Journal of the Energy Institute xxx (2017) 1–20

Contents lists available at ScienceDirect

Journal of the Energy Institute

journal homepage: http://www.journals.elsevier.com/journal-of-the-energy-institute

Sensitivity analysis of skeletal reaction mechanisms for use in CFD simulation of oxygen enhanced combustion systems

Q5 Rene Prieler [a,*], Bernhard Mayr [a], Daniela Viehböck [b], Martin Demuth [c], Christoph Hochenauer [a]

[a] Institute of Thermal Engineering, Graz University of Technology, Inffeldgasse 25/B, A-8010 Graz, Austria
[b] University of Applied Sciences Upper Austria, Stelzhamerstraße 23, A-4600 Wels, Austria
[c] Messer Austria GmbH – Kompetenzzentrum Metallurgie, Industriestraße 5, A-2352 Gumpoldskirchen, Austria

A R T I C L E I N F O

Article history:
Received 26 September 2016
Q1 Received in revised form
2 February 2017
Accepted 6 February 2017
Available online xxx

A B S T R A C T

Oxygen enhanced combustion (OEC) techniques are supposed to be a fuel saving alternative to conventional air-fired combustion, due to the reduction or removal of nitrogen from the combustion system, which causes a higher flame temperature and radiation intensity. Therefore, more heat is available in OEC for heating, melting and annealing processes, and subsequently, increases the process efficiency. The main aim of the present study is the numerical investigation of different reaction mechanisms under air-fuel and oxy-fuel conditions using 1D simulation of laminar counter-flow diffusion flames. The mechanisms are further used in 3D CFD simulation with the steady laminar flamelet model for the development of a time efficient numerical approach, applicable in air-fuel and OEC. Three skeletal reaction mechanisms were tested and compared to the GRI3.0 mechanism. The calculated temperatures and species concentrations revealed that a skeletal mechanism with 17 species and 25 reversible reactions predicts a faster fuel conversion into the reaction products under oxy-fuel conditions, which leads to higher temperatures in the flame compared to the GRI3.0. Sensitivity analysis showed that two reversible reactions are mainly responsible for the faster fuel conversion. Furthermore, the reaction mechanisms investigated, were used for 3D CFD simulation of a lab-scale furnace under different OEC conditions and air-fuel combustion. Up to concentrations of 30% O_2 in the O_2/N_2 mixture, all reaction mechanisms were able to predict the temperatures in the furnace with a close accordance to measured data. With higher oxygen enrichment levels, only the mentioned skeletal mechanism with 25 reactions calculated good results, whereas the GRI3.0 failed for oxy-fuel combustion.

1. Introduction

A high amount of energy is required for high temperature processes in several industries. To cover the energy demand, the combustion of fossil fuels (e.g. natural gas, oil and coal) is crucial for high temperature processes in the steel, cement or glass industries. Since the combustion of fossil fuels is the main source of the anthropogenic greenhouse gas CO_2, operation of combustion processes has to be optimized. Therefore, furnace operators in the industry are highly interested in increasing the overall efficiency of combustion processes, and, subsequently, reduce the fuel consumption to face the rising fuel prices and environmental issues. The combustion of fuels with pure oxygen or oxygen enriched air, which is called oxygen enhanced combustion (OEC), provides an opportunity to achieve these goals. In conventional air-fuel combustion, the nitrogen in the oxidant is ballast during the combustion, which absorbs a huge amount of the heat released by the chemical reaction in the flame. Since nitrogen is removed in oxy-fuel combustion, only the reaction products, mainly CO_2 and H_2O, are heated up in the gas phase, resulting in a higher flame temperature. In high temperature processing and power generation, the main heat transfer mode is radiation. The higher flame temperature in OEC leads to a higher radiation intensity and improved heat transfer. Furthermore, the radiative property of the flue gas is changed by the increased level of H_2O and CO_2. Since a higher radiative heat transfer is

* Corresponding author.
E-mail address: rene.prieler@tugraz.at (R. Prieler).

http://dx.doi.org/10.1016/j.joei.2017.02.004

achieved in OEC, more heat from the combustion process can be transferred to the load, which increases the process efficiency and production rate. Additionally, direct flame impingement on the load and refractory can be avoided by shorter oxy-fuel flames compared to air-fuel combustion, which enhances the product quality. In addition, the higher radiation intensity leads to a more homogeneous temperature distribution of the load [1]. The costs of oxygen production are a major drawback, and require further improvements in oxygen production technology to make the use of OEC more attractive in the future. More detailed information about OEC are summarized in Ref. [2].

