Applied Energy 189 (2017) 449–459

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Prediction of air-fuel and oxy-fuel combustion through a generic gas radiation property model

Chungen Yin

Department of Energy Technology, Aalborg University, 9220 Aalborg East, Denmark

HIGHLIGHTS

- A gas radiation model for general combustion CFD presented, programmed & verified.
- Its general applicability/practical accuracy demonstrated in air-fuel and oxy-fuel.
- Useful guidelines for air-fuel and oxy-fuel combustion CFD suggested.
- Important to include the impact of CO in gas radiation for oxy-fuel combustion CFD.

ARTICLE INFO

Article history:
Received 30 September 2016
Received in revised form 9 December 2016
Accepted 10 December 2016

Keywords:
Combustion
CFD
Gas radiation
Heat transfer
Radiative property model

ABSTRACT

Thermal radiation plays an important role in heat transfer in combustion furnaces. The weighted-sum-of-gray-gases model (WSGGM), representing a good compromise between computational efficiency and accuracy, is commonly used in computational fluid dynamics (CFD) modeling of combustion processes for evaluating gaseous radiative properties. However, the WSGGMs still have some limitations in practical use, e.g., unable to naturally accommodate different combustion environments, difficult to accurately address the variations in species concentrations in a flame, and inconvenient to account for the impacts of participating species other than H_2O and CO_2. As a result, WSGGMs with different coefficients have been published for specific applications. In this paper, a reliable generic model for gaseous radiation property calculation, which is a computationally efficient exponential wide band model (E-EWBM) applicable to combustion CFD and able to naturally solve all the practical limitations of the WSGGMs, is presented, programmed and verified. The model is then implemented to CFD simulation of a 300 kW air-fuel and a 0.8 MW oxy-fuel combustion furnace, respectively, to demonstrate its computational applicability to general combustion CFD and its capability in producing reliable CFD results for different combustion environments. It is found that the usefulness of the WSGGMs in oxy-fuel combustion CFD is compromised if the important impacts of high levels of CO under oxy-fuel combustion cannot be accounted for. The E-EWBM that appropriately takes the impacts of H_2O, CO_2, CO and CH_4 into account is a good replacement of the oxy-fuel WSGGMs for oxy-fuel combustion CFD.

1. Introduction

Gas radiation modeling has received unprecedented attention in the past decade, primarily due to the enhanced gas radiation heat transfer by the elevated levels of CO_2 and H_2O under oxy-fuel combustion conditions, as comprehensively reviewed in [1]. Consequently, different weighted-sum-of-gray-gases models (WSGGMs) with model coefficients refined for specific applications have been published.

For oxy-fuel combustion, several new WSGGMs are derived by using different models or databases as the reference models [2–7], in which the variations in H_2O and CO_2 concentrations in a flame are also taken into account in different ways. For the WSGGMs which have model coefficients for only one single gas composition, the effect of species variations in a flame is virtually neglected. More commonly, the variations in gas compositions in a flame are addressed via discrete coefficient tables. For instance, the oxy-fuel WSGGM [2] accounts for the species variations by using 7 coefficient tables, each of which corresponds to a typical H_2O and CO_2 condition. Based on the local gas composition, different tables will be used to evaluate the local radiative properties. The use of discrete coefficient tables may result in discontinuity, i.e., a small change in gas composition may induce a sharp change in the radiative properties. To eliminate the discontinuity problem,

E-mail address: chy@et.aau.dk

http://dx.doi.org/10.1016/j.apenergy.2016.12.051
0306-2619/

smooth coefficient functions of H_2O/CO_2 molar ratio are proposed recently to address the species variations in a flame [3,4,6,7].

For air-fuel combustion CFD, the Smith et al. WSGGM [8] is commonly used. This model is revisited, based on which a refined air-fuel WSGGM of better accuracy and applicability is derived [9]. Both the air-fuel WSGGMs use the EWBM as the reference model.

Despite being commonly used in combustion CFD, the WSGGMs still have limitations in practical use. For example, they cannot be naturally adjusted to accommodate different combustion environments, which is also the reason efforts are made to develop oxy-fuel WSGGMs. Moreover, it is not convenient to accurately address inhomogeneous H_2O–CO_2 mixture in a flame. Smooth coefficient functions of H_2O/CO_2 molar ratio [3,4,6,7] are a good attempt and oxy-fuel WSGGMs based on the molar ratio of H_2O/CO_2 have been used in oxy-fuel combustion CFD. For example, the line-by-line based WSGGM for inhomogeneous H_2O–CO_2 mixture [6] is successfully implemented in simulation of oxy-fuel combustion in circulating fluidized bed furnaces [10,11]. Special treatments may be needed in the use of such WSGGMs; otherwise, the local absence of CO_2 in a furnace can induce some solution difficulties. New implementation of the discrete coefficient tables by linear interpolation could be a solution. If the local gas composition is in-between two composition conditions, the two corresponding coefficient tables are used to obtain two emissivity values first, and the emissivity of the gas mixture under consideration is then calculated from the two values by interpolation [1,12]. Another limitation of WSGGMs is that currently they only account for the impacts of H_2O and CO_2 under atmospheric pressure. CO concentration can reach as high as 12 vol% under deep staging combustion conditions [13] and can be much higher under oxy-fuel conditions, which is expected to make remarkable contribution to gas radiation. Many high-pressure combustion conditions, in which the pressure can be up to tens or hundreds of bar [14], also call for appropriate radiation property models in CFD analysis. These limitations, though not fundamental, truly induce difficulties in practical uses of the WSGGMs: the model coefficients have to be constantly refined to address these issues.

