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New methodology for the spectrally reduced integration method based on the spectral radiative source term

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Abstract. *The spectrally reduced integration (SRI) is a recently developed methodology to generate highly accurate solutions for the radiative transfer equation (RTE) in participating gas mixtures. Recent studies have shown that the method is capable of obtaining benchmark levels of accuracy three to five times faster than line-by-line (LBL) solutions. The SRI solves the RTE using a non-uniform spectral mesh that employs higher levels of refinement only in the most important wavenumber regions for the radiative transfer. Therefore, the method is able to become considerably less computationally costly than the reference LBL while still retaining great levels of accuracy. In its original formulation, the non-uniform discretization schemes are generated based on quantities defined as the spectral contributions of the bands. The present work proposes a more simplified alternative methodology to generate SRI discretization schemes based on the maximum spectral radiative source term. Discretization schemes based on from this new methodology, the SRI-*S_r*, are developed and compared to the ones obtained through the original SRI methodology available in the literature for two different test cases that consider non-homogeneous gas mixtures of H2O and CO2. Results show that the SRI-*S_r* method is capable of ensuing highly accurate solutions - similar to the ones obtained by the standard SRI methodology. Moreover, the only instance where the SRI-*S_r* resulted in a more significant loss in performance, this was followed by a considerable increase in the solution speed. One of the key SRI methodologies to avoid the need of a pre-processed reference LBL solution was also tested along with the SRI-*S_r*, showing results as accurate as the ones from the original SRI solutions. Overall, it can be concluded that the SRI-*S_r* is competitive with the original SRI method, but further testing is recommended.*

Keywords: *Spectrally reduced integration, line-by-line, radiative transfer equation, participating gas mixtures, discretization schemes*

1. INTRODUCTION

Thermal radiation is often regarded as the dominant heat transfer mechanism in combustion applications, mainly due to the high temperatures involved in such scenarios (Modest, 2013). However, including the wavenumber dependence inherited when considering the radiative transfer considerably increases the computational cost of combustion simulations, especially when these are coupled with other complex phenomena. This rise in CPU time is further aggravated by the presence of partipating gas mixtures that compose the chemical reaction products – such as CO_2 and H_2O –, which present highly irregular spectral behaviors. To account for this erratic wavenumber dependence in detail, the spectral integration of the radiative transfer equation (RTE) needs to be performed in considerably high wavenumber resolution. The most accurate spectral integration methodology of the RTE is the line-by-line (LBL) method, which considers the contributions of every significant absorption line of the partipating gas medium.

Nonetheless, its high computational cost hinders the applicability of the LBL method in combustion scenarios, especially in multidimensional problems. Thus, in such applications, it is significantly more common to solve the RTE using approximated gas models, which considerably simplify the spectral behavior of participating gases. Examples of spectral models that are broadly utilized in the literature and are able to reproduce satisfactory results in combustion scenarios are:

the narrow band models (Soufiani and Taine, 1997; Rivière and Soufiani, 2012; Cai and Modest, 2014), the weighted-sum-of-gray-gases (WSGG) (Bordbar *et al.*, 2014; Coelho and França, 2018), the spectral-line-based WSGG (SLW) (Pearson *et al.*, 2014; Solovjov *et al.*, 2017), and the full-spectrum k-distribution (FSK) (Zhang and Modest, 2002; Modest and Riazzi, 2005). Among them, the WSGG model is the simplest and, depending on the methodology that is employed, it can also be the least computationally costly – although at the cost of resulting, in general, in higher deviations than the alternatives. The SLW and the FSK are more accurate, especially for a moderate number of gray gases, but this often means that the CPU time will be higher than the simplest WSGG methodologies. Finally, the narrow band models usually perform better than all of the previous methods and are often in the literature used as more affordable alternatives to obtain approximate benchmark solutions. Their computational cost is higher than the WSGG, the SLW, and the FSK, but still significantly lower than the LBL.

