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Scale-adaptive simulation on the reactive turbulent flow in a partial combustion lance: Assessment of thermal insulators

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HIGHLIGHTS

- The SAS captures the turbulent eddies better than URANS models.
- The non-premixed flame with detailed chemistry yielded the best prediction.
- The discrete ordinates model gave the best prediction of radiative heat transfer.
- Installation of thermal insulation enhanced 20.4% of peak outlet temperature.

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ABSTRACT

This paper presents a scale-adaptive simulation (SAS) of a partial combustion lance (PCL) aiming to evaluate the influence of thermal insulation on the performance of syngas combustion. Standard k–ε (SKE) and Reynolds stress model (RSM) were used for comparison. The combustion reaction was modelled using eddy dissipation model (EDM), non-premixed and partially premixed flame models. Discrete ordinates (DO) and spherical harmonics (P-1) were used to calculate the radiative heat transfer. The finding suggests that SAS provides a better prediction for reactive turbulent flow. In the present work, simulation of syngas combustion using non-premixed flame with a DO approach showed the best agreement with experimental data by about 5.3%. Installation of an insulator increases the peak outlet temperature by about 20.4%.

1. Introduction

Fluid transport in a PCL is typically unstable and turbulent inducing intense mixing between syngas and oxygen, promoting fast chemical reaction, hence enhancing combustion performance. Thus, it is vital to have an accurate prediction of turbulent flows in a PCL. Ideally, experimental measurement is the best method to observe and understand the fluid flow phenomena inside the combustion system. However, a non-intrusive fluid flow measurement via particle image velocimetry (PIV) or laser Doppler anemometer (LDA) is impractical in PCL since the wall is made of opaque material. In addition, it is dangerous to perform measurements on a PCL at extreme temperatures (above 1000 K). Alternatively, computational fluid dynamics (CFD) can be employed to provide comprehensive information on the turbulent reactive flow, heat and mass transfer in PCL. Most of the previous works reported that accuracy and reliability of the CFD prediction depends on the choice of turbulence model, combustion model and modelling approach. Simulation of the partial combustion of syngas at extreme temperatures is challenging owing to the coupling between the flame chemistry, turbulence, species transport and heat transfer. Thus, a CFD model for PCL must be validated before it can be routinely used.

Reynolds-averaged Navier–Stokes (RANS) model and large eddy simulation (LES) were mostly used to predict turbulent flow in the combustion system. For instance, SKE was employed to model oxy-fuel combustion in fluidized bed [1], whereas renormalized k–ε (RNG) was employed by Khaleghi et al. [2] for the natural gas combustion. The more elaborate RANS model such as RSM was used by Krieger et al. [3] and Yan et al. [4] for oxy-syngas non-premixed combustion and natural gas combustion, respectively. Comparison between various URANS models for syngas combustion was studied by Law and Gimbun [5]. They reported that turbulence models can significantly affect the accuracy and

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reliability of the CFD simulation. Miltner et al. [6] show that no single turbulence model can be universally applied for all cases. The LES model often provides better predictions, but it requires excessive computational effort. For instance, di Mare et al. [7] took up to 36 months to solve a combustion model via LES. This is due to the high resolution grid required by LES to resolve the turbulence flow feature [8]. The URANS model suffers from isotropic eddy viscosity assumption, although it is easier and economical to run. While, LES simulation is relatively expensive at high Reynolds number whereby the grid requirement at the boundary layer does not differ to that of direct numerical simulation (DNS) [9], besides the fact that LES is sensitive to computational grid. The new model such as SAS was proposed to overcome these issues [10], since it is capable to provide a LES-like solution for the unsteady flow regions. Unlike the LES, SAS is not sensitive to computational grid [11]. To our best knowledge, SAS was employed on spray drying [12], centrifugal pump [13] and wake flow around a circular cylinder [14]. Nevertheless, there is no study available using SAS simulation on the reactive flow in a combustion process, and hence this is one of the aims of this work.

