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A REPORT ON THE IMPLEMENTATION OF NEW SPECTRAL MODELS FOR RADIATIVE HEAT TRANSFER CALCULATIONS IN THE SOFTWARE FIRE DYNAMICS SIMULATOR

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Abstract. *Fire Dynamics Simulator (FDS) is a software developed for the numerical simulation of fire-driven flows, widely used in problems involving smoke and in fire reconstructions. Because it is an open-source code, FDS is well-suitable for modifications to its subroutines in order to add new physical or numerical models or to improve existing ones. In this framework, this paper study the implementation of a series of spectral models for the solution of the radiative heat transfer problem in participating media in that software. The models include two formulations for computing local absorption coefficient for a gray gas model, a weighted-sum-of-gray-gases model suitable for non-gray media, and the line-by-line integration methodology. A verification of each model is performed through comparisons with a one-dimensional reference solution obtained by an in-house code for a set test cases consisting of non-homogeneous, non-isothermal mixtures of carbon dioxide and water vapor with different optical thicknesses. Results show a very good agreement between the models implemented to FDS and the reference code, attesting that the implementation was successful.*

Keywords: *Spectral models, verification, Fire Dynamics Simulator, weighted-sum-of-gray-gases model, line-by-line integration*

1. INTRODUCTION

Fire Dynamics Simulator (FDS) is an open-source computational fluid dynamics solver focused on numerical simulations of fire-driven flow, developed by the National Institute of Standards and Technology (NIST) of the United States in collaboration with the VTT Techinical Research Centre of Finland. Its major areas of applications are in problems involving smoke and in activation studies of sprinklers and fire detectors (McGrattan *et al.*, 2017b), though the software is often also used in residential and industrial fire reconstructions (for example, Guedri *et al.* (2011)), simulations of pool and jet diffusion flames (Wen *et al.*, 2007; Lin *et al.*, 2010), and even in more fundamental investigations of specific phenomena such as turbulence-radiation interaction (Fraga *et al.*, 2017a,b). The code is written in Fortran 90 programming language, with its source code consisting in a main routine, which contains the overall solution algorithm, and a series of subroutines, each responsible for modeling a specific physical process (e.g., turbulence, radiation or combustion) or performing pre- or post-processing tests, such as mesh generation and printing of output data (McGrattan *et al.*, 2017a).

The fact that the entire Fire Dynamics Simulator source code is available free of charge encourages users to improve and modify it as to better suit the simulation of specific problems. In this framework, this study presents an investigation into the coupling of a series of spectral models dedicated to the solution of the radiative heat transfer in participating media to the radiation subroutine of FDS. The choice in this work of focusing on FDS's radiation subroutine is motivated first by the fact that radiation plays an important role in all scenarios for which the solver is most commonly used, thus it would be useful to have available a variety of techniques to model this process. Furthermore, the default spectral models shipped with the Fire Dynamics Simulator base code—a gray gas formulation where the absorption coefficient of the medium is computed based on a narrow-band model and (for specific cases) a wide-band model—are relatively simple and are not adequate for detailed simulations of radiative heat transfer in participating gases; therefore, there is much room, and even necessity, to improve.

As far as the authors' knowledge, the have only been a couple of attempts of including other spectral models to FDS. Guedri *et al.* (2011) implemented a narrow-band based weighted-sum-of-gray-gases model originally developed by Kim and Song (2000) to the solver, reporting a good agreement with measurements. More recently, in a series of studies on turbulence-radiation interaction, the weighted-sum-of-gray-gases (WSGG) model (Modest, 1991) and an alternative formulation to compute the gray gas mean absorption coefficient have been used in FDS simulations of non-reacting flows (Fraga *et al.*, 2017a,b); however, even though the results obtained were physically sound, no verification analysis nor comparisons with experimental data were performed.

