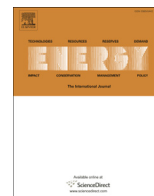




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The usability and limits of the steady flamelet approach in oxy-fuel combustions

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ABSTRACT

This paper investigates two furnaces which work under oxy-fuel condition with natural gas. One is a 0.8 MW furnace where detailed inflame measurements are available. The other furnace is an 11.5 kW lab-scale furnace with temperature measurements. The furnaces were investigated by CFD (Computational fluid dynamics) analysis. The main focus was on using combustion models that are not computationally demanding. Therefore the SFM (steady flamelet) approach was used with two detailed mechanisms. The advantage of the SFM is that the calculation time can be reduced from 4 weeks to 4 days on 8 CPU-cores. The applicability of two detailed mechanisms under oxy-fuel condition is pointed out in this paper. The investigation showed that the skeletal25 mechanism and the SFM are in very good accordance with measurements. If the strain rate between CH₄ and O₂ stream is too low, the SFM fails to predict the flame shape correctly. The influence of three different turbulence models was also investigated. Furthermore simulations with the eddy dissipation model and numerically expensive eddy dissipation concept model were conducted. Different WSGGM (weighted sum of grey gases model) were applied. The comparison of the WSGGMs showed that the difference between them is insignificant for small furnaces.

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1. Introduction

In times of rising fuel prices and global warming, oxy-fuel combustion can be seen as a vast opportunity to optimize the processes of many industrial applications. Oxy-fuel combustion is also a promising technology to reduce global CO₂ emissions. CO₂ is mainly produced by fossil fuels, which are accountable for 85% of global energy production [1]. CO₂ can also be emitted by chemical reaction in industrial processes i.e. cement clinker formation, 68% CO₂ is emitted from carbonates and only 32% by combustion [2]. Flue gas mainly consists of CO₂ and H₂O when using pure oxygen as an oxidant. This can be used to reduce CO₂ emission into the atmosphere by CCS (carbon capture and storage) technologies. Some technical and economic studies show that oxy-fuel and CCS could be an upcoming technology in the near future [3–5]. In industries with high temperature application, like glass, steel or cement industries, oxy-fuel or oxygen-enriched air combustion technologies are already used [6]. The absence of N₂ leads to a higher combustion temperature in comparison to conventional air-firing, and this also

enhances the energy efficiency, e.g., Oliveira et al. [7] showed that in metal reheating furnaces with a temperature level of 1200 °C the fuel consumption could be reduced by 46% if pure oxygen was used instead of air for the combustion. Experiments carried out by Bělohorský et al. [8] on a test facility with a natural gas burner showed a similar trend. With increasing oxygen concentration in the oxidizer the energy efficiency increased from 60% at 21% O₂ to 78% at 38% O₂. Numerical calculations and experiments carried out on a lab-scale furnace with a thermal load by Prieler et al. [9] also showed an increase of the efficiency from 44% at 25% O₂ to 67% at 100% O₂. In conventional power generating processes, the maximum temperature is limited through high stresses, i.e. for gas turbines 1600 K [10]. To control the flame temperature and to substitute missing N₂, the oxidant in power plants is a mixture of oxygen and recycled flue gas (wet or dry flue gas). Through recycling flue gas, the heat transfer in the convection zone of the boiler should be approximately the same as under air fired condition. The total heat transfer characteristic is considerably different compared to air combustion under oxy-fuel condition, with or without recycling of flue gas, the radiative heat transfer is strongly promoted by the much higher level of CO₂ and H₂O [11–13]. Despite the above mentioned reviews about CCS and the use of oxy-fuel in power plants, the main focus of this work was to investigate high

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temperature processes under oxy-fuel conditions. In high temperature processes, as in melting processes, NG (natural gas) is mainly used as fuel. Due to the higher concentration of H_2O therefore, flue gas is considerably different than in CCS and in power plants under oxy-fuel condition. The ratio of H_2O and CO_2 is 0.125 for CCS (i.e. dry flue gas recycling) and for oxy-fuel combustion of NG the ratio equals 2 and is therefore considerably different.

