Bordbar, Hadi; Fraga, Guilherme C.; Hostikka, Simo

An extended weighted-sum-of-gray-gases model to account for all CO_2 - H_2O molar fraction ratios in thermal radiation

Published in:
International Communications in Heat and Mass Transfer

DOI:
10.1016/j.icheatmasstransfer.2019.104400

Published: 01/01/2020

Document Version
Peer-reviewed accepted author manuscript, also known as Final accepted manuscript or Post-print

International Communications in Heat and Mass Transfer

An Extended Weighted-Sum-of-Gray-Gases Model to Account for All CO2-H2O Molar Fraction Ratios in Thermal Radiation

--Manuscript Draft--

Manuscript Number:	ICHMT-D-19-00767R2
Full Title:	An Extended Weighted-Sum-of-Gray-Gases Model to Account for All CO2-H2O Molar Fraction Ratios in Thermal Radiation
Article Type:	Research Paper
Keywords:	Thermal radiation, gas spectral radiation, Weighted sum of gray gases (WSGG), CFD, fire dynamics modeling,
Corresponding Author:	Hadi Bordbar Aalto University FINLAND
Corresponding Author Secondary Information:	
Corresponding Author's Institution:	Aalto University
Corresponding Author's Secondary Institution:	
First Author:	Hadi Bordbar
First Author Secondary Information:	
Order of Authors:	Hadi Bordbar
	Guilhereme Fraga
	Simo Hostikka
Order of Authors Secondary Information:	
Abstract:	All published weighted sum of gray gases models (WSGGM) were either developed for a limited number of molar fraction ratios, MR, or include MR as a variable in their formulations. Either way, they are not able to adequately support moisture rich regions of combustion environments, such as the outer regions of unwanted fires, fires during water-based suppression, and some air-injection regions of furnaces. In this article, we provide an extension to a previously published WSGGM by coupling it to a new accurate set of WSGGM coefficients for pure carbon dioxide and water vapor. The coupling follows a linear interpolation methodology, which is justified by a detailed analysis of the line-by-line (LBL) absorption spectra and by plotting the total emissivity of CO2-H2O mixtures with large and small values of MR for various temperatures and path lengths. The proposed model is discussed and validated in three benchmarks, using as reference a solution obtained by LBL integration. The results indicate that, while the previously available WSGGMs either have excessive computational costs or yield inaccurate results in the regions of large MR, the new model can be safely used for all gas compositions in a computationally efficient manner.
Suggested Reviewers:	Francis H. R. França Professor, Instituto Federal de Educacao Ciencia e Tecnologia do Rio Grande do Sul frfranca@mecanica.ufrgs.br He is perhaps the best well known researcher in development of WSGG model
	Kari Myöhanen kari.myohanen@lut.fi due to his background in heat transfer modeling in combustion systems
	Huaqiang Chu Professor, Huazhong University of Science and Technology

	hqchust@ahut.edu.cn He is an expert of the feild
	Ankit bansal Assistant Professor, Indian Institute of Technology Roorkee Mahatma Gandhi Central Library abansfme@iitr.ac.in He is an expert of the field
	Masood Darbandi Professor darbandi@sharif.edu He is an expert of the feild
Opposed Reviewers:	
Response to Reviewers:	
Additional Information:	
Question	**Response**
Please enter the **Word Count** of your manuscript	2527

An Extended Weighted-Sum-of-Gray-Gases Model to Account for All CO_2-H_2O Molar Fraction Ratios in Thermal Radiation

H. Bordbar[a,*], G.C. Fraga[b], S. Hostikka[a]

[a] *Department of Civil Engineering, Aalto University, Finland*
[b] *Mechanical Engineering Department, Universidade Federal do Rio Grande do Sul, Brazil*

Abstract

All published weighted sum of gray gases models (WSGGM) were either developed for a limited number of molar fraction ratios, *MR*, or include *MR* as a variable in their formulations. Either way, they are not able to adequately support moisture-rich regions of combustion environments, such as the outer regions of unwanted fires, fires during water-based suppression, and some air-injection regions of furnaces. In this article, we provide an extension to a previously published WSGGM by coupling it to a new accurate set of WSGGM coefficients for pure carbon dioxide and water vapor. The coupling follows a linear interpolation methodology, which is justified by a detailed analysis of the line-by-line (LBL) absorption spectra and by plotting the total emissivity of CO_2-H_2O mixtures with large and small values of *MR* for various temperatures and path lengths. The proposed model is discussed and validated in four benchmarks, using as reference a solution obtained by LBL integration. The results indicate that, while the previously available WSGGMs either have excessive computational costs or yield inaccurate results in the regions of large *MR*, the new model can be safely used for all gas compositions in a computationally efficient manner.

*Corresponding author
Email address: hadi.bordbar@aalto.fi (H. Bordbar)

Table 1: Range of molar fraction ratio supported by recent WSGGMs that account for varying MR.

Johansson et al. [7]	Kangwanpongpan et al. [8]	Bordbar et al. [9]	Guo et al. [10]
$0.125 \leq MR \leq 2.0$	$0.125 \leq MR \leq 4.0$	$0.01 \leq MR \leq 4.0$	$0.05 \leq MR \leq 2.0$

1. Introduction

As a member of a more generic category of global spectral models, the weighted-sum-of-gray-gases model (WSGGM) aims at obtaining total radiative quantities such as the radiative heat source and heat flux by solving the spectrally-integrated radiative transfer equation (RTE) for a small number of gray gases [1]. Due to its simplicity compared to other global models (such as the spectral line-based WSGGM [2] and the full-spectrum k-distribution method [3]), the WSGGM has been more widely used for radiative transfer calculations involving CO_2-H_2O mixtures in large-scale combustion systems. Most WSGGMs (e.g., [4–6]) were obtained for a few specific molar fraction ratios $MR = Y_w/Y_c$ (where Y_w and Y_c are the molar fractions of water vapor and carbon dioxide, respectively), which restricts their range of application. More recent WSGGMs [7–10] have attempted to overcome this limitation by including a dependence on MR in their formulations, but the difficulty of fitting emissivity data over all possible molar ratio values—i.e., from $MR \to 0$ for pure CO_2 to $MR \to \infty$ for pure H_2O—makes even these models limited to a certain range of MR. A summary of the applicability range of the most widely used varying MR WSGGMs is provided in Table 1.

