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A line by line based weighted sum of gray gases model for inhomogeneous CO_2–H_2O mixture in oxy-fired combustion

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ABSTRACT

The HITEMP 2010 spectral emissivity database has been employed in line by line (LBL) calculation to produce an accurate total emissivity database for H_2O–CO_2 mixtures of the composition characteristics for the oxy-fired combustion. A wide range of temperatures, pressure-path length products and molar fraction ratios have been covered in the database. By using the LBL based emissivity database, an accurate set of coefficients has been obtained for the weighted sum of gray gases model (WSGGM). Compared to the standard WSGGM, the present model includes the molar ratio of H_2O–CO_2 mixtures in its formulation which leads to one set of coefficients required to represent the entire range of molar ratio. This simplifies the implementation of the model in the simulation of radiative heat transfer in high inhomogeneous media providing higher accuracy. The model is validated against the benchmark solutions for oxy-fired conditions. Obtained results have been compared with some of the previously reported WSGGMs.

1. Introduction

Radiative heat transfer is the dominant heat transfer mechanism in high temperature enclosures such as boilers and furnaces [1]. Since the radiative heat transfer physics is mathematically complex to describe, an analytical solution of radiative heat transfer exists only for a certain limited number of simple cases [2]. Due to this, significant attention has been paid to the development of numerical methods to simulate radiative heat transfer. Recent improvements in available computer resources and power have increased the use of numerical models for solving this mode of heat transfer both in the process of designing the new heat transfer equipments and in the analysis of the performance of existing equipments improving working conditions.

The governing equation of radiation heat transfer in the participating media has the form of an integro-differential equation which is defined for a particular wavelength. The radiation heat transfer occurs within the electromagnetic wave spectrum from a point in the ultraviolet region (0.1 μm) to a point in the infrared region (100 μm). Within this part of the spectrum, the gas spectral absorption coefficient is rapidly changing with the wavelength forming a histogram containing millions of absorption lines. The radiation intensity of the absorption lines changes with the temperature, composition and pressure of the gas mixture. In addition, the absorption lines overlap each other [3]. Due to these facts, considering the effect of all individual absorption lines, the modeling of radiative heat transfer is still infeasible by the currently available computers.

The most simplified models of the gas radiative properties are the gray gas models in which the absorption coefficient of the gas is assumed constant in the entire spectrum. Its average value is obtained and used in solving the radiative heat transfer equation. On the other side, the non-gray gas models take the spectral radiative behavior of gases into account.

The most accurate method for calculating the radiative properties of the gases is the line by line integration which uses spectroscopic databases. The databases contain a set of spectral line parameters required to calculate spectral absorption coefficient for specified spectral location.

Although the results of the LBL calculations are most accurate nowadays, their use is still limited because of high computational costs. Therefore, the LBL calculations are usually the benchmark generator used for the accuracy evaluation of other models.

Another highly accurate property model is the statistical narrow band model (SNBM) in which the radiative properties of the gas are integrated into narrow wave number intervals [4,5]. A widely used radiation code based on narrow band data is RADCAL [6] which provides the average spectral transmissivity of gas mixtures in narrow bands with width varying between 5 cm^{-1} and

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Nomenclature

Roman letters

a	weighted factors (–)
b, c, d	the coefficient of the present WSGGM (–)
E_{bvj}	the Planck function (W m^{-2})
g_ig_j	gas to gas direct exchange area (m^2)
g_is_j	gas to surface direct exchange area (m^2)
K	absorption coefficient (atm^{-1} m^{-1})
L	path length (m)
M	number of surface zones in the computational domain (–)
M_r	molar fraction ratio of H_2O to CO_2 (P_{H2O}/P_{CO2}) (–)
N	number of gas zones in the computational domain (–)
N_g	number of gray gases used in WSGGM (–)
N_v	total number of absorption coefficients stored in its histogram (–)
P_t	total pressure of the mixture: Sum of P_{CO2} and P_{H2O} (atm)
q	radiative heat flux (W m^{-2})
RST	radiative source term (W m^{-3})
s_ig_j	surface to gas direct exchange area (m^2)
s_is_j	surface to surface direct exchange area (m^2)
T	temperature (K)
T_r	normalized temperature (–)
T_{ref}	reference temperature (1200 K)
Y_C	molar fraction of CO_2 (–)
Y_H	molar fraction of H_2O (–)

Greek letters

ε	total emissivity of H_2O–CO_2 mixture (–)
σ	Stefan-Boltzmann constant (5.672×10^{-8} W m^{-2} K^4) (W m^{-2} K^{-4})

Abbreviations

CFD	computational fluid dynamics
DO	discrete ordinate method
EWBM	exponential wide band model
FSK	full spectrum correlated-K method
LBL	line by line integration method
SNBM	statistical narrow band model
RTE	radiative transfer equation
WSGGM	weighted sum of gray gases model

50 cm^{-1}. Five molecular bands of CO_2, five molecular bands of H_2O, three molecular bands of CH_4, and one molecular band of CO are modeled in RADCAL based on the available experimental data in addition to soot which is modeled assuming that it is in Rayleigh limit with zero albedo (no scattering). There are number of other codes available for narrow band calculations based on more recent high resolution spectral properties databases [5]. Although, the narrow band approaches are among the most accurate available tools for prediction of spectral radiative properties, they require a few hundred to thousands of spectral evaluations [3] which restrict their usage in three-dimensional CFD simulations. Recently, Chu et al. [7] reported that SNBM can produce results as accurate as LBL, and therefore, it can produce the benchmark solutions for the evaluation of other methods. However, it is still computationally expensive, and its practical usage is limited. Liu [8] has used SNBM with a ray tracing method to produce a benchmark solution for a system with air-fired combustion which represents the thermal conditions of artificial flame. Using the same methodology and the same geometry and thermal conditions, a benchmark for oxygen fired combustion has recently been reported by Porter et al. [9]. They later used the benchmark to evaluate the obtained results of the full spectrum correlated-K method (FSK).

Some of the simpler models, which generally provide lower accuracy, are the box model [10] and the exponential wide band model (EWBM) [11]. The main idea of these models is based on the fact that gas absorption takes place in certain wave number intervals: in the "absorption bands". In the EWBM, an exponential function for the line intensity is assumed around the center of the absorption bands [12,13]. The box model approximates the band absorption even with a simpler shape of a rectangular box of a certain width and height. Although the box model has been used widely in engineering calculations because of its simplicity, its accuracy is very sensitive to the correct choice of the effective band width, especially when the emission from a hot gas is desired [3].

A group of global models including the full spectrum correlated-K method (FSK) [14,15], the spectral line based weighted sum of gray gas method (SLW) [16,17] and the absorption distribution function method (ADF) [18] have received a lot of attention during last two decades due to their high accuracy and low computational costs. They are based on reordering the absorption lines on the wave number spectrum in order to avoid its irregular variation. While the SLW and ADF methods integrate the absorption cross section in the full absorption spectrum of the absorbing gases, the FSK method integrates over the Planck-weighted function using the Gaussian quadrature [17]. It is proven that these methods are able to exactly predict the radiation heat transfer in homogenous media. Solovjov and Webb [17] described the limitations of these global methods and the relation between them. Liu et al. [19] has recently derived the SLW transfer equation from the FSK transfer equation and confirmed that the SLW is equivalent to the FSK in the k-distribution form [19]. Although, these global methods provide fast and accurate non-gray calculations, implementing them in modeling of gas mixtures is not straight forward since the correlation of FSK, ALBDF and ADF are usually offered for single gas species. Due to reordering of wave numbers in these methods, the spectral position information is lost [20]. In addition, combining the spectra of different gas species is difficult and needs some approximations which in turn cause some inaccuracy and computational costs while applying these methods to the cases with more than one gas species. Two commonly used mixing models are multiplication method [15] or using uncorrelated mixture model [21].