Aiming to address this limitation of the LBL, Ziemniczak *et al.* (2019) developed a reduction technique make the highly irregular behavior of the absorption coefficient distributions smoother, resulting in an approximate LBL methodology with lower computational cost while maintaining satisfactory accuracy. This approach was later called the direct spectral integration (DSI) by Rodrigues *et al.* (2019), who employed the method to solve the RTE in axisymmetric laminar non-premixed flames. The authors chose to apply the DSI since the computational cost of required for a reference LBL solution was not viable at the time. However, despite this ability of the DSI to considerably reduce of the CPU time of the solution, the deviations that result from its application are often still higher than what is desired in highly accurate benchmark solutions. From the various results and analysis available in the literature, it is also known that some regions of the absorption spectrum are considerably more impactful to the radiative transfer than other, which, therefore, means that the uniform spectral reduction employed by the DSI is not the most efficient approach.

With this in mind, Coelho *et al.* (2021) developed a more accurate line-by-line based methodology to reduce the computational cost of benchmark solutions of the RTE, the spectrally reduced integration (SRI). Since – as previously discussed – some regions of the spectrum are more important than others to the overall raditive transfer, the SRI considers non-uniform wavenumber discretization schemes based on the spectral contributions of the bands. Results showed that the most accurate schemes were able to obtain solutions with benchmark levels of accuracy three to five times faster than the reference LBL method. The work from Coelho *et al.* (2021) also proposed two methodologies to address the main limitation of the SRI: the need of a pre-processed LBL solution to evaluate the spectral contributions of the bands. Both methodologies were able to present highly accurate solutions for the test cases that were evaluated. Another work on the SRI, now from Coelho *et al.* (2020), was able to extend the method – together with one of its methodologies to avoid calculating the spectral contributions from a previous LBL solution – to variable mole ratio gas mixtures composed of H_2O and CO_2, which aimed to represent typical scenarios observed in oxy-fuel combustion. The conclusion was that the SRI is also able to result in highly accurate benchmark solutions when the mole ratio between the participating gases vary considerably throughout the domain.

Based on these recent works, the present study proposes a new methodology for the SRI method based on the spectral radiative source term. Instead of developing the non-uniform discretization schemes based on the spectral contributions of the bands – as in the studies from Coelho *et al.* (2020, 2021) –, they are now developed based on the maximum value of the spectral radiative source term throughout the domain of the problem. Despite its simpler approach, it is expected that this new SRI methodology, the SRI-S_r, should also be able to result in highly accurate solutions considerably faster than the LBL method. In order to verify this claim, the newly proposed SRI-S_r method is evaluated in two non-homogeneous test cases and its performance is compared to the one displayed by the original SRI method in the study from Coelho *et al.* (2021). Moreover, one of the two methodologies to avoid the need of generating discretization schemes based on a pre-processed LBL solution is also tested in the present work.

2. METHODOLOGY

For the H_2O and CO_2 participating gas mixture considered in this study, the scattering effect is low and can be neglected, such that – if thermodynamic equilibrium and steady state are assumed – the RTE is given by (Modest, 2013; Howell *et al.*, 2016)

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

in which I_η is the spectral radiation intensity, $I_{b\eta}$ is the blackbody spectral radiation intensity, κ_η is the mixture absorption coefficient, and s is the path length along a line of sight. Since the participating medium is composed of only H_2O and CO_2, the mixture absorption coefficient κ_η is calculated as

$$\kappa_\eta = \kappa_{\eta,c} + \kappa_{\eta,w} \tag{2}$$

where $\kappa_{\eta,w}$ and $\kappa_{\eta,c}$ are, respectively, the absorption coefficients of the individual species H_2O and CO_2. The absorption coefficient for a single gas i, such as H_2O or CO_2, is then calculated as

$$\kappa_{\eta,i}(p,T,Y_i) = N(p,T)Y_i C_{\eta,i}(p,T,Y_i) \tag{3}$$

in which N is the gas molar density and $\kappa_{\eta,i}$, Y_i and $C_{\eta,i}$ are, respectively, the absorption coefficient, the mole fraction and the absorption cross-section of the generic species i.

