Simulation of Oxy-combustion co-firing Coal and Biomass with ASU and Steam Turbine using Aspen Plus

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1. Introduction

Oxy-combustion is one of the main options being considered for the capture of CO_2 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 CO_2 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 O_2 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, including oxygen generation (95% mol, purity) in the Air Separation Unit (ASU), and a steam turbine to transform the thermal energy of the combustion gases into mechanical work. 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 efficiency between the air-firing and oxy-firing combustion for the base case. Additionally, an analysis of the gas composition for different case studies is presented.

2. Description of the system

This study of the oxy-combustion process has been carried out through the definition of three subsystems: air separation unit (ASU); oxy-combustion and steam turbine (power generation unit). The ASU is the section of the process where the oxygen to be fed to the oxy-combustor is generated with a specified purity. In the oxy-combustor section, the fuel and the oxygen are supplied so the combustion process occurs. The high temperature flue gas generated enters into a heat exchanger to produce the steam that will be fed to the last section, the steam turbine. Here, the pressurised steam provides the thermal energy to the turbine which will extract it as mechanical work.

2.1. Air separation unit (ASU)

The ASU process simulated consists, basically, of a multi-stage compressor, a multi-stream heat exchanger, and two distillation columns (one at low and one at high pressure). For the definition of this section it has been taken into account the suggestions made by several authors: Hu *et al.*, (2010), Raibhole and Sapali,(2012), and Amarkhail, (2010).

The four-stage intercooling compressor produces air at 6.3 bar, pressure necessary to generate a stream of oxygen with 95%mol purity. The pressurised air is split into two streams and fed to the multi-stream heat exchanger (HE1) where it works as the hot fluid and its exit temperature is -130 ^{o}C. The stream of air with higher flow rate is supplied to the high pressure column (HPC), which is defined by 40 stages, a total condenser and a reflux ratio of 1.2. Note that the condenser of the HPC provides with the heat needed by the reboiler of the low pressure column (LPC). The stream that exits the HPC in the distillates section has more content of nitrogen as this specie has higher vapour pressure than the oxygen. The stream of the bottom of the HPC is, consequently, enriched in oxygen, having around 47% mol purity. Both streams are cooled in a multi-stream heat exchanger (HE2) and expanded using valves prior to feed them to the LPC. The LPC has a total of 56 stages, and the streams are fed as follows: the air on the 10th stage, the oxygen rich stream (bottom of HPC) on the 23rd stage, and the nitrogen rich stream (top of HPC) on the 1st stage. The reflux fration value for this column is 0.5712. The diagram used for the ASU simulations can be seen on Figure 1.