One of the engineering approaches which has received a lot of attention during the last few decades is the weighted sum of gray gases model (WSGGM). For the first time it was proposed by Hottel and Sarofim [22] in the framework of their development of the zonal method to include the spectral radiative behavior of gases. Because of its simplicity and its great performance, it has been further developed and used by many researchers [1,23–27]. For instance, Kim et al. [27] used this model to predict the self-absorption on an opposed diffusion and partially premixed flame and reported significant self-absorption in their studied flame, especially on the fuel side of reaction zone. The basic idea of the model is that the non-gray behavior of gas mixtures, mainly H_2O–CO_2, can be modeled by a weighted sum of several gray gases and one transparent gas. While different gray gases represent the different levels of spectral absorption coefficients existing in the wavelength spectrum, the transparent gas represents the windows between the absorption bands. The weighted factors are representing the black body fractional function accompanied by each gray gas absorption coefficient. The absorption coefficients of the gray gases and their weights are calculated by fitting the model into the total emissivity

database. The accuracy of WSGGM depends on the accuracy of the total emissivity database, the accuracy of the curve fitting process and the number of gray gases used in the model. However, it cannot provide more accurate results than the total emissivity database used for obtaining its coefficients.

The suitable number of gray gases in the model depends on the available computational power and the needed accuracy. Hottel and Sarofim [22] have reported that for some applications, even considering one gray gas with one transparent gas leads to a significant accuracy. Yin et al. [25] and Johansson et al. [26] have used four gray gases in their recently reported models. Ströhle [28] has tested up to 19 gray gases and reported that considering even three gray gases is an efficient option. Based on this, the combination of four gray gases and one transparent gas has been used to develop the new WSGGM presented in this paper.

The combustion systems which are working based on oxygen fired combustion instead of traditional air-fired combustion are getting more popular because of their better combustion performance and lower greenhouse gas emissions. Several experimental studies have been carried out in order to address the effect of higher level of oxygen in oxidizer of normal and inverse diffuse flames [29–31]. The oxygen inverse flame is found to be more effective in generating radiative heat flux than the normal flame [29]. Krishnan et al. [30] reported that with the same heat release rate, the radiative heat loss fractions of oxygen inverse diffuse flame is four to five times of those for the oxygen normal diffuse flame and generally radiative heat loss fraction increases with the level of oxygen enhancement in both types of flames. Sunderland et al. [31] experimentally examined the effect of gravity and oxygen enhancement on the laminar jet diffusion flame and reported that luminosity, soot production, and soot emission are increased with oxygen enhancement for both normal and inverse diffuse flames.

The change in the combustion atmosphere requires the models of gas properties which are specifically developed for non-gray modeling of oxy-fired combustion systems. Most of the previously developed coefficients of WSGGM have been derived for the air-fired combustion scenario [22,32], and using them in the oxy-fired conditions may lead to uncertain levels of inaccuracy.

Based on this demand, Yin et al. [25] have recently presented new sets of coefficients for the WSGGM that are applicable for the oxy-fired scenario. However, they used EWBM to produce the emissivity database needed for obtaining the model coefficients. EWBM has a limited accuracy especially when it is used for producing the total emissivity of the gas mixture [33,34].

Traditionally, the coefficients of WSGGMs have been obtained for a certain ratio of molar fractions. In other words, the coefficients of WSGGM have been obtained and tabulated for some limited molar fraction ratios. The use of this kind of WSGGMs for the molar fractions in which the coefficients are not tabulated needs the interpolation or extrapolation between the tabulated coefficients of other molar fraction ratios, and therefore, enhances the inaccuracies in the predictions of the model. The WSGGM reported by Yin et al. [25] for oxy-fired combustion was presented in the same way.

Johansson et al. [26] used a second order polynomial to include the effect of the molar fraction ratio in the formulation of their WSGGM. The total emissivity database used for fitting in their model is obtained by SNBM. Although their model is based on a more accurate emissivity database than the one used in Yin's model, the range of applicability is limited, and it does not support the H_2O–CO_2 mixtures with molar fraction ratios larger than two.

A new weighted sum of gray gases model is presented in this article. It is based on the most accurate available emissivity database, HITEMP 2010 [35]. In order to support most of the possible practical combustion conditions, the ranges of effective parameters, which are temperature, molar fraction ratio and pressure path length product, are selected wider than in the two previously oxy-fired WSGGMs proposed by Yin et al. [25] and Johansson et al. [26]. The molar fraction ratio is included in the formulation of the model using a polynomial of fourth order, and therefore, only one set of coefficients has been reported for the entire range of molar fraction ratios in contrast with the traditional models such as the ones developed by Smith et al. [32] and Yin et al. [25] which present a set of coefficients for every molar fraction ratio. The model is verified by comparing it with the LBL emissivity database and also with other previously reported WSGGMs. Two 1D benchmark is used to validate the applicability of the present model in inhomogeneous conditions. In addition, the new model is implemented in the radiative zonal code to solve a 3D oxy-fired benchmark problem recently presented by Porter et al. [9]. The results of the simulations have been compared with the benchmark solutions and also with the results of the implementation of the other WSGGMs in the zone method.

It should be noted that the WSGGM is now known equivalent to the simplest form of SLW [3]. Therefore this WSGGM presents a good straight forward correlation of a four-gas SLW implementation of H_2O–CO_2 mixtures while previously presented SLW correlations support the single gas species and using them in mixtures needs further computational efforts.

The presence of soot in flame increases the radiative heat transfer due to high values of soot's spectral absorption coefficient comparing to the combustion gases. The spectral soot absorption coefficient is usually obtained using the Rayleigh small particle limit and the soot scattering is neglected. The details can be found in many literatures [3,36].

2. Line by line emissivity database

The absorption coefficient of the optically active gases is a property which depends on the type of the molecule, wave number, temperature, the partial pressure of the gas and the total pressure of the gas mixture. To complete this work, the procedure of evaluating absorption coefficient histogram as a function of wave number is provided. The linear absorption coefficient at an arbitrary wave number for a particular spectral line, assuming pressure broadening is evaluated by

$$\kappa_\nu^i = \frac{S_i}{\pi}\frac{\gamma_i}{\gamma_i^2 + (\nu - \nu_i)^2} \tag{1}$$

where κ_ν^i is the absorption coefficient for the i-th spectral line at the ν wave number location, S_i is the intensity of the i-th spectral line, γ_i is the broadening of the spectral line and ν_i is the spectral line location. The intensity of each spectral line is temperature dependent

$$S_i = S_{ref,i}\frac{Q(T_{ref})}{Q(T)}\frac{\exp(-E_{\nu_i}/kT)}{\exp(-E_{\nu_i}/kT_{ref})}\frac{[1-\exp(-hc\nu_i/kT)]}{[1-\exp(-hc\nu_i/kT_{ref})]} \tag{2}$$

where Q is internal partition function of the molecule at temperatures T and T_{ref}, E_ν is the lower state energy of the line, k is Boltzmann constant and h is the Planck constant. The collisional broadening of the spectral line depends on the temperature, partial pressure and total pressure:

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n [\gamma_{air}(p_T - p_s) + \gamma_{self}p_s] \tag{3}$$

In order to calculate the absorption coefficient for an arbitral wave number, the contribution of all neighboring lines needs to be taken into account. We simply sum up all the contributions of the spectral lines at the wave number ν.

$$\kappa_\nu = \sum_i \kappa_\nu^i \tag{4}$$

The spectral line location, its intensity, air and self-broadening are taken from the spectroscopic database HITEMP 2010 [35]. The CO_2 content of the HITEMP database is based on CDSD-1000 [37] database parameters after rescaling the reference temperature from 1000 K to 296 K to be compatible with the other molecules included in HITEMP. The three most abundant isotopic species are used here for the calculation of $^{12}CO_2$, $^{13}CO_2$, $^{16}O^{12}C^{18}O$ corresponding to around 9.89 million line locations. Only the lines with temperature scaled intensities $S > 10^{-10}$ are used for the calculations. The H_2O content of the HITEMP is based on HITRAN 2008 [38] combined with selected lines from BT2 dataset [39]. The three most abundant isotopic species are used here for the calculation of $H_2^{16}O$, $H_2^{18}O$, $H_2^{17}O$ corresponding to 114.2 million line locations. Similarly as for CO_2, only the lines with temperature scaled intensities $S > 10^{-10}$ are used for the calculations. In case of CO_2 and H_2O, three minor isotopes correspond to almost 100% of their natural abundance [40]. These isotopes have been selected similarly as in latest work on SNBM by Rivière and Soufiani [41]. The air and self broadening parameters γ_{air} and γ_{self} (see Eq. (3)) are taken also from HITEMP database [35].