In the present paper, the implementation of four spectral models to the Fire Dynamics Simulator code is studied: two formulations of the gray gas model, the WSGG model, and the line-by-line integration methodology. A verification analysis of each model is performed by comparing the FDS results with a reference solution, given by a dedicated in-house code, for a set of one-dimensional test cases with predefined temperature and species concentration profiles.

2. METHODOLOGY

2.1 Radiative Heat Transfer Models

To determine the thermal radiation field, the radiative heat transfer equation (RTE) is solved. For a non-scattering medium, as it is assumed for the cases studied here, the RTE is given by (Modest, 2013; Howell *et al.*, 2016):

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

in which η is the radiation wavenumber, s is the coordinate along the path of radiation, κ_η is the spectral absorption coefficient of the medium, and I_η and $I_{b\eta}$ are the spectral radiation intensity and the blackbody spectral radiation intensity, respectively. The spatial integration of this equation is resolved using the finite volume method in FDS (Raithby and Chui, 1990) and the discrete ordinates method in the reference in-house code (Chandrasekhar, 1960). For the spectral integration of Eq. (1)—i.e., its integration over the entire radiation spectrum—four approaches are tested: two formulations of the gray gas assumption, both different from the default FDS model, the weighted-sum-of-gray-gases model, and the line-by-line integration method. These approaches are described next.

2.1.1 Gray Gas (GG) Formulations

Integrating Eq. (1) over the radiation spectrum and considering a constant gray gas absorption coefficient κ for the medium yields:

$$\frac{dI}{ds} = \kappa I_b - \kappa I \tag{2}$$

where $I = \int_0^\infty I_\eta \, d\eta$ is the total radiation intensity and I_b is the blackbody radiation intensity. The accuracy of the simplification introduced by Eq. (2) is greatly dependent on how the gray gas absorption coefficient is calculated. In the first formulation tested in this paper, κ is computed following a polynomial expression proposed by Cassol *et al.* (2015), which was obtained from curve-fittings based on the Planck-mean absorption coefficient. For an arbitrary species α, this formulation gives:

$$\kappa_{p,\alpha} = \sum_{i=0}^{5} c_i T^i \tag{3}$$

where $\kappa_{p,\alpha}$ is the pressure-based absorption coefficient of species α, defined as the ratio between the absorption coefficient of this species and its partial pressure. The values of c_i for carbon dioxide and water vapor are extracted from Cassol *et al.* (2015) and the total absorption coefficient of the participating medium is given as $\kappa = \kappa_{p,c} p_c + \kappa_{p,w} p_w$, in which $\kappa_{p,c}$ and $\kappa_{p,w}$ are the pressure-based absorption coefficients of CO_2 and of H_2O, respectively, and the partial pressures p_c and p_w of these species are determined from their molar fraction following Dalton's model.

In the second gray gas formulation, the absorption coefficient of the medium is directly calculated from its total emittance ε as:

$$\kappa = -\frac{\ln(1-\varepsilon)}{S} \tag{4}$$

where S is a characteristic path length, whose value is set as equal to the mean beam length of the medium (Howell *et al.*, 2016). In this study, S is taken as five times the smallest grid cell dimension, following the methodology recommended by McGrattan *et al.* (2017a). The total emittance of the medium is computed using the WSGG model (Modest, 1991):

$$\varepsilon = \sum_{j=1}^{J} a_j \left[1 - \exp(-\kappa_j S)\right] \tag{5}$$

in which all terms in this equation are defined in Section 2.1.2.

Applications of the approach given by Eqs. (4) and (5) for computing the gray gas absorption coefficient are common in the literature (for example, Ravelli *et al.* (2008) and Shakeel *et al.* (2018)) and even in well-established commercial softwares for numerical simulation of reacting and non-reacting flows, such as ANSYS Fluent. Conversely, although the gray gas formulation of Eq. (3) is not as well widespread, it has been studied and successfully employed in a small number of previous works (Fraga *et al.*, 2017a; Sun *et al.*, 2017).