A number of models such as eddy dissipation concept (EDC) [15] and EDM [5] have been studied for syngas and natural gas combustion. Their findings are tinged with confusion with Guo et al. [15] concluding that EDC is unsuitable for methane combustion as it produces large prediction error. In contrast, Christo and Dally [16] found that EDC performs better than EDM. Meanwhile, it was reported that EDM is capable of giving reasonable predictions for fast combustion process [17], especially for gas-fired furnace [18]. In this work, EDM was employed since the reaction rate is faster compared to the mixing rate (Damkohler number > 1, i.e. ≈35.9). Adamczyk et al. [1] performed oxy-fuel combustion modelling using EDM. They concluded that EDM cannot provide accurate prediction due to simplification in the reaction mechanism. Similar findings are also reported by Almeida et al. [8], who found that the single-step reaction mechanism for methane combustion by EDM can be further improved by taking into account the intermediate species reaction (detailed chemistry). The chemistry involved in the partial combustion of syngas consists of a number of different reactions with numerous intermediate stages. Hence, a multi-step reaction model with intermediate species is needed. In addition, a literature review showed a lack of published works dealing with flamelet models in oxy-fuel combustion. Non-premixed and partially premixed flame approaches were used for comparison in this work, since both models are suitable for fast reaction.

Radiation dominates the heat transfer process in most combustion systems such as PCL. Previous studies concluded that radiation accounts for over 90% of heat transfer in a combustion system [19], whereas the rest is attributed to convection. Recently, DO with the weighted sum of gray gas model (WSGGM) was used to estimate the radiative heat transfer in oxy-fuel combustion [20] and natural gas combustion [4]. Both works indicated that radiation absorptive species like carbon monoxide, carbon dioxide and hydrogen affects the radiative heat transfer. Thus DO with WSGGM was used in this work. P-1 can provide reasonable predictions for higher-order CFD simulation with lesser computational demand [21], thus P-1 with WSGGM was tested for comparison.

Heat loss through the rigid wall may significantly affect the overall performance of the combustion process. According to Sanli et al. [22], eliminating the heat loss through insulation saves up to 15% of the fuel requirement. Glouannec et al. [23] shows that increasing the multi-layer insulator thickness reduced the energy consumption in a heat transfer system. However, no prior work on the effect of various types of insulators on temperature distribution in a PCL, and hence this is one of the aims of this work. The present work considers the effectiveness of several types of insulators, i.e., brick, cast iron, ceramic fibre and graphite felt. The mean flow in PCL was validated with PIV measured data by Lourenco and Shih [24]. The predicted flame temperature of the PCL was compared with the experimental measurement [25].

2. Geometry and grid

The PCL in this work is part of the Tenova HYL direct reduction process, which was installed between a gas heater and an oxide removal reactor. The syngas combustion temperature in the PCL was measured at 1293 K by a type-K thermocouple which was installed at 5.85 m from the inlet and 0.373 m from the centreline of PCL. The detailed dimensions of the PCL is shown in Fig. 1 [5]. The computational grid consists of tetrahedral and hexahedral meshes with sufficient refinement around the nozzle wake region (volume $\approx 5 \times 10^{-6}$ m^3) whereas the bulk region of the domain consisted of grid volume ranging from 1×10^{-5} to 1.5×10^{-4} m^3.

3. Combustion modelling

3.1. Eddy dissipation model

The EDM was used to account for turbulence and chemistry interaction in the PCL since the process involved fast reaction. Five simplified chemical kinetic mechanisms were introduced in this work to reduce the complexity of the simulation as shown in Table 1 [26]. Reactions 1–3 are the partial oxidation of methane, carbon monoxide and hydrogen, respectively, while reaction 4 is the complete oxidation of methane. Carbon dioxide decomposition is represented by reaction 5. All reactions are exothermic except for the carbon dioxide decomposition in reaction 5.

3.2. Flamelet approach

A multi-step chemical mechanism was used to develop the flamelet libraries to account for the flame strain and non-equilibrium chemistry effects. A modified GRI-MECH 1.2 reaction mechanism [27] which consisted of over 82 reactions and 20 species equipped with associated rate and thermodynamic data was used for the non-premixed and partially premixed models. Laminar flamelet approach was applied where the realistic chemical kinetic effect was incorporated into the turbulent flames. The non-premixed flame model is based on the solution of transport equations for the mixture fraction. The reaction source terms are not required in the governing transport equation since the atomic elements are conserved in the chemical reactions. Individual species concentrations are derived from the predicted mixture fraction fields. The partially premixed flame model is a combination of the non-premixed (mixture fraction model) and premixed (progress variable) approaches. Flame front position is defined by the progress variable (c). Mixture fraction model determines the reaction behind the flame front while unburnt mixture fraction is used ahead the flame front.

4. Radiation modelling

4.1. Discrete ordinates

In DO model, a finite number of discrete solid angles was solved. The solid angle at a certain point of the domain is splitted into a number of discrete directions and the radiative intensity is assumed constant within each division of solid angle. DO model takes into account the scattering and particulate effects. DO provides accurate prediction for an anisotropic heat transfer, although it can be CPU-intensive to solve [21].