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A gas radiation property model applicable to general combustion CFD and its demonstration in oxy-fuel combustion simulation

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Abstract

As a good compromise between computational efficiency and accuracy, the weighted-sum-of-gray-gases model (WSGGM) is often used in computational fluid dynamics (CFD) modeling of combustion processes for evaluating gas radiative properties. However, the WSGGMs still have practical limitations (e.g., difficult to naturally accommodate different combustion environments or accurately address species variations in a flame or properly account for the impacts of participating species other than H_2O and CO_2) fostering different WSGGMs. In this paper, a gas radiation model, computationally efficient and practically accurate and applicable to general combustion CFD, is presented, programmed and verified. The model is implemented in CFD simulation of a 0.8 MW oxy-fuel furnace, via which the applicability and usefulness of the model in combustion CFD is demonstrated. On the contrary, the usefulness of the WSGGMs in oxy-fuel combustion CFD is found to be compromised, mainly because that the important impacts of the high levels of CO under oxy-fuel combustion cannot be accounted for in the current framework of the WSGGMs.

Keywords: CFD; Combustion; Radiation; Weighted-sum-of-gray-gases model; Exponential wide band model

1. Introduction

Gas radiation modeling gains a lot of concerns in the recent years especially for oxy-fuel combustion, primarily due to the enhanced radiative heat transfer by the elevated levels of CO_2 and H_2O. The weighted-sum-of-gray-gases

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model (WSGGM) represents a good compromise between computational efficiency and accuracy, and is widely used in computational fluid dynamics (CFD) modeling of combustion processes.

For oxy-fuel combustion, new oxy-fuel WSGGMs have been derived based on different reference models or databases, e.g., [1-5]. Besides the reference model, another major difference among the new WSGGMs is the way to address the variations in H_2O and CO_2 concentrations in a flame. The species variation in a flame cannot be considered when only one single coefficient table for the entire flame is proposed in some WSGGMs. More commonly, the species variations are accounted for by using discrete coefficient tables. For instance, the new 4-gray-gas-1-clear-gas oxy-fuel WSGGM accounts for the species variations in a flame by using 7 discrete coefficient tables, each of which corresponds to a representative H_2O and CO_2 concentration condition [1]. However, switching to different parameter tables based on the local gas composition may result in discontinuities, i.e., a sharp change in the gaseous radiative properties induced by a small change in local gas composition. Recently, smooth coefficient functions of H_2O/CO_2 molar ratio, instead of discrete coefficient tables, are derived in a few oxy-fuel WSGGMs with the aim to better address the species variations in a flame [2-5].

For air-fuel combustion CFD, the WSGGM with model coefficients proposed in [6] is commonly used. A refined air-fuel WSGGM of better accuracy and applicability is recently derived [7], in which more discrete coefficient tables are also used to better address the variations in H_2O and CO_2 concentrations in a flame. Both the air-fuel WSGGMs are derived by using the EWBM as the reference model.

Although the WSGGMs are widely used in combustion CFD, they still have some limitations in practical use. First, they cannot be naturally adjusted to accommodate different combustion environments, spurring interest in developing new oxy-fuel WSGGMs recently. Second, it is not convenient to accurately address the variations in H_2O and CO_2 in a flame. Smooth coefficient functions of H_2O/CO_2 molar ratio [2-5] are a new attempt, which, however, may cause solution difficulties under some circumstances. Without special treatments, the local absence of CO_2 in a real furnace may crash the WSGGM calculation in the related cells and then crash the entire CFD simulation. Third, all the existing WSGGMs only account for the impacts of H_2O and CO_2 under atmospheric pressure, even though H_2O and CO_2 are truly by far the most important participating gas species in conventional air-fuel combustion furnaces. Other participating gas species (e.g., CO) and other pressure conditions may also play an important role in some scenarios. For instance, the much higher levels of CO in oxy-fuel combustion are expected to contribute to gas radiation and ignoring the impacts of CO in the current WSGGMs may compromise their usefulness in oxy-fuel combustion CFD.