From Equation 3, it can be noticed that the spectral dependency from κ_η comes solely from the $C_{\eta,i}$. In this study, these absorption cross-sections of the individual gases are calculated through the Lorentz profile, such that

$$C_\eta = \sum_{k=1}^{K} C_{\eta,k} = \sum_{k=1}^{K} \frac{S_k}{\pi} \frac{\gamma_k}{{\gamma_k}^2 + (\eta - \eta_k)^2} \tag{4}$$

where K is the total number of significant spectral lines for the wavenumber interval located at the η, $C_{\eta,k}$ is the contribution of the spectral line k to the absorption cross-section, S_k is the integrated line intensity, γ_k is the line half-width for the chosen line profile, and η_k is the wavenumber position of the center of the spectral line that is being considered. The line half-width γ_k is calculated using the high-resolution spectroscopic database HITEMP2010 (Rothman *et al.*, 2010) and is given by

$$\gamma_k = \left(\frac{T_{ref}}{T}\right)^{n_i} (p_i \gamma_{self,k} + (p - p_i)\gamma_{air,k}) \tag{5}$$

where $T_{ref} = 296\,\mathrm{K}$ is the reference temperature of the HITEMP2010 database, n_i is the temperature dependence coefficient, p_i is the partial pressure of species i, $\gamma_{self,k}$ is the half-width due to the line self-broadening, and $\gamma_{air,k}$ is the half-width due to the broadening caused by air. Finally, the integrated line intensity S_k is then obtained through (Rothman *et al.*, 2010)

$$S_k(T) = S_k(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\exp(-C_2 E_k/T)}{\exp(-C_2 E_k/T_{ref})} \frac{[1 - \exp(-C_2 \eta_k/T)]}{[1 - \exp(-C_2 \eta_k/T_{ref})]} \tag{6}$$

in which Q is the total internal partition sum, E_k is the energy of the lower state, and η_k is the wavenumber location of line k. The line parameters η_k, n_i, $\gamma_{self,k}$, $\gamma_{air,k}$, $S_k(T_{ref})$, Q, and E_k are taken from the high resolution spectroscopic database HITEMP2010 (Rothman *et al.*, 2010).

In this work, the absorption cross-sections C_η of both H_2O and CO_2 are calculated considering a total pressure of $1\,\mathrm{atm}$, temperatures ranging from $300\,\mathrm{K}$ to $2500\,\mathrm{K}$, and mole fractions $Y_c = 1$ and $Y_w = 0.01, 0.1, 0.2$. To obtain other values of Y_w, a linear interpolation methodology is employed between the listed discrete values. For CO_2, a simple linear relation is enough to obtain any value of Y_c ranging from 0 to 1 (Cassol *et al.*, 2014). The absorption spectrum of the gases is considered ranging from 0 to $10\,000\,\mathrm{cm}^{-1}$, discretized in spectral intervals of $\Delta\eta = 0.0667\,\mathrm{cm}^{-1}$. All these parameters are the same as the ones employed in the work from Coelho *et al.* (2021), which, through a detailed spectral grid analysis, showed that they are sufficient to obtain accurate LBL solutions.

Analogously to the analysis performed by Coelho *et al.* (2021), all the test cases studied here consist of 1D slabs containing gas mixtures of H_2O and CO_2 surrounded by two infinite and parallel black walls. For this configuration, when Eq. (1) is solved using the discrete ordinates method (DOM) for angular discretization, the spectral radiative heat flux and source term are given by

$$q_{r,\eta}(x) = \sum_{l=1}^{n_d} [2\pi \mu_l \omega_l (I^+_{\eta,l}(x) - I^-_{\eta,l}(x))] \tag{7}$$

$$S_{r,\eta}(x) = \sum_{l=1}^{n_d} [2\pi \kappa_\eta \omega_l (I^+_{\eta,l}(x) - I^-_{\eta,l}(x))] - 4\pi \kappa_\eta I_{b\eta} \tag{8}$$