In this paper, a reliable gas radiation model applicable to general combustion CFD, i.e., a computationally efficient EWBM (E-EWBM), is presented. It can naturally and properly accommodate all the above issues in combustion CFD, with no need to constantly revise its coefficients. First, the formulation of the E-EWBM is briefly described, in which the differences with the original EWBM are emphasized. The model is programmed and verified by comparing its prediction results for given gas mixtures against the benchmark data in the literature. Then, the E-EWBM code is implemented to CFD simulations of a natural gas air-fuel furnace and a natural gas oxy-fuel furnace, respectively, in both of which the CFD results based on the E-EWBM are compared with those based on the alternative models as well as the experimental data.

2. E-EWBM: model formulation and code verification

The EWBM, first developed in [15,16], is by far the most successful of the wide band models and is capable of accommodating different combustion conditions [17]. A computer code is developed to calculate the total emissivity of any gas mixture at any condition using the EWBM. The code is validated first and then used to generate emissivity database for the derivation of the new oxy-fuel WSGGM [2] and the refined air-fuel WSGGM [9]. The model equations and stepwise calculation procedure of the original EWBM, as well as the intermediate calculation results of the EWBM code for a given gas mixture, are detailed in [2]. The verified EWBM code is also implemented to CFD of a natural gas flame, which is found to slow down the simulation to a nearly computationally prohibitive degree. As a result, it is necessary to improve its computational efficiency while retain its accuracy in order to make it applicable to real combustion CFD.

Few efforts have been made to improve the computational efficiency of the EWBM for its use in CFD, e.g., [18,19]. For instance, two main refinements are made in [19]. First, the integrated band intensity α_{ij} and the line width to spacing ratio parameter β_{ij} for band j of participating species i are recalculated by fitting the emissivity values to those evaluated by the line by line model with the HITEMP-2010 spectral database in the temperature range of 300–2500 K. Second, lookup tables are used to calculate the blackbody intensity to speed up the computation. The refined EWBM is implemented in CFD of natural gas combustion under air-fuel conditions in a 300 kW burner furnace [20], which is found to work well in the temperature range of 300–2500 K.

Based on the stepwise calculation procedure and the verified computer code of the original EWBM in [2], changes are made mainly following [18] to improve its computational efficiency while retain its accuracy.

First, the calculation of the integrated band intensity α_{ij} in the second step, Eq. (1), is simplified by using approximate expressions for $\psi(T)$, instead of the computationally expensive, analytical expressions. Table 1 shows the simplified relations for the calculation of the integrated band intensity $\alpha_{ij}(T)$.

$$\alpha_{ij}(T) = \alpha_0 \frac{\left[1 - \exp\left(-\sum_{k=1}^{m} u_k\ \delta_k\right)\right] \cdot \psi(T)}{\left[1 - \exp\left(-\sum_{k=1}^{m} u_{0,k}\ \delta_k\right)\right] \cdot \psi(T_0)} \tag{1}$$

In the equation, u_k and $u_{0,k}$ are defined as $u_k \equiv (h \cdot c_0/k_B) \cdot (\eta_k/T)$ and $u_{0,k} \equiv (h \cdot c_0/k_B) \cdot (\eta_k/T_0)$. The symbols, h, c_0, k_B, T, T_0, α_0, η_k, and δ_k, represent the Planck's constant, speed of light in vacuum, Boltzmann constant, gas temperature, reference temperature of 100 K, integrated band intensity constant, vibrational quantum number (or fundamental band wave number), and vibrational transition quantum step for species i, band j, respectively.

Second, the calculation of the mean line-width to spacing ratio parameter β_{ij}, also in the second step, is simplified by using an approximate expression, Eq. (2), instead of the analytical expression.

Table 1
E-EWBM: simplified relations for the calculation of the integrated band intensity $\alpha_{ij}(T)$.

	Bands (μm)	$\psi(T)$	$\alpha_{ij}(T)$ ($cm^{-1}/(g\ m^{-2})$)
H_2O	Rotational > 10	–	$\alpha_0 \cdot \exp(-9\ (T_0/T)^2)$
	6.3	S_2[a]	α_0
	2.7[b]	$2 \cdot S_2^2$	Eq. (1)
		S_1	α_0
		S_3	α_0
	1.87	$S_2 \cdot S_3$	Eq. (1)
	1.38	$S_1 \cdot S_3$	Eq. (1)
CO_2	15	$2 \cdot S_2$	α_0
	10.4	$e^{-u_1}(2 - e^{-u_1}) \cdot S_1 \cdot S_3$	Eq. (1)
	9.4	$e^{-u_1}(2 - e^{-u_1}) \cdot S_1 \cdot S_3$	Eq. (1)
	4.3	S_3	α_0
	2.7	$S_1 \cdot S_3$	Eq. (1)
	2	$2 \cdot S_1^2 \cdot S_3$	Eq. (1)
CO	4.7	S_1	α_0
	2.35	$2 \cdot S_1^2$	Eq. (1)
CH_4	7.66	$3 \cdot S_4$	α_0
	3.31	$3 \cdot S_3$	α_0
	2.37	$3 \cdot S_1 \cdot S_4$	Eq. (1)
	1.71	$6 \cdot S_1 \cdot S_2 \cdot S_4$	Eq. (1)

[a] $S_k \equiv (1 - e^{-u_k})^{-1}$, where $u_k \equiv (h \cdot c_0/k_B) \cdot (\eta_k/T)$.
[b] The 2.7 μm H_2O band consists of three overlapping bands. The overall integrated band intensity is obtained by summing the three bands contributions for this band, $\alpha_{2.7} = \sum_j \alpha_{2.7,j}(T)$.