In the paper, a reliable gas radiation model applicable to general combustion CFD is presented, which is a computationally efficient EWBM (E-EWBM). The E-EWBM can naturally and properly address all the above practical limitations of the WSGGMs. The formulation of the E-EWBM is briefly described, for which the computer code is developed and verified. The E-EWBM code is then used in CFD simulations of a 0.8 MW oxy-fuel combustion furnace as a demonstration, in which the CFD results based on the E-EWBM and the commonly used WSGGM are compared against each other as well as the available experimental data.

2. E-EWBM: Calculation procedure

The EWBM [8] is by far the most successful of the wide band models and can accommodate different combustion environments [9]. A computer code is developed and validated to calculate the total emissivity of any gas mixture at any condition using the EWBM, based on which the new oxy-fuel WSGGM [1] and the refined air-fuel WSGGM [7] are derived. The EWBM code is also implemented to CFD of a natural gas flame, making the simulation nearly computationally prohibitive. As a result, the computational efficiency of the EWBM needs to be largely improved in order to make it applicable to general combustion CFD.

The EWBM code developed and validated in our previous works [1,7] is reformulated into an E-EWBM code which can correctly evaluate the total emissivity of *any* gas mixture at *any* condition. The required input parameters are the gas temperature (T), the total gas pressure (P_T), the mean beam length or path-length (L), and the molar fractions of different species in the gas mixture (x_i). The stepwise procedure for the calculation of total emissivity using the E-EWBM is same as that for the original EWBM [1,10].

1. For each gas i : calculate the mass-path length product, $\chi_i = \rho_i \cdot L$;

2. For band j of gas i: calculate the parameters $P_{e,ij}$, ω_{ij}, α_{ij} and β_{ij}, which represents effective pressure, bandwidth parameter, integrated band intensity and a parameter related to the mean line-width to spacing ratio, respectively;
3. For band j of gas i: calculate the total band absorptance A_{ij}, defined as $A_{ij} \equiv \int_{\eta_{L,ij}}^{\eta_{U,ij}} \alpha_{\eta,ij}\, d\eta$, from the above evaluated (χ_i, $P_{e,ij}$, ω_{ij}, α_{ij}, β_{ij});
4. For band j of gas i: calculate the band transmissivity τ_{ij} from ($P_{e,ij}$, β_{ij}, ω_{ij}, A_{ij}) and then evaluate the upper and lower limits of each band, $\eta_{U,ij}$ and $\eta_{L,ij}$;
5. After all the band limits are calculated, sort them in blocks and arrange in ascending order [$\eta_{L,k}$, $\eta_{U,k}$], $k = 1, 2, \cdots, N$: the lower limit of block $k+1$ being the same as the upper limit of block k;
6. By comparing whether the limits of a given block belongs to none, one or several absorption bands, compute the block transmissivity as the product of the band transmissivity to which the block belongs by $\tau_b = \tau_1 \times \tau_2 \times \cdots$;
7. Multiply each block emissivity $(1-\tau_b)$ by the fraction of blackbody radiation in the block limits and sum over all the blocks. The summation result gives the total emissivity, ε.

To improve the computational efficiency, the calculation of a few parameters is simplified, compared to the original EWBM. Specifically, the calculation of the integrated band intensity α_{ij} and the mean line-width to spacing ratio parameter β_{ij} in step 2 is simplified by following [11], instead of the computationally expensive analytical expressions as used in [1]. The fractional function in step 7 is calculated by following [10] also to somehow speed up the calculation. These approximate expressions are summarized in [12].

