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A Study of an oxy-coal combustion with wet recycle using CFD modelling

Diego Perrone[a,*]

[a]Department of Mechanical, Energy and Management Engineering University of Calabria, 87036 Rende, Italy

Abstract

Coal use presents challenges for reducing emissions of air pollutants and carbon dioxide (CO_2). In response to these challenges the research is focused on technologies that significantly reduce emissions of SO_2, NO_x, particulate matter (PM), and mercury (Hg), in order to develop toward "near zero emission" power plants. CO_2 emissions are gaining significant attention. Greater reduction of CO_2 emissions can be achieved by CO_2 capture and geological sequestration (CCS). One of the most important technologies for CCS is the oxy-combustion, which, due to its almost N_2-free flue gases, reduces the CO_2 capture cost. The main aim of this work is to study, using the CFD commercial code FLUENT, the performances of pulverized coal combustion with exhaust gas recirculation, to evaluate the gas temperature and NO_x emissions. Three dimensional steady-state simulations of a quarter of the IFRF no.1 furnace have been performed, for high-volatile bituminous coal. The Eddy Dissipation Model and Discrete Ordinates model have been used for turbulence-chemistry interaction and radiation respectively. The turbulence has been modeled using the standard k-ε model, with standard wall functions. A Lagrangian description has been used for the solid phase and empirical sub-models have been implemented for devolatilization and char burnout. Different combustion cases have been considered in several oxy-coal combustion environments, with different CO_2/H_2O concentrations in the gas recirculation. The effect of dry and wet recycle conditions on combustion characteristics has been considered. The results show the benefits in term of NO_x emission in oxy-coal combustion. The temperature and emission profiles are influenced by the mixture of gas recycled, in fact the gas temperature and Thermal-NO_x decrease when N_2 is replaced by CO_2. The simulations were performed with the same mass flow rate of oxygen at inlet in order to evaluate also the effect of CO_2 and H_2O.

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Keywords: Oxy-coal Combustion - Wet Recycle - NO_x Emissions – Computational Fluid Dynamics.

* Corresponding author. Tel.: 3206868006; fax: +039 0984 494673.
E-mail address: diego.perrone@unical.it.

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1. Introduction

Coal has played and continues to play a significant role in our day-to-day lives. According to International Energy Agency (IEA) coal provides 30.1% of global primary energy needs and generates over 40% of the world's electricity. It is also used in the production of over 70% of the world's steel. In fact coal, being the most abundant, available, and affordable fuel, has the potential to become the most reliable and easily accessible energy source, thus able to make a crucial contribution to world energy security [1].

The negative impacts on environment of Coal are due to the release of pollutants such as oxides of sulphur and nitrogen (SO_x and NO_x), particulate matter (PM), carbon monoxide (CO) and trace metals (Hg). Thus, it is very important to develop control technologies to reduce these pollutant emissions. Potential reductions in greenhouse gas (GHG) emissions, particularly CO_2, are gaining considerable attention. Carbon capture and geological sequestration (CCS) is the key enabling technology for the reduction of CO_2 emissions from coal based power generation. In this context, the oxy-coal combustion technology is almost ready to provide solution to the CO_2 capture.

In this technology, pure oxygen produced by ASU is used for fuel combustion, thereby producing a CO_2 enriched flue gas ready for sequestration once water is condensed from the flue gas. The ASU consumes a significant fraction of the oxy fired PC plant's output and reduce its efficiency. The challenge is the development of a low energy intensity oxygen production process.

This paper is focused on the pulverized oxy-coal combustion with recycle of a H_2O-CO_2 mixture, in order to analyze the effect of these combustion products on NO_x respect to the recycle without vapor water.

From point of view of combustion process, the flame temperature and stability are strongly affected by this technology as showed by several experimental investigations with oxy-firing pulverized coal burners [2-6].