2.1.2 The Weighted-Sum-of-Gray-Gases (WSGG) Model

The WSGG model, first introduced by Hottel (1954) and later generalized and consolidated by Modest (1991), is a spectral model relatively simple to implement and with low computational cost, which has shown good agreement with line-by-line integration results for a number of different situations (Dorigon *et al.*, 2013; Cassol *et al.*, 2014; Fonseca *et al.*, 2018). In this model, the spectrum of radiation is replaced by a total of J gray gases with uniform absorption coefficients and by an undetermined number of transparent windows. Following this procedure and invoking a set of assumptions that are explained elsewhere (Modest, 1991; Dorigon *et al.*, 2013), the RTE for the jth gray gas may then be written as:

$$\frac{dI_j}{ds} = \kappa_j a_j I_b - \kappa_j I_j \quad (6)$$

where I_j and κ_j are the radiative intensity and the absorption coefficient of gas j, respectively. The term a_j is denominated the temperature coefficient and represents the fraction of blackbody radiation emitted at the local temperature of the medium in the wavenumber interval correspondent to the jth gas; its dependence on the medium temperature T is described by a polynomial function (Dorigon *et al.*, 2013; Cassol *et al.*, 2014):

$$a_j = \sum_{k=0}^{4} b_{j,k} T^k \quad (7)$$

The polynomial coefficients $b_{j,k}$ in Eq. (7), as well as the pressure-absorption coefficient $\kappa_{p,j}$ of each gray gas (defined similarly to the pressure-absorption coefficient of species α discussed in Section 2.1.1), are obtained from fitting global radiation data, typically of total emittance (cf. Eq. (5)). In the present study, the values of those coefficients to be used in the framework of the WSGG model are taken from Dorigon *et al.* (2013), while the set of correlations generated by Cassol *et al.* (2014) are adopted for the GG model based on Eqs. (4) and (5).

For the solution of the radiative heat transfer problem in the WSGG model, Eq. (6) is solved $J + 1$ times and the total radiation intensity is obtained as a summation over the intensities I_j of each gray gas and transparent window—i.e., $I = \sum_{j=0}^{J} I_j$, where $j = 0$ denotes the transparent windows. To determine the temperature coefficient for the transparent windows, a_0, the constraint $\sum_{j=0}^{J} a_j = 1$ is used, derived from the conservation of energy principle.

2.1.3 The Line-By-Line (LBL) Integration Method

The LBL integration is a more sophisticated method for the RTE solution, in which Eq. (1) is directly solved for each spectral line that composes the radiation spectrum. To evaluate κ_η, the high-resolution spectroscopic database HITEMP2010 (Rothman *et al.*, 2010) is used. More details on this methodology and the parameters adopted for generating spectral absorption coefficient data may be found in Dorigon *et al.* (2013) and Cassol *et al.* (2014).

2.2 Description of the Test Cases

The verification of each model implemented to FDS is based on comparisons with an already well-established (or reference) solution for a set of test cases. All these cases revolve around the radiative heat transfer problem occurring in a one-dimensional medium slab bounded by two infinite parallel walls, as depicted in Fig. 1a. The walls are treated as black surfaces with fixed temperature and the medium is a non-homogeneous, non-isothermal mixture of carbon dioxide and water vapor kept at a total pressure of 1 atm; a mixture of CO_2 and H_2O is chosen for the analyses because these are the two of the most common participating species in the products of hydrocarbon fuels combustion. Temperature and species concentration are known in every point of the medium, following predefined spatial distributions. As such, the problem requires only the solution of the RTE without the need of solving the remaining governing equations that would be solved in a traditional coupled FDS computation. This is deliberate, in order to avoid the influence of models and approximations associated with these other equations on the comparison between the modified Fire Dynamics Simulator code (with the different spectral models implemented on) and the reference solution.