The E-EWBM code is then verified. For the gas mixture whose temperature, total pressure, beam length, molar fractions of H_2O, CO_2, CO and CH_4 are $T_g = 1500$ K, $P_T = 101325$ Pa, $L = 0.5$ m, $x_{H_2O} = 0.160$, $x_{CO_2} = 0.085$, $x_{CO} = 0.020$ and $x_{CH_4} = 0.005$, respectively, the detailed calculation results of the EWBM are available in [1,10]. The total emissivity of the original EWBM and the E-EWBM is 0.167257 and 0.167252, respectively. All the step-by-step calculation results of the two EWBMs are nearly identical. Such a comparison shows that the E-EWBM is correctly implemented and programmed. If more benchmark data are available in the literature, the similar verification can be made.

3. CFD demo: Applicability and impacts of the E-EWBM

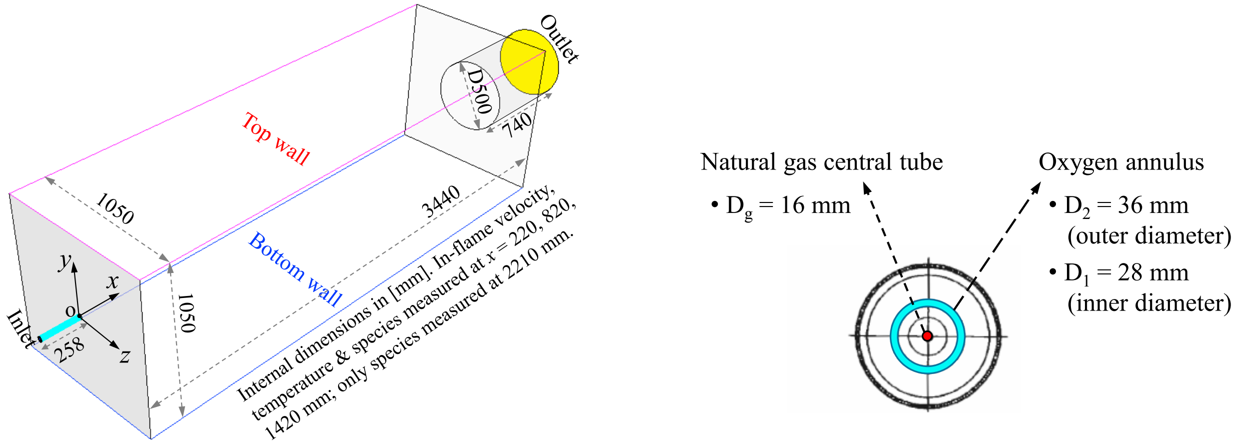
The main purpose of the CFD simulation is to demonstrate the applicability of the verified E-EWBM code in real combustion CFD in terms of computational efficiency, rather than to demonstrate the accuracy of the E-EWBM in combustion CFD. Actually, it is less likely to conclude the accuracy of a particular model via such a CFD study, unless all others (e.g., mesh, experimental data, and other models) are perfectly done or perfectly accurate. In general combustion CFD, the turbulence and combustion models are expected to induce more uncertainties than the gas radiation model does.

3.1. The furnace used for demonstration

The IFRF 0.8 MW oxy-natural gas flame furnace is used for the CFD demo, which has been simulated in quite some CFD studies in the past. However, none of them is very successful in terms of the agreement with the measured data. This furnace is used here, partly because there is very limited experimental data available in the literature on gaseous fuel combustion under oxy-fuel conditions and partly because the CFD study is to demonstrate the applicability of the E-EWBM rather than to conclude its accuracy in combustion CFD.

As shown in Fig. 1(a), the high-momentum jet flame is issued from the burner into the refractory-lined furnace. In the burner, natural gas and oxygen are issued from the central tube and the outer annulus, respectively, as seen in

Fig. 1(b). The same flame in the same furnace is also numerically studied to investigate the impacts of the new oxy-fuel WSGGM [1] and the impacts of meshes and combustion mechanisms [13], in which the new oxy-fuel WSGGM and the commonly used air-fuel WSGGM are not found to make remarkable difference in the CFD results. The natural gas composition, operational conditions and furnace wall temperatures are presented in [13]. More details about the flame and the 0.8 MW furnace can be found in [14-16].