One of the advantages of this technology is the capability to prevent the formation of NO_x due to the absence of nitrogen. Several researchers showed that a reduction in NO_x emissions can be achieved in oxy-fuel combustion. Okazaki and Ando [7] studied the separate effects of CO_2 concentrations, reduction of Recycled NO_x, and interaction between fuel-N and recycled NO_x on the reduction of the final overall NO_x exhausted from coal-combustion systems with recycled CO_2. They reported that the amount of NO_x exhausted from the O_2/CO_2 combustion system was reduced to less than one third of that with combustion in air, because the conversion of fuel-N to NO_x decreased and the recycled NO_x reduced in the flame zone. Ikeda et al. [8] carried out experimental investigations on NO_x emissions from oxy-coal pilot plant of Institute of Heat and Mass Transfer (WSA) at RWTH Aachen University, Germany. They showed that NO_x emissions in O_2/CO_2 mode are about 20% lower than in air mode. This causes high temperatures in the burner vicinity to form large amounts of thermal NO_x in air mode. On the other hand, NO_x emissions in O_2/RFG mode are strongly reduced, by approximately 50%. This is due to the NO_x contained in RFG, which is supplied back by secondary stream to the flame and thus destructed by reduction gas in volatile matter.

In this work, a pulverized coal swirl burner has been used in order to study the combustion in CO_2/O_2 atmosphere in term of gas temperature profile, and NO_x profile. The addition of steam has also been evaluated in order to study the effect of the wet recirculation of flue gas.

Acronyms

ASU	Air Separation Unit

CCS	Carbon Capture Sequestration
CFD	Computational Fluid Dynamics
DO	Discrete Ordinates
EDM	Eddy Dissipation Model
GHG	Green House Gas
IEA	International Energy Agency
IFRF	International Flame Research Foundation
RFG	Recycled Flue Gas
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations

2. Mathematical model and methodology

Numerical simulation of pulverized oxy-coal combustion under air-fired and the O_2/CO_2 combustion has been carried out by a commercial computational fluid dynamics code (CFD), ANSYS® FLUENT, rel. 14.5. The CFD code has been used to model and simulate a 3-D computational domain of IFRF furnace no.1, in order to predict turbulent flow, coal particle motion, burnout of coal, temperature of gas and the NO_x emissions. The Numerical approach used for gas-solid flow is the Eulerian/Lagrangian.

The gas phase has been described by steady state partial differential equations (PDE's) for mass, momentum, enthalpy and species in order to predict flow, temperature and concentration of species. The algorithm used is the SIMPLE (Semi-Implicit Method for Pressure Linked Equations). The turbulence has been modeled by standard k-ε model. The trajectory of pulverized coal particles have been solved by integrating the force balance on the particle, which is written in a Lagrangian reference frame. The dispersion of particles due to turbulence in the fluid phase has been predicted using the stochastic tracking model. The stochastic tracking (random walk) model allows to include the effect of instantaneous turbulent velocity fluctuations on the particle trajectories through the use of stochastic methods. The interaction between gas and coal particles has been considered every 50 iterations for fluid flow. The radiative heat transfer has been included in the overall computational domain using the discrete ordinates radiation model (DO), while the absorption coefficients of the gas phase has been calculated using the weighted-sum-of-gray-gases model (WSGGM).

The mixing and transport of chemical species has been modeled by solving the conservation equations describing convection, diffusion, and reaction sources for each component species. To model the mass diffusion has been used the Fick's law instead of Maxwell-Stefan equations because in this work the dilute approximation can be acceptable. In fact the results show that there is not much difference between the two models.

For the interaction of turbulence and chemistry in gas phase, the EDM, proposed firstly by Spalding [9] and modified later by Magnussen and Hjetager [10], has been used. This model is based on the concept that burning is fast, and turbulent mixing controls the overall rate of reaction.

Coal combustion has been modeled according to the following phenomena sequence: drying, devolatilization, volatile combustion and char burnout.

In order to validate the experimental results predicted by Weber [11] the two-competing-rates model for coal devolatilization model proposed by Kobayashi et al. [12] has been modelled with different kinetic rate parameters. The char combustion is computed according to the kinetics/diffusion-limited model of

Baum and Street [13] and Field [14] where the surface reaction rate is determined either by kinetics or by diffusion rate.

In this work the fuel and thermal NO_x have been considered. The transport equations for nitric oxide (NO) and for intermediate species (HCN) have been solved. For the thermal NO, the extend Zeldovich mechanism [15] have been used, the concentrations of O-radical and OH-radical are calculated using the partial equilibrium approach as suggested by Westenberg [16]. For the fuel NO, it is assumed that all fuel nitrogen, both volatiles and char, is converted into HCN. The HCN release and depletion rates are given by De Soete expressions [17].

The used kinetic mechanism is the same as the work of Weber [11]. Detailed formulations of the models can be found in the FLUENT 14.5 Theory Guide [15].