Although the domain-average value of MR in combustion systems usually lies within the limits of the models in Table 1, it is possible that the molar fraction ratio locally exceeds their limits, such as in moisture-rich regions of flames and in the outer regions of unwanted fires. In these cases, these WSGGMs can not be safely applied. Another approach for dealing with this limitation is to adopt the double integration methodology, in which WSGGM coefficients for the individual

species are combined using probabilistic arguments (see, for example, [11, 12]). However, while this in principle allows for considering the full range of *MR*s, it entails a significant increment in the computational cost as the radiative transfer equation must be solved for each gray gas of H_2O and CO_2. Andre et al. [13] and Consalvi et al. [14] presented the detailed assessment of computational performance of the double integration WSGGM [12] for high temperature [13] and high pressure [14] combustion systems in comparison with some other global models such as different versions of full spectrum correlated-k method (FSCK).

In this regard, the present study proposes an extension to the previously published WSGGM of Bordbar et al. [9], originally developed for $0.01 \leq MR \leq 4.0$, to cover all values of *MR*. The accuracy of the WSGGM of [9] has been proven by several comparative studies [15, 16]. To the best of the authors' knowledge, this is the first attempt to provide a WSGGM that is applicable for the entire range of *MR* beside the computationally demanding double integration models.

2. Methodology

2.1. WSGGM coefficients for pure species

Following the same methodology used in [9], two new sets of WSGGM coefficients are generated for pure CO_2 and pure H_2O to support cases where only one of these species exist. First, line-by-line (LBL) absorption spectra at atmospheric pressure are obtained for each species from the HITEMP 2010 database [17] as described in [18], adopting a spectral resolution of $0.02\,\mathrm{cm}^{-1}$ within a wavenumber range $150\,\mathrm{cm}^{-1} \leq \eta \leq 15\,000\,\mathrm{cm}^{-1}$. A resolution of $0.02\,\mathrm{cm}^{-1}$ is reported as the optimal spectral resolution for obtaining the LBL absorption spectra of combustion gases, and using finer spectral resolution has found to have a negligible influence on the results of LBL spectral data while significantly increasing the computing time [19]. Considering 43 evenly distributed temperature points between 300 K and 2400 K and by using the LBL

Table 2: WSGGM coefficients for pure CO_2 at 1 atm.

i	$\kappa_{p,i}$ ($m^{-1}\,atm^{-1}$)	$b_{i,1}$	$b_{i,2}$	$b_{i,3}$	$b_{i,4}$	$b_{i,5}$
1	3.272772×10^{-2}	8.495135×10^{-1}	-1.496812	1.361406	-5.551699×10^{-1}	8.076589×10^{-2}
2	4.229655×10^{-1}	-1.103102×10^{-1}	9.363958×10^{-1}	-1.250799	6.527827×10^{-1}	-1.206959×10^{-1}
3	4.905367	1.731716×10^{-1}	-5.174223×10^{-1}	8.256840×10^{-1}	-4.998864×10^{-1}	1.008743×10^{-1}
4	1.085440×10^{2}	3.995426×10^{-2}	1.423006×10^{-1}	-1.649481×10^{-1}	5.140768×10^{-2}	-3.497246×10^{-3}

spectra, a total emissivity ε database is constructed, where ε is given as [3]

$$\varepsilon = \frac{\int_0^\infty I_{b\eta}[1 - \exp(-\kappa_{p\eta} p_t Y L)]}{\int_0^\infty I_{b\eta}\,\mathrm{d}\eta}\,, \tag{1}$$

in which $I_{b\eta}$ is the Planck function, $\kappa_{p\eta}$ is the pressure-based spectral absorption coefficient, p_t is the total pressure, Y is the molar fraction, and L is the path length. The emissivity database is generated by LBL integration for 20 path lengths between 0.01 m and 60 m, with $p_t = 1\,\mathrm{atm}$ and $Y = 1$. Then, the following equation, which expresses the total emissivity for the WSGGM, is fitted to the database to obtain the weighting factors a_i and pressure-based absorption coefficients $\kappa_{p,i}$ of each gray gas i,

$$\varepsilon = \sum_{i=1}^{N_g} a_i[1 - \exp(-\kappa_{p,i} p_t Y L)]\,. \tag{2}$$

Similarly to [9], the number of gray gases N_g of the model is taken as 4 and the weighting factor of the gray gases is given as a polynomial function of the temperature T,

$$a_i = \sum_{j=1}^{5} b_{i,j} \left(\frac{T}{T_{ref}}\right)^{j-1}\,, \tag{3}$$

with $b_{i,j}$ the polynomial constants of the model and $T_{ref} = 1200\,\mathrm{K}$. As is common in the WSGGM, the weighting coefficient for the transparent windows ($i = 0$) is determined from energy conservation considerations as $a_0 = 1 - \sum_{i=1}^{N_g} a_i$. Tables 2 and 3 report the obtained coefficients for pure CO_2 and pure H_2O, respectively.

It should be noted that WSGGM coefficients for these individual species already exist in the literature—for example, in [4, 5, 12]. However, they have

Table 3: WSGGM coefficients for pure H_2O at 1 atm.

i	$\kappa_{p,i}$ (m^{-1} atm^{-1})	$b_{i,1}$	$b_{i,2}$	$b_{i,3}$	$b_{i,4}$	$b_{i,5}$
1	8.047859×10^{-2}	6.670204×10^{-1}	-1.228413	1.428908	-6.267906×10^{-1}	9.628539×10^{-2}
2	9.557208×10^{-1}	2.343433×10^{-1}	-3.192256×10^{-1}	8.867348×10^{-1}	-5.927787×10^{-1}	1.185824×10^{-1}
3	8.005283	-1.793041×10^{-1}	1.683454	-2.136989	1.020422	-1.723960×10^{-1}
4	7.613186×10^{1}	3.455969×10^{-1}	-7.510442×10^{-1}	6.313180×10^{-1}	-2.416500×10^{-1}	3.530972×10^{-2}

been developed with different conditions than those of [9] (e.g., different number of gray gases or distinct ranges of temperature applicability), thus making the coupling to already existing correlations not sensible.

2.2. Coupling methodology

For conditions where $0 < MR < 0.01$ or $MR > 4.0$ (i.e., outside the applicability range of the WSGGM of Bordbar et al. [9]), the correlations in Tables 2 and 3 are coupled to those of [9] by linearly interpolating the values of $\kappa_{p,i}$ and a_i. For $0 < MR < 0.01$, the upper and lower bounds of this interpolation are the results of the WSGGM of [9] for $MR = 0.01$ and the coefficients of Table 2 for $MR = 0$, respectively. For $MR > 4.0$, the lower bound is again the results of [9] for $MR = 4.0$, while the upper bound is taken as the coefficients of Table 3 for a very large molar fraction ratio represent pure H_2O. Our numerical tests showed that using a value of $MR = 10^8$ to represent this upper bound (H_2O) consistently provides very good accuracy in all of our validation tests.

