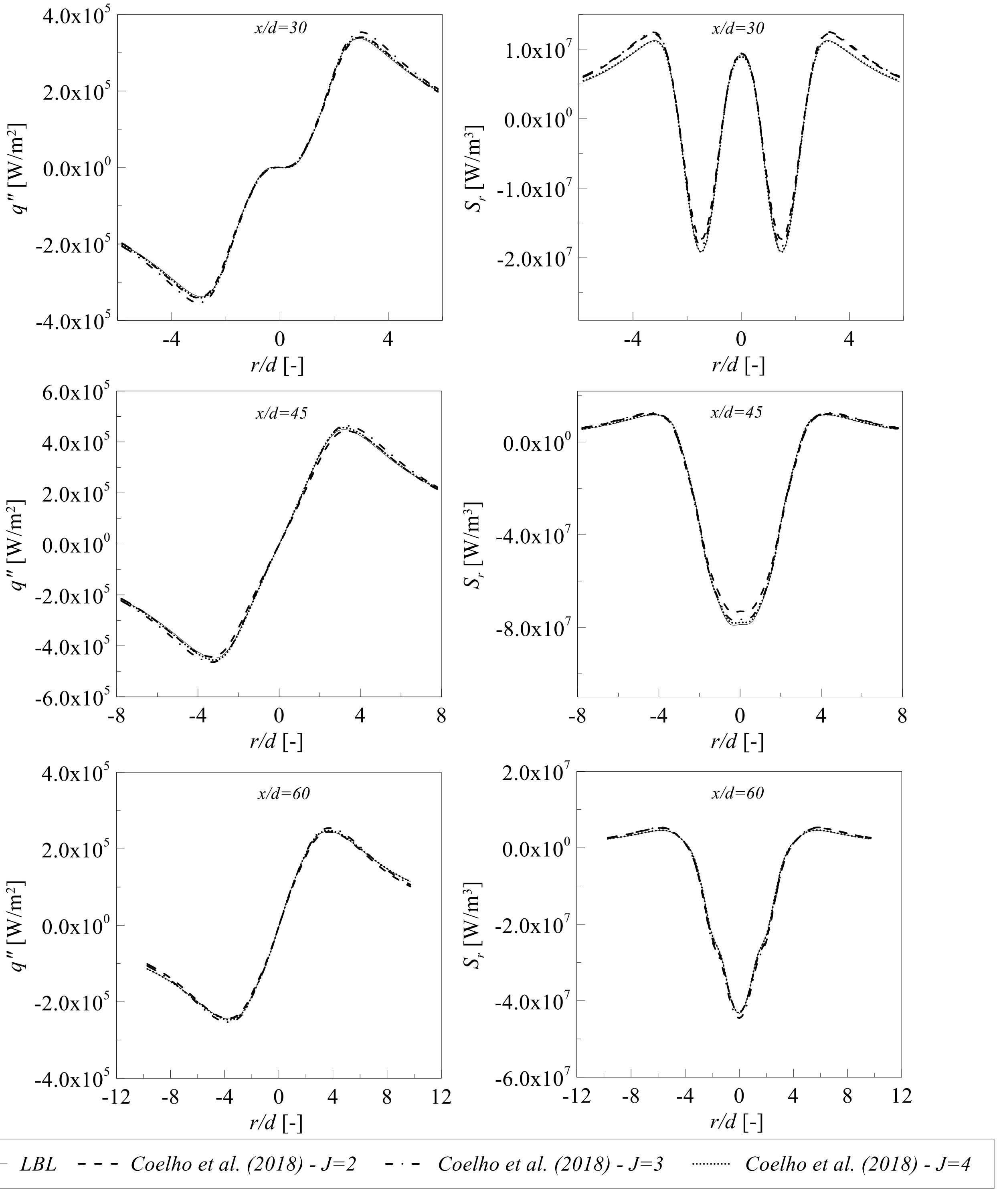

Figure 3. Radiative heat flux results (left) and radiative heat source (right) results for the flame cross sections x/d=30 (top), x/d=45 (center) and x/d=60 (bottom).