where w_l is the quadrature weight for the lth direction, n_d is the total number of directions l, μ_l is the direction cosine associated with the lth direction, and $I^+_{\eta,l}$ and $I^-_{\eta,l}$ are, respectively, the spectral radiation intensity for outward ($\mu_l > 0$) and inward ($\mu_l < 0$) fluxes. If a sufficiently refined spectral mesh is employed, Eqs. (7) and (8) represent the LBL solution of the RTE for the spectral radiative heat flux and source term. In this work, apart from the wavenumber resolution of $\Delta\eta = 0.0667\,\mathrm{cm}^{-1}$, Eqs. (7) and (8) are solved considering a spatial discretization of 200 uniform elements in x and a directional discretization of 15 l directions in both inward and outward fluxes, which results in a total of 30 directions when considering the whole hemisphere. These are the same parameters as the ones employed in the other two previous works on the SRI method by Coelho *et al.* (2020) and Coelho *et al.* (2021).

In the original SRI methodology proposed by Coelho *et al.* (2021), the non-uniform discretization schemes are generated based on the spectral contributions of the bands to the radiative heat flux and source term, which are obtained through

$$\zeta_{q_r}(\eta) = \frac{1}{L} \int_0^L |q_{r,\eta}(x)|\, dx \tag{9}$$

$$\zeta_{S_r}(\eta) = \frac{1}{L} \int_0^L |S_{r,\eta}(x)|\, dx \tag{10}$$

in which L is the distance between the two parallel black walls and ζ_{q_r} and ζ_{S_r} are, respectively, the spectral contributions of each wavenumber η to the radiative heat flux and source term. These quantities represent how each wavenumber interval from the absorption spectrum of the participating gas mixture impacts the overall radiative transfer through the medium. In order to facilitate the comparison between spectral contributions based on different quantities or problems, having them in dimensionless form is more convenient, such that (Coelho *et al.*, 2021)

$$\zeta^*_{q_r}(\eta) = \frac{\zeta_{q_r}(\eta)}{\zeta_{q_r,max}} \tag{11}$$

$$\zeta^*_{S_r}(\eta) = \frac{\zeta_{S_r}(\eta)}{\zeta_{S_r,max}} \tag{12}$$

where $\zeta_{q_r,max}$ and $\zeta_{S_r,max}$ are, respectively, the maximum values of ζ_{q_r} and ζ_{S_r} throughout the entire spectrum.

Furthermore, to attenuate the highly oscillatory behavior of the $\zeta^*_{q_r}$ and $\zeta^*_{S_r}$, Coelho *et al.* (2021) suggest that these quantities should face an initial spectral reduction in samples of n_{red} wavenumber intervals, resulting in

$$\zeta^*_{q_r,red} = \frac{1}{\Delta\eta_{red}} \int_{\Delta\eta_{red}} \zeta^*_{q_r}\, d\eta \tag{13}$$

$$\zeta^*_{S_r,red} = \frac{1}{\Delta\eta_{red}} \int_{\Delta\eta_{red}} \zeta^*_{S_r}\, d\eta \tag{14}$$

where $\Delta\eta_{red}$ is the reduced spectral interval – given by $\Delta\eta_{red} = n_{red} * \eta$ –, η_{red} is the wavenumber location from the center of the reduced interval, and $\zeta^*_{q_r,red,}$ and $\zeta^*_{S_r,red}$ are, respectively, the reduced spectral contributions to the radiative heat flux and source term. The present study employs the same value of initial reduction $n_{red} = 100$ as in the work from Coelho *et al.* (2021). The originally proposed SRI method generate non-uniform spectral discretization schemes based on the magnitude of the quantities $\zeta^*_{q_r,red,}$ and $\zeta^*_{S_r,red}$, employing higher wavenumber resolutions on the most important regions to radiative transfer and coarser discretizations on the least important ones. An example of how two discretization schemes proposed by (Coelho *et al.*, 2021) divide the spectral contributions spectrum based on the values of $\zeta^*_{q_r,red,}$ is illustrated in Figure 1.