(a) The furnace used in simulation

(b) The cross-section of the inlet tube

Figure 1. The 0.8 MW oxy-natural gas flame furnace: (a) the furnace used in simulation; (b) the inlet tube.

3.2. Computational cases

Compared to our previous studies [1,13], the following items are principally the same: a high-quality mesh of 608,864 hexahedral cells; the Discrete Ordinates model for radiative heat transfer; the species transport method for species mass fractions and the Eddy-Dissipation Concept for turbulence-chemistry interaction; the refined 2-step oxy-CH_4 combustion mechanism [17] for natural gas combustion; wall emissivity set to 0.9 and the measured wall temperature profile used as the wall thermal condition.

Differently, the SST k-ω model and the E-EWBM are used here for turbulence and gaseous radiative properties, respectively, instead of the standard k-ε model and the oxy-fuel WSGGM used in our previous studies. Two computational cases are presented here with detailed results and discussion. The only difference between them is with the gaseous radiative property model: the Smith et al. WSGGM [6] in one case *vs*. the E-EWBM in the other case. All the CFD simulations are performed using Ansys Fluent v16.1 [18], in which the new models/mechanisms and the measured profiles of wall temperatures are implemented via the user-defined functions.

3.3. Impacts of the E-EWBM

The E-EWBM is found to be computationally efficient and applicable to real combustion CFD, although it slows down the CFD simulation to some extent compared to the WSGGM. On an identical computer, it takes about 10 hours and 1.1 hours to complete 1000 iterations for the two computational cases based on the E-EWBM and the WSGGM, respectively. Such a computational efficiency of the E-EWBM is acceptable for general combustion CFD, especially with the fast growing capacity of computers.

Before discussing the CFD results, the CFD predictions are compared with the measured data. Among the in-flame measurement data, the velocity and species concentration have good quality while the temperatures have large errors [14-16]. Overall, the CFD results and the in-flame measurements show a consistently, reasonably good agreement. Here, only the comparison at 82 cm downstream of the burner quarl is given in Fig. 2, as an example, from which some interesting phenomena are observed.