This interpolation approach is based on the assumption that the absorption spectra of CO_2-H_2O mixtures with $MR < 0.01$ or $MR > 4.0$ are linearly scalable with MR; thus, for instance, for large MR values (>4.0) one could obtain the absorption spectrum of a mixture by a linear interpolation between the spectra of $MR = 4.0$ and of pure H_2O. This is physically justified because, in these ranges of MR, the mixture mainly consists of only one species (H_2O for large MR and CO_2 for small MR), so the effect of mixing of the absorption spectra of the individual gases is marginal. Nonetheless, this, like any other similar assumption used in development of global models—such as the correlation or

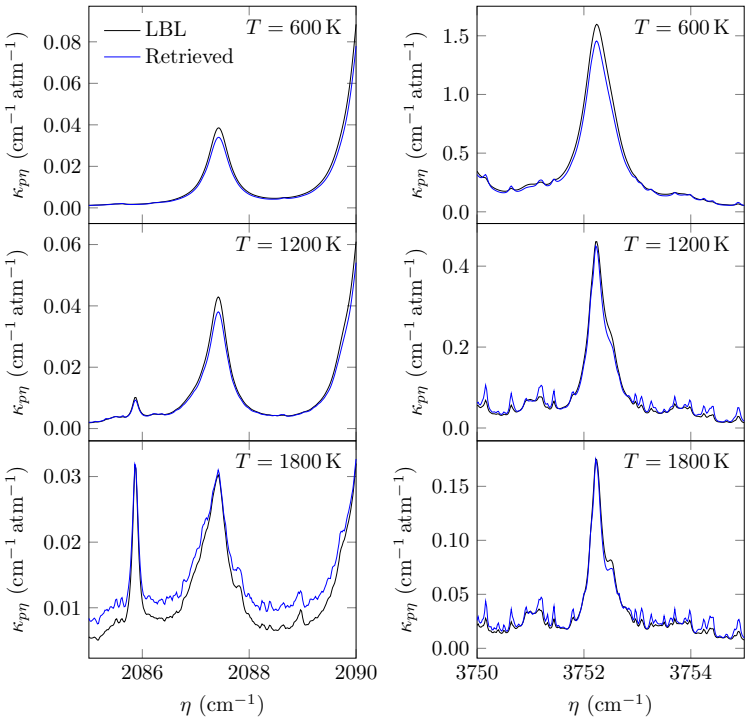

Figure 1: The spectral absorption of a mixture with $MR = 10$: comparison of the real LBL profiles with those retrieved by linear interpolation between $MR = 4.0$ and pure H_2O.

scaling assumption used in FSCK or FSSK methods [3]—is not completely true and its accuracy needs to be checked. For that purpose, Fig. 1 compares the real LBL absorption spectra of a CO_2-H_2O mixture with $MR = 10$ and the spectra recreated by linearly interpolating between $MR = 4.0$ and pure H_2O. Two spectral regions with strong H_2O or CO_2 absorption lines are shown in this figure, and for both of them, as well as for the three different medium temperatures considered, the retrieved spectra of the mixture exhibit a good agreement with the LBL data.

The linear interpolation assumption is further assessed by examining the total emissivity of CO_2-H_2O mixtures with $MR > 4.0$. This is done in Fig. 2, where ε predicted by the extended WSGGM is compared to results obtained by LBL integration. For small and intermediate path lengths, the extended

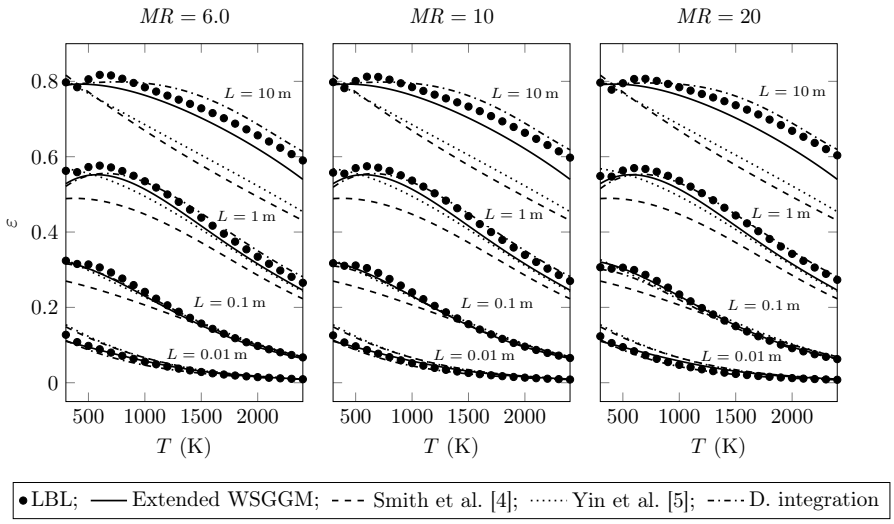

Figure 2: Comparison of the total emissivity predicted by the extended WSGGM proposed in this paper and by existing models that comport $MR > 4$ with ε generated by LBL integration.

WSGGM gives a very accurate approximation of the total emissivity for the entire temperature range for which the model was developed. Moreover, compared to the WSGGMs presented by Smith et al. [4] and Yin et al. [5] that are also applicable to $MR > 4$ and are briefly described in Section 3, the present model performs significantly better for all the temperatures, path lengths and molar fraction ratios. Both the present extended WSGGM and the double integration model perform equally good in most of the temperature and path length range especially in small to intermediate path length. However, as expected the double integration WSGGM [12], provides slightly more accurate total emissivity in large path length but in the price of higher computational time as will be explained more in the results of 1D test cases in the next section. Similar results are observed for mixtures with $MR < 0.01$ and are omitted here for brevity.