In this work, the idea of discrete summation is employed. The part of spectrum in which the radiative heat transfer occurs is divided into equally spaced discrete values of wave number ν_j. For each wave number ν_j, we evaluate the value of the absorption coefficient for all spectral lines which wings span selected lines wings width and then sum up their contributions. Such a procedure results in omitting the peaks of the spectral lines from the calculation. In order to account for the peak values, it is necessary to discretize the spectrum in a non-uniform way which is not practical since it is rather expensive for computing and requires too many discrete wave number locations. For controlling the accuracy of the lines generated at each discrete value of wave number ν_j (equally spaced), the numerical integration of the line intensity has been performed using rectangle rule and compared to the value calculated with Eq. (2). The spectral line reproduction error is assumed to be lower than 10^{-4}. After performing lines generation for all lines spectral locations, the selected wave number distribution is assumed to be equal to 0.01 1/cm. Another issue affecting the accuracy is the proper selection of the spectral line wings width. This controls the influence of the particular line on the entire absorption coefficient histogram. After extensive testing, the wings width equal to 500 1/cm has been used in left and right direction from the ν_j line center.

The generated histograms of the absorption coefficient are used to prepare total emissivity database. This database is used for evaluation of the coefficient of new WSGGM. Total emissivity has been calculated according to Eq. (5).

$$\varepsilon = \frac{1}{\sigma T^4}\sum_{j=1}^{N_\nu} E_{bvj}(1 - e^{-\kappa_j L}) \tag{5}$$

where N_ν is total number of absorption coefficients stored in its histogram, E_{bvj} is the Planck function evaluated for wave number ν_j and interval of $\Delta\nu = 0.01$ 1/cm.

Total emissivity is calculated for temperature range from 500 K to 2400 K with the spacing of 100 K. Fifteen different molar fraction ratios ($M_r = Y_{H2O}/Y_{CO2}$) are selected as 0.01, 0125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0. For each of these molar fraction ratios, the mole fraction of H_2O and CO_2 are calculated by considering $Y_{H2O} + Y_{CO2} = 1$ and therefore, $Y_{CO2} = 1/(1 + M_r)$ and $Y_{H2O} = 1 - Y_{CO2}$. The following path lengths (m) have been used: 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.75, 1.0, 1.5, 2.0, 3.0, 5.0, 10.0, 15.0, 20.0, 30.0, 40.0, 50.0, 60.0. Totally 6800 emissivity values have been generated.

3. New WSGGM

The WSGGM is proposed for the calculation of the total emissivity of the mixture of H_2O and CO_2. The model can be easily implemented in CFD calculations and supports the various combustion conditions. In the standard WSGGMs, the coefficients of the model are reported for some certain molar fraction ratios of H_2O to CO_2 ($M_r = Y_{H2O}/Y_{CO2}$), and therefore, their best accuracy is limited to the mixtures in which the coefficients are tabulated. For other mixtures, the inter/extrapolations of the calculated emissivity is needed which imposed some errors especially for the models which are presented just for a limited number of mixtures such as the one reported by Smith et al. [32] and Krishnamoorthy [42]. When considering the flame area of the combustion system, the concentration of both CO_2 and H_2O changes with the position,

Table 1
The model coefficients to be used in Eqs. (10) and (11). The coefficients, as a data file with a Matlab code for the formulations, can be provided by the corresponding author upon request by email.

Coef. name	I	J	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$
c	1	0	0.7412956	−0.5244441	0.5822860	−0.2096994	0.0242031
c	1	1	−0.9412652	0.2799577	−0.7672319	0.3204027	−0.0391017
c	1	2	0.8531866	0.0823075	0.5289430	−0.2468463	0.0310940
c	1	3	−0.3342806	0.1474987	−0.4160689	0.1697627	−0.0204066
c	1	4	0.0431436	−0.0688622	0.1109773	−0.0420861	0.0049188
d	1	–	0.0340429	0.0652305	−0.0463685	0.0138684	−0.0014450
c	2	0	0.1552073	−0.4862117	0.3668088	−0.1055508	0.0105857
c	2	1	0.6755648	1.4092710	−1.3834490	0.4575210	−0.0501976
c	2	2	−1.1253940	−0.5913199	0.9085441	−0.3334201	0.0384236
c	2	3	0.6040543	−0.0553385	−0.1733014	0.0791608	−0.0098934
c	2	4	−0.1105453	0.0464663	−0.0016129	−0.0035398	0.0006121
d	2	–	0.3509457	0.7465138	−0.5293090	0.1594423	−0.0166326
c	3	0	0.2550242	0.3805403	−0.4249709	0.1429446	−0.0157408
c	3	1	−0.6065428	0.3494024	0.1853509	−0.1013694	0.0130244
c	3	2	0.8123855	−1.1020090	0.4046178	−0.0811822	0.0062981
c	3	3	−0.4532290	0.6784475	−0.3432603	0.0883088	−0.0084152
c	3	4	0.0869309	−0.1306996	0.0741446	−0.0202929	0.0020110
d	3	–	4.5707400	2.1680670	−1.4989010	0.4917165	−0.0542999
c	4	0	−0.0345199	0.2656726	−0.1225365	0.0300151	−0.0028205
c	4	1	0.4112046	−0.5728350	0.2924490	−0.0798076	0.0079966
c	4	2	−0.5055995	0.4579559	−0.2616436	0.0764841	−0.0079084
c	4	3	0.2317509	−0.1656759	0.1052608	−0.0321935	0.0033870
c	4	4	−0.0375491	0.0229520	−0.0160047	0.0050463	−0.0005364
d	4	–	109.81690	−50.923590	23.432360	−5.1638920	0.4393889

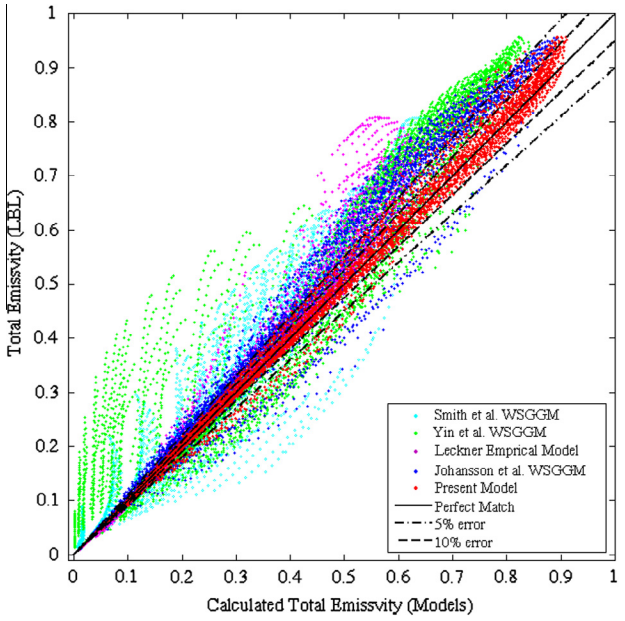

Fig. 1. Deviation plot of the total emissivity calculated by different methods. The emissivity calculated by line by line calculation is used as the reference data.

and a constant molar fraction ratio cannot be assumed. In the large scale oxy-fired combustion systems where the oxidizer is the pure oxygen mixed with wet or dry recycled flue gases, the M_r is also not constant. In the present model, the molar fraction ratio (M_r) is taken into account as an effective parameter in the formulation of WSGGM, and therefore, the radiative heat transfer of such inhomogeneous oxygen fired combustion systems can be more accurately modeled.