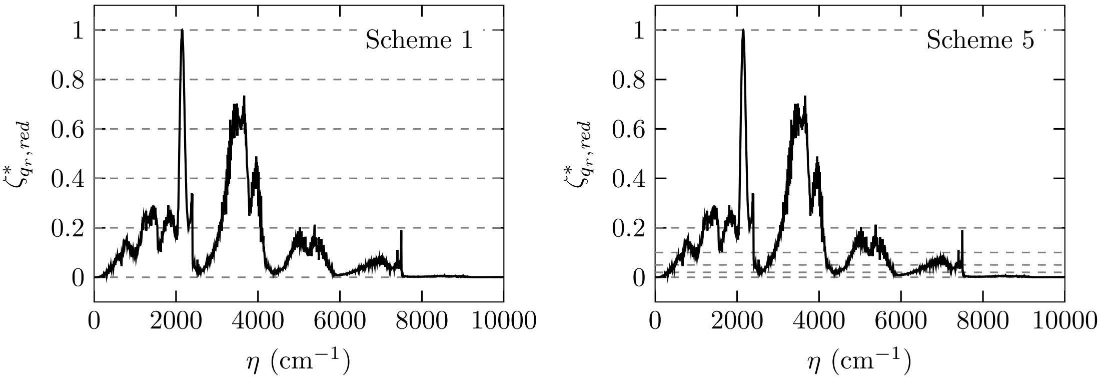

Figure 1. Example of how two discretization schemes, Scheme 1 and Scheme 5, divide the spectrum according to the spectral contributions of the bands to the radiative heat flux (Coelho *et al.*, 2021).

However, instead of employing this originally proposed SRI methodology, the present study generates SRI discretization schemes based on the maximum spectral radiative source term throughout the domain, which is a slightly more simplified approach. From now on, this alternative methodology will be referred to as SRI-S_r. Since all the test cases studied in the work consider a hot medium surrounded by cold walls, most of the radiative transfer in these problems is due to the emission of the high temperature regions of the gas mixture. Thus, the maximum spectral radiative source term $S_{r,\eta,max}$ is always located in the region of highest temperature and it can be calculated by simply evaluating Eq. 8 for the position $x(T_{max})$, where T_{max} is the maximum temperature throughout the domain. Following this, the SRI-S_r discretization schemes are generated based on the $S_{r,\eta,max}$ spectral distribution by employing an analogous methodology to the one shown in Figure 1, but now for $S_{r,\eta,max}$ instead of $\zeta^*_{q_r,red,}$. Analogously to the original SRI method proposed by Coelho *et al.* (2021), the SRI-S_r solution is then obtained by evaluating Eqs. (7) and (8) with these non-uniform discretization schemes.

Up to this point, both the SRI methodologies presented here are based on LBL solutions of Eqs. (7) and (8). However, if a prior LBL solution is needed to obtain an accurate SRI method, then the advantages of the SRI in terms of computational cost are meaningless. With this in mind, Coelho *et al.* (2021) proposed two alternative methodologies to obtain SRI solutions without the need of a previous LBL solution of the problem: one where the SRI discretization schemes are based on a sufficiently similar problem and the other where SRI discretization schemes are generated based on approximated LBL methodologies, such as the DSI method Ziemniczak *et al.* (2019); Rodrigues *et al.* (2019). This first methodology, which is referred to as M1 from now on, was very successful for the test cases evaluated in both the SRI studies from Coelho *et al.* (2020, 2021). This high performance of M1 was mainly attributed to the fact that the problems presented a sufficient degree of similarity between them. In particular, the work from Coelho *et al.* (2020) extended M1 methodology to participating gas media with variable mole ratio between H_2O and CO_2, concluding that a sufficient degree of similarity is met when both cases consider a hot medium bounded by cold walls and present the same value of $M_r = Y_w/Y_c$ in the region of highest temperature.

