

CFD SIMULATION OF THE OXY-NG EXPERIMENTS IN A 3 MW FURNACE

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Abstract

The problem of greenhouse gases and pollutant emissions from combustion devices is moving the attention towards the development of new combustion technologies. In this context, oxy-fuel combustion, in which the fuel is fed with an oxygen-enriched gas mixture instead of air, represents a promising solution.

Two of the most important advantages are represented by the reduction of nitrogen oxide (NO_x) formation and the ability to capture CO_2 from power plants and, more generally, to control the corresponding emissions. The reduction of N_2 content during combustion makes easier the CO_2 capture for its successive storage.

In this work the numerical simulation of the semi-industrial FoSper furnace, fed with natural gas and a mixture of oxygen and recycled flue gases is presented and discussed. The combustion chemistry is described through a revised detailed kinetic mechanism and the Eddy Dissipation Concept (EDC) model is adopted for the description of chemistry-turbulence interactions. The role of the unavoidable air leakage and the drawbacks of global kinetic mechanisms are also discussed.

Introduction

Oxy-fuel combustion is considered an interesting technology for reducing greenhouse gases emission through CO_2 capture and storage (CCS) techniques [1]. In oxy-fuel combustion, a mixture of O_2 and recycled flue gases is used instead of air for the fuel oxidation, producing a nearly sequestration-ready CO_2 effluent. Flue gases are recycled in order to control the flame temperature and make up the volume of the missing N_2 to ensure a sufficiently large amount of gas flow rate in the furnace.

In recent years there has been a large increase of the use of simulation tools, such as those based on Computational Fluid Dynamic (CFD). These numerical codes appear especially relevant for combustion processes, for which scale-up procedures are generally complicated by the strong interaction between turbulence, reaction kinetics, heat release and radiation. However the application of CFD to novel combustion systems needs a validation of the sub-models (combustion models, kinetic schemes) as they have been generally developed for air.

CFD simulations at the industrial scales are computational demanding so that simplified models have to be generally adopted for the chemistry and radiative

properties treatment. Global oxidation mechanisms are likely to be used. However, the substitution of CO₂ to N₂ in oxy-fuel conditions changes the relevance of different elementary reactions thus modifying the global rates [2]. Andersen et al. [3] observed an unsatisfactory performance of the 2-step mechanisms of Westbrook and Dryer, WD [4], and the 4-step mechanism of Jones and Lindstedt, JL [5], when predicting CO in a plug flow reactor in oxy-conditions (28% O₂, 72% CO₂). Frassoldati et al. [6] investigated the performance of the JL scheme for oxy-fuel combustion without flue gas recycle (thus using pure O₂ as oxidizer) by performing calculations in laminar counter-flow diffusion flames. The authors concluded that the water vapour dissociation reactions should be included in the mechanism to address the high temperature conditions with pure O₂.

In the present work, CFD simulations of experiments conducted with a 3 MW low-NOx burner installed in the FoSper furnace, a replica (placed at the ENEL experimental facility of Livorno, Italy) of the IFRF furnace n.1, in oxy-fired conditions fed with natural gas, NG [7] are performed. Even though coal is the main fuel considered for oxy-fuel units, the gas-fired oxy-fuel conditions may help shedding light into some modelling aspects.

Importantly, when retrofitting a real furnace of such a scale from air to oxy-fuel conditions, air leakage unavoidably occurs. The implications for that will be discussed.

Experimental tests

The FoSper furnace has an internal square cross-section (2 m x 2 m), is approximately 6.25 m long and is made of 11 independently water-cooled refractory-lined sections (Figure 1a). Seven cooling loops are used to extract energy from the combustion chamber and maintain a temperature history comparable to a radiant section of a full-scale boiler operating with air. The standard suction pyrometer is used to measure temperature and concentration of CO, CO₂, NO, O₂ inside the furnace.

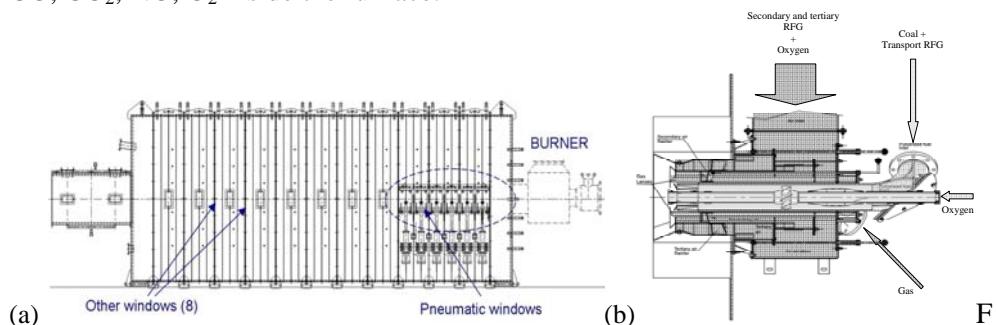


Figure 1. (a) Fo.Sper furnace and (b) TEA-C burner

The TEA-C (Figure 1b) is a Low NOx burner developed by Enel and Ansaldo used in industrial utility boilers; to allow the testing on the FoSper furnace, a scaled-down prototype of 3MW thermal power was used. The oxidizer goes into the

burner through two separate ducts (secondary and tertiary) both having an axial movable swirler and a damper that controls the flow rate distribution. The primary duct, positioned on burner axis, is aimed at providing the oxidizer/coal mixture with pulverized coal experiments (not considered here); however the primary oxidizer flow is maintained active even with NG configurations. For the NG firing operation, 8 lances inject the fuel through nozzles having two holes with an axis which forms a 45 degrees angle with the burner axis.