3. Numerical simulations

The furnace geometry is the IFRF furnace no. 1 [11]. The profile of the burner quarl is defined by a cubic equation in term of radius. The inlet consists of two ducts: the primary air, transporting pulverized coal, enters from internal one and secondary swirled air enters from the external one. For further details about the geometry, it can refer to the work of Weber [11]. The governing equations have been solved using the finite volume technique. The computational domain has been discretized by about 60000 rectangular cells. The grid size is finer near the burner, where take place the combustion of coal.

The second order upwind scheme has been used to discretize the convective term for the all transport equations, while the selected solver algorithm is the SIMPLE (Semi-Implicit Method for Pressure Linked Equations).

The following figures show the properties of coal sand the boundary conditions for the analyzed cases.

Table 1. Proximate analysis of Göttelborn hvBp coal

Proximate analysis	Weight % dry
Volatile matter	37.4
Fixed carbon	54.3
ash	8.3

Table 2. Ultimate analysis of Göttelborn hvBp coal

Ultimate analysis	Weight % daf
C	80.36
H	5.08
N	1.45
S	0.94
O	12.17
LHV daf	32.32 MJ/kg

Table 3. Göttelborn hvBp coal properties

Density	1000 kg/m^3
Specific heat	1100 J/(kg K)

Coal particle size distribution	Rosin-Rammler
Mean diameter	45 μm
Smallest diameter	1 μm
Largest diameter	300 μm
Spread	1.36

Table 4. Boundary Condition for the secondary inlet

Conditions at inlet	18% O_2 – 82% CO_2	18% O_2 – 52% CO_2 – 40% H_2O	18% O_2 – 42% CO_2 – 30% H_2O
Gas flow rate [kg/h]	3312	3312	3312
Temperature, [K]	573	573	522
Mean axial velocity, [m/s]	37.68	53.76	53.76
Mean tangential velocity, [m/s]	49.4	49.4	49.4
Turbulence Intensity, %	20	20	20
Lenght scale, m	0.047	0.047	0.047

The boundary conditions, for the primary inlet and for the wall temperatures, are the same used by Weber [11]. In particular, the coal flow rate at primary inlet is 263 kg/h.

All simulations were performed maintaining, at secondary inlet, both the same O_2 excess and the gas flow rate, in order to evaluate the effect of CO_2 and H_2O on the gas temperature and NO_x emissions.

In order to keep constant the gas flow rate for all cases, the axial gas velocity at inlet has been set with different values. For the cases 2 and 3, it is important to highlight that both the molecular weight and the gas temperature are different, thus the axial velocity have to be the same value to obtain the same gas flow rate.

4. Results and discussion

This section is focused on the results and discussion of three different combustion cases specified in the table 4. The fig. 1(a) shows the gas temperature profile along the axis of combustor. The aim of this figure is to visualize the comparison between the combustion in O_2/CO_2 environment and that one in $O_2/CO_2/H_2O$. The gas temperature in presence of H_2O is lower than that in presence of pure CO_2. This trend is due to specific heat of H_2O, which is almost twice those of CO_2 and N_2 when the temperature is around the typical flame one.

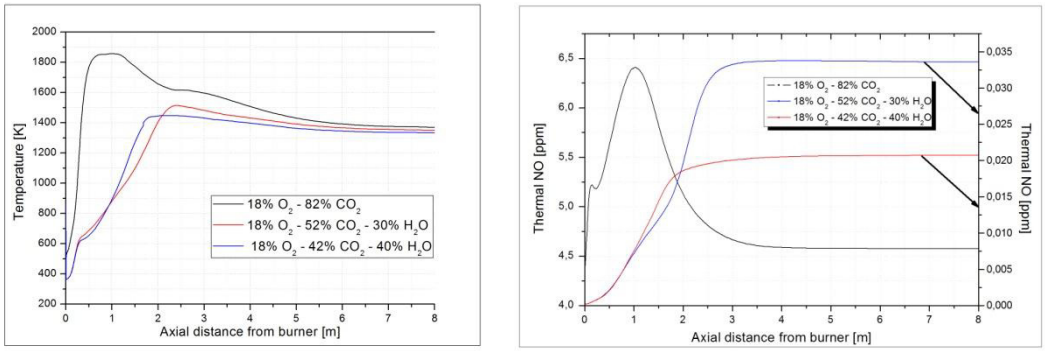

Fig. 1. (a) Gas temperature profiles and (b) Thermal NO profiles along the axis of combustor for the three cases: the red and blue lines refer to the right axis.

