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Application of the steady flamelet model on a lab-scale and an industrial furnace for different oxygen concentrations

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ABSTRACT

In the present study a numerical and experimental investigation was done on the impact of oxy-fuel combustion in a lab-scale furnace. For combustion and radiation modelling the steady flamelet approach with 17 species and 25 reactions associated with a WSGG (weighted sum of grey-gases) model was used. CFD (computational fluid dynamics) model was validated by measured temperatures and heat fluxes with different O_2 concentrations. It was found that simulated temperatures and heat fluxes were in close agreement with the measurements in the full range of oxygen enrichment. Although 17 species were considered the calculation time was significantly reduced by the steady flamelet approach compared to commonly used eddy dissipation concept models. Predicted and measured data revealed gas savings of 8.2% by an O_2 concentration of 25 vol% instead of 21 vol%. Maximum gas savings were determined for 100 vol% O_2 with a value of 16.7%. The CFD model was also applied to a simulation of an 18.2 MW walking hearth furnace under air-fired conditions which should be adapted for oxy-fuel combustion in the future. Results from CFD showed a heat flux of 9.15 MW compared to the required 9.33 MW according to the material data and production rate.

1. Introduction

The combustion of fossil fuels, currently the most important source of the anthropogenic greenhouse gas CO_2, is a key process in a number of different applications like power generation, transportation and several industrial sectors. Nowadays, proven by several studies, the reduction of CO_2 emissions is identified as main topic to reduce the global warming. The IPCC (Intergovernmental Panel on Climate Change) determined the total amount of CO_2 emissions from fossil fuels in the year 2000 to be 23.5 Gt/a, where about 60% were produced by large scale plants with emissions of more than 0.1 Mt/a [1]. CO_2 can also arise as a side product in several industries like cement and glass melting. Manickam et al. [2] quantified that about 68% of the CO_2 in cement clinker formation is formed by carbonates and that the rest emerges by combustion. The same trend was observed by Falcitelli et al. [3] in two glass melting furnaces where 30 to 36 vol% of the overall CO_2 emissions was emitted from the glass bath. Therefore, decreasing CO_2 emissions is inevitable for the main emitting industries to slow down the global warming. Oxy-fuel or oxygen enriched combustion represents a technological option for CCS (carbon capturing and storage) to avoid CO_2 emissions besides pre- and post-combustion. Actually, most investigations regarding oxy-fuel combustion have been related for application in power plants which use pulverized coal as fuel. Detailed reviews for oxy-coal combustion were already published by Chen et al. [4], Scheffknecht et al. [5] and Wall et al. [6].

Besides environmental issues, for high temperature processes like melting and annealing furnaces, with a huge demand on fossil fuels, the increase of the energetic efficiency is also crucial. Due to the absence of nitrogen in the oxidizer for oxy-fuel combustion a lower fuel input is needed to reach the same flame temperature as for the conventional air-fired case. Furthermore, high H_2O and CO_2 concentrations lead to improvements on the heat transfer in boilers and furnaces through enhanced radiation intensity which causes a more homogeneous temperature distribution and product quality (i.e. cement, glass, steel …). Moreover, the flow-rate of the flue gas and CO_2 emission can be decreased. On that account, oxy-fuel

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technology can be an upcoming technology to reduce greenhouse gas emissions and simultaneously reach higher efficiency levels. Oliveira et al. [7] carried out an analysis with simple energy balances about fuel saving in metal reheating furnaces using oxy-fuel combustion. It was calculated that at a temperature level of 1200 °C the fuel consumption could be reduced by 46% if pure oxygen is used instead of air (without pre-heating of the oxidizer). Oxygen enhanced combustion was also investigated by experiments on a test facility by Bělohradský et al. [8]. Increasing the oxygen content in the oxidizer up to 46 vol% leads to an improvement of the combustion efficiency of 22%. Beside the advantages of oxy-fuel combustion some technical efforts, like O_2 production or an additional process unit to obtain the desired O_2 concentration in the oxidizer, has to be conquered on the implementation in existing firing systems in industry. Commercial production technologies for O_2 are cryogenic air separation, vacuum swing adsorption etc. and are summarized in Baukal [9]. Nevertheless, many industrial processes use oxygen and therefore on-site oxygen production is available for example in steel industry. Further consideration has to be done on the furnace to prevent air leaking and overheating of the burners and refractory due to higher flame temperature in oxy-fuel combustion. An overview about the advantages and implementation of oxy-fuel combustion is given in Ref. [9].