The experimental campaigns considered in the present paper regard NG combustion oxy-fired conditions with a flue gas recycle ratio $R = 0.69$. Operating conditions are reported in details in [7]

Numerical model

The numerical model was developed with the fluid dynamics package Fluent by Ansys Inc. Due to the burner/furnace symmetries, just one quarter of the furnace was modeled. Fluid domains were used for the burner and the furnace, whereas the cooling loops were modeled as solid domains, to facilitate the setting of heat extraction BCs from the cooling loops. Much effort was devoted to the optimization of the grid. A complete domain, in which the burner was represented in all details, was used to perform preliminary runs in non-reactive conditions. Obtained profiles of velocity and turbulence characteristics were then used to set proper BCs at the secondary and tertiary duct inlets of a reduced domain, generated by representing just a portion of the secondary and tertiary ducts.

The grid was hybrid, as many tetrahedrons were needed for the burner, whereas a structured grid was adopted in the furnace. 4.5M elements were required for the complete domain (Figure 2a), whereas 3.4 M for the reduced one (Figure 2b), providing a 30% reduction of computational cost.

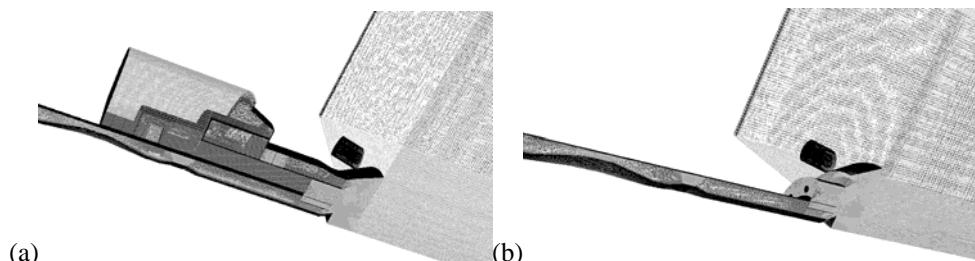


Figure 2. Grids for the (a) complete and (b) reduced domain.

Physical model

Favre-averaged Navier-Stokes equations were resolved with a stationary solver. The turbulence model used for the reactive runs shown here is the shear stress transport (SST) $k-\omega$ model. The Eddy Dissipation Concept (EDC) by Magnussen was used for the turbulence-chemistry interaction, as it allows considering

reversible reactions which may play an important role under oxy-fuel conditions due to CO₂ decomposition at high temperatures.

Two different kinetic schemes were employed:

1) the global kinetic mechanism of Westbrook and Dryer [4] consisting of fuel oxidation to CO and subsequently reversible oxidation of CO to CO₂ is employed and will be denoted as WD;

2) a revised version of the Kee 58 mechanism [8] (discussed in the next section).

The P1 radiation model was employed although some simulations were performed also with the Discrete Ordinates model. The gas phase spectral properties were evaluated through a revised version of WSGG proposed by Johansson et al. [9] for oxy-fuel conditions, which was added to the code through a C++ subroutine. In particular it was chosen the 1-clear/4-gray gas model optimized for H₂O to CO₂ partial pressure ratio of 0.125, which better approximates the dry flue gas recirculation of the present oxy-NG campaigns.

The second order discretization scheme was applied. To help solution convergence, such a scheme was initialized on results obtained with a first order scheme.

Typically, the run with WD needed about 30 days using 24 processors, whereas the one with the revised KEE needed about 4 months with 72 processors.

Boundary conditions

Some boundary conditions (BCs) have to be properly set as not directly available from the experimental campaign. This is the case of air leakage, which unavoidably occurs when retrofitting existing air-fired furnaces to oxy-fired conditions. The amount of air leakage is reconstructed by performing a mass balance on the system based on the flue gas composition; however uncertainties still exist on the location of the air leakage. In the present work the air leakage was evaluated to be 194 kg/hr by performing mass balances and trying to minimize the errors on both CO₂ and O₂ measurements. For the BCs at the walls, it was set a wall temperature profile (and emissivity) from measurements.

