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Evaluation of FSK models for radiative heat transfer under oxyfuel conditions

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ABSTRACT

Oxyfuel is a promising technology for carbon capture and storage (CCS) applied to combustion processes. It would be highly advantageous in the deployment of CCS to be able to model and optimise oxyfuel combustion, however the increased concentrations of CO_2 and H_2O under oxyfuel conditions modify several fundamental processes of combustion, including radiative heat transfer. This study uses benchmark narrow band radiation models to evaluate the influence of assumptions in global full-spectrum k-distribution (FSK) models, and whether they are suitable for modelling radiation in computational fluid dynamics (CFD) calculations of oxyfuel combustion. The statistical narrow band (SNB) and correlated-k (CK) models are used to calculate benchmark data for the radiative source term and heat flux, which are then compared to the results calculated from FSK models. Both the full-spectrum correlated k (FSCK) and the full-spectrum scaled k (FSSK) models are applied using up-to-date spectral data. The results show that the FSCK and FSSK methods achieve good agreement in the test cases. The FSCK method using a five-point Gauss quadrature scheme is recommended for CFD calculations in oxyfuel conditions, however there are still potential inaccuracies in cases with very wide variations in the ratio between CO_2 and H_2O concentrations.

1. Introduction

Oxyfuel is a promising technology to abate CO_2 emissions from combustion facilities. The process replaces air with high purity oxygen as the oxidant for fuel combustion. The oxygen supply is often diluted with recycled flue gas to control the flame temperature. The resulting flue gas from the oxyfuel process is composed entirely of the products from combustion, with a very high CO_2 concentration that can be purified to a level suitable for storage. Oxyfuel combustion has been successfully demonstrated at small scales [1–3], and there are further projects in development aiming to demonstrate the technology at much larger scales, such as the White Rose,[1] FutureGen 2.0[2] and Youngdong projects.

There are several changes to the fundamental properties of combustion under oxyfuel, where the transparent and inert bulk gas N_2 is replaced with radiatively participating and potentially reactive CO_2 and H_2O. Furthermore, there are additional avenues of control available in the oxyfuel process, as the gas composition of the inlets is completely defined by the operator. Drying or cooling the flue gas recycle, or changing the oxygen enrichment level, could result in drastic changes to the combustion process.

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1 http://www.whiteroseccs.co.uk/
2 http://futuregenalliance.org/futuregen-2-0-project/

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0022-4073/

In the development of oxyfuel technology it would be extremely useful to be able to accurately predict the influence of these changes to optimise the process, however models developed for predicting air-fired combustion may not be suitable for oxyfuel, with the models used for radiative heat transfer being repeatedly identified as a key area of research for oxyfuel modelling [4–6].

Radiation is the most significant thermal transfer mechanism at combustion temperatures. Failure to accurately account for the effects of thermal radiation will significantly affect further modelling predictions such as heat flux, gas velocity and species concentration predictions. The process of radiative transfer is influenced by the medium, where participating species, such as CO_2 and H_2O, will emit and absorb radiative energy. Accurate consideration of gas-phase radiation is important even in atmospheres where highly emissive particles, such as soot, are present due to strong self-absorption [7].

Combustion modelling has often made use of the grey weighted sum of grey gases (WSGG) method to account for gas absorption/emission in radiative transfer. The grey WSGG model has been successfully applied to air-fired combustion, but is only valid for predetermined environments, and the traditional models are unable to predict key radiative quantities in an oxyfuel environment [8,9]. The FSK models offer an alternative approach to accurately calculate radiative heat transfer for arbitrary gas mixtures, and can be evaluated fast enough to be applied in complex computational fluid dynamics (CFD) calculations [9,10]. Previous modelling studies have shown a significant influence of using a FSK model in CFD calculations, highlighting the need to accurately account for radiation heat transfer [7,11,12]. In addition to the FSK models that are the focus of this study, other global methods, such as the absorption distribution function (ADF) [13] and spectral line-based weighted sum of grey gasses (SLW) [14], are also potentially viable for calculating radiative transfer in novel environments within CFD calculations. These additional global models have been shown to be related to the FSK models [15,16], and so the conclusions of this study may also be applicable to the ADF and SLW models.

