Kinetic Simulation of a 100kWth Oxy-Combustor using Aspen Plus

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TWELFTH ANNUAL CONFERENCE ON CARBON CAPTURE, UTILIZATION AND SEQUESTRATION
May 13 – 16, 2013 David L. Lawrence Convention Center Pittsburgh, Pennsylvania

Abstract

Oxy-fuel combustion is a clean coal technology based on firing fuel in an enriched oxygen atmosphere to obtain high CO2 concentrations in the exhaust gas. Experimental tests were performed at Cranfield University using a 100kWth retrofitted oxy-combustor. In parallel, a kinetic simulation model using Aspen Plus was designed and validated to serve as a computer tool to predict the behaviour of the oxy-combustion process for a wide range of fuels and conditions.

The main input parameters varied in the simulation study were: fuel type (El Cerrejon coal, Daw Mill coal, Cereal Co-product biomass, and coal/biomass blends); percentage of recycled flue gas (55, 60, and 65%); type of recycled flue gas(wet or dry); percentage of excess oxygen (0 and 5%), and the amount of air ingress into the process (0, 2, 10, and 18% of the total flue gas fed to the oxy-combustor). The last input condition, percentage of air ingress, is of greater importance as a result of the unit being a retrofitted oxy-combustor; for which air ingress is more probable and this represents a situation likely to be an issue for any boiler retrofitted for oxyfuel firing. Results from the simulations as well as the definition of the operating conditions that best represents the behaviour of the rig are presented.

1. Introduction

Oxy-combustion is one of the main options being considered for the capture of CO2 from fossil fuel-fired power generation. This is required to satisfy the current regulations regarding reduction of greenhouse emissions. The generation of a current of flue gas with a high percentage of CO2 in the combustor, or a smaller size of flue gas conditioning equipment downstream of the furnace are examples of the advantages that this technology presents over other carbon capture technologies (pre-combustion and post-combustion). However, the main disadvantage of the use of the oxy-fuel combustion technology is the elevated cost associated with generating high purity O2 by cryogenic distillation.

Oxy-combustion can be combined with the use of biomass as fuel to allow a near-zero emission process to produce electricity.

The oxy-combustion process has been widely studied using different commercial software. The importance of using computational and simulation models to predict the behaviour of a particular process is based on that it requires less economic investment than performing research on the same process through experiments. Some of the commercial packages used to carry out these studies are: Fluent, Chemkin Pro, Aspen Plus, gPROMS, Thermoflex or Hysis. By using simulation models, faster study of the key parameters of a process can be completed and less cost is associated with performing a sensitivity analysis to determine which inputs have more effects on the outputs to optimise the process. This is part of the work that is being carried out at CERT in Cranfield University, where simulations using Aspen Plus are being developed to have a tool with which select the most significant experimental tests with operation parameters based on the prediction of the simulation model.

This paper presents the latest results using Aspen Plus for the oxy-combustion process, implementing dry recycled flue gas.

The parameters varied for the oxy-combustion process have been: excess of oxygen supplied to the furnace, percentage of flue gas recirculated, and type of fuel used. The results generated will compare the gas composition obtained for air-firing and oxy-firing combustion, with and without the implementation of water vapour and acid species removal.

2. Description of the system

The oxy-combustor system designed consists of several sub-sections. In first place, the drying process has been defined so 5% of the moisture present in the fuel is taken by inert gas. The oxy-combustor is simulated using five reactors: the first one to convert the fuel, nonconventional solid, to a conventional one; then, a reactor to perform the combustion of the volatiles species of the fuel (where the fraction of C that reacts is Xc =VM-H-S, according to the proposal made by Sotudeh-Gharebaagh et al., (1998)); a reactor to simulate the combustion of the char; a reactor where thermal NOx is generated; and, lastly, a reactor to simulate the generation of NOx from the N of the fuel. The hot combustion products go to the super heater (SH), with an exit temperature of the flue gas of 370 ºC. After this, a cyclone removes the suspension solids from the gas. The flue gas enters into a heat exchanger, where it will be cooled down to 90 ºC; the heat released will be used to pre-heat the gases to be fed to the combustor later on. To simulate the condenser, used to remove water vapour and acid species (SOx, HCl, NOx) from the flue gas, an additional heat exchanger and a component separator have been implemented. The purified flue gas is split into two streams: part of the gas is recirculated to the oxy-combustor and another part goes to the exhaust. The fractions of recycled flue gas defined for this study have been set on 55, 60 and 65% of the total flue gas generated in the combustion. The stream of pure oxygen (95% mol, purity) is injected to the recycled flue gas at this point. The oxygen is fed to the process stoichiometrically or with a 5 % excess, depending of the case study. The gas containing the oxygen necessary for the combustion of the fuel passes by the gas pre-heater and is fed to the oxy-combustor.