Counterflow diffusion flame analysis

Calculations of counter-flow diffusion flames with concentration and temperature characteristics of the oxy-NG run were performed using OpenSMOKE [10], a simulation code specifically conceived to manage large, detailed kinetic schemes (with hundreds of species and thousands of reactions) in numerical simulations of reacting flows. The fuel was injected with a temperature of 287 K and a composition of CH₄=0.934, CO₂=0.011, N₂=0.055 (by vol.). The oxidizer was fed with a temperature of 430 K and a composition of O₂=0.307, CO₂=0.447 and N₂=0.246. The high N₂ content simulates the air-leakage in the furnace, which was evaluated through mass balances. The inlet velocity of the fuel was set equal to 100 cm/s, whereas that of the oxidizer was evaluated through momentum balance.

Figure 3 shows the temperature and CO predicted with the San Diego mechanism [11] and the WD scheme. It can be observed that the global mechanism over-

predicts the temperature by of about 400K and under-predicts CO concentration by of about 33%. The original KEE58 mechanism, which consists of 17 species and 58 reversible reactions [8] was found to provide results which agree well with those from the San Diego scheme.

A sensitivity analysis was carried out and indicated a minor effect of CH, H₂O₂, H₂ and CH₂ on the temperature and species predictions. Thus such species (and related reactions) were removed from the original scheme, leading to a modified version of the scheme with 13 species (CH₄, O₂, CO₂, H₂O, CO, H, O, H, HO₂, CH₃, HCO, CH₂O, N₂) and 24 reversible reactions.

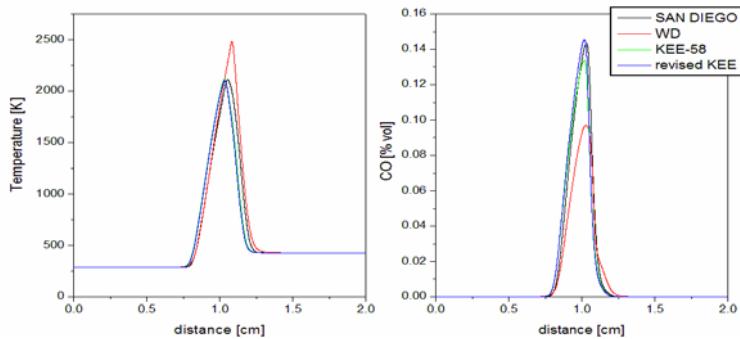


Figure 3. Counterflow flame: predicted Temperature (a) and CO (b).

Results

Figure 4 shows the temperature distribution in the furnace symmetry plans. It is possible to observe the larger temperature peak (~2570 K) of the simulation performed using the WD global scheme, while the detailed mechanism gives a maximum temperature of ~2350 K.

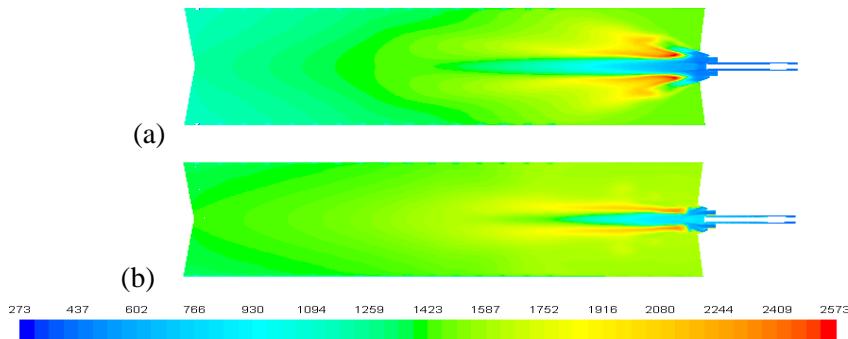


Figure 4. Predicted temperature field (in K) for (a) WD and (b) revised KEE schemes.

Figure 5 shows a comparison between model predictions and measurements. As expected from the analysis of Figure 3, the comparison with the measured temperature profiles confirms the tendency of global models to largely overestimate the flame temperature in oxy-fuel conditions.

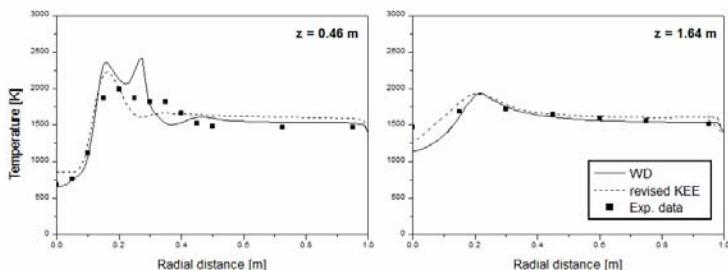


Figure 5. Predicted and measured radial temperature profiles at two axial distances from the burner.

Conclusions

This work discusses the results of numerical simulations of a semi-industrial furnace fed with natural gas and a mixture of oxygen and recycled flue gases. The simulations were carried out using the EDC model coupled with both global and detailed kinetic mechanisms. The results showed the need to account for intermediate combustion products in order to obtain realistic and reliable predictions. The simulations indicated that boundary conditions have to be carefully defined and that the effect of the air leakage is relevant and cannot be disregarded. The agreement with measurements was satisfactory, even if some observed discrepancies highlight the need of further investigations.

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