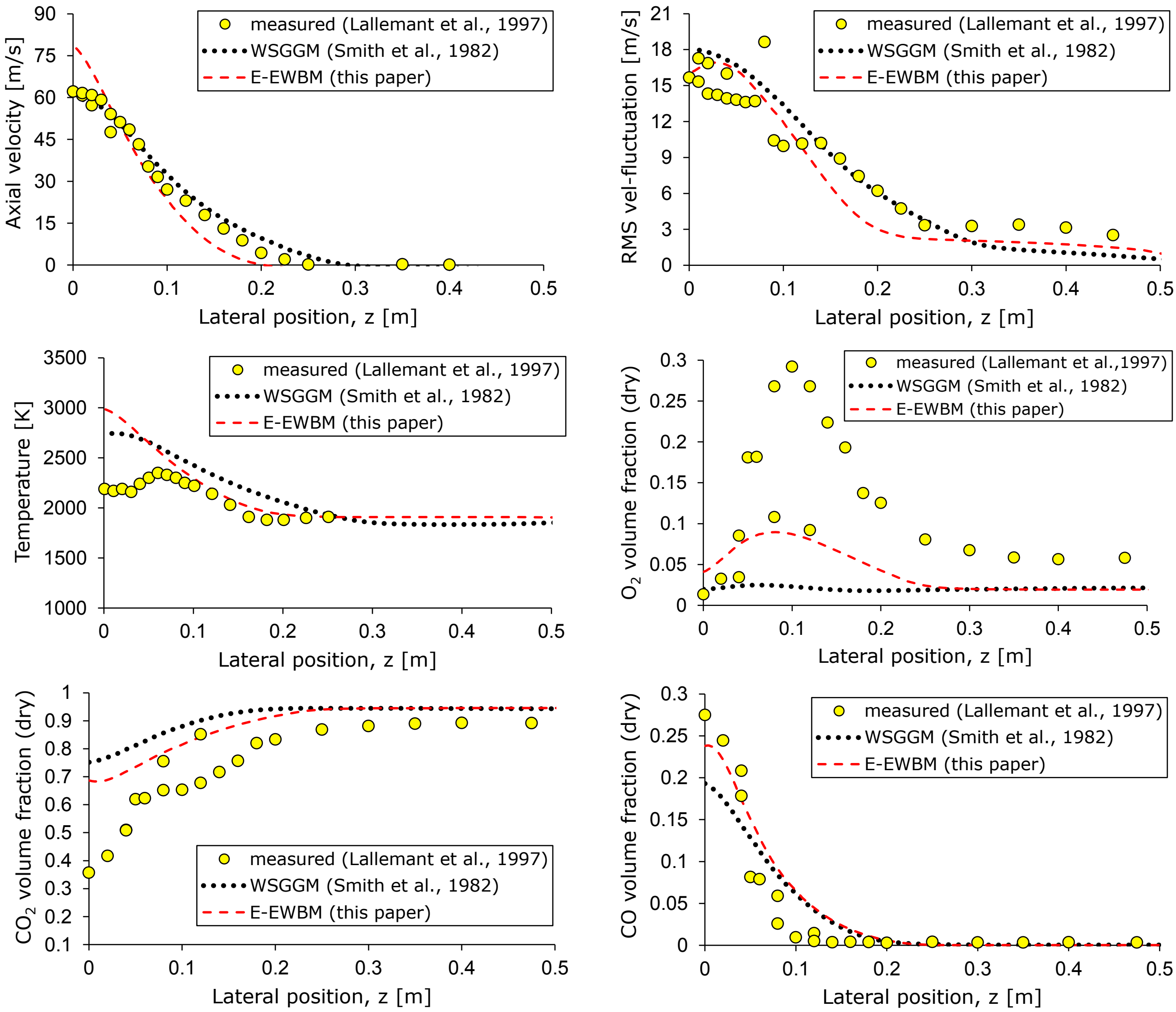
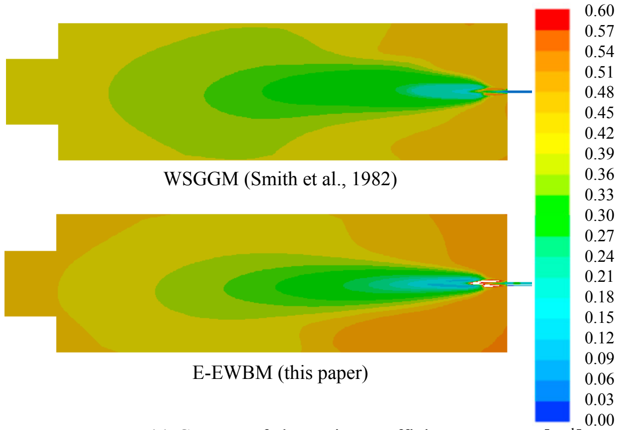


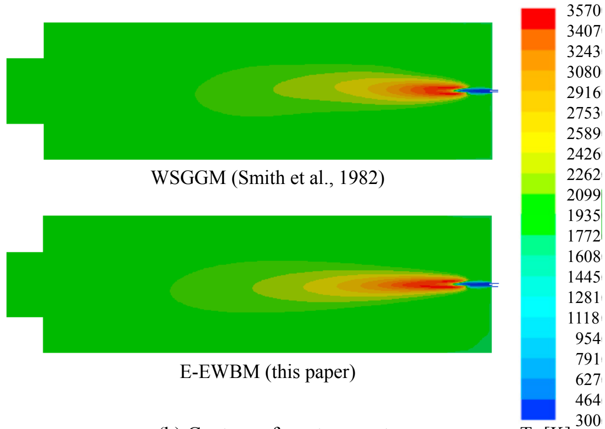
Figure 2. Predictions of the two cases *vs*. the measured results at 82 cm downstream of the burner quarl.