Based on the results presented on Figure 3, it can be observed that the results are in good correlation with the benchmark (LBL) solution, with small variations close to the radiative heat flux and radiative heat source peaks. These variations are evident for the optical paths representing x/d=30 and x/d=45. With the increase of the number of gray gases used on each simulation, the errors encountered for the radiative heat source decreased as expected, where for the case of x/d=30 using the Cassol *et al.*, 2014 model the average error encountered achieved a value of 4,35% when J=2 where used, and when J was increased to 4, the average error reduced to 0,64%. For the same case, using the Coelho and França (2018) model, the average errors went from 4,22% for J=2, to 0,72% for J=3. The errors encountered for all the simulation runs were compiled on Table 1.

An interesting behavior was observed for some results, where increasing *J* from 2 to 3 increased the error encountered by the WSGG method, but then reduced from *J*=3 *to J*=4. This phenomenon occurred for the lower portion of the flame, *x/d*=30 and 45 and only for the radiative heat flux result. This could be addressed to the WSGG fitting coefficients for the number *J* studied, alongside the nonuniformity of the temperature and molar fraction profiles of the Sandia D flame. From the results obtained it can be shown that using 4 gray gases in the WSGG method is sufficient to achieve very good correlation with the benchmark solutions for a sooting medium, common for combustion applications, which matches the findings of Cassol *et al.*, (2014) and Coelho and França (2018).

Table 1. Summary of maximum and average errors of the WSGG models when compared to their respective LBL solution.

		Cassol *et al.*, (2014)		Coelho and França (2018)	
		q” (Avg.) Max.	S_r (Avg.) Max.	*q”* (Avg.) Max.	S_r (Avg.) Max.
	J=2	(1.22%) 2.54%	(4.35%) 9.59%	(1.19%) 2.39%	(4.22%) 9.55%
x/d=30	J=3	(2.97%) 5.92%	(3.90%) 7.31%	(2.89%) 5.78%	(3.77%) 7.16%
	J=4	(0.80%) 1.30%	(0.64%) 1.29%	(0.72%) 1.14%	(0.72%) 1.54%
	J=2	(1.58%) 3.92%	(2.02%) 6.96%	(1.58%) 3.95%	(2.07%) 7.25%
x/d=45	J=3	(2.53%) 5.37%	(1.42%) 2.59%	(2.49%) 5.30%	(1.45%) 2.87%
	J=4	(1.16%) 1.87%	(0.36%) 0.89%	(1.12%) 1.78%	(0.40%) 1.17%
	J=2	(1.96%) 5.25%	(1.34%) 2.95%	(2.01%) 5.29%	(1.29%) 2.82%
x/d=60	J=3	(1.90%) 3.86%	(2.04%) 4.28%	(1.88%) 3.79%	(1.96%) 4.04%
	J=4	(0.51%) 0.97%	(0.22%) 0.51%	(0.46%) 0.88%	(0.16%) 0.33%

3.2 WSGG model comparison

With the determination of the sufficient number of gray gases to represent accurately the heat transfer by radiation on the studied domain, a comparison between the models was conducted, in order to evaluate the efficacy of each one to represent the sooting medium of the studied flame profiles. Both of the models, Cassol *et al*., 2014, and Coelho and França 2018, are based on superposition methods, where the absorption coefficients are calculated for each individual species, in this case water, carbon dioxide and soot. Then the computation of the mixture absorption coefficient is calculated by the summation of these quantities. The difference lies on the validation of each model, while Cassol *et al*., validated their model at atmospheric conditions and to a temperature range of 400 to 2500K, Coelho and França evaluated the influence of pressure, in a range from 1 to 40 atm at the same temperature range.