The interface of Aspen Plus for the kinetic model with flue gas purification is shown in Figure 1.

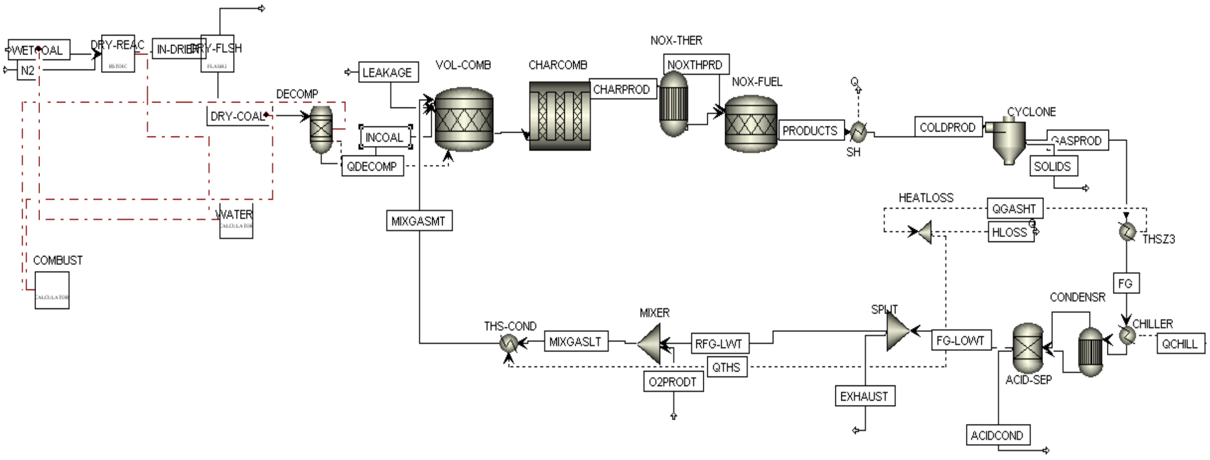

Figure 1.Oxycombustion process interface in Aspen Plus with dry RFG

Additional inputs parameters used in the simulations related to the geometry of the combustor, and fuel flow rates are shown in Table 1.

Table 1.Input data and assumptions for the simulations

	Value	Unit
Oxy-combustor		
Flow rate $_{\text{El Cerrejon}}$	13.5	kg/h
Flow rate $_{\text{CCP}}$	22.03	kg/h
Flow rate $_{\text{El Cerrejon50\%-CCP50\%}}$	17.8	kg/h
Combustor geometry (flame section)		
- Cross section	0.09	m^2
- Length	3.71	m
Cyclone efficiency	99	%
Air ingress (of total gas supplied to the oxy-combustor)	10	%
$T_{\text{exit SH}}$	370	^oC
Condenser efficiency		
- H_2O	95	%
- HCl	98	%
- H_2SO_4	100	%
- HNO_3	100	%

The composition of the fuel supplied to the oxy-combustor has been varied, using: El Cerrejon coal, Cereal Co-Product biomass, and blends of these two fuels. The analysis of the parent fuels is shown in Table 2.

Table 2. Analysis of El Cerrejon and Cereal Co-Product (CCP).

	El Cerrejon	CCP
CV, kJ/kg (as received)		
- Gross	27850	17610
- Net	24107	16340
Proximate analysis (% (w/w))		
- Moisture	5.8	8.1
- Fixed carbon	53.9	18.39
- Volatile matter	36.9	77.04
- Ash	9.1	4.57
Ultimate analysis (% (w/w))		
- C	69.20	47.22
- H	4.80	6.46
- N	1.42	3
- Cl	0.02	0.18
- S	0.58	0.17
- O	9.98	38.4
Sulphur analysis (% (w/w))		
- Pyritic	0.27	0.06
- Sulfate	0.07	0.05
- Organic	0.27	0.06

This simulation study has been carried out using the software Aspen Plus ™ V7.3. The property methods used have been: Peng-Robinson (PENG-ROB), National Bureau of Standards steam table equation of state (STEAMNBS), and General Solid and Pyrometallurgy Applications (SOLIDS). For the convergence, Broyden method was selected for the oxy-combustor.