The three spatial profiles of temperature T and carbon dioxide molar fraction X_c considered in this study are given in Tab. 1 and Fig. 2 ; these profiles try to mimic temperature and species concentration distributions typical of flames, and are similar to the ones used in previous studies (Dorigon *et al.*, 2013; Cassol *et al.*, 2014; Fonseca *et al.*, 2018). Both T

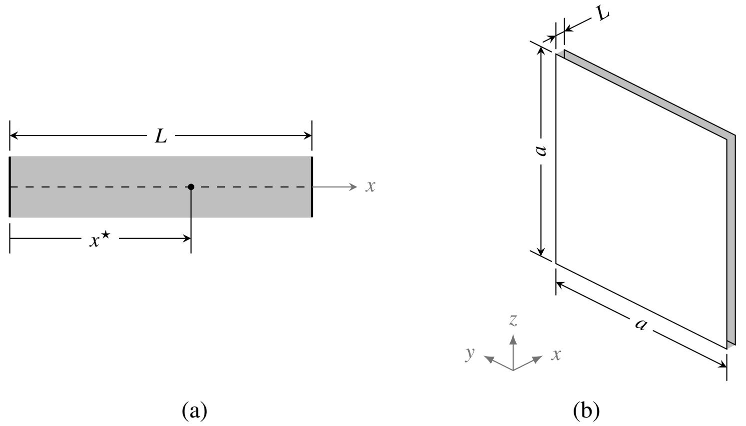

Figure 1: Schematic representation of the one-dimensional problem used for the reference solution (a) and three-dimensional adaptation adopted for the FDS simulation (b).

Table 1: Profiles of temperature and molar fraction of carbon dioxide used for the test cases.

	Temperature profile, $T(x^\star)$	Molar fraction of CO_2 profile, $X_c(x^\star)$
Profile 1	$400\,\mathrm{K} + 1400\,\mathrm{K}\sin^2(\pi x^\star)$	$0.2\sin^2(\pi x^\star)$
Profile 2	$400\,\mathrm{K} + 1400\,\mathrm{K}\sin^2(2\pi x^\star)$	$0.2\sin^2(2\pi x^\star)$
Profile 3	$\begin{cases} 800\,\mathrm{K} + 920\,\mathrm{K}\sin^2(2\pi x^\star), & \text{if } x^\star \leq 0.25 \\ 400\,\mathrm{K} + 1400\,\mathrm{K}\left\{1 - \sin^{3/2}\left[\frac{2\pi(x^\star-0.25)}{3}\right]\right\}, & \text{if } x^\star > 0.25 \end{cases}$	$\begin{cases} 0.25\sin^2(2\pi x^\star), & \text{if } x^\star \leq 0.25 \\ 0.25\left\{1 - \sin^{3/2}\left[\frac{2\pi(x^\star-0.25)}{3}\right]\right\}, & \text{if } x^\star > 0.25 \end{cases}$

and X_c are expressed as functions of the dimensionless length of the domain $x^\star = x/L$, where x is the spatial coordinate normal to the walls and L is the total length of the medium slab (cf. Fig. 1a). The spatial distribution of water vapor molar fraction X_w is determined by defining a constant ratio between the partial pressures of H_2O and CO_2 equal to 2, which is a ratio commonly found in the combustion methane. Additionally, for each case, three total distances between the walls are tested as a means of including the effect of different optical thicknesses of the participating medium: L =0.5, 1.0 and 2.0 m.