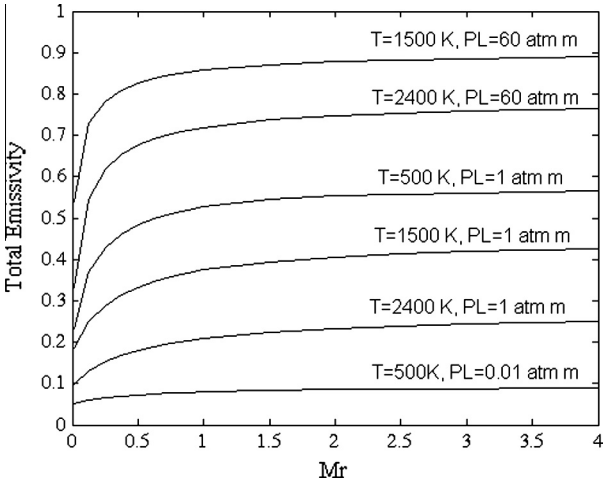

Fig. 3. Changes of total emissivity with molar fraction ratio in fixed temperature and pressure path length product.

In the formulation of the WSGGM, the total emissivity of H_2O–CO_2 mixture is calculated by

$$\varepsilon = \sum_{i=0}^{N_g} a_i (1 - e^{-K_i P_t (Y_C + Y_H) L}) \tag{6}$$

where N_g, a, K, P_t, Y_C, Y_H and L represent the number of gray gases used in the model, the weighting factors, the absorption coefficients of gray gases, total pressure of the mixture, molar fraction of CO_2, molar fraction of H_2O and path length, respectively. Based on the values reported for a sufficient number of gray gases in the WSGGM [25,26,28], four gray gases ($N_g = 4$) with a transparent gas is used to develop the present WSGGM. $i = 0$ represents the transparent gas in

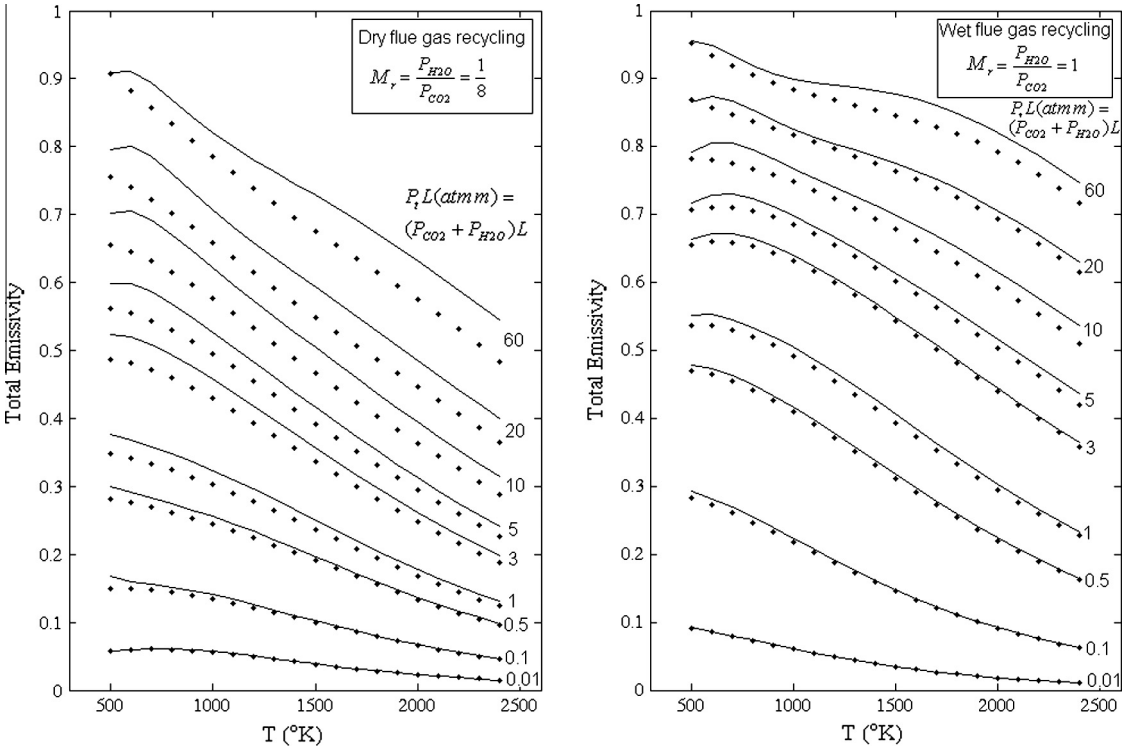

Fig. 2. The emissivity chart of CO_2–H_2O mixture in two practical cases of oxygen fired combustion ($Y_{CO2} + Y_{H2O} = 1$). The solid lines illustrate the LBL results and the dots show the results of the present WSGGM.

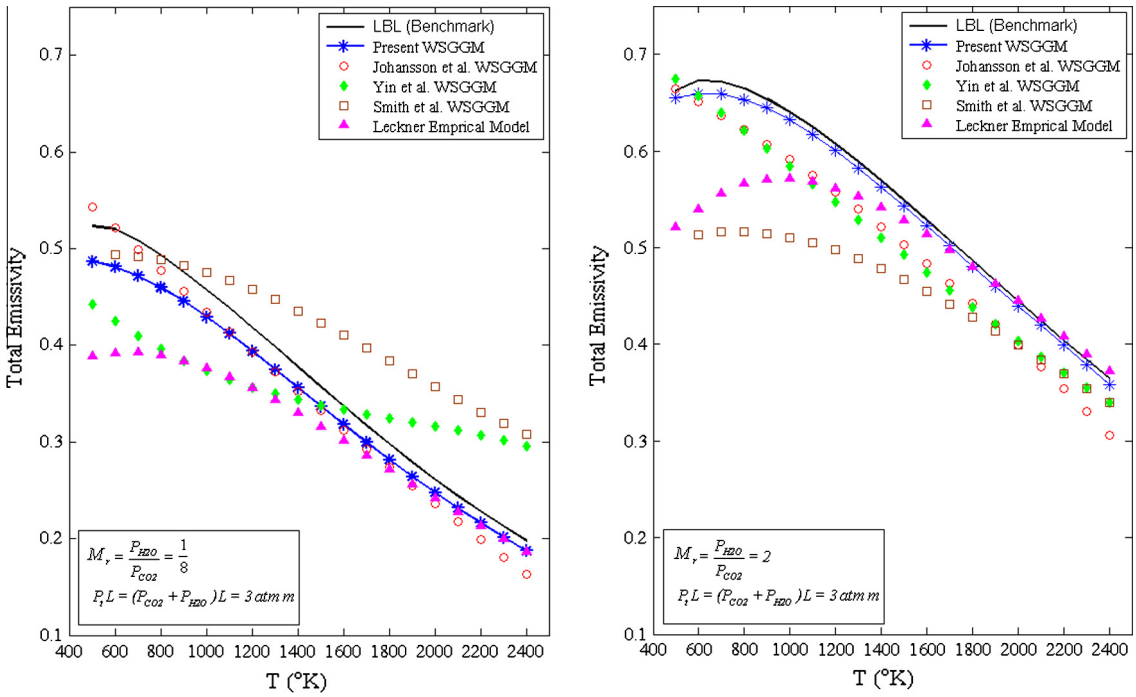

Fig. 4. Emissivity of the H_2O–CO_2 mixture in two different molar fraction ratios calculated by different methods compared with the benchmark solution.

the formulation. For a very long path length, when $L \to \infty$, the emissivity equals to unity. Therefore, the sum of weighted factors is unity:

$$\sum_{i=0}^{N_g} a_i = 1 \tag{7}$$

and the weighting factor which corresponds to the transparent gas ($K_0 = 0$) is

$$a_0 = 1 - \sum_{i=1}^{N_g} a_i \quad a_0 > 0 \tag{8}$$

The transparent gas ($K_0 = 0$) actually represents the spectral windows between the absorption bands.

