CFD simulation of a turbulent oxy-fuel flame

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Abstract

The problem of 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 (NOₓ) formation and the ability to capture CO₂ from power plants and, more generally, to control the corresponding emissions. The reduction of N₂ content during combustion makes easier the CO₂ capture for its successive storage. Additional advantages can be clearly identified in terms of higher temperature, higher flame speed and stability.

In this work numerical simulations of a semi-industrial furnace, fed with natural gas and pure oxygen, both containing N₂ in traces, are presented and discussed. The combustion chemistry is described through a detailed mechanism and the Eddy Dissipation Concept (EDC) model is adopted for the description of chemistry-turbulence interactions. The attention is devoted to the estimation of NOₓ formation in the furnace by the application of a newly conceived kinetic post-processor, able to manage very large kinetic schemes.

Key words: oxy-fuel combustion, nitrogen oxides, turbulent flames

1. Introduction

Turbulent non premixed flames are largely used in many practical combustion devices to convert chemical energy into work, because of their high efficiency, large heat releases and for safety reasons. However diffusion flames produce more pollutant species (in particular NOₓ and soot) than premixed flames. Since combustion devices need to respect always more stringent limitations concerning the emissions of pollutants, a number of new combustion technologies are being investigated. The most important are the flameless combustion (or MILD combustion) and the oxy-fuel combustion. Both these two technologies are energy efficient and strongly reduce the formation of NOₓ. However, the flameless combustion do not address the problem of CO₂ reduction. On the contrary, one of the most important advantages of oxy-fuel combustion, in which the fuel is fed in a nitrogen-free environment, is its ability to make the capture CO₂ from power plants easier. Moreover, the global efficiency is greatly enhanced, because no unnecessary N₂ has to be heated. Additional advantages can be clearly identified in terms of higher temperature, faster flame propagation speed and better flame stability. Of course oxy-fuel combustion finds several applications where high temperatures are required, like in the iron and steel industry. In the glass industry, the conversion of natural-gas-fired furnaces from air to oxygen has reduced fuel consumption by 15% to 50% and simultaneously decreased NOₓ emissions by 50% to 90% [1].

The numerical modeling of oxy-fuel turbulent flames is a very challenging task. There are several crucial physical processes that need to be accurately addressed for reliable numerical...
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simulations: chemical dissociations, turbulence-chemistry interactions, radiative heat transfer, soot formation and oxidation, turbulence-radiation interactions, etc. Because of the complexity of these phenomena, only in the last ten years numerical simulations of oxy-fuel flames were published. In most cases, the oxy-flames were modeled using ad hoc physical models (with a large number of tuning parameters) and simplified sub-models (both from a physical and chemical point of view), often resulting in questionable predictions. Brink et al. [2] and Breussin et al. [3] numerically modeled the same oxy-natural gas flames of 0.78 MW thermal input studied in the present work using two different turbulent combustion models: an eddy break-up model accompanied with a global chemistry and an Eddy Dissipation Concept (EDC) model coupled with a thermodynamic equilibrium procedure, specifically conceived for oxy-natural gas combustion. NOx formation was estimated through a post-processing technique. Good predictions were obtained with both models, especially for temperature and main chemical species (CO₂ and H₂O). The equilibrium model resulted superior to the mixed-burned model, especially for CO predictions, because of the importance of molecular dissociation. The predicted concentrations of H₂ and CO in the flame were generally higher than the measured ones and in some cases appeared unrealistic. The importance of taking into account intermediate combustion products was clearly showed. In particular, the inclusion of the O, OH and H radicals resulted necessary for realistic and reliable predictions. The limited capabilities of the existing combustion models were evidenced, showing that usually they cannot be reliably applied to the furnace/burner design process.

In this work CFD simulations of a semi-industrial furnace fed with natural gas and oxygen are discussed. The combustion chemistry is described through a detailed scheme and the attention is focused to the prediction of NOx emissions using kinetic post-processing techniques.