3. Results and discussion

The extended WSGGM proposed in this paper is tested for four test cases, all consisting of a one-dimensional medium slab bounded by two parallel black walls

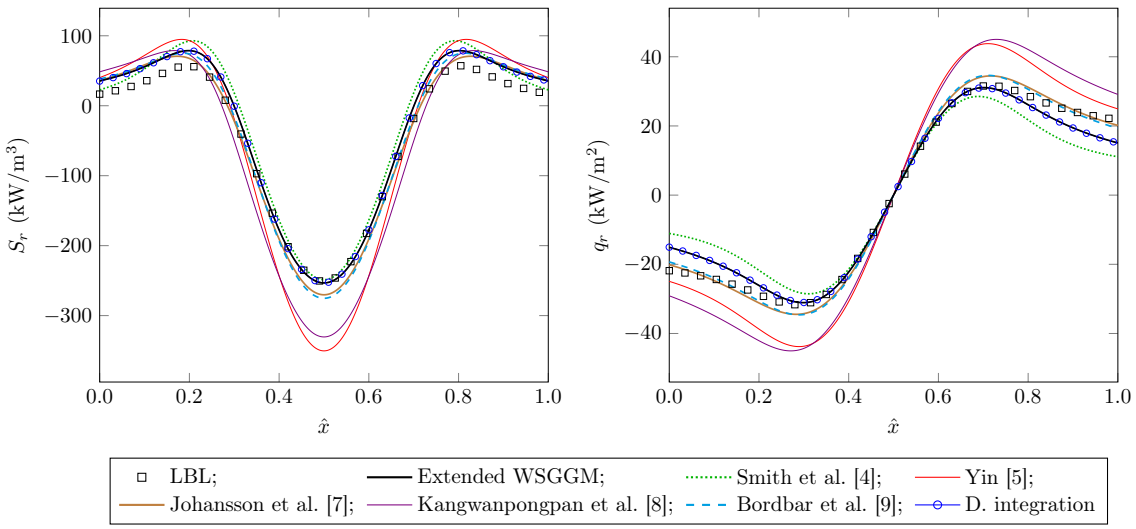

Figure 3: Results of the first test case ($MR \to 0$).

at 400 K and separated by a distance $X = 1$ m for test cases 1-3 and $X = 10$ m for the test case 4. All the cases are subjected to the same non-homogeneous, symmetrical temperature profile, given as $T(\hat{x}) = 400\,\mathrm{K} + 1400\,\mathrm{K}\sin^2(2\pi\hat{x})$, where $\hat{x} = x/X$ is the dimensionless distance from the left wall. The medium composition of each case is defined as to consider the conditions $MR < 0.01$ (case 1), $MR > 4.0$ (case 2 and 4), and $0 \leq MR \leq \infty$ (case 3).

The RTE is solved with the discrete ordinates method, following the methodology and discretization parameters outlined in [6]. The reference solution, to which all WSGGMs are compared, is provided via the LBL integration method as described in [20].

The first test case represents a scenario in which $MR \to 0$, where the medium is a homogeneous CO_2-H_2O-N_2 mixture with $Y_c = 0.5$ and $Y_w = 10^{-4}$. Figure 3 compares the extended WSGGM proposed in this paper to the variable-MR correlations presented in Table 1 in terms of the predicted radiative heat source, S_r, and radiative heat flux, q_r. The figure also reports the results obtained by three additional formulations: the one by Yin [5], in which fixed-MR coefficients are provided for a number of different gas compositions alongside an algorithm

to define which of them to be used; a linear interpolation (carried out following a similar procedure as described in Section 2.2) between the more outdated set of coefficients of Smith et al. [4], which were generated for $MR = 1.0$, $MR = 2.0$, $MR \to 0$ and $MR \to \infty$; and a double integration methodology similar to the one outlined in [11], but employing the pure CO_2 and H_2O coefficients in Tables 2 and 3.

For the first case, all WSGGMs yield physically sensible results, even though the medium has a molar ratio well below the recommended MR ranges of the correlations in Table 1. A normalized error of each model can be defined as $\delta\phi = |\phi^{\mathrm{WSGGM}} - \phi^{\mathrm{LBL}}| \,/\, \max(|\phi^{\mathrm{LBL}}|)$, where ϕ^{WSGGM} and ϕ^{LBL} are the values of the radiative quantity ϕ (S_r or q_r) obtained with the WSGGM and the LBL method, respectively, and $\max(|\phi^{\mathrm{LBL}}|)$ is the maximum absolute value of ϕ^{LBL} in the domain. Table 4 reports the maximum and domain-average δS_r and δq_r for all WSGGMs, where it can be seen that for test case 1 the most accurate radiative transfer solutions are achieved with the model of [7], with the extended WSGGM developed in this paper and with the double integration model.

Figure 4 shows the results of the second test case, which consists of a homogeneous CO_2-H_2O-N_2 mixture with $Y_c = 10^{-4}$ and $Y_w = 0.5$, illustrating the condition of $MR \to \infty$.

Note that results of the WSGGMs in Table 1 are not included in Fig. 4 because those models yield physically unrealistic profiles of S_r and q_r (i.e., the values of these quantities are several order of magnitudes larger than the LBL results). Conversely, the models based on fixed-MR correlations [4, 5] are able to provide fairly accurate results; however, as indicated by the errors reported in Table 4, they are much less accurate than the extended WSGGM. Finally, the results of the double integration approach are almost as accurate as the current extended model but with much higher computational cost, as it will be discussed later.

In the third test case, the medium is a non-homogeneous CO_2-H_2O mixture with $Y_w(\hat{x}) = 10^{-4} + (1 - 10^{-4})\sin^2(\pi\hat{x})$ and $Y_c(\hat{x}) = 1 - Y_w(\hat{x})$, representing a scenario where both $MR \to 0$ and $MR \to \infty$ occur in the domain. Figure 5 and

Table 4: Domain-average and maximum (in parenthesis) normalized error of and average computational time required for the different WSGGMs.

	Case 1		Case 2		Case 3		Case 4		$\bar{t}$
	$\delta S_r(\%)$	$\delta q_r(\%)$	$\delta S_r(\%)$	$\delta q_r(\%)$	$\delta S_r(\%)$	$\delta q_r(\%)$	$\delta S_r(\%)$	$\delta q_r(\%)$	$(\times 10^{-3}\,\mathrm{s})^{\mathrm{a}}$
Extended WSGGM	5.79	7.20	5.52	4.60	6.57	8.16	4.76	10.4	5.9
	(9.14)	(21.3)	(7.54)	(8.33)	(11.1)	(23.8)	(6.58)	(21.8)	
Smith et al. [4]	8.53	16.3	8.20	6.21	12.9	25.3	7.38	25.4	3.2
	(16.3)	(34.0)	(12.0)	(14.1)	(31.9)	(51.3)	(27.8)	(30.6)	
Yin [5]	17.0	24.9	11.5	9.24	12.6	7.47	7.26	26.8	3.8
	(39.5)	(38.3)	(21.5)	(17.5)	(43.1)	(19.0)	(26.5)	(32.3)	
Johannson et al. [7]	5.79	5.21	–	–	–	–	–	–	2.6
	(9.65)	(8.80)							
Kangwanpongpan et al. [8]	16.1	30.8	–	–	–	–	–	–	3.2
	(31.5)	(43.2)							
Bordbar et al. [9]	6.81	5.54	–	–	–	–	–	–	5.1
	(9.56)	(9.45)							
Guo et al. [10]	60.4	90.1	–	–	–	–	–	–	2.7
	(154)	(138)							
Double integration	5.77	7.28	4.50	5.24	2.74	3.02	6.68	7.26	16
	(9.18)	(21.5)	(6.34)	(8.92)	(6.55)	(5.81)	(10.6)	(19.5)	

[a] For the LBL integration method, $\bar{t} = 66\,\mathrm{s}$.