In the standard WSGGMs, the weighting factors are considered as a function of temperature only, and the absorption coefficients are assumed constant. In the present approach, the weighting factors are considered as a polynomial function of temperature, and the molar fraction ratio and absorption coefficients are polynomial of molar fraction ratio as:

$$a_i = \sum_{j=0}^{4} b_{i,j} T_r^j \quad a_i > 0 \tag{9}$$

where T_r is the normalized temperature defined as $T_r = T/T_{ref}$. T_{ref} is selected as 1200 K. The normalized temperature is used as suggested by Yin et al. [25], and it improves the accuracy of the model and simplifies the multivariate regression analysis [25].

The $b_{i,j}$ in Eq. (9) is a polynomial function of the molar fraction ratio as:

$$b_{i,j} = \sum_{k=0}^{4} C_{i,j,k} M_r^k \tag{10}$$

In the same way, the absorption coefficient of gray gases in Eq. (6) is defined as:

$$K_i = \sum_{k=0}^{4} d_{i,k} M_r^k \tag{11}$$

To find the WSGGM coefficients, the multivariate regression has been done in two steps. For the molar fraction ratio between 0.01 and 4, a database of the total emissivity for the temperature range of 300–2400 K and pressure-path length product between 0.01 and 60 atm m has been generated using HITEMP 2010 spectroscopic databank.

In the first step of fitting for each M_r, $b_{i,j}$ and K_i from Eqs. (6) and (9) have been found. The LSQCURVEFIT function of Matlab software with lower band of $a_i > 0$ has been used for the curve fitting, This function solves the nonlinear curve fitting problems, and its algorithm is based on the nonlinear least square method which obtains the best curve parameters in which the square of error between the evaluated values by the fitting equation and the target vector is minimized.

In the second step of the multivariate regression, the polynomial functions expressed by Eqs. (10) and (11) have been fitted on $b_{i,j}$ and K_i found in the first step of fitting. By this way the dependency of the model coefficients on the temperature and pressure-path length product is obtained in the first step of fitting while the dependency of the model coefficients on the molar fraction ratio is taken into account in the second step of fitting.

The model coefficients which are $c_{i,j,k}$ and $d_{i,k}$ are reported in Table 1.

The existence of soot in practical flames is of great importance in radiative heat transfer. The WSGGM can be extended to include the effect of soot. It is well described in the previous works, see for instance [43,44].

4. Results and validation

4.1. Total emissivity comparison

The WSGGM has been practically used in gray gas radiative heat transfer modeling to obtain the total emissivity of a mixture, especially in commercial CFD solvers such as Fluent. In such a case, the advantage of the model in modeling spectral radiative behavior of the gases is not gained. To compare the new model with the previously published ones in calculating the total emissivity of

the mixture, the LBL emissivity database has been used as the benchmark. Figure 1 shows the result of the comparison in the form of a deviation plot. The total emissivity of the H_2O–CO_2 mixtures in all the points of the database, calculated by WSGGMs developed by Johansson et al. [26], Yin et al. [25], Smith et al. [32] and the empirical model developed by Leckner [45], has been compared with those obtained by the present WSGGM.

Figure 2 shows the total emissivity charts corresponding to two practical cases of oxygen fired combustion: the wet and dry flue gas recycling. The results of the present WSGGM have been shown in the same chart with the exact emissivity obtained by LBL. In a specified temperature and pressure-path length product, with increment of molar fraction ratio, total emissivity varies more smoothly as shown in Fig. 3; hence, the considered WSGGM function approximates the database better in higher molar fraction ratios. However, even in low molar fraction ratios which are the weakest region of the present model, the accuracy is better than that of the other models as shown in Fig. 4.

Figure 4 shows the changes of the total emissivity of the mixture with temperature for two different molar fraction ratios of 1/8 and 2. For both cases, the present WSGGM shows better accuracy than the other models. However, the performance of the present model is better in larger molar fraction ratios.

4.2. 1D benchmarks

The radiation heat transfer in a plane layer filled with non-isothermal and inhomogeneous mixture of Carbone dioxide and water vapor which is bounded by two black walls are analyzed using the discrete ordinate method as the RTE solver together with the present WSGGM, Johansson WSGGM [26], Yin WSGGM [25] and LBL.

In the first case, the walls are black with temperature of 400 K. The temperature and gas compositions are defined to present a case of inhomogeneous benchmark in which there is not any non-participating species ($Y_H + Y_C = 1$). The distributions of temperature and CO_2 and H_2O along the distance between two infinite walls are shown in Fig. 5(a). Implementing the LBL data in non-gray formulation of DO method provides the benchmark solution. This benchmark solution is used to evaluate the results of the present WSGGM. Figure 5(b) shows the distribution of radiative source term along the distance between two infinite walls by using different spectral models, i.e. LBL, the WSGGM by Yin et al. [25], WSGGM by Johansson et al.[26] and the present WSGGM, together with DO. Figure 5(c) shows the radiative heat flux along the distance between two walls.

The distributions of CO_2 and H_2O in the second 1D benchmark is defined to present the existence of non-participating media ($Y_H + Y_C < 1$). This 1D benchmark is proposed by Chu et al. [46] and is an oxy-fired benchmark. The distributions of CO_2 and H_2O and temperature is given by Chu et al. [46] and shown in Fig. 6(a) while the calculated radiative heat source by using DO as the RTE solver and different WSGGMs are shown in Fig. 6(b), The result of using LBL data is used as the benchmark solution to evaluate the WSGGMs. As Fig. 6 shows the present model can be used for the oxygen fired cases in which there is some non-participating species such as Nitrogen.

4.3. 3D benchmark

To provide an insight into how different WSGGMs work in the overall modeling of radiative heat transfer in participating media, a three dimensional benchmark problem for radiative heat transfer in participating media has been solved using the modified radiative zone method. Radiative zone method was proposed by Hottel and Cohen [47] and has been widely used and modified by others [1,2,48,49]. Bordbar and Hyppänen [2] have recently improved the performance of radiative zonal theory by introducing the multi-scale radiative exchange method (MREM) in which the variable size of integration elements is used in the calculation of exchange factors between cells in a coarse radiative mesh structure.