Figure 4 presents the comparison between the models simulated for 4 gray gases, alongside a comparison to the LBL integration method. The three different flame sections were simulated and the radiative heat flux and radiative heat source along the domain are plotted.

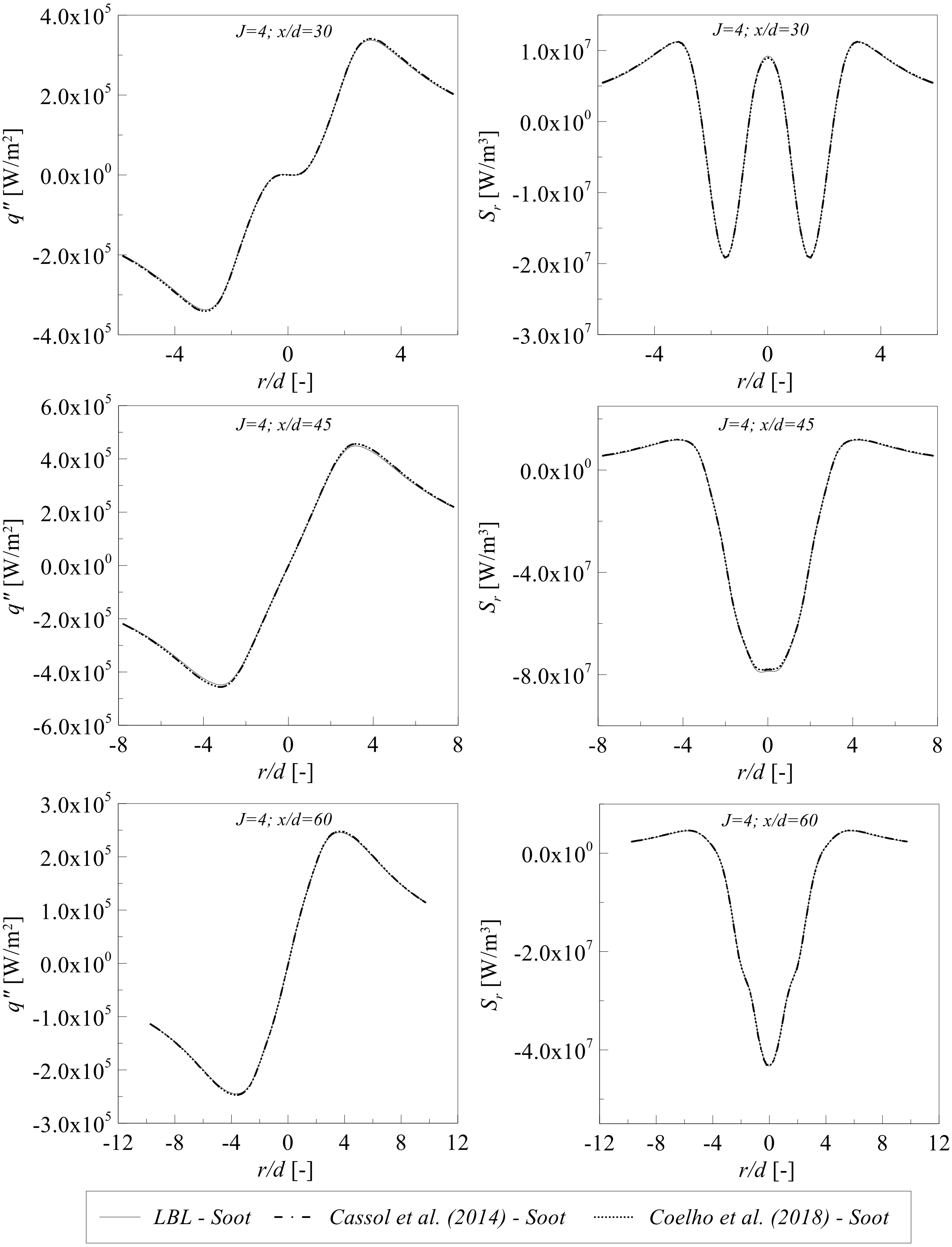

Figure 4. Radiative heat flux results (top) and radiative heat source (bottom) results for the flame cross sections x/d=30 (left), x/d=45 (center) and x/d=60 (right) for both WSGG models studied.