Table 4 present the results and the associated errors for this case, respectively. As in the second test case, all WSGGMs in Table 1 lead to nonphysical results, so they are omitted. Similarly, the WSGGMs of Smith et al. [4] and Yin [5], although capable of capturing well the overall spatial variation of S_r and q_r, fail at particular locations, where the radiative source experiences abrupt peaks or valleys and, correspondingly, the radiative heat flux profile has quick changes in its slope. Such locations correspond to regions where the formulations of [4] and [5] transition from one set of fixed-MR WSGGM coefficients to another, resulting in a mismatch in the values calculated for $\kappa_{p,i}$ and a_i in one grid point to the next and yielding large local errors (especially for S_r), as depicted in Table 4. The same does not happen for the double integration and the extended

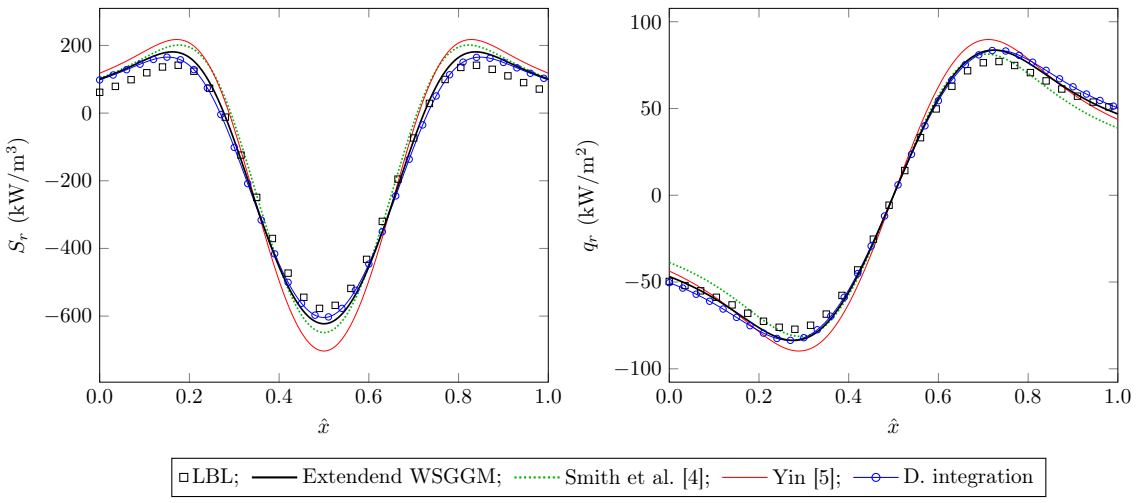

Figure 4: Results of the second test case ($MR \to \infty$).

WSGGMs, and no spurious oscillations of S_r and q_r can be seen in the results of theses models.

As the WSGGMs are most widely used to model thermal radiation in practical large scale combustion systems where the medium are usually optically thick, the performance of the present extended WSGGM is assessed in test case four with $X = 10\,\mathrm{m}$ representing the optically thick conditions. All the other settings of the fourth test case are the same as the second test case and therefore $MR > 4.0$. The radiative heat flux and heat source of test case 4 are shown in Fig. 6. As seen the accuracy of the present extended WSGGM is quite good and in a similar level of double integration method. This figure and the errors reported in Table 4 for this test case prove that the present extended WSGGM perform equally good in optically thin and thick regimes. Finally, the computational cost of different models should be checked and compared. Table 4 reports the average computational time $\bar{t}$ required by each WSGGM for simulating the three test cases, from which one may conclude that all but the double integration model have similar processing costs; differences in $\bar{t}$ between these models are attributed to the different number of gray gases used in the different models and the amount of operations necessary for determining $\kappa_{p,i}$ and a_i. Conversely,

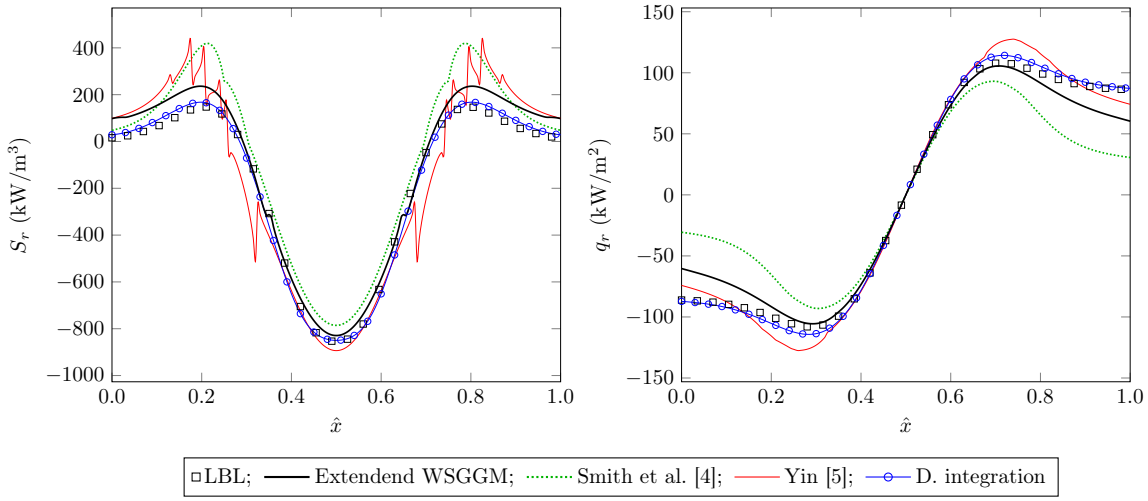

Figure 5: Results of the third test case ($0 \leq MR \leq \infty$).

the average computational time associated to the double integration model is 3 to 6 times that of the other WSGGMs, due to the need of accounting for a much greater number of gray gases—5 gases and transparent windows for both CO_2 and H_2O, totaling $N_g = 24$ (besides a global transparent window for the mixture), compared to $N_g = 4$ for the extended WSGGM, for instance. However, despite this substantially longer $\bar{t}$, the gained accuracy of double integration model compared to the extended WSGGM for the third case is quite small, while for the first, second and fourth cases both models perform similarly.