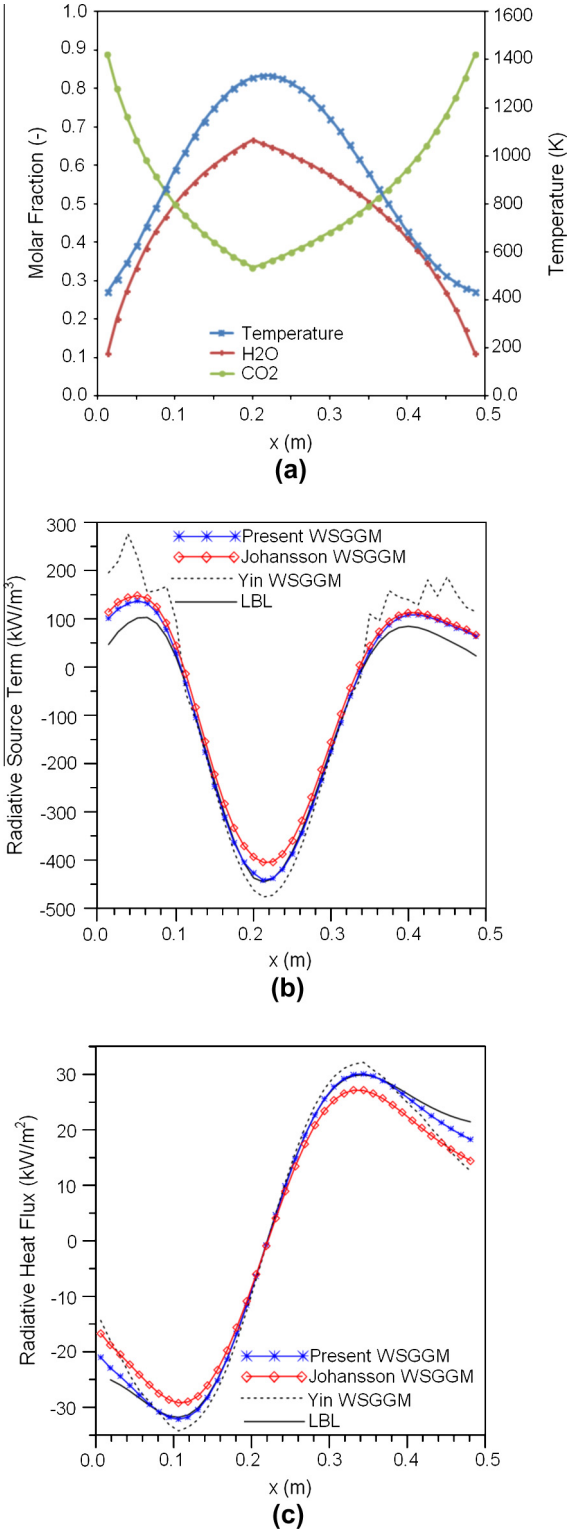

Fig. 5. The first 1D Benchmark in which $Y_H + Y_C = 1$, (a) the distributions of temperature and molar fraction of gases, (b) the radiative heat source calculated by different spectral models, and (c) the radiative heat flux by the present model and LBL.

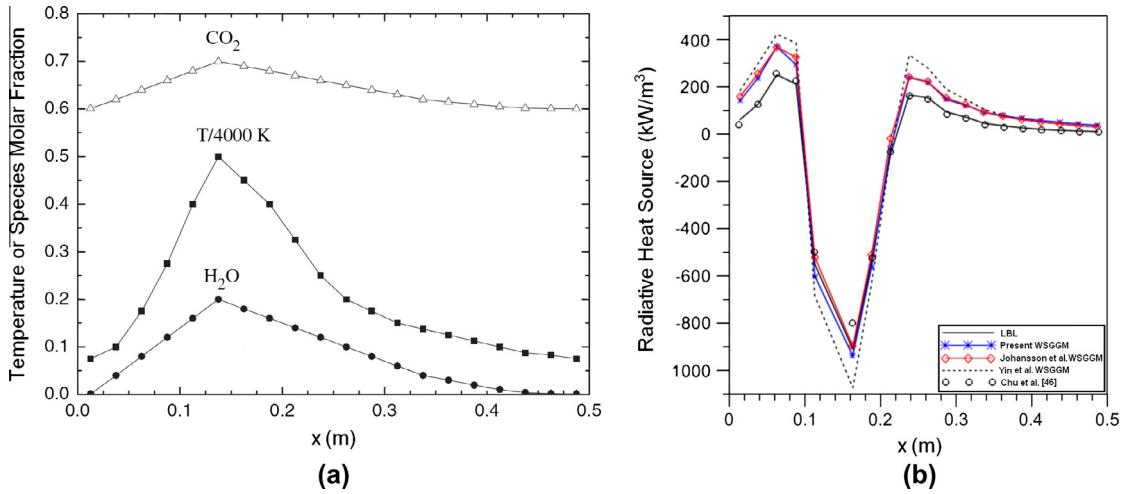

Fig. 6. The third 1D Benchmark in which $Y_H + Y_C < 1$ proposed by Chu et al. [46], (a) the distributions of temperature and molar fraction of gases reproduced from Chu et al. [46] and (b) the radiative heat source calculated by different spectral models.

A 3D benchmark representing the thermal condition of an oxygen fired flame has been presented recently by Porter et al. [9]. The geometry of the benchmark problem is a box of gas mixture with dimensions of $2m \times 2m \times 4m$ surrounded by black walls at $T = 300$ K. The system total pressure is 1 bar, and the gas concentration is assumed to be 85% CO_2, 10% H_2O and 5% of other gas species which are assumed to be neutral to radiation heat transfer. This gas concentration corresponds to the practical condition of dry flue gas recycling in oxygen fired combustion systems.

The temperature distribution in the gas is expressed by $T = (T_c - T_e)f(r/R) + T_e$ where T_c and T_e are the centerline temperature and the temperature at the end of the geometry ($z = 4m$), respectively. The function $f(r/R)$ is defined as $f(r/R) = 1 - 3(r/R)^2 + 2(r/R)^3$ where r and R are the shortest distance from the geometry centerline and the radius of a circle of 1 m, respectively. The temperature of centerline T_c is changing linearly from 400 K at the bottom of the container to the maximum of 1800 K in $z = 0.375m$, and decreasing linearly from this point to 800 K (T_e) at the top wall of the enclosure. This temperature distribution simulates roughly the temperature distribution of a flame. The contours of temperature in three cross sections of the geometry ($x = 1m$, $y = 1m$, and $z = 0.375m$) are shown in Fig. 7.

Porter et al. [9] have solved this benchmark problem by using the ray tracing approach for solving RTE and SNBM for calculating the radiative properties of the gas. They have used the $17 \times 17 \times 24$ grid points with a greater concentration of nodes in z direction around $z = 0.375m$. Since Porter et al. [9] did not report the tabulated benchmark solution, the solution of the benchmark is reproduced by image processing of the figures reported by Porter et al. [9].

To verify the present WSGGM and to compare the accuracy of different WSGGMs, the radiative source term in the enclosure centerline calculated by the zonal approach using different WSGGMs has been compared with the benchmark solution reported by Porter et al. [9] in Fig. 8. A uniform cubical mesh structure with $17 \times 17 \times 34$ grid points has been used to solve the benchmark problem with the zonal approach. The WSGGMs is implemented into zonal theory not to calculate the total properties of the gas mixture (gray gas modeling) but to solve the non-gray radiative heat transfer. For a system of absorbing, emitting and non-scattering media surrounded by black walls, the radiative source term in the volume zones can be calculated by

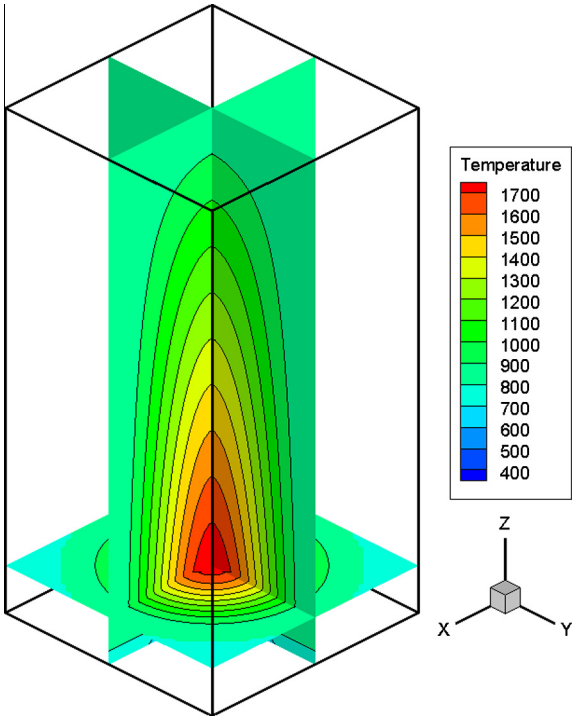

Fig. 7. The temperature distribution in three cross sections of the benchmark problem.

$$RST_i = \sum_{l=0}^{N_g}\left[\sum_{j=1}^{M}\left[(s_j s_i)_l\left(a_l(T_i)\sigma T_i^4 - a_l(T_j)\sigma T_j^4\right)\right] + \sum_{j=1}^{N}\left[(g_j s_i)_l\left(a_l(T_i)\sigma T_i^4 - a_l(T_j)\sigma T_j^4\right)\right]\right] \quad (12)$$