3. RESULTS

The two test cases studied here, Cases 1 and 2, are taken from Coelho *et al.* (2021) (Cases 3 and 5 from that work) and represent two distinct configurations for approximate scenarios of stoichiometric methane combustion in air. Case 1 considers a symmetric sinusoidal temperature distribution ranging from 300 to 2500 K, which is given by

$$T = 300\,\mathrm{K} + 2200\,\mathrm{K}\sin^2(\pi x/L) \tag{15}$$

and CO_2 mole fraction distribution ranging from 0 to 0.1, such that

$$Y_c = 0.1\sin^2(\pi x/L) \tag{16}$$

where $Y_w = 2Y_c$ throughout the whole domain. Case 2 employs a symmetrical sinusoidal profile, but now presenting two peaks and ranging from 300 to 1800 K, such that

$$T = \begin{cases} 300\,\mathrm{K} + 1500\,\mathrm{K}\sin^2(2\pi x) & \text{if } x \leq 0.25\,\mathrm{m} \text{ or } x > 0.75\,\mathrm{m} \\ 1050\,\mathrm{K} + 750\,\mathrm{K}\sin^2(2\pi x) & \text{if } 0.25\,\mathrm{m} < x \leq 0.75\,\mathrm{m} \end{cases} \tag{17}$$

Similarly, the mole fraction distribution of CO_2 in Case 2 also presents two peaks, but still ranges from 0 to 0.1 as in Case 1, being given as

$$Y_c = \begin{cases} 0.1\sin^2(2\pi x) & \text{if } x \leq 0.25\,\mathrm{m} \text{ or } x > 0.75\,\mathrm{m} \\ 0.05 + 0.05\sin^2(2\pi x) & \text{if } 0.25\,\mathrm{m} < x \leq 0.75\,\mathrm{m} \end{cases} \tag{18}$$

in which, once more, $Y_w = 2Y_c$ throughout the whole domain. It is important to notice that, as also concluded by Coelho *et al.* (2021), Cases 1 and 2 meet the degree of similarity needed for M1 to be applicable: both consider a hot medium surrounded by cold walls and present the same value of $M_r = 2$ in the region of highest temperature.

In order to establish a comparison between the standard SRI-S_r method – based on a prior LBL solution of the problem that is being solved – and the SRI-S_r solution using the M1 approach, both these methodologies are evaluated for Cases 1 and 2 and compared to the LBL solutions of these same problems. The SRI discretization scheme chosen for this analysis is Scheme 4 (S4), first developed in the work by Coelho *et al.* (2021). S4 is a scheme aimed for highly accurate solutions and was also employed by Coelho *et al.* (2021) to obtain results of the originally proposed SRI method for these two exact same cases, which facilitates the comparison with the SRI-S_r solutions presented here. The main goal is to contrast these two methodologies in terms of accuracy – when compared to the reference LBL solutions of Cases 1 and 2 –, computational cost, and applicability of the M1 approach. Similarly to the work by Coelho *et al.* (2021), the M1 methodology is only tested here for Case 2, when S4 is based on the sufficiently similar Case 1 instead – referred to as $\mathrm{S4_{C1}}$ from now on. However, independent studies show that employing schemes based on Case 2 – e.g. $\mathrm{S4_{C2}}$ – to solve Case 1 leads to similar levels of accuracy for the M1 approach.

To start off this analysis, Fig. 2 presents the comparison between the LBL and the SRI-S_r S4 and $\mathrm{S4_{C1}}$ solutions, in terms of radiative heat flux and source term distributions along the x position, for Cases 1 and 2. According to this figure, the results from the LBL and the SRI-S_r S4 methods are so close to each other that their curves piratically coincide through the whole domain. This level of agreement evidences that S4 – similarly to what is observed in the results from Coelho *et al.* (2021) for the original SRI methodology – is also able to generate highly accurate solutions when the SRI-S_r is employed. Moreover, the high proximity between the SRI-S_r S4 and $\mathrm{S4_{C1}}$ curves in Case 2 illustrates the the M1 methodology is also able to generate high levels of accuracy when applied to the SRI-S_r method proposed in the present work.