4. Conclusions

An extension to a published WSGGM has been proposed, making it able to cover all possible molar fraction ratios for gas mixture of carbon dioxide and water vapor. The extension is based on a linear interpolation between the existing formulation and newly developed WSGGM coefficients for pure CO_2 and pure H_2O. The validity of this interpolation approach has been justified by a detailed analysis of the absorption spectra of gas mixtures with large (> 4.0) or small (< 0.01) molar fraction ratios, which showed that the spectra of the mixture

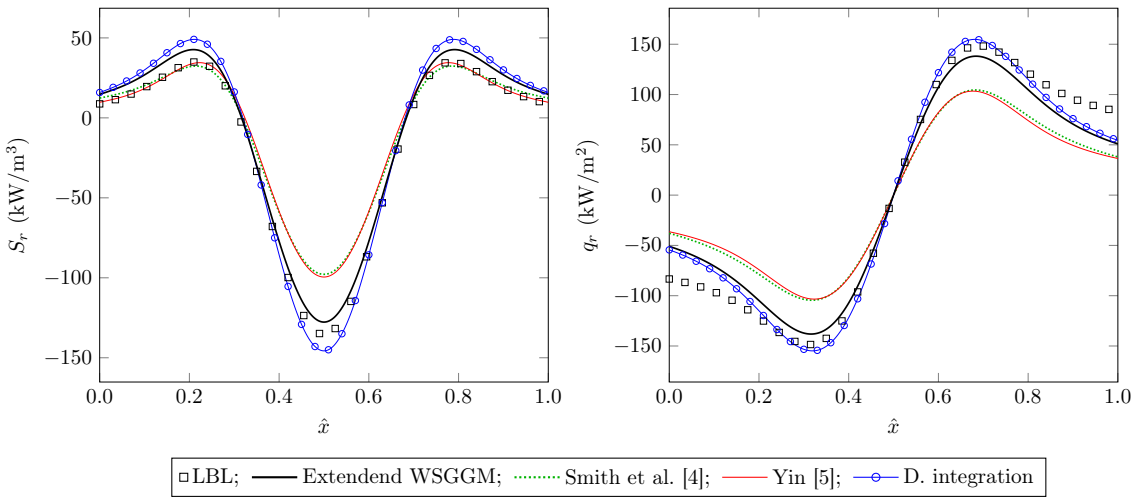

Figure 6: Results of the fourth test case ($MR \to \infty$, $X = 10\,\mathrm{m}$).

is approximately linearly scalable with MR. Furthermore, a good agreement between the total emissivity predicted by the extended WSGGM developed in this paper and results obtained by LBL integration for $MR > 4.0$ and $MR < 0.01$ was also verified.

The extended model was then tested for four non-isothermal cases and compared to a reference solution provided by the LBL integration method, as well as to other WSGGMs developed for a wide range of MR. For a case where $MR \to 0$, most models performed well, while none of the varying-MR WSGGMs available in literature were capable of providing physically realistic results in a scenario with $MR \to \infty$. Two other WSGGMs based on fixed-MR correlations were also tested and obtained fairly accurate solutions for the latter case, but were outperformed by the extended WSGGM proposed in this paper. Finally, for a more challenging case with a varying molar fraction ratio, in which both $MR \to 0$ and $MR \to \infty$ occur in the domain, only the extended WSGGM and a model based on the double integration of the pure CO_2 and H_2O coefficients provided physically realistic and reasonably accurate results. While the double integration model led to similar (as in cases 1, 2 and 4) or more accurate (as in case 3) results than the present extended WSGGM, its computational cost was significantly

higher, which limits its usage in large scale industrial cases. Therefore, the new extended WSGGM provides a computationally efficient solution with sufficient accuracy for most engineering applications that require the calculation of radiative transfer, and can be particularly useful for the modeling of combustion systems with heterogeneous conditions of gas concentrations, including locally moisture rich regions.

Acknowledgments

Authors HB and SM greatly acknowledge the support of the Academy of Finland under grant no. 314487. Authors GCF thanks CNPq for a doctorate scholarship.

References

References

[1] M. F. Modest, Journal of heat transfer 113 (1991) 650–656. doi:10.1115/1.2910614.

[2] V. P. Solovjov, B. W. Webb, F. Andre, in: Handbook of Thermal Science and Engineering, Springer International Publishing, 2017, pp. 1–74. doi:10.1007/978-3-319-32003-8_59-1.

[3] M. F. Modest, Radiative Heat Transfer, Academic Press, 2013.

[4] T. F. Smith, Z. F. Shen, J. N. Friedman, Journal of Heat Transfer 104 (1982) 602–608. doi:10.1115/1.3245174.

[5] C. Yin, L. C. R. Johansen, L. A. Rosendahl, S. K. Kær, Energy and Fuels 24 (2010) 6275–6282. doi:10.1021/ef101211p.

[6] L. J. Dorigon, G. Duciak, R. Brittes, F. Cassol, M. Galarça, F. H. França, International Journal of Heat and Mass Transfer 64 (2013) 863–873. doi:10.1016/j.ijheatmasstransfer.2013.05.010.

[7] R. Johansson, B. Leckner, K. Andersson, F. Johnsson, Combustion and Flame 158 (2011) 893–901. doi:10.1016/j.combustflame.2011.02.001.

[8] T. Kangwanpongpan, F. H. França, R. C. da Silva, P. S. Schneider, H. J. Krautz, International Journal of Heat and Mass Transfer 55 (2012) 7419–7433. doi:10.1016/j.ijheatmasstransfer.2012.07.032.

[9] M. H. Bordbar, G. Węcel, T. Hyppänen, Combustion and Flame 161 (2014) 2435–2445. doi:https://doi.org/10.1016/j.combustflame.2014.03.013.

[10] J. Guo, X. Li, X. Huang, Z. Liu, C. Zheng, International Journal of Heat and Mass Transfer 90 (2015) 218–226. doi:10.1016/j.ijheatmasstransfer.2015.06.052.

[11] M. K. Denison, B. W. Webb, Journal of Heat Transfer 117 (1995) 788. doi:10.1115/1.2822652.

[12] F. Cassol, R. Brittes, F. H. França, O. A. Ezekoye, International Journal of Heat and Mass Transfer 79 (2014) 796–806. doi:10.1016/j.ijheatmasstransfer.2014.08.032.

[13] F. Andre, F. R. Coehlo, J.-L. Consalvi, F. H. R. Franca, M. Galtier, F. Nmira, V. P. Solovjov, B. W. Webb, in: 9th International Symposium on Radiative Transfer, RAD-19, pp. 407–414.

[14] J.-L. Consalvi, F. Andre, F. R. Coehlo, F. H. R. Franca, M. Galtier, F. Nmira, V. P. Solovjov, B. W. Webb, in: 9th International Symposium on Radiative Transfer, RAD-19, pp. 423–430. doi:10.1615/RAD-19.520.