Recent developments in computer power allow numerical investigations of a huge number of manufacturing processes with reasonable effort. Several studies about the modelling of combustion processes were carried out with different approaches like reactor network systems or CFD (computational fluid dynamics). Reactor network systems offer a simple method to analyse gas phase combustion in furnaces. Ponsich et al. [10] carried out a reactor network analysis of a glass melting furnace to predict the residence time distribution of the gas phase and the glass bath. A comparison with a CFD simulation showed similar results with the benefit of a lower computational demand. Important spatial information about the flow field, temperature distribution and species concentration are not calculated by such reactor network analysis. Falcitelli et al. [3] conducted a hybrid CFD/reactor network analysis of two different glass melting furnaces (5 and 10 MW fuel input) to predict the NOx emissions. First, a CFD simulation was done with a reduced reaction mechanism, involving the main species. Based on the CFD results a reactor network analysis was performed with detailed chemical kinetics for the combustion of natural-gas including a sub-model for nitrogen (about 3200 reactions and 240 species overall). NOx values at the furnace outlet showed a close agreement of measured and calculated data. In high temperature applications knowledge about the heat transfer is essential for the dimensioning and operating of the furnace. The CFD model is able to predict the heat transfer as well as detailed resolution of the flow field inside the combustion chamber especially when measurements of temperature and species concentrations are difficult. Habibi et al. [11] for example, investigated the heat flux and NOx concentrations in a steam cracking under air-fired conditions. Another study on flow, combustion and heat transfer was done by Guihua et al. [12] for an ethylene cracking furnace. The effect of the heat transfer on the cracking process was shown by coupling of the CFD model with the thermal cracking process. With regard on oxy-fuel combustion, several numerical studies were carried out on lab-scale and industrial furnaces for different applications. A rotary kiln for cement manufacturing was simulated by Manickam et al. [2] with oxygen enriched combustion of coal with special emphasis on the flame shape. Furu et al. [13] tested the impact of different oxygen enrichments on the heat transfer to aluminium samples in a pilot scale furnace by measurement and CFD. Improved heat transfer to the samples was determined using the oxy-fuel conditions in the furnace.

Nowadays, most commercial CFD codes offer a big selection of models to consider transport phenomena in furnaces. Depending on the application and combustion environment, the choice of appropriate models to describe the combustion is important for accurate predictions of transport problems. It was found that chemistry and radiation modelling are the crucial parts in CFD simulations of combustion processes. The majority of the models for radiation and chemistry calculation in CFD were developed and optimized for air-fired conditions. High flame temperature, H_2O and CO_2 concentrations in oxy-fuel combustion lead to different combustion phenomena due to dissociation effects and the radiative properties of the flue gas. The aim is to find suitable combustion and radiation models which are applicable in the full range of oxygen enrichment as well as air-firing systems.

Computational costs for detailed CFD analysis of the chemical kinetic in a combustion chamber are still high, especially when the furnace exceeds lab-scale sizes. On that account most researchers use reduced chemical reaction mechanisms to predict the combustion. Although detailed mechanisms like the GRI3.0 [14] involve more than 300 reactions and 50 species, global mechanisms with just a few reaction steps seem to be sufficient for air-natural-gas combustion. For example WD (Westbrook and Dryer) [15] and JL (Jones and Lindstedt) [16] proposed 2-step and 4-step mechanisms which were successfully used in the past for combustion with air. In such global mechanisms only the main species are included. Due to high flame temperature in oxy-fuel combustion the formation of radicals like H, O and OH has to be considered. This statement was demonstrated by simulations for an oxy-fuel and air-fuel counter-flow diffusion flame by Frassoldatti et al. [17]. A comparison with a detailed chemical kinetic showed that WD and JL mechanisms failed to predict the adiabatic flame temperature of the oxy-fuel case in a range of 0.4–2 for the equivalence ratio. The flame temperature was overestimated by the global mechanisms due to the neglected radicals. However, results with global and detailed mechanisms were similar for air-fired conditions. An adaptation of the JL mechanism, which involves radicals, leads to improved prediction of the adiabatic flame temperature. Yin et al. [18] calculated same the results for the adiabatic flame temperature in oxy-fuel and air-fuel combustion between equivalence ratios of 0.6 and 1.4. A CFD simulation with a refined JL mechanism calculated close results to measurements of temperature and species on a 0.8 MW IFRF furnace. Glarborg and Bentzen [19] also considered hydrocarbon radicals in their investigations. It was found that CO occurs at high temperatures due to dissociation of CO_2 because of the presence of radicals and thermal dissociation. Andersen et al. [20] performed calculations on an isothermal plug-flow reactor as well as a CFD simulation of a propane-oxygen flame with refined mechanisms. Results for both calculations determine the influence of radicals in oxygen enriched combustion. The impact of chemical kinetics on the calculation time was investigated by Tihay et al. [21]. Global and skeletal reaction mechanisms, up to 20 species and 49 reactions, were tested in the study. A skeletal mechanism proposed by Peters and Kee [22] showed the best results with reasonable computational demand, however it was stated that detailed skeletal mechanisms are still too time intensive for use in combustion modelling. Since the impact of radicals on oxy-fuel combustion was determined, Prieler et al. [23] tested three detailed reaction mechanisms with 17 and 53 species respectively. The steady flamelet approach was used, where chemistry calculations were done before the CFD simulations to keep the computational effort to a minimum. Results revealed that the skeletal25 mechanism [24] was able to predict the flame shape and achieved good accordance with temperature measurement. Based on the mentioned publications, it can be concluded that the presence of