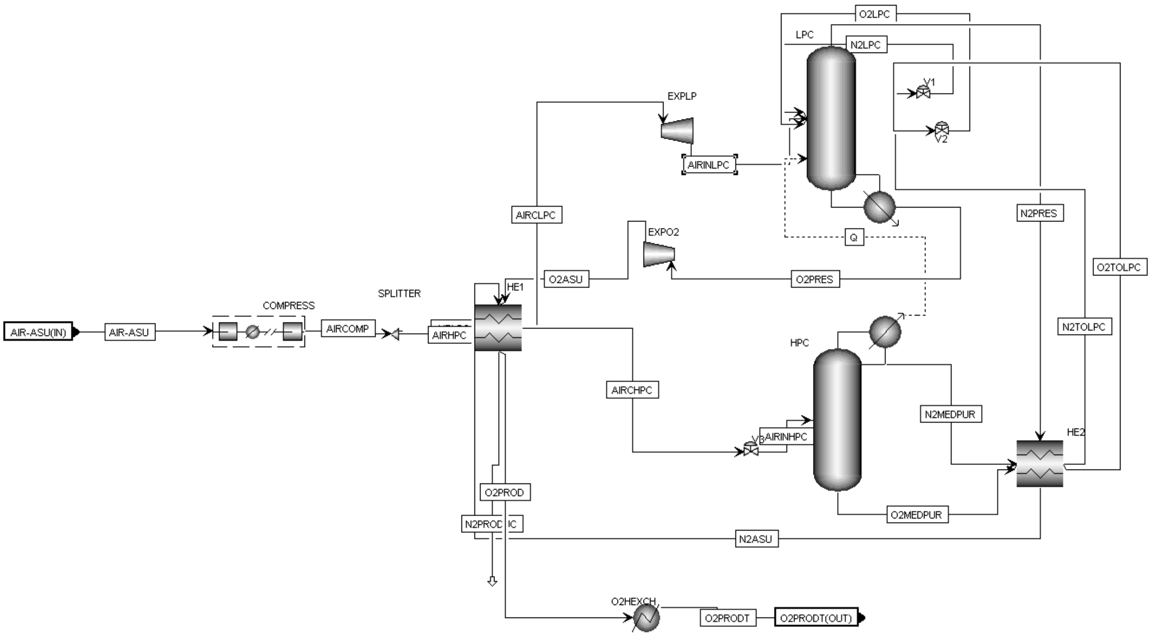

Figure 1.ASU process interface in Aspen Plus

2.2. Power generation unit

The power generation unit consists of the oxy-combustor and the steam turbine.

To define the oxy-combustor system in Aspen plus, a kinetic model was designed. 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), where the heat is transferred to the steam that will be fed to the steam turbine. From the SH, the exit temperature of the flue gas is 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 SOx 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 oxygen generated in the ASU hierarchy is injected to the recycled flue gas at this point. The purity of the oxygen supplied by the ASU is 95%mol, but will be fed to the process at the stoichiometric amount or with 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 2.

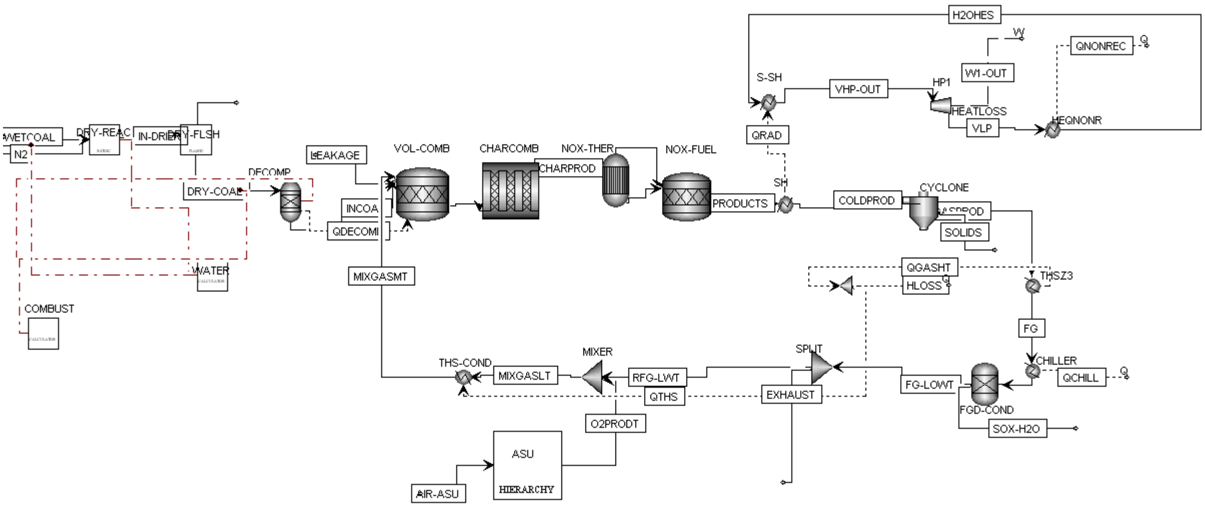

Figure 2.Oxycombustion process interface in Aspen Plus

Additional inputs parameters used in the simulations related to the geometry of the combustor, and fuel flow rates are shown in Table 1.The analysis of the fuels can be seen in Table 2.

For the steam turbine subsection, two heat exchangers and a turbine were defined. The first heat exchanger, has as input the heat released by the products of combustion. This heat is used to increase the temperature and the pressure of the steam that will be fed to the turbine. The thermal energy of the steam is converted into mechanical work in the steam turbine, as the steam is expanded down to 0.06 bar, as it is proposed by Xiong *et al*., (2011). The low pressure vapour is fed to another heat exchanger to return to the pressure and temperature conditions at which is set to be fed to the first heat exchanger (S-SH).

3. Input data and assumptions

Some assumptions have been made for the power generation and ASU process definition. These assumptions and other input data used for the simulations are summarized in Table 1.