Since low enrichment levels can already lead to significant differences to air-fuel combustion, some research has been done on oxygen enhanced flames between 21 and 30% O_2 in the O_2/N_2 mixture. Merlo et al. [3] did experiments on a 25 kW lab-scale burner, investigating flame stability, lift-off and NO_x emissions for different O_2 concentrations. The OH chemiluminescence revealed higher flame stability and lower lift-off with oxygen enhancement. Additional tests on a lab-scale furnace were done by Wu et al. [4] in two steps. First, experiments were done to investigate the time needed to heat up the furnace to 1200 °C with OEC and air-fuel combustion. A significant increase in the heating rate was determined between 700 and 1200 °C for 30% O_2 compared to air-fuel combustion. Below 700 °C, the difference on the heating rate was low. The second experiments revealed the fuel savings when a steady-state of the furnace is achieved at a fixed temperature level of 1220 °C. There, a 26.1% reduction of fuel consumed was detected, with 30% oxygen due to higher heat fluxes to the walls. Similar effects were found by Bělohradský et al. [5,6] in a 750 kW combustion chamber. Besides OEC with low oxygen enrichment levels, also investigations were done for the combustion of natural gas with pure oxygen (oxy-fuel). For example, Yin published a ForskEL report [7] where a 0.8 MW IFRF furnace was investigated under oxy-fuel conditions. Measured data were used to develop new WSGGM coefficients [8] for oxy-fuel conditions. Another work from Leicher and Giese was carried out for the combustion of natural gas with pure oxygen on a lab-scale furnace with special consideration for glass melting applications [9]. Since this work is dealing with OEC for high temperature applications, it is important to note the difference to oxy-fuel combustion for power generation. For such applications high flue gas temperatures from the oxy-fuel combustion have to be avoided, because of the material limits (e.g. gas turbine, heat exchanger). For this purpose, the flue gas recirculation is applied to control the temperature in the boiler. In the past some review papers on oxy-fuel combustion mainly dealing with power generation including flue gas recirculation were published by Chen et al. [10], Scheffknecht et al. [11], Wall et al. [12] and Yin and Yan [13].

Since test runs on large scale furnaces represent additional costs, experiments should be avoided. In recent years, computational methods have evolved for the prediction of combustion processes and heat transfer in furnaces. Thus, numerical analyses are used with increasing regularity for the investigation of combustion and radiation in high temperature applications. Computational methods are able to provide detailed insight into temperature distribution and species concentrations in furnaces, especially when measurement techniques are limited due to high temperatures and challenging accessibility. Computational fluid dynamics (CFD) is commonly used to investigate the transport phenomena in combustion, solving the governing transport equations. Local information about the scalars (temperature, species, etc.) can be predicted with a high spatial resolution for different furnaces in industrial applications. For example, Stallinger [14] used the experimental results from Ref. [9] for comparison with CFD simulations of an oxy-fuel glass melting furnace. The simulations showed that one flame was deflected in the furnace resulting in an inhomogeneous temperature distribution on the melting glass. In the aluminium industry, Furu et al. [15] carried out several experiments and CFD simulations on a small scale furnace to predict the heat transfer to aluminium samples. The heat transfer was determined for air-fuel and oxy-fuel conditions for further application in aluminium melting. Not only furnaces for different industrial applications have been tested, but also pilot scale furnaces with various fuels. Al-Abbas and Naser [16,17] published experiments and CFD results of a 100 kW furnace lignite and propane. The results of co-firing of biomass in a 0.5 MW furnace were published by Naser and Bhuiyan in Ref. [18]. Temperatures and species concentrations can also be calculated with high accuracy for large scale furnaces or boilers with CFD simulations (e.g. steam cracking [19], ethylene cracking [20] and a rotary kiln furnace for cement production [21]). Thus, the local prediction of relevant thermo-physical information in the furnace can be achieved by available commercial or free CFD codes without test runs. A more detailed overview of CFD modelling of OEC and oxy-fuel combustion can be found in Refs. [2,13].

1.1. Aim of this study

Computational fluid dynamics (CFD) represents a useful tool for predicting the fluid flow, gas phase reaction as well as radiative and convective heat transfer in furnaces. Besides solving the fluid flow within a furnace, the crucial elements for a numerical analysis of combustion are the chemistry within the main reaction zone and the heat transfer, mainly due to radiation. Several combustion (including reaction mechanisms) and radiation models are already available to predict temperature, species concentrations and the heat transfer in furnaces, but these have to be tested for their applicability in OEC (without flue gas recirculation).

The aim of the present paper is to analyse different skeletal reaction mechanisms for their applicability in CFD simulations with the steady laminar flamelet model (SFM). The SFM was chosen because of low calculation time for modelling combustion processes in contrast to the eddy dissipation concept (EDC) approach, which was already tested by Prieler et al. [22,23]. 1D simulations, using CHEMKIN, of counter-flow diffusion flamelets with different reaction mechanisms will be carried for air-fuel and oxy-fuel conditions. Differences on the temperature and species concentrations between the reaction mechanisms will be revealed for both operating conditions. Sensitivity analysis will show the effect of the elementary reactions of the mechanisms on temperature, as well as the production/destruction rates of the different species involved. The reaction mechanisms will be further used with the SFM for 3D CFD simulations of OEC in a lab-scale furnace. The simulations are carried out with the commercial software package ANSYS Fluent. Four OEC cases, as well as the air-fuel combustion will be simulated and the predicted temperatures will be compared to measured data from the experiments. The study will present the differences between the reaction mechanisms when oxygen enriched air is used for the combustion process in conjunction with the SFM. Furthermore, limitations of the reaction mechanisms with regard to the oxygen enrichment level will be highlighted.

2. Experimental setup

The investigated lab-scale furnace is shown in Figs. 1 and 2, where the positions of the burner, the thermocouples and dimensions of the main combustion chamber are displayed. Furthermore, the position of the coordinate system was arranged in the middle of the chamber