2.3 Reference Solution

The reference solution is given by an in-house Fortran-based code developed by the research group on thermal radiation of the Universidade Federal do Rio Grande do Sul, which has been successfully employed in a number of previous studies (Dorigon *et al.*, 2013; Cassol *et al.*, 2014; Fonseca *et al.*, 2018). The code solves the one-dimensional radiative heat transfer problem for specified fields of temperature and species concentration, adopting for the spatial integration of

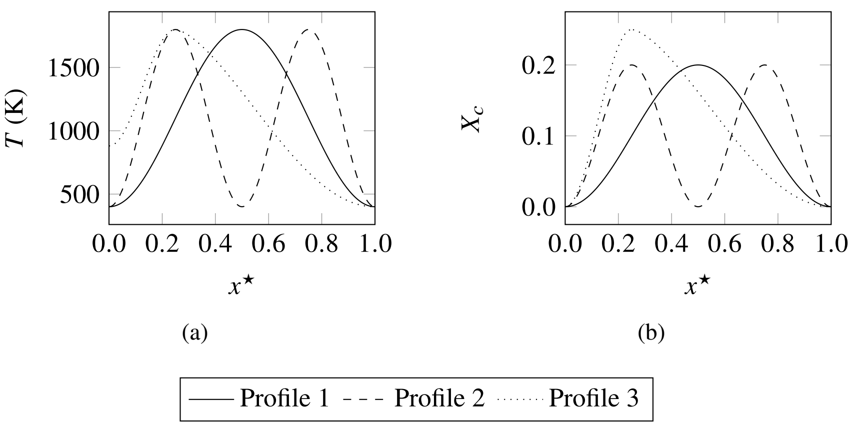

Figure 2: Spatial distributions of temperature (a) and CO_2 molar fraction (b) for each profile considered in this study.

the RTE the discrete ordinates method (DOM) coupled with a finite differencing methodology. A Gauss-Legendre quadrature is used to determine the weights and direction cosines of the DOM (Modest, 2013). Following mesh quality studies, twelve discrete ordinates and a uniformly spaced grid of 400 cells (the medium length was found to not significantly influence the mesh quality) are chosen for the reference computations.

2.4 Adaptation of the Test Problem to the FDS Simulations

The geometry shown in Fig. 1a needs to be adapted for a numerical solution in FDS, since this software is not capable of directly solving one-dimensional problems. For this purpose, a three-dimensional configuration is proposed, consisting of two large square-shaped parallel plates of side a bounding a thin volume layer of participating medium, as illustrated in Fig. 1b. The idea behind this is that, if the area a^2 of the plates is sufficiently large compared to the distance L between them, then the radiative heat transfer may be approximated as a one-dimensional problem and results along a line that passes through the center of both plates could be satisfactorily compared to the one-dimensional reference solution. Preliminary testing showed that a domain with $a = 50L$ is adequate for the computations, yielding errors in local quantities at the centerline of the plates of less than 5×10^{-3} % compared to a domain with $a = 100L$.

Temperature and species concentration are assumed to be constant along the y- and z-directions and to vary along direction x according to the profiles introduced in Section 2.2 (cf. the coordinate system in Figure 1b). The boundary conditions at the parallel plates are the same as in the one-dimensional problem and, at the lateral surfaces (the surfaces normal to the y- and z-axes, shown in gray in Fig. 1b), a constant temperature equal to 1100 K is prescribed, which is equal the average medium temperature for the three profiles in Tab. 1; like the parallel plates, the lateral surfaces are also treated as black to thermal radiation.

The three-dimensional domain is spatially discretized using a rectangular, structured, uniformly spaced mesh. Along direction x, the same spatial refinement level as the reference solution is adopted, while a coarser discretization is employed at the cross-sectional yz plane, since the radiative heat transfer in these directions should be negligible; following a mesh quality analysis, 50 grid cells in the y- and z- directions (independently of the domain size) were shown to be sufficient to provide negligible errors relative to a finer discretization. For the angular discretization required for the RTE solution in the finite volume method, a total of 400 control angles are used, which was found to yield maximum errors of approximately 5 % compared to a discretization with 800 control angles (further refinements in the angular discretization increase substantially the computational cost of the calculations).

