

## Thesis Review. Oxyfuel combustion for CO<sub>2</sub> capture. Application of computational fluid dynamics techniques

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### Objectives and novelty

The use of coal in power plants generates a large amount of CO<sub>2</sub>, which is the chief contributor of global climate change. A diverse power generation portfolio including Carbon Capture and Storage (CCS) technologies and renewable energies is needed to reduce atmospheric CO<sub>2</sub> to below 1990 levels. Oxy-coal combustion is one of the most promising CO<sub>2</sub> capture technologies since it could be adapted to both new and existing pulverized coal-fired power stations. During oxy-coal combustion, coal is burnt in a mixture of oxygen and recycled flue gas (mainly CO<sub>2</sub> and H<sub>2</sub>O), to yield a rich CO<sub>2</sub> stream. Successful implementation of oxy-coal combustion depends on fully understanding the difficulties arising from replacing nitrogen by a mixture of CO<sub>2</sub> and water vapour in the oxidizer stream. Thus, the first objective of this thesis was to study the influence of the combustion atmosphere, i.e., air or oxy-firing conditions, on several combustion aspects such as coal devolatilisation, particle ignition, char reactivity or pollutant formation in an entrained flow reactor (EFR) of 30 kW<sub>t</sub>.

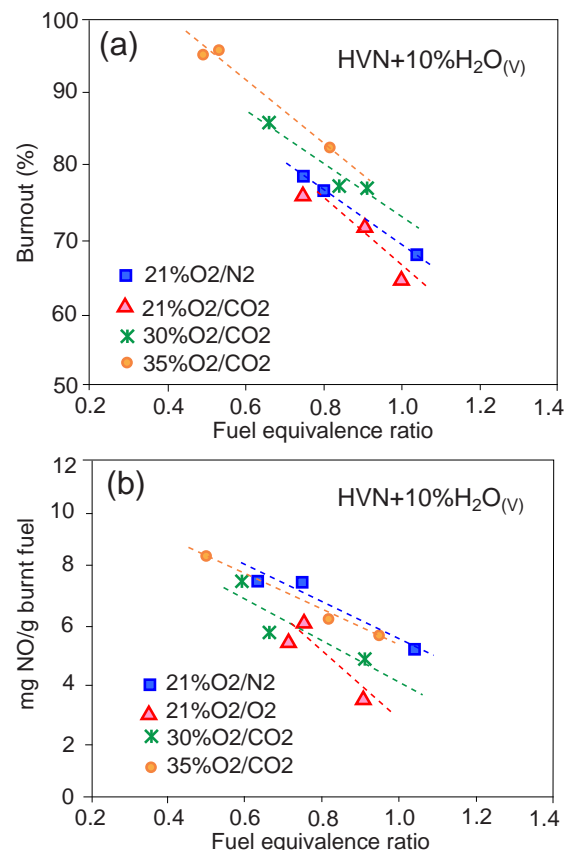
Computational Fluid Dynamics (CFD) models have been widely used as a design tool for coal fired power stations. Those CFD models include several sub-models (e.g., char and volatile combustion, heat transfer, etc.) which are perfectly established and developed for air-firing conditions. With the accumulated knowledge on the fundamental differences between air-fuel and oxy-fuel conditions, an important effort has been gone into developing and validating sub-models for the new environment. Thus, the second objective of this thesis was the development of a CFD model which adequately described overall combustion behaviour in both air and oxy-firing conditions.

### Results

First, the influence of the devolatilisation environment on volatile and nitrogen yield, for coals of different rank, was studied at 1000 °C in the EFR. In all cases, the apparent volatile yields measured after devolatilisation under CO<sub>2</sub> were greater than those obtained in N<sub>2</sub>, probably caused by char-CO<sub>2</sub> gasification reaction. In addition, the volatile-N yield for the CO<sub>2</sub>-chars was found to be higher than that for the N<sub>2</sub>-chars. The devolatilisation atmosphere also affected the structure and the subsequent reactivity of the char. The thermal reactivity and kinetics of the N<sub>2</sub>-chars and CO<sub>2</sub>-chars in 30% O<sub>2</sub> / 70% CO<sub>2</sub> was studied using a thermobalance, and three nth-order representative gas-solid models were employed to describe the reactive behaviour of oxy-char combustion. It was found that the N<sub>2</sub>-chars presented a slightly higher reactivity over the CO<sub>2</sub>-chars.