Both models provided excellent correlation to the LBL solution when calculating the RTE over the one-dimensional Sandia D flame profile, with marginal divergence between them. As mentioned in the previous subsection, the maximum divergence between the LBL and WSGG models occurs close to the points of maximum absolute heat flux and sources, but even with this difference, the maximum error encountered on the models were 9,59% for the heat source at *x/d*=30 using the Cassol *et al., (2014)* model, and 9,55% at the same situation for the Coelho and França model. The average error for the source term at this location is 4,35% and 4,22% for Cassol and Coelho methods respectively.

3.3 Flame sections evaluation

The present study evaluates the radiative heat transfer across an experimental flame profile, which is not uniform on its radius nor its axis. Hence the need to evaluate different profiles of the flame, which represent effectively cuts at multiple flame heights, which in this work were divided by the nozzle diameter, *d*, in order to obtain a non-dimensional value. The flame heights evaluated were *x/d*=30, *x/d*=45 and *x/d*=60, following the work developed by Gomes *et al.*, (2020). The temperature and concentration profiles between these sections, as seen on Figure 2, vary significantly, indicating the importance of the evaluation of multiple locations to better understand the heat transfer by radiation in these types of flames. Figure 5 presents the radiative heat flux and source term across the simulation domain for the different flame heights, comparing the WSGG models against the LBL solution when *J*=4.