Table 1.Input data and assumptions for the simulations

	Value	Unit
ASU		
Compressor isentropic efficiency	80	%
Compressor mechanical efficiency	97	%
Pressure loss in the heat exchangers	0.1	bar
Pressure in the HPC	5.5	bar
Pressure in the LPC	1.35	bar
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	2	m
Cyclone efficiency	99	%
Air ingress (of total gas supplied to the oxy-combustor)	10	%
$T_{\text{exit SH}}$	370	^{o}C
Condenser efficiency	100	%
Steam turbine		
Turbine mechanical efficiency	92.5	%
S-SH Steam	100;100;400	kg/h;bar; ^{o}C

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

4. Methodology

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). As convergence methods, Cryogenic has been set for the ASU section, and Broyden for the power generation section.

5. Results and discussion

The base case has been defined as the process in which 13.5kg/h (necessary to produce $100kW_{th}$) of El Cerrejon coal 100% (weight) is oxy-fired using oxygen generated in the ASU with 95%mol purity, an excess of oxygen of 5%(vol) and 55% of RFG. A reference case has been also defined as the air-firing case of the same amount of El Cerrejon coal 100% (weight) to generate $100kW_{th}$ through a conventional combustion process. The results from simulations completed for these cases are presented in Table 3.

Table 3.Simulation results for the air and oxy-firing Base Case.

	Air-firing	Oxy-firing
Power generated (kW)	23.77	25.01
Power consumed ASU(kW)	--	8.05
Net fuel input (kW)	100	100
O_2 stoichiometric (kmol/h)	0.8973	0.8973
O_2 excess supplied (%)	21	5
Raw air to ASU (kmol/h)	--	4,70

Observing this set of data, it could be deduced that the air-firing process is more efficient for the generation of the same amount of power per unit of fuel burnt. However, it is important to consider that after the conventional combustion would be necessary to carry out the carbon capture process to have a higher content in CO_2 of the combustion gases. This process of removing the nitrogen from the exhaust gas, would have an associated power consumption. Consequently, the accurate comparison should be made by having the net efficiency of conventional combustion with capture process to have the same final CO_2 concentration in the gas product, as in the oxy-firing case (four times more concentrated, as illustrated on Table 4).

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 4.

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

	CO_2 (%)	H_2O (%)	O_2 (%)	SO_2 (ppm)	CO (ppm)	NO_2 (ppm)	NO (ppm)	N_2O (ppm)	Cl_2 (ppm)
El Cerrejon (CC)	14.42	6.06	3.09	448	0	2523	3716	0	6.64
El Cerrejon (OC)	61.12	10.34	7.15	759	0	4276	7537	0	28
El Cerrejon50%-CCP50% (OC)	58.17	17.16	2.40	563	16630	7466	3838	0	163
Cereal Co-Product (OC)	55.68	22.41	1.79	300	0	12133	3036	0	359

Attending to the CO_2 content in the oxy-firing cases, the highest concentration is produced when burning the 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. Regarding the relatively high CO concentration reached for the blend El Cerrejon50%-CCP50%, the possible cause is that there was not enough 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 noticeably lower than for the 100% El Cerrejon case. The NOx concentrations generated are high, although following the theoretical prediction. NO_2 can be generated as product of the thermal and fuel NOx reactions. This together with the higher content of nitrogen in the biomass, makes that the maximum concentration for this specie is generated when burning 100% biomass. On the other hand, the NO is generated during the thermal NOx generation and this process is encouraged by higher temperatures reached when using 100% coal as fuel. The reason for the high concentrations of NOx in the combustion products is likely to be associated with these compounds are not removed in the condenser, whereas water vapour and SO_2 are removed. However, if the SO_2 condenses due to the cooling under the acid dew point temperature of the flue gas, the NOx should condense as well. Consequently, this is a modification that needs to be implemented in the simulation model to generate more realistic results.

Nomenclature

ASU	Air Separation Unit
CC	Conventional combustion
CCP	Cereal Co-Product
H	Hydrogen content of the fuel
HPC	High Pressure Column
LPC	Low Pressure Column
OC	Oxy combustion
RFG	Recycled Flue Gas
S	Sulphur content of fuel
VM	Volatile matter
Xc	Fractional conversion of carbon

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