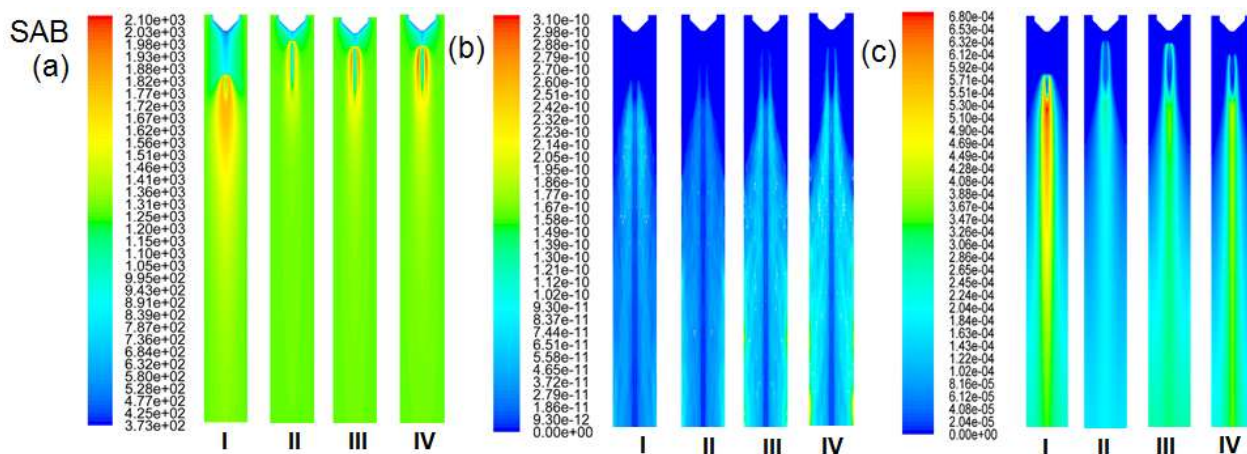
The effect of the combustion atmosphere was evaluated for coals of different rank at different levels of oxygen excess at 1000 °C in the EFR, as shown in Figure 1. The fuel equivalence ratio, defined as the ratio between the coal mass flow rate and the stoichiometric value, was used to assess the oxygen

excess during the combustion. A worsening on coal burnout was observed when replacing N<sub>2</sub> for CO<sub>2</sub> for the same oxygen concentration, due to difference in gas properties. Also lower NO emissions were observed during oxy-fuel combustion. Complementary to combustion experiments, ignition tests were also carried out. A significant ignition delay was observed when nitrogen was replaced by CO<sub>2</sub>, not only due to the higher heat capacity of the CO<sub>2</sub>, but also to the persistence of a thick volatile cloud around the particle which prevented its ignition. While for oxy-firing conditions with oxygen content up to 30 or 35%, better ignition and combustion properties than those for air-firing conditions were observed. This is due to the higher mass flux of oxygen promotes the consumption rate of volatiles, providing extra heat feedback to the coal particles to enhance their ignition and combustion.



**Figure 1.** Burnout values and NO emissions of coal HVN (semi anthracite) vs. fuel equivalence ratio during its combustion in air and oxy-fuel atmospheres with 10% H<sub>2</sub>O(v) and different oxygen content.

Finally, a CFD model for oxy-coal combustion was developed for both air and oxy-firing conditions. The inputs for volatile yield and nitrogen partitioning between char and volatiles were those determined during the devolatilisation experiments, and the kinetics implemented in the char combustion sub-model were based on the values previously obtained for each char. For the CFD model the calculation domain is the reaction zone of the entrained flow reactor. A three dimensional structured grid consisting



**Figure 2.** (a) Predicted temperature (K), (b) char burnout rate ( $\text{kg s}^{-1}$ ) and (c) NO emissions (%) inside the entrained flow reactor during SAB (high-volatile bituminous coal) combustion for each atmosphere: 21% $\text{O}_2$ /79% $\text{N}_2$  (I), 21% $\text{O}_2$ /79% $\text{CO}_2$  (II), 30% $\text{O}_2$ /70% $\text{N}_2$  (III) and 35% $\text{O}_2$ /65% $\text{N}_2$  (IV). Length scale for (a), (b) and (c) is 40 cm.

of ~75,000 cells was employed to describe a quarter of the total volume. The boundary conditions, mass flow inlets and wall temperatures were established using measurements made during the experimental tests. Figure 2 presents the temperature contours, char burnout rates and NO emissions in the mid plane of the reactor during SAB (high-volatile bituminous coal) combustion.

As can be seen in Figure 2 (a) and (b), the temperatures and the burning rates, dropped significantly when  $\text{N}_2$  is replaced by  $\text{CO}_2$  for the same oxygen concentration (cases I and II), due to the higher specific heat of  $\text{CO}_2$ . To counteract the negative effect of  $\text{CO}_2$  on temperature and burning rate, the oxygen concentration in the  $\text{CO}_2$  mixture must be up to 30 or 35% (cases III and IV). The NO simulations were carried out as a post-processing stage once a solution for the global combustion problem was obtained. As observed during the experimental tests, lower NO emissions were produced in the oxy-fuel environment with 21% oxygen in comparison to those for air-firing conditions. An increase on NO production was observed with increasing oxygen concentrations, due to the higher fuel-N conversion to NO. Coal burnout values and NO emissions were predicted and compared with the experimental values. A good agreement between both experimental and predicted values was found, evidencing the accuracy of the model.

## Conclusions

The overall combustion behaviour for coals of different rank was experimentally and numerically studied in air and oxy-fuel conditions in an entrained flow reactor. High  $\text{CO}_2$  concentrations seemed to affect volatile yield and nitrogen distribution, and also the subsequent char reactivity. To obtain similar or better ignition and combustion properties under oxy-firing conditions to those attained in air, the oxygen concentration in the  $\text{CO}_2$  and  $\text{H}_2\text{O}_{(v)}$  mixture must be about 30%. During oxy-fuel combustion, lower NO emissions were produced in comparison with air-firing conditions, although an increase on fuel-N conversion to NO was observed when increasing the oxygen concentration. The experimental findings related to coal burnout and NO emissions were used to test the accuracy of the CFD model developed for oxy-coal combustion. The CFD model predicted accurately oxy-coal combustion in the entrained flow reactor, and it was a useful tool for describing the differences in temperature, species concentration and burning profiles, during the combustion of

different coals in both air and oxy-firing conditions.

## Related publications

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