However, despite the highly accurate results displayed in Fig. 2, it is still unknown how the original SRI and the SRI-S_r compare in terms of computational cost. Similarly to the LBL method and other gas models, the CPU time of an SRI solution is directly proportional to the number of RTEs that are being solved in the spectrum – i.e. the number of wavenumber values required for Eqs. (7) and (8) evaluation. Thus, the computational cost of the SRI method is directly proportional to the number of points $n_{p,t}$ that results from the discretization scheme employed (Coelho *et al.*, 2020,

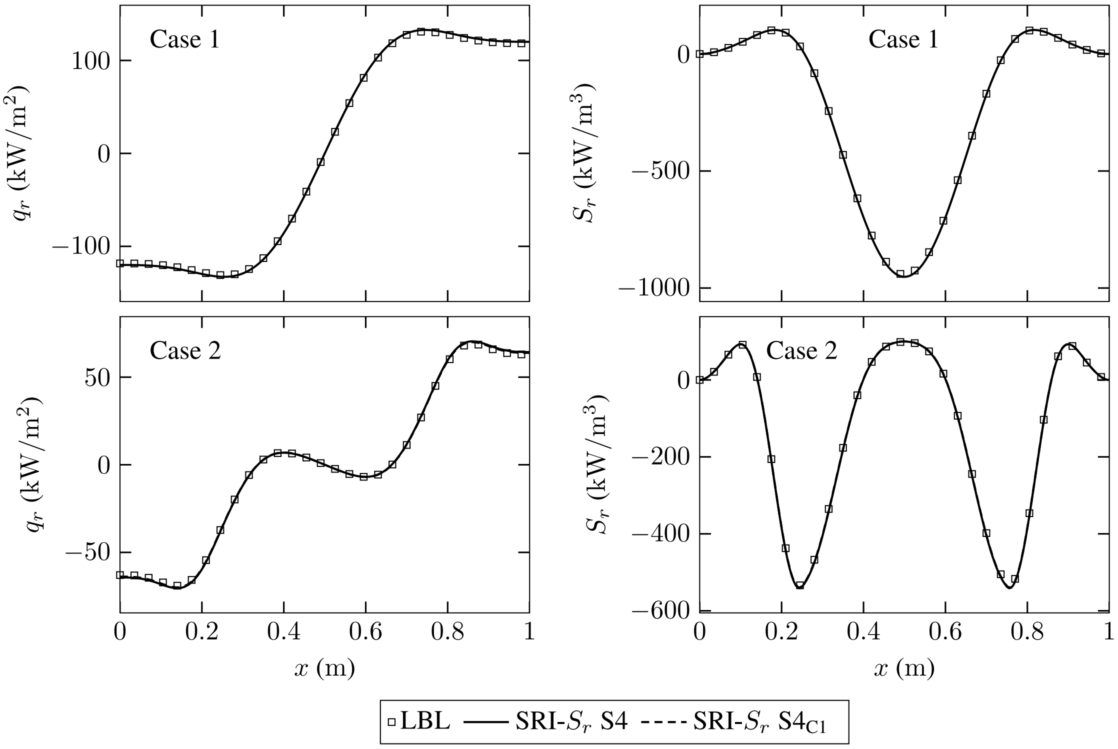

Figure 2. Radiative heat flux (left) and source term (right) solutions obtained by the LBL and the SRI-S_r S4 and S4$_{\mathrm{C1}}$ methods for Cases 1 and 2.

2021). Moreover, due to the fact that the curves from Fig. 2 basically coincide throughout the whole domain, calculating numerical deviations between the LBL and the SRI-S_r solutions allows for a better comparison between the accuracy of the two SRI approaches.