3. RESULTS

Comparisons between the Fire Dynamics Simulator code with each new model implemented into it and the reference solution are based on the spatial distribution of the volumetric radiative heat source S_r (given as the negative value of the local radiative heat flux divergence (Modest, 2013; Howell *et al.*, 2016)) along the medium slab. As previously noted, in the three-dimensional configuration adopted for the FDS computations the one-dimensional spatial profile of this quantity is extracted from a line that passes through the center of both parallel plates that bound the medium.

Figure 3 shows, for all test cases studied in this work, the distribution of S_r obtained by the FDS and reference solutions for the WSGG model and for the gray gas formulations; for the latter, the two approaches studied in this paper are denoted as $GG_{Eq.(3)}$ and $GG_{Eq.(4)}$, where the subscripts indicate the equation used to calculate the gray gas absorption coefficient. To facilitate readability, results of the LBL integration method are shown separately, in Fig. 4. In both these figures, there is a clear agreement between the FDS and the reference solutions, indicating that all models were correctly implemented to the Fire Dynamics Simulator code. It is also interesting to note that, while the two gray gas formulations are reasonably similar, the difference between them and the WSGG and the LBL solutions is of an order of magnitude in most of the domain. Conversely, the radiative heat source predicted by the WSGG model is remarkably close to results of the LBL integration method, in agreement with what is reported by (Dorigon *et al.*, 2013).

The difference between the FDS and the reference solutions can be quantified by defining a normalized deviation ψ:

$$\psi = \left| \frac{{S_r}^{\mathrm{FDS}} - {S_r}^{\mathrm{ref}}}{\max({S_r}^{\mathrm{ref}})} \right| \tag{8}$$

where ${S_r}^{\mathrm{FDS}}$ and ${S_r}^{\mathrm{ref}}$ are the local values of the radiative heat source obtained by the FDS code (with any of the studied models implemented to it) and by the reference solution, respectively, and $\max({S_r}^{\mathrm{ref}})$ is the maximum value of ${S_r}^{\mathrm{ref}}$ in the medium slab.

Following this methodology, Tab. 2 presents the maximum and medium-averaged values of ψ ($\psi_{\max}$ and ψ_{avg}, respectively) for each implemented model and for each test case. No medium-averaged difference exceeds 1.5 % and, even for the cases where the Fire Dynamics Simulator code deviates the most from the reference results, the maximum local deviation between the two solutions is of approximately 3 %. Observing that this difference is similar to the errors attributed to the angular discretization for the FDS computations, all models are considered to have been successfully implemented into this code.