In the same way, the radiative heat flux in the walls is obtained by:

$$q_i = \sum_{l=0}^{N_g}\left[\sum_{j=1}^{M}\left[(s_j g_i)_l\left(a_l(T_i)\sigma T_i^4 - a_l(T_j)\sigma T_j^4\right)\right] + \sum_{j=1}^{N}\left[(g_j g_i)_l\left(a_l(T_i)\sigma T_i^4 - a_l(T_j)\sigma T_j^4\right)\right]\right] \quad (13)$$

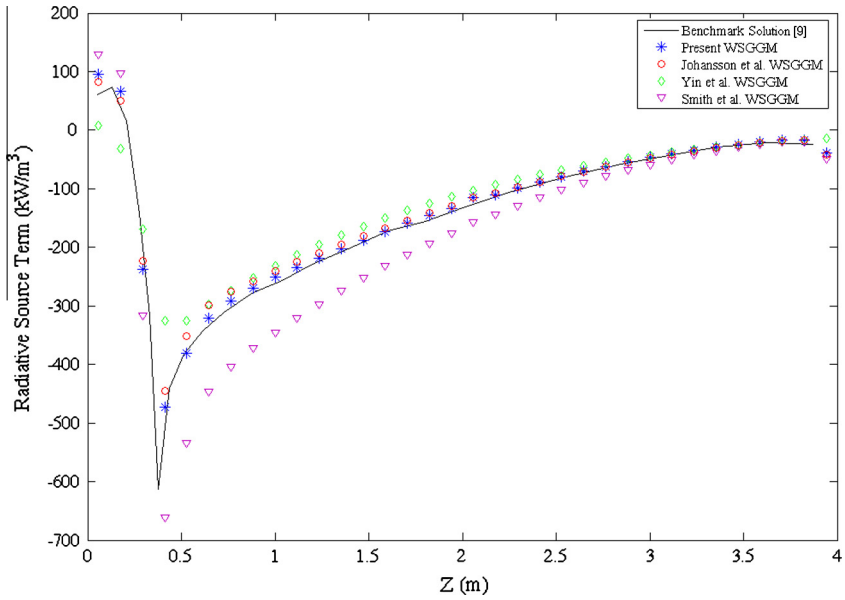

Fig. 8. The radiative source term in the center line of oxy-fired benchmark geometry shown in Fig. 7 obtained by the non-gray modeling using different WSGGMs.

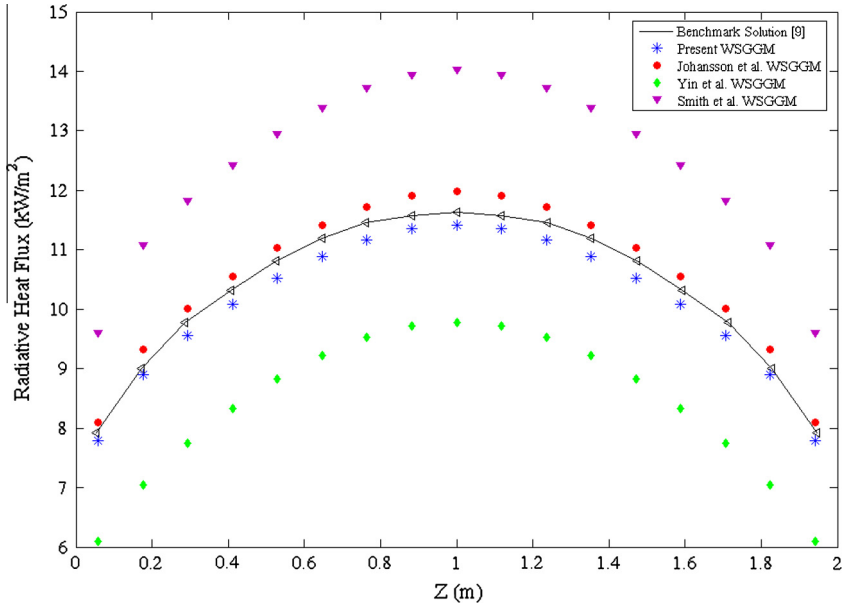

Fig. 9. Radiative heat flux in the centerline of the top wall of the oxy-fired benchmark geometry shown in Fig. 7 obtained by the non-gray zone method using different WSGGMs.

The last two equations are limited to no scattering media and black walls. The terms $s_j s_i$, $s_j g_i$, $g_j g_i$, and $g_j s_i$ represent the pre-calculated direct exchange areas between the zones. The use of zone method for non-gray gas modeling can be extended to the cases with reflecting walls and scattering media approximately by replacing direct exchange area with total exchange area in Eqs. (12) and (13) [3]. The theory of zone method and the way of calculating direct exchange area used in this research is well described in the Refs. [1,3,22].

Although the molar fraction ratio of the benchmark problem is equal to 0.1137 which is in the weakest region of the present WSGGM, the values predicted by the present WSGGM are the closest ones to the benchmark solutions. As it is expected, the minimum point of the radiative source term is in the maximum temperature point in $z = 0.375m$. Since the used mesh structure in the zonal code does not have any grid point exactly in $z = 0.375m$, this minimum point is not predicted by different methods. However, in the other parts, the present WSGGM is in a very good agreement with the benchmark solution.

Figure 9 shows the radiative heat flux at the top wall of the geometry calculated by different WSGGMs in comparison with the exact solution of the benchmark. The present WSGGM shows its better accuracy in comparison with other WSGGMs, especially with the one reported by Smith et al. [32] which is currently used in the commercial CFD software Fluent as a representative of WSGGMs for all the applications. It should be noted that the current versions of Fluent are using the WSGGM only to calculate the total properties of the gas mixture which is in use for gray

gas radiative heat transfer calculations, and practically they do not take advantage of WSGGM in non-gray radiative heat transfer modeling.

As Figs. 8 and 9 show, in this low molar fraction ratio, the present WSGGM provides just slightly better accuracy than the WSGGM proposed by Johansson et al. [26]. However, the small molar fraction ratios, especially those below 1/8, are the weakest region of the present model, and the better relative accuracy of the present model is expected in other ranges of molar fraction ratios. In addition, the range of parameters considered in the development of the present model is much wider than those used by Johansson et al. [26].

5. Conclusions and remarks

One of the recent widely used techniques for improving the performance of combustion equipment is the oxygen fired scenario in which the combustion is done by using pure oxygen instead of air used in the conventional systems. In the new oxygen fired systems, the mixtures usually include higher molar fractions of H_2O and CO_2 than in the conventional air-fired combustion systems. Thus, the previously established WSGGMs which were proposed for limited number of molar fraction ratios corresponded to air-fired combustion scenario may not provide good accuracy level when applied to oxygen fired systems.

The most well-known coefficients for WSGGM are those reported by Smith et al. [32] which are basically found based on the total emissivity of H_2O–CO_2 mixtures obtained by EWBM in the range of air-fired combustion scenario for limited number of molar fraction ratios. Using this kind of coefficients in the modeling and analysis of oxygen fired systems may lead to some inaccuracy.

Traditionally the coefficients of WSGGMs have been reported for a certain number of molar fraction ratios. However, in real applications, due to the progress of combustion, the molar fraction ratios are not constant, and therefore the implementation of traditional WSGGMs for such inhomogeneous conditions might be a practical problem. Usually, for not tabulated molar fraction ratios, the interpolation or extrapolation between the coefficients of tabulated molar fraction ratios is needed. However, it might impose large error in the results of the models, especially if the number of molar fraction ratios in which the coefficients are tabulated is small.

In the present WSGGM, the coefficients of the model are obtained by using the most accurate emissivity database which is based on line by line calculation employing the latest HITEMP 2010 database. The line by line integration is performed in discrete way for the mixture of H_2O and CO_2. The parameters of the integration have been selected in such a way that the value of particular line intensity is reproduced with an accuracy of 10^{-4}. Presenting new formulations for WSGGM, the molar fraction ratio is included in the formulation of WSGGM, and therefore the model accounts the variation of the molar fraction ratio in the mixture. The coefficients of the model are obtained for a wide range of different combustion conditions in the temperature range of 300–2400 K, the pressure-path length product of 0.01–60 atm m and the molar fraction ratio of 0.01 and 4 supporting different practical combustion conditions which may occur in the oxygen fired combustion systems.