First, the E-EWBM and the WSGGM yield distinctly different CFD results. However, in our previous numerical study of the same flame in the same furnace, the new oxy-fuel WSGGM and the WSGGM are found to produce the same CFD results in velocity, temperature and species, which is attributed to the less apparent thermal radiation impacts in small furnaces [1]. Such a different observation is mainly because that the high levels of CO in the oxy-fuel furnace (as shown Fig. 3) are neglected in both the WSGGMs in our previous study while are properly accounted for in the E-EWBM in this study. For air-fuel combustion in which the CO level is significantly lower, the E-EWBM and the WSGGM are expected not to induce clearly different CFD results for small furnaces, as demonstrated in [12].

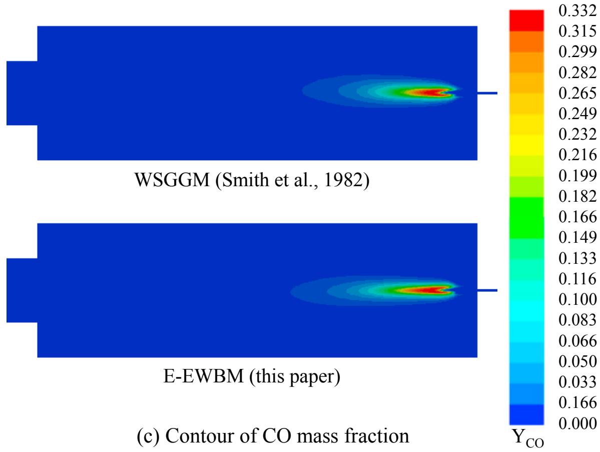
Second, the E-EWBM tends to improve the CFD results in terms of agreement with the measurements, even though the superiority of a sub-model cannot be readily concluded from such a CFD-measurement comparison. Remarkable discrepancy between the CFD predictions and the measurements still exists in both the computational cases. Besides the uncertainties with the experimental data, on the CFD side the turbulent combustion model seems to over-estimate the mixing and reaction in the furnace, which could be the main reason why the existing CFD simulations of this furnace have failed in the past. To further improve the agreement between the CFD results and experimental data for the furnace, unsteady calculations on much more refined mesh may be needed, which is beyond the scope of this study.



(a) Contour of absorption coefficient



(b) Contour of gas temperature



(c) Contour of CO mass fraction

Figure 3. Contour of absorption coefficient, temperature and CO on the horizontal centerplane.

Figure 4 plots the lateral profiles of the absorption coefficient and radiation source at the axial position of x=82 and 142 cm for the two cases. Differences are also observed. The first is the discontinuity in the plot using the WSGGM which consists of five discrete parameter tables. As explained previously, a small spatial change in the local gas composition may induce a large change in the absorption coefficient due to the switch to a different parameter table in the WSGGM calculation. The E-EWBM does not have such a problem. The second is the distinctly different absorption coefficient and radiation source for the two cases. The WSGGM yields somehow accurate results only for five composition conditions in terms of H_2O and CO_2, while can only give a rough estimate by using the closest parameter table for other composition conditions.