CFD (Computational fluid dynamics) are mainly used to investigate heat transfer, fluid flow and combustion behaviour. With the aid of computer power that has strongly increased in recent years, it is now possible to perform numerical calculation of industrial processes, which also provides a good opportunity to get a better understanding of combustion behaviour and heat transfer under oxy-fuel conditions. Commercial CFD codes have many models for transport and heat transfer problems in furnaces. The main goal is to find the right models to simulate combustion accurately. In combustion modelling, chemistry and radiative heat transfer were identified to have the greatest impact on the solution. The aim is to find radiation and combustion models that are in good accordance with measurements and are not computationally demanding. Global mechanisms have been successfully used in the past for simulations of air-fired furnaces. Very popular are the two global mechanisms by Westbrook and Dryer (WD) [14], which is a 2-step mechanism, and the mechanism postulated by Jones and Lindstedt (JL) [15] which contains 4-steps. In oxy-fuel combustion, the formation of radicals is mainly promoted by the high temperature. In the WD and JL mechanisms these radicals are only considered in the burning rates and not explicitly in the reactions. That means that for the radicals no conservation equations are solved explicitly. Yin et al. [16] performed chemical calculation with WD and JL mechanisms under oxy-fuel and air-fuel condition and compared it with a detailed mechanism. The results of this calculation showed that the adiabatic flame temperature for the WD and JL mechanism are in a good agreement with the detailed mechanism for air-fuel condition. In the case of oxy-fuel combustion, the adiabatic flame temperature was massively overestimated (300–500 K). It was concluded that neglected radical formation in the reactions was the reason for the overestimation of the adiabatic flame temperature. Frassoldati et al. [17] did a similar investigation and came to the same conclusion as Yin et al. They refined the JL mechanism to consider the radicals H, OH and O in the reactions. The temperature profile calculated with the refined mechanism fits well with the detailed mechanism. Glarborg and Bentzen [18] conducted further investigations on the influence of radicals under oxy-fuel condition. They studied the dissociation of CO_2 with the radicals H, OH, O as well as hydrocarbon radicals. The study showed that CO also occurred at higher temperatures due to the thermal dissociation of CO_2 . It can be concluded that the presence of radicals and high temperature in oxy-fuel combustion has a great influence on the correct prediction of CO concentration in the furnace but it must not be overlooked that most of the CO production occurs before CO_2 production (see equations (1) and (2)). Andersen et al. [19] performed simulation in a plug-flow reactor under oxy-fuel condition with the WD and JL mechanism. As a reference they also calculated the plug-flow reactor with the detailed mechanism proposed by Glarborg and Bentzen [18]. The global mechanisms were refined to improve the prediction of the species concentration in the plug-flow simulation and as well as in the CFD simulation of a propane oxy-fuel flame. The adapted mechanisms showed a good prediction of the CO concentration with a lower computational time compared to detail mechanism.

As mentioned before, radiation heat transfer is a very crucial part in modelling furnaces. The models for the radiative properties of gases, which are implemented in the most commercial CFD codes, are developed for air-fuel condition. In air-fuel condition the

concentration of radiative active gases like CO_2 and H_2O is low due to the high concentration of N_2 . This makes it possible to consider the flue gases as a grey gas without spectral dependence. It also has to be mentioned that this assumption can lead to a temperature under prediction of 100 up to 150 K even in air-fuel condition [20,21]. The concentration of CO_2 and H_2O are far higher under oxy-fuel condition due to the lack of N_2 which leads to a strong spectral dependence. Therefore, most models for radiative properties used in commercial CFD codes are out of their validation range. There are mainly three different types of models to describe the radiative properties of gases. These are the line-by-line method, band models and global methods. For CFD calculation, global methods are widely used due to the low computational effort. One of these global methods is the WSGGM (weighted sum of grey gases model) first proposed by Hottel and Sarofim [22]. In this model, the non-grey gas is assumed to be a mixture of a number of grey gases, weighted by factors. These factors are derived from more accurate models like the line-by-line methods or the banded models, which are computationally highly demanding. Becher et al. [12] compared different LBL (line-by-line) models (HITEMP2010 [23], HITEMP1995 [24], HITRAN2008 [25], HITRAN2004 [26]) and band models (EM2C [27], RADCAL [28], EWB [29]) with gas cell experiments. The comparison showed that the HITEMP2010 is the most accurate one with regard to concentration and temperature. The band models are less accurate but not so computationally demanding. In CFD codes, the WSGGM proposed by Smith et al. [30] is widely used. This WSGGM was derived for a $\text{H}_2\text{O}/\text{CO}_2$ ratio of 1 and 2, path lengths up to 10 m and for temperatures between 600 and 2400 K from a banded model (EWB). Yin et al. [31] investigated the WSGGM from Smith for different $\text{H}_2\text{O}/\text{CO}_2$ ratios, path lengths and temperature. The WSGGM showed high deviation for small $\text{H}_2\text{O}/\text{CO}_2$ ratios and large beam lengths. Similar investigations were done by Becher et al. [32]; they compared the WSGGM with the very accurate LBL model (HITEMP2010). The WSGGM showed a maximum deviation of 59% under oxy-fuel conditions. This is the reason why many new WSGGM have been published for oxy-fuel condition recently [13,31,33–37]. These new chemical approaches and the new radiation models were tested for different furnaces. Yin et al. [16] simulates a 0.8 MW furnace (which will be investigated in this study as well) and a 609 MW boiler with different combustion mechanisms and two WSGGMs. The simulation showed that the different WSGGMs make a negligible difference for small-scale furnaces because of the small beam length. For bigger furnaces, the WSGGMs showed a higher deviation from each other. Another work published by Galletti et al. [38] focused on oxy-fuel combustion. The authors investigated a 3 MW semi-industrial furnace equipped with a low NO_x burner. The aim of this study was to validate the different sub models (e.g. combustion/kinetics and radiation/spectral) under oxy-natural-gas fired conditions by comparing of prediction and measurements. Global combustion mechanisms were applied just like WD and JL as well as the refined mechanism proposed by Anderson et al. [19]. They used two WSGGM models with coefficients from Refs. [13,39] to calculate the radiative properties. Results showed a better agreement with the refined global mechanism and with WSGGM model optimized for oxy-fuel conditions.

It can be seen that lots of investigations have been done so far on oxy-fuel combustion and radiation under oxy-fuel condition. Most researchers used global mechanisms with a maximum of 6-steps to reduce the calculation time. However, most of these global mechanisms were derived for air-fuel combustion and were therefore insufficient for oxy-fuel combustion. New refined global mechanisms were derived for oxy-fuel combustion, but these mechanisms are not as good as detailed mechanisms. The aim of this paper is to use detailed chemical kinetic by using the SFM

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