This work focusses on the application and validation of FSK models to predict radiation heat transfer in oxyfuel environments within a commercial CFD code. The FSK models are validated against narrow-band predictions on a 3D enclosure that represents potential oxyfuel combustion environments. Calculations of the radiation energy source term and heat flux are compared between the benchmark narrow-band models, the standard grey WSGG model and the FSK models. A previous study identified FSK models as being accurate in potential air and oxyfuel cases [9]; this study updates the validation data and FSK parameters to recently developed spectral database values, and validates both the FSCK and FSSK models against two cases that test the underlying assumptions in the models for non-isothermal and non-homogeneous media. This study also identifies the optimal number of transfer equations that are required for the FSK models in the identified cases. The WSGG and FSK methods are implemented so that they are directly applicable to CFD calculations, allowing the conclusions from this study to be directly applicable to cases of practical interest.

2. Modelling radiative heat transfer

The directional radiative transfer equation (RTE) for an emitting, absorbing and non-scattering medium, assuming radiative equilibrium, is given as

$$\frac{dI_\eta}{d\hat{\mathbf{s}}} = \kappa_\eta\left(\underline{\phi}\right)\left(I_{b\eta} - I_\eta\right) \tag{1}$$

where η denotes wavenumber, I_η is the spectral radiative intensity, $\hat{\mathbf{s}}$ is a ray direction through the medium, $I_{b\eta}$ is the spectral blackbody intensity, κ_η is the spectral absorption coefficient of the medium and $\underline{\phi}$ is a vector of the local gas properties that affect the absorption coefficient, namely pressure, temperature and gas composition. This study focuses on methods that evaluate the radiative intensity of a participating gas-phase medium, where absorption and emission are significant and scattering effects are negligible, so the RTE formulation in Eq. (1) is adequate.

Radiation is coupled to the energy solution in CFD calculations through the radiation source term and the radiative heat flux. The radiation source term is the divergence of radiative heat flux through the medium, and can be calculated from the radiation intensity field as

$$\nabla \cdot \mathbf{q}_R = \int_0^\infty \kappa_\eta(\underline{\phi})\left(4\pi I_{b\eta} - \int_{4\pi} I_\eta \, d\Omega\right) d\eta \tag{2}$$

where $\nabla \cdot \mathbf{q}_R$ is the radiative source term, $\mathbf{q}_R$ is the radiative heat flux at a position in the domain and Ω denotes solid angle. The radiation source term is important in calculating the temperature field, which has a significant impact on fluid dynamics and chemical reaction rates. The radiative contribution to the total heat flux at a surface can be calculated as

$$\mathbf{q}_R \cdot \hat{\mathbf{n}} = \int_0^\infty \int_{4\pi} I_\eta \hat{\mathbf{s}} \cdot \hat{\mathbf{n}} \, d\Omega \, d\eta \tag{3}$$

where $\hat{\mathbf{n}}$ is the inward surface normal. Most of the surface heat flux in combustion systems is due to radiation, making the accurate treatment of this quantity important in evaluating the performance of the operating parameters for combustion.

Determining the quantities in Eqs. (2) and (3) across the whole spectral dimension is computationally expensive due to the variability of the absorption coefficient, which oscillates at very small spectral intervals – the exhaustive line-by-line (LBL) method typically requires over 10^6 RTE evaluations. The behaviour of the absorption coefficient for a potential oxyfuel environment is shown in Fig. 1. This study uses statistical narrow band (SNB) and correlated-k (CK) models to generate benchmark data to validate the global FSK models, which are also compared to the more standard grey WSGG model.

The SNB model is able to reach LBL accuracy in special cases within an acceptable time-frame, making it suitable for 3D calculations. The SNB model is often used to generate data for validating more time-efficient and widely-applicable models [17,9,10]. The CK model offers an alternative source of benchmark data to the SNB model, and the model provides a more amenable representation of absorption and emission, and is therefore applicable to more general RTE solvers. Global models, such as the