The total emissivity predicted by the present model is verified by comparing it with the LBL benchmark values and the predictions of other WSGGMs. The present model showed the most accurate result among all other WSGGMs.

To validate the present model, the radiative heat transfer in non-isothermal and inhomogeneous slab layer of CO_2–H_2O mixture bounded by black walls is analyzed by the present WSGGM using the DO method as the RTE solver. Three different conditions for the distributions of gas species and temperature have been considered which demonstrate the inhomogeneous oxygen fired combustion cases in which there are some non-participating species such as N_2. The results showed a good conformity and proved the applicability of the model for the inhomogeneous and non-isothermal cases.

The present model is also implemented in the modeling of radiative heat transfer in a three dimensional oxygen fired benchmark. The results proved the privileges of the new model.

While one of the difficulties of the global models such as FSK and SLW is in using them in gas mixtures, the present WSGGM can also be expressed as the simplest form of SLW which offers a good correlation for four gas implementation of SLW. The present WSGGM does not require special treatment for the gas mixtures since the approximation formula is a function of molar fraction ratio.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.combustflame.2014.03.013.

References

[1] M.H. Bordbar, T. Hyppänen, Adv. Stud. Theor. Phys. 1 (2007) 71–84.
[2] M.H. Bordbar, T. Hyppänen, Heat Transf. Eng. 34 (2013) 54–69.
[3] M.F. Modest, Radiative Heat Transfer, second ed., Academic Press, New York, 2003.
[4] R. Goody, Quart. J. R. Meteorol. Soc. 78 (1952) 165–169.
[5] A. Soufiani, J. Taine, Int. J. Heat Mass Transf. 40 (1997) 987–991.
[6] W.L. Grosshandler, "Radcal: a Narrow-Band Model for Radiation Calculations in a Combustion Environment", Technical Report NIST Technical Note 1402, National Institute of Standards and Technology, 1993.
[7] H. Chu, F. Liu, H. Zhou, Int. J. Heat Mass Transf. 54 (2011) 4736–4745.
[8] F. Liu, J. Heat Transf. 121 (1999) 200–203.
[9] R. Porter, F. Liu, M. Pourkashanian, A. Williams, D. Smith, J. Quant. Spectrosc. Radiat. Transf. 111 (2010) 2084–2094.
[10] S.S. Penner, Quantitative Molecular Spectroscopy and Gas Emissivities, Addison Wesley, Reading, 1959.
[11] D.K. Edwards, Adv. Heat. Transf. 12 (1976) 115–193.
[12] A. Maximov, M.H. Bordbar, T. Hyppänen, Int. Rev. Mech. Eng. 6 (2012) 411–419.
[13] A. Maximov, Spectral Analyses and Reliable Calculations of the Radiative Properties of H_2O –CO_2 Mixtures Under Oxy- and Air-Fired Conditions, PhD thesis, Dec. 2012, Lappeenranta University of Technology, Finland.
[14] M.F. Modest, H. Zhang, J. Heat Transf. 124 (2002) 30–38.
[15] M.F. Modest, R.J. Riazzi, J. Quant. Spectrosc. Radiat. Transf. 90 (2005) 169–189.
[16] M.K. Denison, B.W. Webb, J. Heat Transf. 115 (1993) 1004–1012.
[17] V.P. Solovjov, B.W. Webb, J. Heat Transfer 133 (2011) 042701-1–042701-9.
[18] P. Rivière, A. Soufiani, M.Y. Perrin, H. Riad, A. Gleizes, J. Quant. Spectrosc. Radiat. Transf. 56 (1996) 29–45.
[19] F. Liu, H. Chu, J.L. Consalvi, in; 7th International Symposium on Radiative Transfer, ICHMT-RAD-13, Turkey, June 2013.
[20] J. Cai, R. Marquez, M.F. Modest, J. Heat Transf. (in press), http://dx.doi.org/10.1115/1.4026169.

[21] V.P. Solovjov, B.W. Webb, J. Quant. Spectrosc. Radiat. Transf. 65 (2000) 655–672.
[22] H.C. Hottel, A.F. Sarofim, Radiative Transfer, McGraw-Hill Education – Europe, New York, 1967.
[23] M.F. Modest, J. Heat Transf. 113 (1991) 650–656.
[24] O.J. Kim, T.H. Song, J. Quant. Spectrosc. Radiat. Transf. 64 (2000) 379–394.
[25] C. Yin, L.C.R. Johansen, L.A. Rosendahl, S.K. Kær, Energy Fuels 24 (2010) 6275–6282.
[26] R. Johansson, B. Leckner, K. Andersson, F. Johnsson, Combust. Flame 158 (2011) 893–901.
[27] O.J. Kim, J.P. Gore, R. Viskanta, X.L. Zhu, Numer, Heat Transfer, Part A 44 (2003) 335–353.
[28] J. Ströhle, J. Quant. Spectrosc. Radiat. Transf. 109 (2008) 1622–1640.
[29] S.S. Hwang, J.P. Gore, KSME Int. J. 16 (2002) 1156–1165.
[30] S.S. Krishnan, M.K. Saini, Y. Zheng, J.P. Gore, ASME J. Heat Transf. 134 (2012) 022701-1–022701-8.
[31] P.B. Sunderland, S.S. Krishnan, J.P. Gore, Combust. Flame 136 (2004) 254–256.
[32] T.F. Smith, Z.F. Shen, J.N. Friedman, J. Heat Transf. 104 (1982) 602–608.
[33] M. Bahador, B. Sundén, in: Proceeding of IV Conference of Radiative Heat Transfer-IV, 2004, pp. 563–571.
[34] J. Ströhle, P.J. Coelho, Int. J. Heat Mass Transf. 45 (2002) 2129–2139.
[35] L.S. Rothman, I.E. Gordon, R.J. Barber, H. Dothe, R.R. Gamache, A. Goldman, et al., J. Quant. Spectrosc. Radiat. Transf. 111 (2010) 2139–2150.
[36] V.P. Solovjov, B.W. Webb, J. Heat Transf. 123 (2001) 450–457.
[37] S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov, N.N. Lavrentieva, J. Quant. Spectrosc. Radiat. Transf. 82 (2003) 165–196.
[38] L.S. Rothman, I.E. Gordon, A. Barbe, D.C. Benner, P.F. Bernath, M. Birk, et al., J. Quant. Spectrosc. Radiat. Transf. 110 (2009) 533–572.
[39] R.J. Barber, J. Tennyson, G.J. Harris, R.N. Tolchenov, Mon. Not. R. Astron. Soc. 368 (2006) 1087–1094.
[40] http://www.cfa.harvard.edu/hitran/Updated/ref-table.pdf.
[41] P. Rivière, A. Soufiani, Int. J. Heat Mass Transf. 55 (2012) 3349–3358.
[42] G. Krishnamoorthy, Int. Commun. Heat Mass Transf. 37 (2010) 1182–1186.
[43] J.D. Felske, C.L. Tien, ASME J. Heat Transf. 99 (1977) 458–465.
[44] M.J. Yu, S.W. Baek, J.H. Park, Int. J. Heat Mass Transf. 43 (2000) 1699–1713.
[45] B. Leckner, Combust. Flame 19 (1972) 33–48.
[46] H. Chu, F. Liu, H. Zhou, Int. J. Heat Mass Transf. 54 (2011) 4736–4745.
[47] H.C. Hottel, E.S. Cohen, AIChE J. 4 (1958) 3–14.
[48] J.M. Goyhénéche, J.F. Sacadura, J. Heat Transf. 124 (2002) 696–703.
[49] A. Batu, N. Selçuk, Turkish J. Eng. Environ. Sci. 26 (2002) 49–58.