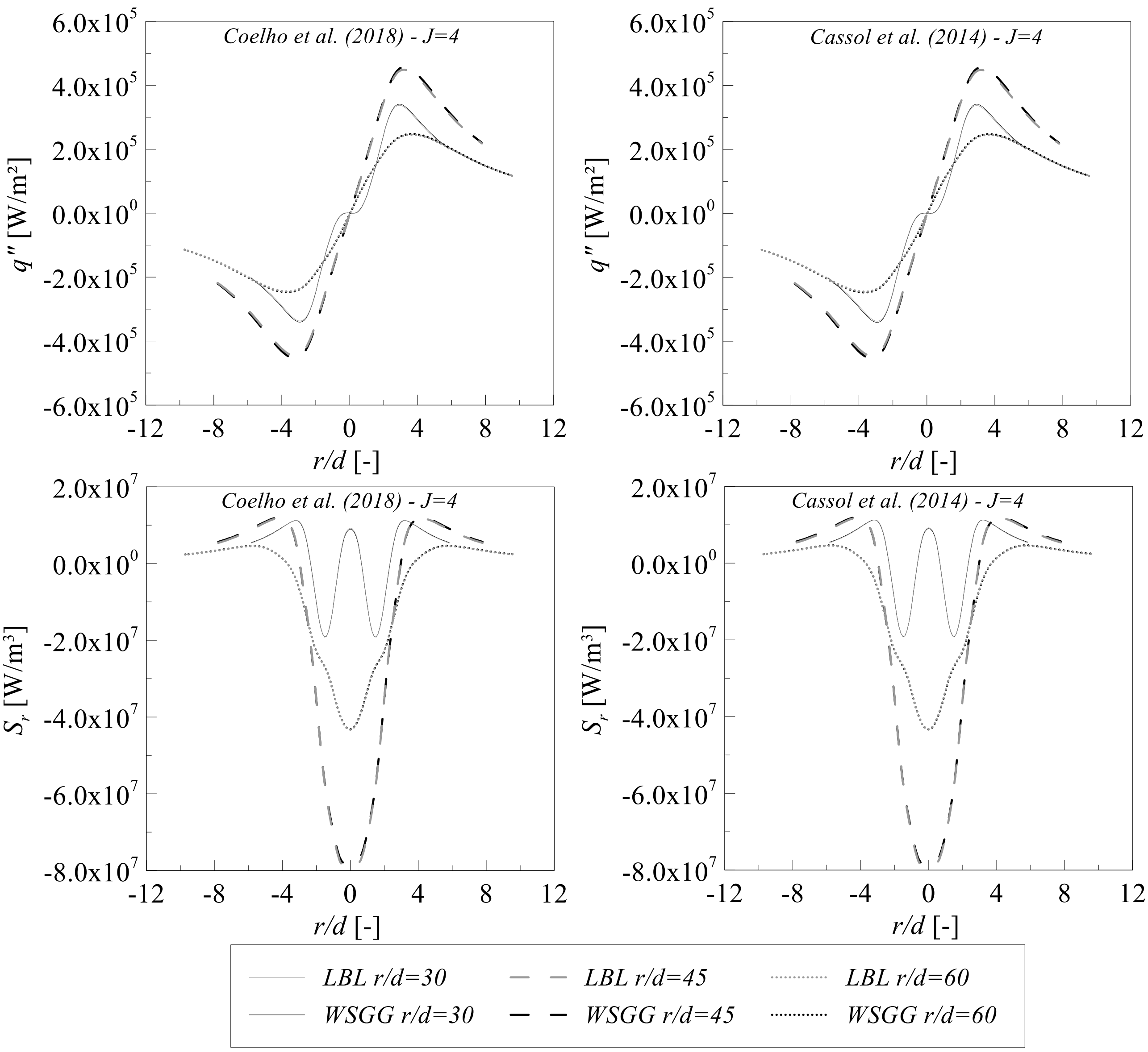

Figure 5. Radiative heat flux results (top) and radiative heat source (bottom) results for the three flame sections evaluated and both WSGG models, Coelho and França 2018 (left) and Cassol *et al.*, 2014 (right).

From the results obtained, it can be observed that WSGG models achieved a better agreement with the LBL integration method for furthest from the jet nozzle, at x/d=60. With an average temperature close to the midrange of applicability of the models, as well as an average ratio between the molar fractions of H_2O and CO_2 closer to 2, which was the proposed molar ratio validated by the model authors. At this location, the radiative heat source average error achieved 0,16%, which is a good agreement to the LBL solution and at a fraction of the computational time.

4. CONCLUSIONS

The present study investigated numerically the behavior of the radiative heat transfer across a premixed methane jet flame in air when considering the presence of soot as a participating species. The radiative transfer equation was solved by means of global models, in this case, two WSGG models within the range of applicability of the flame profiles assessed in this paper. The results for the radiative heat flux, as well as the radiative heat source for the global models were then compared to the benchmark solution, LBL integration; the average and maximum relative errors between the solutions was also obtained. The WSGG models were the ones developed by Cassol *et al*., 2014 and Coelho and França, 2018; the studied flame profile was the Sandia D (Barlow and Frank, 1998).

Results were evaluated first by comparing the number of gray gases used in the WSGG calculation of the RTE in order to determine its appropriate number in order to obtain good agreement with the LBL integration method. The cases were simulated with 2, 3 and 4 gray gases; it was determined that with 4 gray gases is enough to achieve small errors when compared to the benchmark solution, at minimal computational cost.

Moreover, both WSGG models were compared to each other and against the LBL solution. Results showed minimal differences between the models, providing also very good agreement to the benchmark. Therefore, it is possible to implement each of the models for a sooting medium, assuring that the medium temperature and molar fractions are within the applicable range of the model validation.

Then the three flame sections simulated had their results evaluated, and it was determined that the better agreement between these sections was obtained the farthest from the jet nozzle, while the regions close to the flame had higher, but still relatively small, deviations.

5. ACKNOWLEDGEMENTS

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