3. Results and discussions

The data generated regarding the gas composition of the flue gas for the reference case (conventional combustion), and using different types of fuel, supplying 5% (vol) excess of oxygen and 60% of recycled flue gas are presented in Table 3. Note that this table shows the composition of the gas just after the exit of the oxy-combustor, prior to the cyclone and the condenser.

Table 3.Simulation results for gas composition for air and oxy-firing in the combustion products

	CO_2 (%)	H_2O (%)	O_2 (%)	SO_2 (ppm)	CO (ppm)	NO (ppm)	NO_2 (ppm)	HCl (ppm)
El Cerrejon (CC)	14.42	6.05	3.48	447	0	459	32	13
El Cerrejon (OC)	61.14	10.59	7.65	759	1	779	59	23
El Cerrejon50%-CCP50% (OC)	56.73	14.75	7.38	560	1	467	52	128
Cereal Co-Product (OC)	50.47	20.45	2.12	255	4,870	96	40	107

Attending to the CO_2 content in the oxy-firing cases, the highest concentration is produced when burning 100% El Cerrejon, as it was expected from the analysis of the fuels shown in Table 2; the same trend can be observed for the SO_2 concentrations, having a similar explanation. For the water vapour and chlorine content, the results agree with the theoretical prediction, this is: increasing with the content of biomass in the fuel burnt. Although there is a slightly higher content for the HCl generated in the case where burning the blend El Cerrejon50%-CCP50% than in 100% Cereal Co-Product. Regarding the relatively high CO concentration reached for 100% Cereal Co-Product, the possible cause could be the lack of oxygen to perform the total oxidation of the carbon to carbon dioxide, even though when the supply was still with 5% excess of oxygen over the stoichiometric. It can be seen that the content of oxygen in the products of combustion for this case is lower than for the rest of the cases. The NOx concentrations generated are in the range expected.

The results obtained from the simulation in the exhaust stream, after having been purified by the cyclone and the condenser are presented in Table 4. The operating conditions in this case are 5% (v/v) excess of oxygen and 60% of recycled flue gas, as in the previous case.

Table 4.Simulation results for gas composition for air and oxy-firing in the exhaust gas

	CO_2 (%)	H_2O (%)	O_2 (%)	SO_2 (ppm)	CO (ppm)	NO (ppm)	NO_2 (ppm)	HCl (ppm)
El Cerrejon (CC)	15.32	0.32	3.64	0	0	0	9	0.3
El Cerrejon (OC)	68.18	0.58	8.43	0	0	0	8.8	0.5
El Cerrejon50%-CCP50% (OC)	66.12	0.85	8.54	0	0.2	0	4.6	3
Cereal Co-Product (OC)	72.46	1.48	3.47	0	0	0	1.5	3.4

Notice that the maximum content for CO_2 is reached for the case using 100% Cereal Co-Product, while in the combustion products this maximum was achieved oxy-firing 100% El Cerrejon coal. This is due to the water vapour and acid species removal, that have taken place for this stream, together with the higher content of water vapour generated when using biomass. Consequently, once this specie (H_2O) is removed, its effect is more noticeable for the case of 100% CCP. Accordingly, the increase in CO_2 for this case study is of 30%(v/v), while in the case of 100% El Cerrejon is 20% (v/v),comparing results showed in Table 3 and Table 4.

Table 5 presents the composition of the condensates generated in the water vapour and acid species removal system, for different fuels, feeding oxygen to the oxy-combustor with an excess of 5%(v/v) and applying 60% RFG. It can be seen that the composition for the condensates varying the fuel is similar, being the major component water.

Table 5. Simulation results for condensates composition

	H_2O (%)	H_2SO_4 (%)	HNO_3 (%)	HCl (%)
El Cerrejon (CC)	98.37	0.77	0.84	0.02
El Cerrejon (OC)	98.40	0.75	0.82	0.02
El Cerrejon50%-CCP50% (OC)	98.00	0.75	0.82	0.02
Cereal Co-Product (OC)	98.41	0.75	0.82	0.02

The next stage to undertake in the design of the kinetic simulation model will be the implementation of an Air Separation Unit (ASU) and steam turbine system to transform the thermal energy of the combustion gases into mechanical work. Thus, a comparison will be carried out between the energetic efficiency achieved under air and oxy-firing conditions using coal and biomass.

Nomenclature

CC	Conventional combustion
CCP	Cereal Co-Product
H	Hydrogen content of the fuel
OC	Oxy combustion
RFG	Recycled Flue Gas
S	Sulphur content of fuel
VM	Volatile matter
Xc	Fractional conversion of carbon

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