The fig.1 (b) shows the Thermal NO_x profiles. It is noteworthy that the profiles follow that of gas temperature according with the NO formation rate proposed by mechanism of Zeldovich [15]. The amount of them is very low due to both the temperature and the absence of nitrogen in the secondary stream, which is predominant, in most cases, respect the primary one.

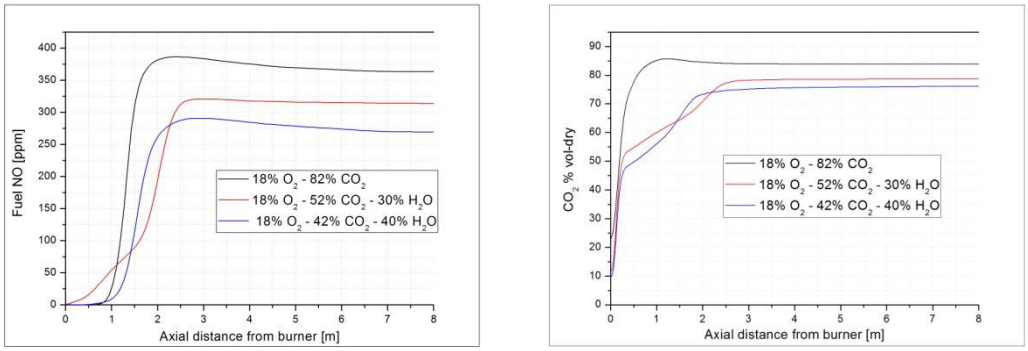

Fig. 2. (a) Fuel NO profiles and (b) Concentration of CO_2 on dry base profiles along the axis of combustor for the three cases.

The fig. 2(a) presents the Fuel NO_x profiles. They depend on the intermediates HCN species. The release rate of these latter depends on the combustion rate of char and volatiles, whereas the depletion rate depends on molar fraction of HCN formed, molar fraction of O_2, temperature and pressure, as shown by De Soete expressions [17]. The temperature play an important role, because influences both the combustion rates of char and volatile matter and the depletion rate of HCN. In case of oxy-coal with wet recycle, the amount of Fuel NO_x is lower than that in dry-recycle. It is due to the combined effect of release and consumption rates of HCN in the combustion chamber, influenced by O_2 concentration and temperature profiles.

In the fig. 2(b) is showed the CO_2 concentration on dry base. The formation of CO_2 is predominant near the burner where take place the relaese of volatiles, the char combustion and the oxidation of CO. It is important to highlight that the amount of CO_2 at outlet is greater when pure CO_2 is recycled. This is an important advantages for the capture of CO_2, because the higher the flue gas CO_2 concentration and easier

is to separe it. In case of high concentration (greater than 90%), it would be enough only condensate the water vapour.

It is necessary to notice that in the cases 2 and 3 the axial velocity at secondary inlet is different. Consequently, the velocity field is different, and leads to the relase of volatiles and char combustion in the external zone of combustor.

5. Conclusions

In this work, numerical simulations were performed to study the effect of CO_2/H_2O mixture on gas temperature and NO_x emissions in oxy-coal combustion. The results show that the recirculation of CO_2/H_2O leads to low temperature respect of CO_2 one. It influences also the thermal NO_x, strongly related to the temperature, and the Fuel NO_x because these latter depend on intermediates HCN species.

These simulations have to be validated by experimental data. Further studies could be to implement, reaction mechanisms of H_2O with HCN as shown by Schäfer and Bonn [18] and other mechanisms related to the reaction of H_2O and CO_2 with the nitrogen presented in the carbon char [19].

It is worthwhile to remind that when steam is added in the mixture at inlet, the concentration of CO_2 decreases. If on the one hand, this effect is not desirable for the separation of CO_2 at downstream, on the other it inhibits the formation of NO_x emissions.

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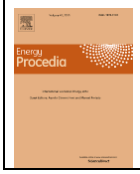

Biography

Diego Perrone graduated in Energy Engineering at University of Calabria. Currently he is a Ph.D. student at the same University. Tha main research fields are the MILD-coal combustion and fluidized bed combustion using the CFD. The focus is to improve the efficiency with application on large scale.