[15] H. Chu, Y. Feng, W. Cao, F. Ren, M. Gu, Acta Physica Sinica 66 (2017) 94207. doi:10.7498/aps.66.094207.

[16] V. Kez, F. Liu, J. Consalvi, J. Ströhle, B. Epple, Journal of Quantitative Spectroscopy and Radiative Transfer 172 (2016) 121 – 133. doi:https://doi.org/10.1016/j.jqsrt.2015.11.002.

[17] L. Rothman, I. Gordon, R. Barber, H. Dothe, R. Gamache, A. Goldman, V. Perevalov, S. Tashkun, J. Tennyson, Journal of Quantitative Spectroscopy and Radiative Transfer 111 (2010) 2139–2150. doi:10.1016/j.jqsrt.2010.05.001.

[18] H. Bordbar, T. Hyppänen, International Journal of Heat and Mass Transfer 127 (2018) 870–884. doi:10.1016/j.ijheatmasstransfer.2018.06.093.

[19] H. Chu, F. Liu, H. Zhou, International Journal of Heat and Mass Transfer 54 (2011) 4736 – 4745. doi:https://doi.org/10.1016/j.ijheatmasstransfer.2011.06.002.

[20] F. R. Coelho, F. H. R. França, International Journal of Heat and Mass Transfer 127 (2018) 105–114. doi:10.1016/j.ijheatmasstransfer.2018.07.075.

Conflict of Interest Statement

11 June, 2019

Reffering to manuscript entitled as "*An Extended Weighted-Sum-of-Gray-Gases Model to Account for All CO_2-H_2O Molar Fraction Ratios in Thermal Radiation*", we wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome. We confirm that the manuscript has been read and approved by all named authors and that there are no other persons who satisfied the criteria for authorship but are not listed. We further confirm that the order of authors listed in the manuscript has been approved by all of us. We confirm that we have given due consideration to the protection of intellectual property associated with this work and that there are no impediments to publication, including the timing of publication, with respect to intellectual property. In so doing we confirm that we have followed the regulations of our institutions concerning intellectual property. We understand that the Corresponding Author is the sole contact for the Editorial process (including Editorial Manager and direct communications with the office). He is responsible for communicating with the other authors about progress, submissions of revisions and final approval of proofs. We confirm that we have provided a current, correct email address which is accessible by the Corresponding Author.

Signed by all authors as follows

Hadi Bordbar

Guilherme Fraga

Simo Hostikka

Response to the review:

We would like to thank the reviewer for his/her fruitful comments which enhanced the quality of the paper. Below please find our detailed responses to the reviewer's comments.

Reviewer 2: The authors have satisfactorily revised the paper following this reviewer's comments. However, some of the new elements added in this version require some further minor (some of them compulsory) modifications. They are listed below:

- Compulsory C1: in Figure 2, total emissivities calculated with the double integration method are required.

Response to C1: Figure 2 is updated as requested. The results of the double integration method for total emissivity are added. For most of the temperature and path length (from short to intermediate), the double integration method and the present extended WSGGM performs equally good in predicting total emissivity of the gas mixture. For larger path lengths, as expected, the double integration model provides slightly better but in the expenses of higher computational time. It is discussed in the manuscript, see the paragraph after figure 2.

- Compulsory C2: in this version, the authors are more reasonable on the possible accuracy of the WSGGM. In this context, and as possible readers of the present paper may need further information about the accuracy of WSGGM compared to other available methods, the following two recent references (in which WSSGM accuracy is compared to other up-to-date modeling approaches) need to be added:
  - [A] F. Andre, F. R. Coelho, J.-L. Consalvi, F. H. R. Franca, M. Galtier, F. Nmira, V. P. Solovjov, B. W. Webb, Accuracy of engineering methods for radiative transfer in CO2-H2O mixtures at high temperature, in: Proceedings of the 9th International Symposium on Radiative Transfer, RAD-19, Begellhouse, Connecticut, 2019, pp. 407-414.
  - [B] J.-L. Consalvi, F. Andre, F. Coelho, F. Franca, M. Galtier, F. Nmira, V. Solovjov, B. Webb, Assessment of engineering gas radiative property models in high pressure turbulent jet diffusion flames, in: Proceedings of the 9th International Symposium on Radiative Transfer, RAD-19, Begellhouse, Connecticut, 2019.

Response to C2: Two references have been added to the paper as instructed. See the first paragraph of page 3.

- Not compulsory NC1: as noticed in Figure 1, the present method seems to be accurate near line centers but produces higher errors in the wings of the spectral lines. If this result is general (the authors can easily check it) then this may explain why the relative inaccuracy of the present method for large optical thicknesses, where radiative transfer is driven by the wings of the lines, is higher than in optically thin cases, for which most of the absorption / emission is due to line centers.

Response to NC1: we checked the other parts of the spectra of different MRs. Generally one cannot conclude that the accuracy of linear interpolation with MR is always better at the centers of the bands and is always worse in the wings.

As seen in Figure 1, the linear interpolation predicts the center of bands more accurately (than wings) for high temperatures but for low temperatures, the accuracy of the method in retrieving the wings is better than the band centers. See for instance the following curve (and the first row of Figure 1).

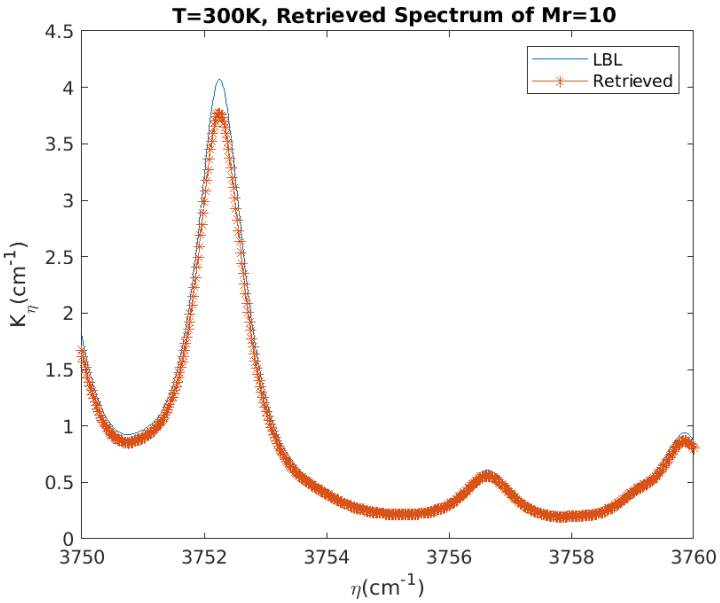

Figure R1: The retrieved spectrum versus LBL spectrum for a mixture of CO2-H2O with Mr=10 at T=300K.