2. Furnace Geometry and Numerical modeling

The turbulent oxy-flames simulated in this work were experimentally investigated in the OXYFLAM Project [4]. During the experimental campaign two different furnaces were used: OXYFLAM1 furnace had walls cooled with water, while OXYFLAM2 furnace was built with refractory walls (see Fig. 1). In both cases the fuel was natural gas, but the composition was slightly different in the two campaigns. The furnace adopted in OXYFLAM1 series had a square section (1200x1200 mm) and a length of 3900 mm, while the OXYFLAM2 furnace a section of 1050x1050 mm and a length of 3740 mm. Both furnaces were equipped with a circular chimney (I.D.=500 mm) and the pressure was maintained ~3 mm H₂O above the atmospheric value to avoid entrainment of external air. Fuel and oxygen streams were injected through a coaxial burner. For each OXYFLAM series 4 different burner diameters were used (called Burner A, B, C and 2), in order to test different jet momenta. The power of OXYFLAM1 and OXYFLAM2 flames of ~1 MW and ~0.78 MW, respectively. For each OXYFLAM2 flames, velocity, main species and temperature profiles inside the furnace were measured at several axial locations. On the contrary, only for OXYFLAM2 B flame measurements inside the furnace were performed. For all the eight flames, composition and temperature of exhaust gases were measured. The numerical simulations were carried out only for the flames for which experimental data in the furnace are available (OXYFLAM1 A, B, C and OXYFLAM2 B). These flames were simulated with the commercial CFD code ANSYS-FLUENT® 6.3.2 [5]. Although the two furnaces have a square section, they were modeled with a circular section (with the same section), in order to exploit the axial symmetry of the computational domain. Structured, non-uniform grids were taken into account, with high resolution in the flame region close to the inlets. The domain was resolved with ~50000
control volumes in a cylindrical coordinate system. For the spatial resolution the Second-Order Upwind Scheme was adopted. The segregated implicit solver was used with the SIMPLE procedure for pressure-velocity coupling. PRESTO! (PREssure Staggering Options) algorithm was used for pressure interpolation. Turbulence was modeled via the RANS approach, using the standard $\kappa$-$\varepsilon$ model with $C_1\varepsilon$ constant modification to better model round jets. The radiative heat transfer was calculated with the DO model \[5\]. For OXYFLAM1 simulations the wall temperature was fixed to 700 K, as suggested by the experimental measurements \[4\]. For OXYFLAM2 B flame a polynomial temperature profile was assigned to the walls, according to the experimental measurements \[4\].

The application of Eddy Dissipation (ED) and Eddy Dissipation Finite Rate (ED-FR) models in oxy-fuel combustion is questionable, since only global schemes can be adopted. Since multi-step or detailed kinetics are needed to obtain accurate predictions, the attention was focused on the EDC model \[6\].

![Fig. 1 OXYFLAM2 furnace and temperature field as predicted by CFD simulations.](image)

3. CFD Simulations and Results

The numerical activities were carried out in two steps. Initially the attention was focused on OXYFLAM2 B flame, which was assumed as a “reference” flame. Most appropriate sub-models (chemistry, radiation, turbulence, etc.) were selected only on this flame, together with tuning of semi-empirical parameters and extensive sensitivity analyses. In this way a “standard” set of sub-models was chosen and applied without changes to the other three flames (second step). Therefore, simulations for OXYFLAM1 A, B and C were obtained without specific tuning of parameters and sub-models. In the following only the details and main results about the simulation activities performed on OXYFLAM2 B are summarized.

3.1. Fuel composition

Most of N$_2$ enters in the furnace through the fuel stream, whose composition (%vol.) is the following: 86% CH$_4$, 5.40% C$_2$H$_6$, 1.87% C$_3$H$_8$, 0.58% C$_4$H$_{10}$, 0.14% C$_5$H$_{12}$, 1.79% CO$_2$, 4.01% N$_2$, 0.21% O$_2$. On the contrary, oxygen stream has only ~100 ppm of N$_2$. In order to avoid the need of very large kinetic schemes (in the context of CFD simulation), C$_3$H$_8$, C$_4$H$_{10}$ and C$_5$H$_{12}$ fractions were transformed in an equivalent amount (in terms of mass flow rate) of C$_2$H$_6$. 
3.2. **Grid sensitivity**
In order to check the sensitivity to the grid resolution, additional simulations were carried out on finer grids with ~100000 and ~400000 cells. The differences were negligible and supported the use of the the coarser grid (~50000 cells) in all the simulations.

3.3. **Kinetic mechanism**
Most of the turbulence-chemistry models that are commonly used for describing combustion in air cannot be extended to oxy-fuel combustion. In particular, global kinetic models usually produce temperature fields much hotter than reality and may lead to unexpected results. At the high temperatures in oxy-fuel combustion, the chemical processes are extremely fast and sufficiently high for the thermal decomposition into radical species such as O, OH and H. At temperatures higher than 2500 K, not only CO-CO$_2$ equilibrium is in favor of CO and H$_2$-H$_2$O equilibrium foresees a significant amount of H$_2$, but also the radical pool has a significant impact in limiting the heat release. Simplified mechanisms do not always account for the dissociation reactions and do not include radicals. The application of detailed chemistry and consequently the adoption of a turbulence-chemistry models able to manage finite rate chemistry appears necessary for the accurate and reliable modeling of oxy-fuel combustion. This result was confirmed by the numerical simulations of OXYFLAM flames. When global mechanisms (Westbrook-Dryer [7] or Dryer-Glassmann [8] mechanisms) were adopted, unrealistic temperatures were obtained. As a consequence, the flames were simulated using semi-detailed kinetic mechanisms for methane combustion: the DRM22 (22 species and 104 reactions) [9] and the Glarborg (33 species and 152 reactions) [10] schemes.