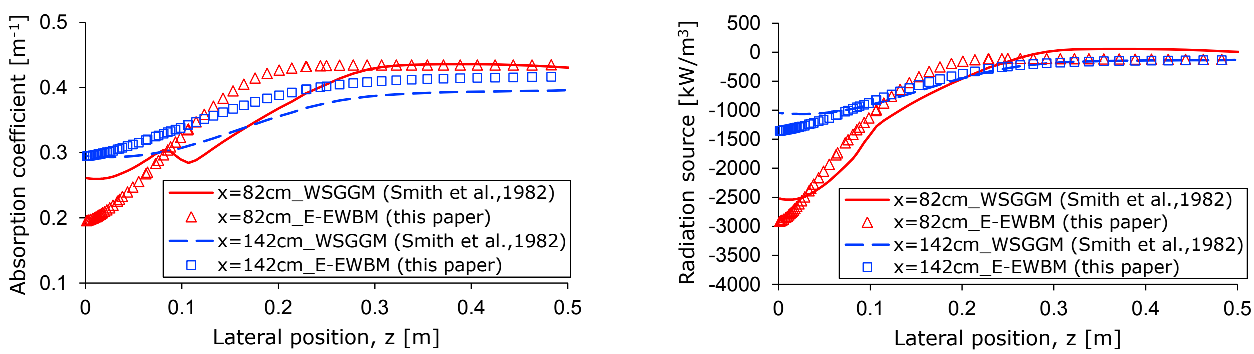


Figure 4. Lateral profiles of radiation at 82 cm and 142 cm downstream of the burner quarl.