- NC2: the cases of section 3 consider geometrical lengths of 1m for which, according to Figure 2, the WSGGM is accurate. It would be informative for the readers to have at least one case for which the distance between the walls is 10m (where the WSGGM should be, again according to Figure 2, less accurate). This question is relevant because, as correctly stated by the authors in the introduction, "the WSGGM…more widely used…large scale combustion systems".

Response to NC2: We tested the model for three new test cases in which the gas concentration and temperature are the same as the first three test cases but the length is X=10m. Figures R2 to R4 show the results. $\hat{x} = \frac{x}{X}$ is the normalized x coordinate. As seen the performance of the present model is in a similar level for optically thick cases as the first three cases with X=1m. For the sake of brevity, we decided to include only one of these new cases in the paper. The new case 4 represents the similar conditions as test case 2 (MR>4) but its length is 10m. Several parts of the text are modified accordingly including Table 4 and the last paragraph of page 11.

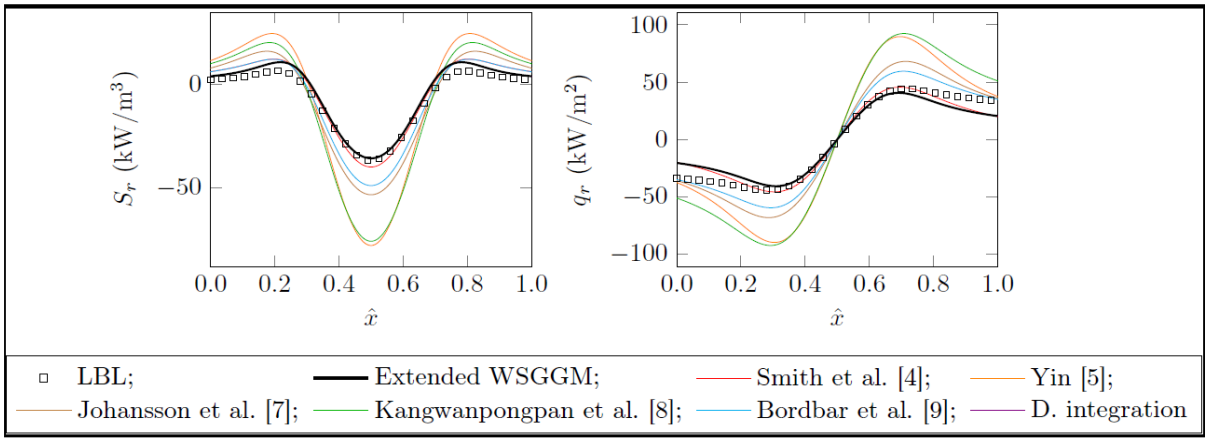

Figure R2: The results of test case 1 with X=10m

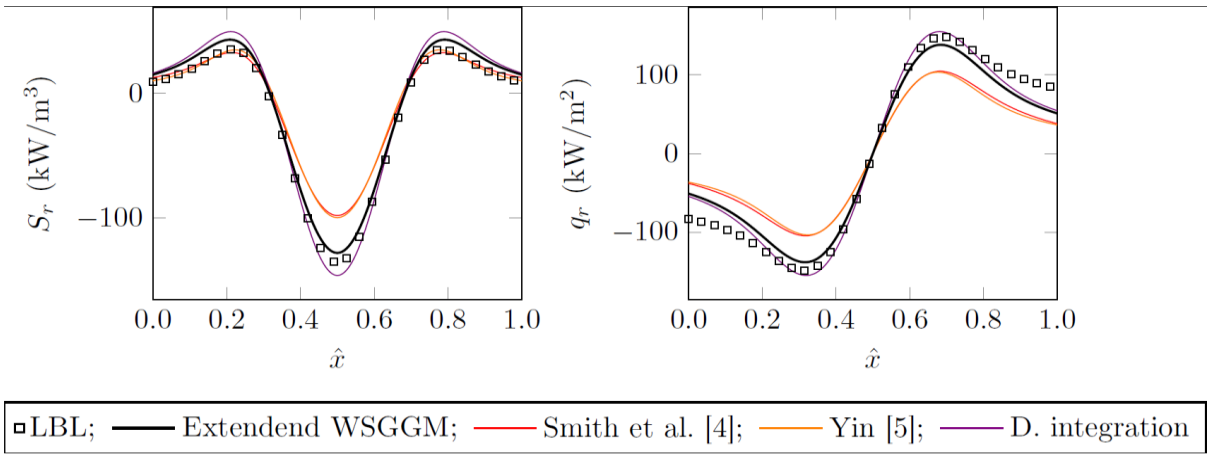

Figure R3: The results of test case 2 with X=10m

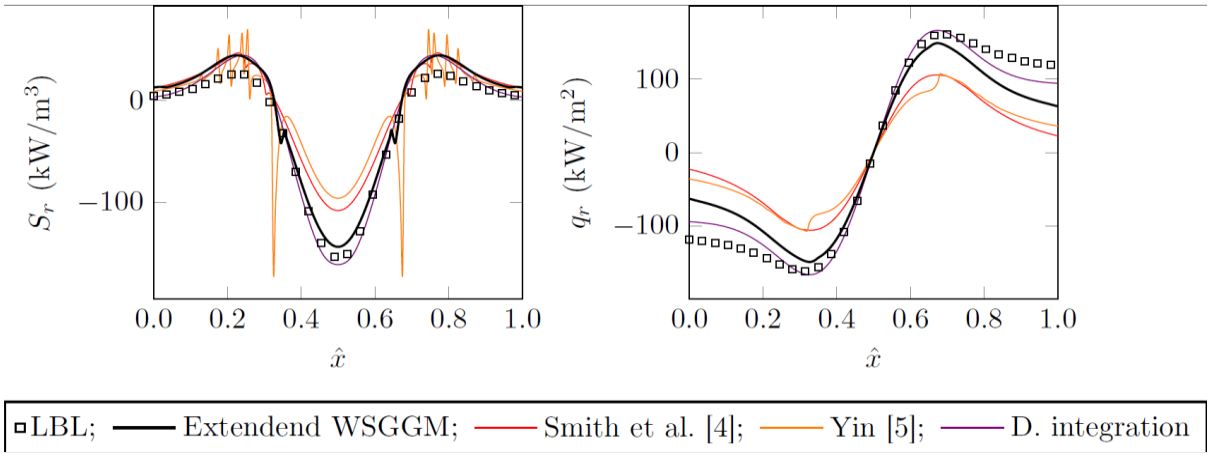

Figure R4: The results of test case 3 with X=10m