Following this discussion, Tab. 1 displays the number of spectral intervals together with the average and maximum deviations – with respect to the reference LBL method – of both the SRI and SRI-S_r solutions of Cases 1 and 2. The results from this table illustrate that the original SRI solutions from Coelho *et al.* (2021) presented higher accuracy in both test cases, even when the M1 approach was applied to Case 2. However, this gain in performance comes at the cost of an increase in the computational time (due to the higher number of spectral intervals) in every solution of the original SRI method. In the solutions where S4 was based on Case 1, it is noticeable that there is only a slight increase in CPU cost – followed by a minor raise in performance. On the other hand, when S4 was based on Case 2, the decrease in both accuracy and computational time is more significant when applying the SRI-S_r methodology. Therefore, it can be concluded that the higher accuracy displayed by the original SRI solutions from Coelho *et al.* (2021) is mainly due to the higher number of wavenumber points that result from the generation of the non-uniform discretization scheme.

Table 1. Number of spectral intervals and average and maximum deviations of the original SRI and the SRI-S_r solutions for the radiative heat flux and source term in Cases 1 and 2. The deviations are evaluated considering the LBL method as the reference solution.

Method	Test case	Scheme	$n_{p,t}$	$\delta_{q_r,avg}$ (%)	$\delta_{S_r,avg}$ (%)	$\delta_{q_r,max}$ (%)	$\delta_{S_r,max}$ (%)
SRI-S_r	Case 1	S4	34 714	1.06	0.41	1.36	1.04
	Case 2	S4	25 796	1.12	0.59	2.11	1.42
		S4$_{\mathrm{C1}}$	34 714	0.74	0.46	1.44	1.08
Original SRI	Case 1	S4	35 737	0.98	0.37	1.26	0.96
(Coelho *et al.*, 2021)	Case 2	S4	35 110	0.67	0.33	1.25	0.81
		S4$_{\mathrm{C1}}$	35 737	0.66	0.38	1.28	0.92

Another conclusion that can be drawn from Tab. 1 is that the M1 methodology is also applicable to the SRI-S_r method proposed in this work. In fact, the accuracy shown by S4$_{\mathrm{C1}}$ is considerably higher than the one from the standard S4 – but this was mainly due to the significantly increase in computational cost, as also discussed in other studies Coelho *et al.* (2020, 2021). The exact cause behind this effect is still unknown, but a reasonable initial guess would be that this is caused by the two temperature and mole fraction peaks that are present in Case 2. As shown in Figure 2, this results in the presence of two peaks and an overall different behavior in the radiative source term distribution. In such scenario, and together with the lower temperatures involved in Case 2, this could make the original SRI discretization schemes based on the spectral contributions a better fit than the ones based solely on the maximum spectral radiative source term from the SRI-S_r. However, Case 2 results alone are not enough to draw such conclusion and, thus, further testing is recommended. Overall, from the results reported in the present work, it can be concluded that both the SRI-S_r approaches are able to generate highly accurate solutions, as even the SRI-S_r S4 solution of Case 2 presented radiative heat flux and source term curves that coincide with the reference LBL method throughout the whole domain – as seen in Fig. 2.

4. CONCLUSIONS

The present study developed a new alternative methodology for the SRI method where the non-uniform discretization schemes are generated based on the maximum radiative source term rather than the spectral contributions of the bands proposed in the original study from Coelho *et al.* (2021). The main goal of was to verify if the new method, the SRI-S_r, was able to compete with the original SRI in terms of accuracy, computational cost, and the applicability of the M1 methodology – which is an important approach to avoid the pre-processing of a previous LBL reference solution by employing discretization schemes based on sufficiently similar problems (Coelho *et al.*, 2021). Results showed that the SRI-S_r presented similar levels of performance and computational cost in most cases. In the only instance where there was a more significant drop in accuracy, this was followed by an also considerable reduction in CPU time. Thus, it was concluded that the loss in performance is mostly due the differences in solution speed rather than the innate accuracy of both the SRI methods. Furthermore, the solutions of the SRI-S_r when applied together with the M1 approach were almost as accurate as the ones displayed by the original SRI method. Overall, from the results reported in the present work, it can be concluded that the newly developed SRI-S_r method is able to generate highly accurate solutions, but further testing is still needed to identify why some test cases result in discretization schemes with lower accuracy and CPU time.

5. ACKNOWLEDGEMENTS

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