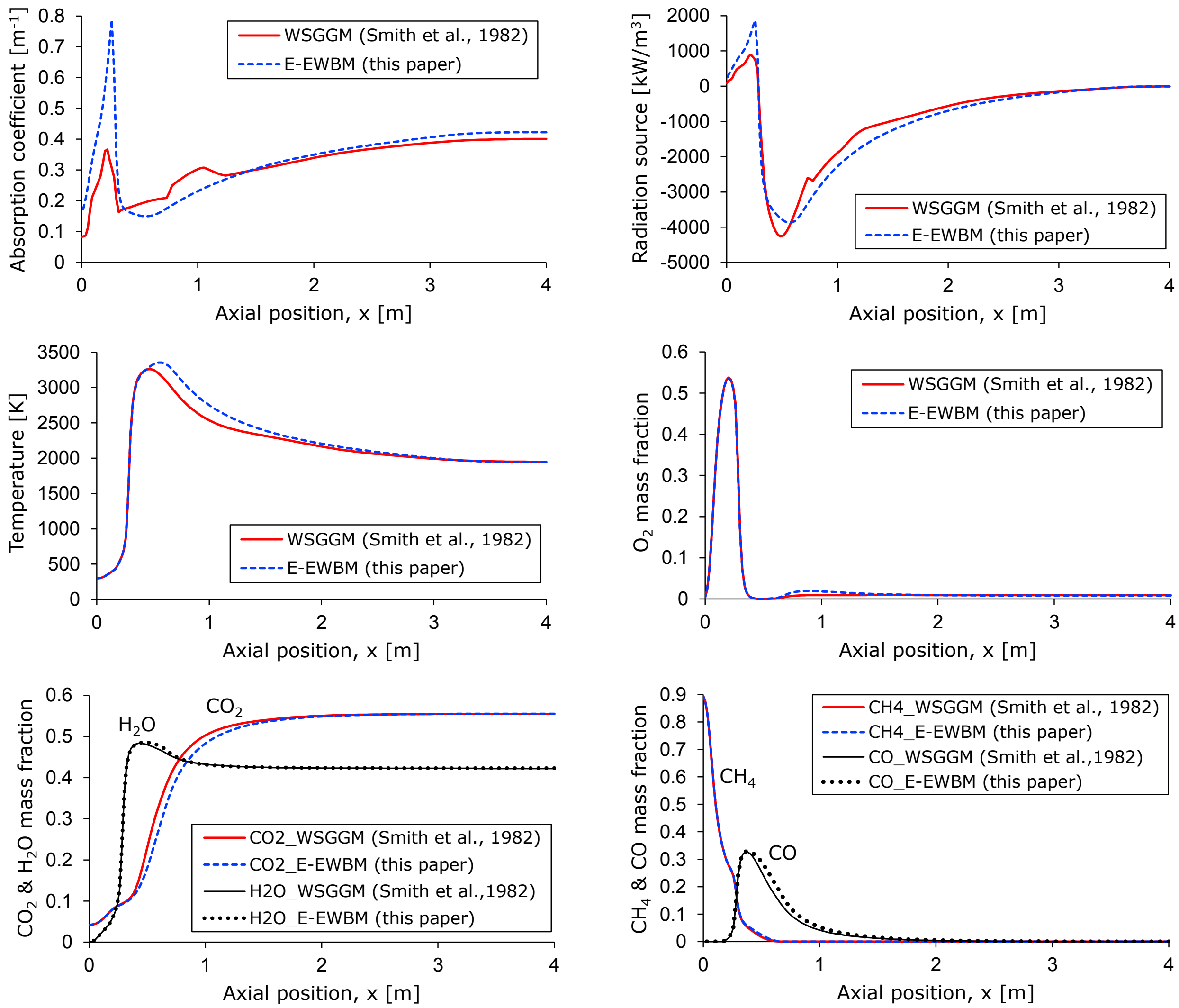


Figure 5. Axial profiles of radiation, temperature and species along the furnace centerline.

The contours in Fig. 3 and the axial profiles of the key variables along the furnace centerline in Fig. 5 for the two computational cases further illustrate the above differences. The existing WSGGMs only account for the impacts of CO_2 and H_2O while neglect other participating gases, which may hinder their usefulness in oxy-fuel combustion due to the high levels of CO and the important contribution to gas radiation.

The E-EWBM is not only applicable to real combustion CFD in terms of computational efficiency but also able to produce reliable CFD results for general combustion processes. Similar to the E-EWBM, the spectral-line-based weighted-sum-of-gray-gases (SLW) and the full-spectrum *k*-distribution (FSK) method [9] are also accurate and computationally competitive and can also readily address the practical limitations of the WSGGMs. As a result, they all can be used in general combustion CFD. The E-EWBM is applicable to both gray and non-gray calculation, although the commonly used gray calculation is performed for both the E-EWBM and WSGGM in the study. Non-gray calculation represents the rigorous implementation of a gas radiation model and can make distinct difference in the CFD results compared to the gray calculation [19]. For the E-EWBM which has about 30 spectral intervals in the entire spectrum, the non-gray calculation will remarkably increase the computational requirements since one set of radiative transfer equations needs to be solved for each of the spectral intervals.

Besides the E-EWBM presented above, other CFD-oriented E-EWBMs exist, e.g., the one in [20] whose integrated band intensity and line width to spacing ratio are recalculated by fitting the emissivity values to those evaluated by the line by line model with the HITEMP-2010 database in temperature of 300–2500 K. The two E-EWBMs are found to produce the same CFD results when applied to air-fuel combustion [12]. When the E-EWBM [20] is used in CFD of this 0.8 MW oxy-fuel furnace, it crashes the simulation, because the peak flame temperature exceeds the upper temperature limit of the model and can crash the calculation of the gas radiative properties.

4. Conclusions

A reliable gas radiation model applicable to general combustion CFD, i.e., a computationally efficient EWBM or E-EWBM, is presented, programmed and verified. The E-EWBM can naturally and properly accommodate different combustion environments (e.g., oxy-fuel or air-fuel) and account for the variations in species concentrations in a flame and the impacts of participating species other than H_2O and CO_2. The ability to properly account for CO is important for the use in oxy-fuel combustion CFD, due to the very high CO concentrations in oxy-fuel furnaces. The existing efforts on refining WSGGMs for oxy-fuel combustion may be compromised, if the impacts of the high levels of CO in oxy-fuel conditions can not be appropriately accounted for.

The applicability of the E-EWBM is demonstrated in CFD modeling of a 0.8 MW oxy-natural gas combustion furnace. Compared to the widely used WSGGM, the E-EWBM slows down CFD simulations by a factor of about 10 but makes distinct difference in the CFD results. The computational efficiency and accuracy of the E-EWBM can be further improved to make it more attractive in general combustion CFD, considering its inherent advantages especially its ability to properly address the impact of participating gases other than H_2O and CO_2 (e.g., CO).

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