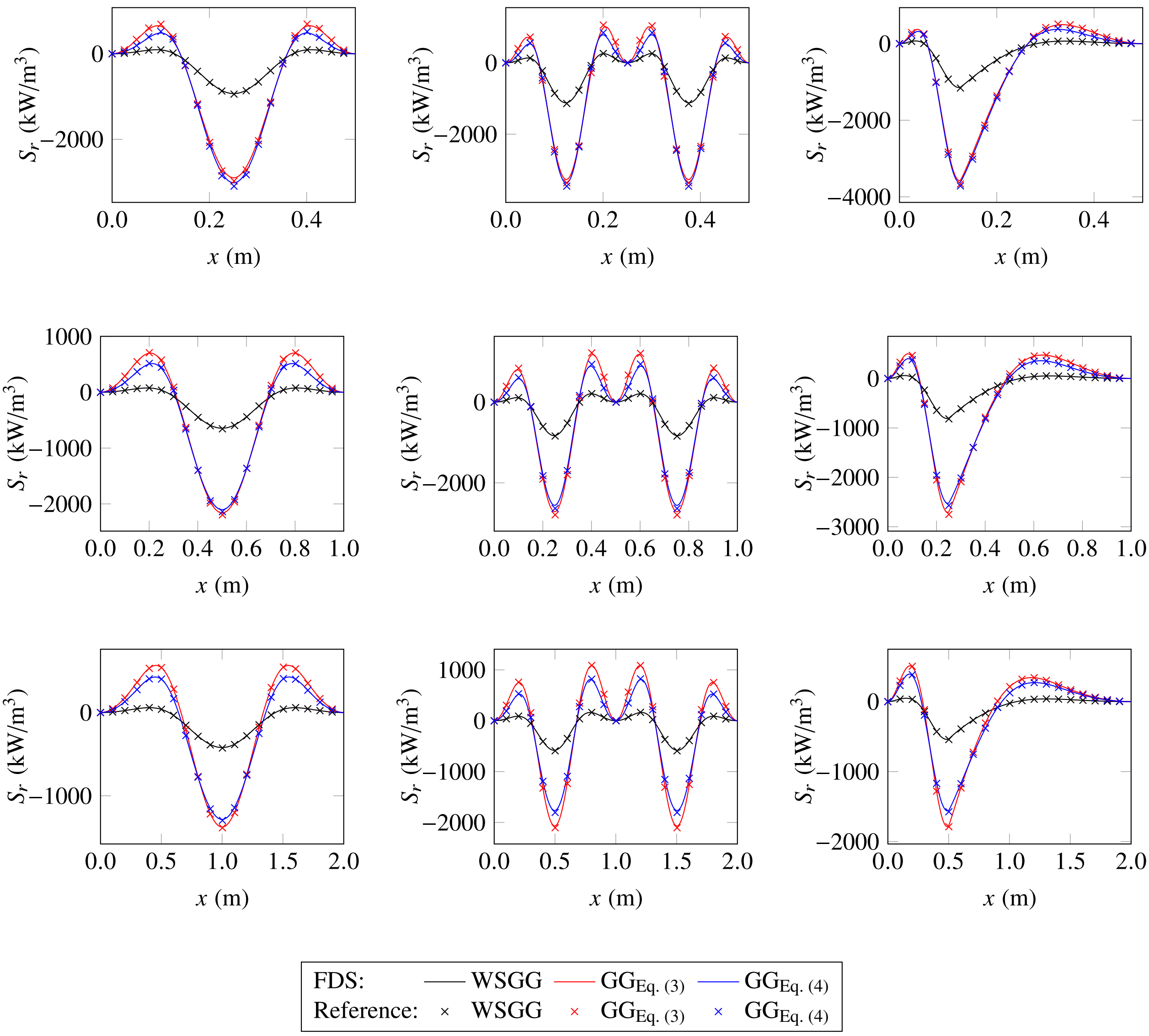

Figure 3: Radiative heat source along the medium slab obtained by FDS and by the reference solution with the WSGG model and the gray gas formulations. From left to right: profiles 1, 2 and 3; from top to bottom: L =0.5, 1.0 and 2.0 m.

A final point concerns the computational time demanded each model when applied to FDS. The gray gas formulation based on Eq. (3) proved to be significantly faster than the other models, solving the radiation field in approximately half the time of the WSGG model. Conversely, the gray gas formulation of Eq. (4) yields computational times comparable to the WSGG model, probably due to the need of performing multiple operations to determine the emittance of the gray medium (cf. Eq. (5)); nevertheless, because the $GG_{Eq.(4)}$ model only requires a single global solution of the RTE, this formulation is expected to be substantially faster than the WSGG model for more refined spatial and angular discretizations. Finally, despite the fact that all calculations with the LBL integration method were conducted in a better machine, they seem to require upwards of two magnitudes more computational time than the remaining models. Therefore, while fully coupled heat transfer, combustion and fluid flow simulations are feasible in FDS with either the WSGG model or any of the gray gas formulations implemented in this study, the LBL method should probably be restricted to frozen field computations such as the ones performed in the present work.

4. CONCLUSIONS

This paper presented a study on the coupling of a series of spectral models for the solution of the radiative transfer equation to the open-source Fire Dynamics Simulator solver. A verification analysis of each implemented model was conducted by comparing the local radiative heat source obtained by the modified FDS code with a reference solution for one-dimension radiative transfer problem.

