International Journal of Thermal Sciences 120 (2017) 289–302

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

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

Assessment of several gas radiation models for radiative heat transfer calculations in a three-dimensional oxy-fuel furnace under coal-fired conditions

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A R T I C L E I N F O

Article history:
Received 4 November 2016
Received in revised form
16 June 2017
Accepted 16 June 2017

Keywords:
Oxy-fuel combustion
Non-grey gas radiation models
NBCK
WBCK
FSCK
WSGG

A B S T R A C T

Oxy-fuel coal combustion is a promising Carbon Capture and Storage technology that allows retro-fitting of existing power plants. Due to high concentrations of CO_2 and H_2O and the strong and irregular spectral variation of their absorption coefficients, prediction of radiative heat transfer in oxy-fuel combustion systems requires a non-grey gas radiation model. Several models, including narrow-band correlated-k (NBCK), wide-band correlated-k (WBCK), full-spectrum correlated-k (FSCK), and weighted-sum-of-grey-gases (WSGG) models, were used to predict radiative heat transfer by CO_2 and H_2O in a three-dimensional real-size virtual coal-fired furnace under air- and oxy-fuel (dry and wet flue-gas recycle) conditions. The best agreement with the benchmark solution calculated by the NBCK model with the updated EM2C parameters is achieved by the FSCK model. The WBCK model is less accurate. The WSGG parameter sets of Kangwanpongpan et al. (2012) and Bordbar et al. (2014) are most suited for oxy-fuel combustion among the six sets considered. The FSCK model offers the best performance in terms of both accuracy and computational efficiency among the considered gas radiation models and is recommended for CFD simulations of real-sized oxy-coal systems.

1. Introduction

Coal-fired power plants are often used to meet the energy demands of the world's increasing population. Since these energy systems produce a large amount of the greenhouse gas carbon dioxide (CO_2), various carbon capture and storage/sequestration (CCS) technologies have been investigated to reduce the CO_2 emissions into the atmosphere. A very promising approach, also applicable to retro-fit existing power plants, is the oxy-fuel combustion technology [1]. In oxy-fuel combustion, the conventional oxidizer (air) is substituted by pure oxygen or a mixture of oxygen and recycled flue gas. The resultant flue gas contains mainly water vapour (H_2O) and CO_2 and is suitable for sequestration or utilization purposes after condensation of water vapour. Depending on the amount of water vapour in the recycled flue gas, dry or wet flue gas recycle is differentiated.

In furnaces of coal-fired power plants, the heat transfer to the walls in regions of high temperatures is mainly due to thermal radiation. Since the concentrations of CO_2 and H_2O are higher in oxy-fuel combustion compared to those in the conventional air-fired systems, the radiation characteristics are changed. To accurately predict the net radiative wall heat fluxes and the source terms, which are crucial for employing computational fluid dynamics (CFD) methods to design new oxy-fuel furnaces or to retro-fit existing ones, the highly irregular distribution of spectral absorption coefficient over the wave number has to be efficiently taken into account. For this purpose, various gas radiation models have been developed. In line by line (LBL) calculations [2], the radiative transfer equation is solved with a spectral resolution of the order of 0.01 cm^{-1} and the spectral absorption coefficient is computed by summing the contribution of all radiating spectral lines. The information concerning spectral lines is taken from a spectroscopic database, such as HITEMP 2010 [3]. This procedure is impractical for CFD simulations of large-scale three-dimensional real combustion systems, since about one million spectral lines have to be considered in the infrared spectrum. For statistical

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http://dx.doi.org/10.1016/j.ijthermalsci.2017.06.017
1290-0729/

narrow-band (SNB) models, the whole wave number spectrum is divided into several tens or even hundreds of narrow-bands with a bandwidth of 25–100 cm^{-1} [4]. The SNB model shows a high accuracy in calculation of radiative properties [5] despite the lower spectral resolution and computational effort in comparison to LBL. But still its computational demand is too high for application in CFD simulations of real systems. Another drawback of this method is that it provides spectrally averaged transmissivities, instead of absorption coefficients, and the resultant RTE has to be solved using a ray-tracing type of method [6]. To overcome this disadvantage, the correlated-k approach can be applied at the narrow-band level (NBCK) [7], providing the absorption coefficient distribution in each narrow-band so that the RTE can be solved with any methods available [8]. This procedure furthermore reduces the computational effort while maintaining a high accuracy. Under conditions relevant to oxy-fuel combustion, solutions obtained with this method were found to agree well with the exact LBL solutions [9] and SNB results [10]. Thus, NBCK model results can serve as reference for evaluation of other gas radiation models in cases where LBL results cannot be obtained with reasonable computing resources.

Since narrow-band models are still very time consuming, wide-band models have been developed. Such models treat each rotation-vibration band as a single band, see e.g. Ref. [11], and thus improve the computational efficiency, but with some loss of accuracy. Applying the correlated-k approach to this model (WBCK) enables the use of the absorption coefficient, rather than transmissivity, as the radiative property [12, 13], which significantly improves the computational efficiency for solving RTE [14].