3.4. **Main results**
In Fig. 2 the calculated radial profiles of temperature, O$_2$ and CO$_2$ concentration are compared with experimental measurements at several distances from fuel nozzle. The numerical results refer to the EDC model with Glarborg kinetic scheme. The agreement is quite satisfactory, especially at larger distances from inlet. Similar results were obtained also for OXYFLAM1 series. The results obtained with the DRM22 scheme were very similar (especially in terms of temperature and main species), but some differences were observed for radical species.

4. **NOx formation modeling**
Pollutant species like NOx only marginally affect the main combustion process and consequently do not significantly influence the overall temperature and flow fields. As a consequence, it is feasible to evaluate the structure of the flame without accounting for the formation of NOx and then post-process the CFD results. This is the approach which was used in the present work to estimate NOx emissions. In particular, the results coming from the post-processing tools available in FLUENT were compared with the calculations performed with the Kinetic Post-Processor (KPP), a numerical tool able to predict pollutant emissions through the coupling between detailed kinetics and fluid dynamics [11].
To predict NOx emissions, FLUENT post-processor solves the mass transport equation for the NO species, taking into account convection, diffusion, and the rates of production and consumption of NO and related species through thermal, prompt and fuel-NOx mechanisms. Radical species which are not available in the CFD simulation are estimated using the quasi-steady assumption. The effects of temperature fluctuations are taken into account through a $\beta$-PDF, while fluctuations of species are neglected. Additional details are reported in [5].
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Fig. 2 Radial profiles of temperature, O\textsubscript{2} and CO\textsubscript{2} concentrations at axial locations reported in Fig. 1: comparison between predictions and measurements [4].

The main advantage of this approach is the computational cost, which is very low, since only a small number of transport equations (NO and related species) have to be solved. However, inaccuracies can arise since the species transported in the CFD simulation are frozen in the post-processing phase. This is particularly important when N\textsubscript{2} is present in traces because it can be largely transformed into NO\textsubscript{x}. The KPP uses the results from CFD calculations to build a network of reactors, with fixed temperature. A detailed kinetic scheme (thousands of reactions) is adopted to solve the reactor network, using the composition fields extracted from the CFD simulation as a first guess solution. Also in this case the effects of turbulent fluctuations are accounted for through a \( \beta \)-PDF. Additional details on the KPP and the kinetic mechanism adopted in the KPP simulations can be found in [11] and [12]. In principle this approach should be more accurate than the procedure adopted by FLUENT, since all the species are transported and no tuning parameters are required. The disadvantage is the computational cost associated to the reactor network solution with detailed kinetics. Numerical predictions of NO\textsubscript{x} concentration are compared with the experimental data in Fig. 3. The agreement can be considered satisfactory, considering the uncertainties on the boundary conditions and the experimental measurements and the modeling simplification adopted. In particular, FLUENT post-processor tends to overestimate the formation of NO\textsubscript{x}. This result was expected, since N\textsubscript{2} consumption is not taken into account in this post-processing procedure. On the contrary, KPP predictions seem to always underestimate NO\textsubscript{x} production, especially at larger distances from the fuel nozzle. Even if the predictions of temperature and main species obtained with DRM22 and Glarborg mechanisms are very
similar, some differences can be observed for NOx predictions. This result depends on the different predictions of radical species, like H, O and OH, which strongly affect NOx formation. This means that the quality of FLUENT post-processor results strongly depends on the detail of the kinetic mechanism adopted in the CFD simulations, which must be able to correctly predict not only the temperature, but also the formation of minor species. KPP approach is less affected by this issue, because it applies a very detailed kinetic scheme directly in the post-processing phase (impossible to apply in complex CFD simulations) and the only requirement is a correct evaluation of the temperature field.

![Fig. 3 Predicted and measured NOx radial profiles at different axial locations.](image)

**5. Conclusions**

This work discussed the results of numerical simulations of a semi-industrial furnace fed with natural gas and pure oxygen. The simulations were carried out using the EDC model coupled with semi-detailed kinetic mechanisms. The results showed the need to account for intermediate combustion products in order to obtain realistic and reliable predictions. NOx emissions were estimated using two different post-processing techniques, whose strengths and weakness were evidenced. In both cases the agreement with experimental measurements was satisfactory, even if some observed discrepancies highlight the need of further investigations.

**6. Acknowledgements**

The authors would like to acknowledge the financial support of Regione Friuli Venezia Giulia.

**7. References**