Nine test cases were studied, combining different prescribed temperature and species concentration profiles and dif-

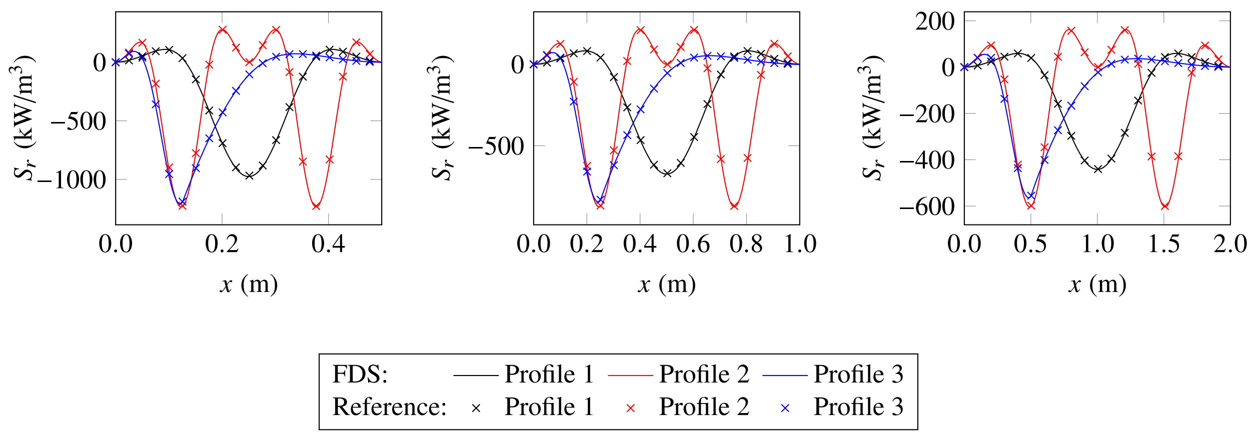

Figure 4: Radiative heat source along the medium slab obtained by FDS and by the reference solution with the LBL integration method. From left two right: $L = 0.5$, 1.0 and 2.0 m.

Table 2: Results of the test cases for the verification of the WSGG model implementation to FDS.

	WSGG		$GG_{Eq.(3)}$		$GG_{Eq.(4)}$		LBL	
	ψ_{max} (%)	ψ_{avg} (%)	ψ_{max} (%)	ψ_{avg} (%)	ψ_{max} (%)	ψ_{avg} (%)	ψ_{max} (%)	ψ_{avg} (%)
$L = 0.5$ m:								
Profile 1	1.43	0.41	2.56	1.07	2.55	0.95	0.84	0.42
Profile 2	2.04	0.62	2.83	1.26	2.68	1.03	2.31	0.71
Profile 3	1.72	0.35	2.71	0.70	2.69	0.67	2.06	0.32
$L = 1.0$ m:								
Profile 1	1.70	0.44	1.58	0.63	1.67	0.61	0.72	0.35
Profile 2	1.62	0.52	2.98	1.27	3.10	1.26	2.31	0.76
Profile 3	1.90	0.36	1.97	0.42	2.07	0.45	2.02	0.29
$L = 2.0$ m:								
Profile 1	1.32	0.38	0.64	0.29	0.91	0.35	0.43	0.24
Profile 2	1.90	0.58	2.08	0.73	2.35	0.92	2.24	0.77
Profile 3	1.72	0.30	1.31	0.21	1.50	0.28	1.96	0.31

ference medium lengths. All models implemented to FDS yielded results very similar to the reference solution, with maximum local deviations of less than 3 %, attesting that the implementations were done correctly. In future works, the authors expect to validate the models by performing comparisons with data from the literature for more complex two- and three-dimensional configurations.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE

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