The computational effort for radiation heat transfer can be further reduced if the spectral properties are integrated over the whole wave number spectrum. Consequently, many different global models have been developed, like the weighted-sum-of-grey-gases (WSGG) model [15], the spectral line based WSGG (SLW) model [16], the absorption distribution function model with fictitious gases (ADFFG) [17], and the full-spectrum correlated-k (FSCK) model [18].

Much effort has recently been devoted to compile updated WSGG model parameters for oxy-fuel conditions valid over a broad application range, see e.g. Refs. [19, 20, 21, 22]. Up to now, the WSGG model has been the gas radiation model of choice to simulate large oxy-fuel boilers because of its simple implementation in commercial CFD software with fair to good accuracy and high computational efficiency. For example, Yin et al. [23] conducted CFD simulations of an oxy-fired natural gas utility boiler with 609 MW_e electrical output and found that non-grey WSGG models with parameters fit to oxy-fuel conditions should be used for large-scale boilers. Guo et al. [24] investigated different oxy-fuel cases of a 200 MW_e bituminous coal-fired boiler incorporating newer WSGG parameters suitable for oxy-fuel combustion conditions derived from k-distributions of the FSCK model [25].

Various gas radiation models have been evaluated by means of virtual test cases under conditions relevant to oxy-fuel combustion. In the work of Porter et al. [26], the SNB results serve as the benchmark for a 3D oxy-fuel combustion test case with a non-uniform temperature distribution between 400 and 1800 K, homogeneous H_2O to CO_2 ratio of about 0.118, and pressure path-lengths up to approximately 5 bar m. They found that results of the FSCK model are in good agreement with the benchmark solution, whereas the use of a grey gas model derived from the WSGG model with the standard parameters of Smith et al. [27], derived for air-combustion, leads to large errors. Clements et al. [28] used the SNB and NBCK models to provide reference results for the same 3D oxy-fuel test case as [26] and a further one with a uniform temperature distribution and an inhomogeneous H_2O to CO_2 ratio ranging between 0.125 and 2. They observed good agreement of the FSCK results with the benchmark data. Kez et al. [10] evaluated the performance of several models, ranging from NBCK, FSCK, different WBCK formulations, as well as the WSGG model with few new parameter sets, for two 3D oxy-fuel test cases of [29] with inhomogeneous temperature and gas concentrations distributions with pressure path-lengths up to about 10 bar m. They also calculated the reference solutions with a SNB model and recommend the use of the FSCK model for CFD simulations of oxy-fuel combustion and the parameter set of Bordbar et al. [22] if the WSGG model is applied.

So far, no NBCK simulations have been carried out for 3D test cases under oxy-fuel conditions with pressure path-lengths above 20 bar m encountered in typical furnaces of coal-fired power plants and used them as a reference to evaluate the accuracy of other approximate gas radiation models. In this study, for the first time, the NBCK simulation results are provided as the benchmark solution for one air-fuel and two oxy-fuel 3D test cases of a virtual furnace with pressure path-lengths up to 55 bar m given in Ref. [30] representing the relevant thermal conditions in a coal-fired power boiler. Using the NBCK results as the benchmark solution, the accuracy of the WBCK, FSCK, and WSGG models is evaluated. All the test cases have the same non-uniform temperature distribution, whereas the inhomogeneous distributions of H_2O and CO_2 mole fractions represent typical conditions for air, dry-, and wet-recycle oxy-fuel combustion, respectively. Particulate radiation, mainly due to coal and fly-ash particles, is not considered, since the aim of this study is to investigate solely the influence of gas radiation models.

In comparison to our previous work [10], the main differences of this study are a) to investigate the influence of much longer path-lengths encountered in real-sized applications on the applied gas radiation model, since to our knowledge no such information is available in the literature, especially for oxy-fuel-fired boilers; b) atmospheric pressure, typical for coal-fired boilers, in contrast to 20 bar encountered in gas turbine combustors, and c) the considered oxy-fuel combustion conditions with higher ratios of H_2O to CO_2, since these molecules directly influence the radiation characteristics. Finally, a recommendation is provided on which gas radiation model should be employed for CFD simulations of such a large-scale furnace.

2. Description of test cases

Radiation heat transfer is investigated in the 3D test cases of a virtual coal-fired furnace from Ströhle et al. [30]. Herein, the furnace is approximated by a rectangular enclosure with the dimensions of $L_x \times L_y \times L_z = 50\,m \times 20\,m \times 20\,m$, enclosed by black walls. The prescribed concentrations and temperature profiles were derived from a simplified combustion calculation for a coal-fired furnace burning a representative bituminous coal. The thermodynamic state of the unburned coal-oxidizer mixture was specified for the all test cases at the inlet of the domain. At the outlet, the whole volatile and carbon matters were burnt and a typical outlet temperature before the first convective heat exchanger, T_E, was assigned. At the side walls, a typical temperature for water-cooled furnaces, T_{wall}, was chosen. Fast release and combustion of volatiles as well as slow char combustion were assumed. With the aforementioned information, the concentrations of water vapour and carbon dioxide as well as the adiabatic combustion temperature could be calculated and used as the thermal input fields.

A physical quantity ϕ of interest, namely temperature and mole fractions of CO_2 and H_2O, is prescribed throughout the domain by the following assumed relation: