Valorization of Waste in a Gasification Plant for Clean Power Production

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ABSTRACT

The purpose of this work is to perform a feasibility analysis of co-gasification using waste materials, petcoke being specifically considered here. From a Life Cycle Assessment (LCA) point of view co-gasification of coal with solid residues is seen beneficial because of transforming a residue into a raw material and further into power. The base work of this paper is a structured and validated conceptual model of an Integrated Gasification Combined Cycle (IGCC) power plant. It comprises steady state models of a Pressurized Entrained Flow (PRENFLO) gasifier, following gas cleaning operations, a Heat Recovery Steam Generator (HRSG) and Combined Cycle (CC) unit operations. The model has been developed using Aspen Hysys[®] and Matlab, which is mainly used for Artificial Neural Network (ANN) training and parameters estimation for electrolytes models implemented in Aspen Plus[®]. Predicted results of clean gas composition and generated power present a good agreement with industrial data.

Keywords: conceptual modeling, LCA, IGCC power plant, waste utilization, syngas cleaning.

1 INTRODUCTION

Although fossil fuels are and will be the main source of energy in a medium-term horizon, their scarce availability raises the question of the increasing need of renewable resources. In gasification, coal can be partially replaced by other fuels such as wood residues, sewage sludge, scrap tires or municipal solid waste. In addition, features like "CO₂ neutrality" (meaning that products from renewable resources contribute less to global warming) and "biodegradability" (meaning that such products may be disposed of with less risk as well as at lower costs) are mainly responsible for the environmental attraction of renewable sources based technologies and products. This work analyzes the use of coal and petcoke mixture from an environmental point of view. The environmental performance indicators used are based on impact assessment schemes currently used in LCA.

2 IGCC POWER PLANT MODEL

The global flowsheet developed in this work includes mainly a PRENFLO gasifier and a series of purification units, i.e. a fabric filter, a venturi scrubber, a COS

hydrolysis reactor, a sour water stripper, a MDEA absorber and a Claus plant. An Air Separation Unit (ASU) is used to obtain oxygen at a purity of 85 wt%. Steam, oxygen and fuel raw materials enter the gasifier and they are converted into syngas, which is cooled down before entering the purification units. Heat is recovered by producing steam in the HRSG, used for CC turbines. In the venturi scrubber, syngas is put into contact with water that absorbs and removes acid and basic pollutants. Main water flow is down to the venturi, decreasing water recycled consumption. The other water fraction needs to be cleaned, in the sour water stripper. After this unit, water is finally treated with ozone (that is not simulated). Syngas is further purified through the COS hydrolysis reactor. This unit converts COS into H₂S, which is removed in the MDEA absorber. Polluted streams from sour water stripper, COS hydrolysis reactor and MDEA absorber are sent to the Claus plant, where sulfur is recovered in liquid form. The obtained clean gas, after the MDEA absorber, is sent to the CC. Heat from exhaust clean gas, after the gas turbine cvcle, is recovered for the steam turbine cvcle in the HRSG. This model has been validated with industrial data from ELCOGAS plant in Puertollano (Spain).

_	Base Case	Mix1	Mix2	Mix3	Mix4	
Input Data						
Coal (%)	50	39	45	54	58	
Petcoke (%)	50	61	55	46	42	
Carbon (%ar)	61.68	68.28	64.93	61.95	60.1	
Hydrogen (%ar)	2.93	3.21	3.16	3.07	3.1	
Nitrogen (%ar)	3.46	1.97	2.71	3.37	3.69	
Oxygen (%ar)	1.42	1.51	1.29	1.47	1.26	
Sulphur (%ar)	3.34	3.79	3.43	3.24	2.97	
Moisture (%ar)	2	0.75	1.04	1.29	0.93	
Ashes (%ar)	25.17	20.49	23.44	25.61	27.95	
Volat. Matter (%dry)	17.3	16.8	17.1	18.2	18.5	
Feed (t/day)	2,600	2,600	2,600	2,600	2,600	
Gasif. T (°C)	1,600	1,600	1,600	1,600	1,600	
Gasif. P (bar)	25	25	25	25	25	
O2/feedstock (mb)	0.175	0.175	0.175	0.175	0.175	
H ₂ O/feedstock (mb)	0.13	0.13	0.13	0.13	0.13	

Table 1: Operating conditions of ELCOGAS plant ("ar": as received basis. "mb": in mass basis).

Model input data and results are showed in Tables 1 and 2 for four different raw materials mixtures and for a base case, obtained from the ELCOGAS operating conditions.

	М	ix1	М	ix2	М	ix3	M	ix4
Output Data	Exp.	Model	Exp.	Model	Exp.	Model	Exp.	Model
Clean gas composition			_		_			
H ₂ (vol. %)	21.11	19.82	21.17	19.53	21.14	19.05	19.8	18.89
CO (vol. %)	62.06	49.76	61.1	49.76	60.36	49.9	60.7	49.88
CO ₂ (vol. %)	1.43	2.55	2.19	2.58	2.29	2.6	3.05	2.61
$N_2 + Ar (vol. \%)$	15.34	27.54	15.47	27.81	16.14	28.11	16.36	28.28
$H_2S + COS (ppm)$	0	0.36	0	0.38	0	0.39	0	0.38
H ₂ O (vol. %)	0.07	0.32	0.07	0.33	0.07	0.33	0.08	0.33
LHV (MJ/m ³)	8.259	7.985	8.126	7.956	8.038	7.923	7.796	7.905
Gas turbine power (MW)	168.7	187.5	173	183.9	163	181.4	137.8	180.6
Steam turbine power (MW)	121.5	112.5	130	109	124.8	108	109.7	105.8
Total power (MW)	290.2	299.7	303	293	287.8	289.4	247.5	286.4
Error (%)		3.27		-3.30		0.56		15.72

Table 2: Power generation and clean gas composition comparison. Error: total power deviation.

Mixtures are made up by different proportions of coal and petcoke. Major final results differences are found for N_2 and water composition in the clean gas stream (after MDEA absorber). Lower volume percentages are predicted for H_2 and CO, while higher values are obtained for H_2S , COS and water. Simulation of produced power is in good agreement with plant data; this comparison is worst in the case of Mix4.

2.1 Simulation Tools and Specific Units Modeling

This modeling framework is implemented using mainly Aspen Hysys[®] due to its capacity of accepting custom models as extensions and of allowing the creation of new components not considered in its database. Aspen Plus[®] calculations, involving ionic species, are used for phase equilibrium problems solution (for venturi scrubber, sour water stripper and MDEA absorber) and are introduced into Aspen Hysys[®] by means of ANN extensions. ANNs have been mainly used as data based models (to train each ANN, data from sensitivity analysis in Aspen Plus[®] are used) and are carried out using the ANN package provided with Matlab 6.5.

The gasification superstructure comprises:

• Conceptual model of the PRENFLO gasifier. The process sequence is pyrolysis, volatiles combustion, char combustion, char gasification and gas equilibrium. Pyrolysis is modeled using experimental correlations from [1,2] which depend on temperature and volatile matter. Production of H₂S, COS, NH₃ and HCN is represented by equations extracted from experimental data from [3,4]. Every set of correlations is inferred from analysis of different coal types. For volatiles combustion, all pyrolysis gases consumption is

assumed. Kinetics of char combustion main reactions are from [5,6], and consider total oxygen consumption. Char gasification comprises heterogeneous reactions of char with H_2O , CO_2 and H_2 . Finally, gas equilibrium reactions are performed by minimizing Gibbs free energy of all species.

- Venturi scrubber and sour water stripper. They are firstly simulated in Aspen Plus[®] using electrolyte properties package. An ANN for the two units is introduced into Aspen Hysys[®]. Main reactions concerns H₂S, CO₂, HCN and NH₃ water reactions.
- COS hydrolysis reactor. It permits the catalyzed reaction of COS with alumina to produce H₂S. Model kinetic expression and parameters are from [7-8]. It is introduced into the software by means of a user extension.
- MDEA absorber. In analogous way to venturi scrubber and sour water stripper, it has been firstly simulated in Aspen Plus[®] and latter introduced into Aspen Hysys[®].
- Claus plant. It is formed by two kilns (in parallel) and two catalytic stages (in series). In the catalyzed step, kinetic reactions are based on [9-10] and they are introduced into Aspen Hysys[®] with a user extension. After the two mentioned steps, a hydrogenator increases the overall sulfur conversion. Liquid sulfur is recovered in every stage after a condensation process and it is collected in a sulfur pit.
- HRSG. Heat from turbine exhaust gases is mainly recovered here, producing water steam at three pressures (high, intermediate and low pressures). In high pressure and intermediate pressure steam

circuits, steam is also heated by syngas cooling before purification units.

• CC. Final power achieved is the sum of gas and vapor turbines power generation.

For all above mentioned units, simulation results and industrial plant data has been compared. It is important to point out the remarkable agreement between both values.



Figure 1: Impact assessment results by echelon. Axis units [yr⁻¹]

3 LCA

Here, a 4-step LCA is realized [11]:

1) First of all, an objective has to be defined. In this case, the study is focused on the environmental contribution change attained by the different raw material composition feeds. Moreover, a system and a functional unit (FU) are defined. The simulated co-gasification plant, considering extraction and processing of raw material, constitutes the system, making this LCA fit a "cradle to gate" approach. A 1MJ-capacity of electricity production FU has been chosen. Regarding system boundary, it is worth mentioning that the wastewater treatment plants are not included, while the sulfur obtained from Claus plant is neglected.

2) To continue with, an emission inventory, called Life Cycle Inventory (LCI), is gathered for the simulated cogasification plant. Simulation results are used to conceptually estimate flue gas emissions. This step constitutes a conservative approach (i.e. it overestimates emissions), given that the industry complies with all legal emission requirements. However, the use of simulation software makes mass balances and energy balances to be met without requiring further data checks; making this approach a robust one. For all other echelons studied, which are production/extraction of raw materials, LCI of emissions are retrieved from the Ecoinvent database [12]. In the current case, production of: coal, petcoke, sulfuric acid and sodium hydroxide is required given their consumption for electricity generation. The results are shown in Table 3.

Inputs	Electricity MIX1	Electricity MIX2	Electricity MIX3	Electricity MIX4
Fuel [kg/FU]	1,00E-01	1,03E-01	1,04E-01	1,06E-01
Water[kg/FU]	2,29E-02	2,34E-02	2,38E-02	2,41E-02
Naoh [kg/FU]	5,05E-04	5,17E-04	5,24E-04	5,32E-04
H2SO4[kg/FU]	4,25E-06	4,34E-06	4,41E-06	4,47E-06
Outputs				
CO2 [kg/FU]	1,93E-01	1,96E-01	1,98E-01	1,99E-01
SO2 [kg/FU]	1,95E-05	2,07E-05	2,10E-05	2,05E-05
NO [kg/FU]	1,55E-03	1,56E-03	1,58E-03	1,57E-03
NO2 [kg/FU]	4,47E-05	4,50E-05	4,55E-05	4,52E-05

Table 3: Illustrative LCI results from LCI Simulation.

3) Afterwards, an impact assessment, based on the LCI considering all echelons, is performed. Several environmental impact indicators are available. For the case of electricity generation broadly used impacts are Global

Warming Potential (GWP), Acidification Potential (AP), and Abiotic Depletion Potential (ADP). The CML 2 baseline 2000 V2.03 [13] with normalization of the values obtained considering emissions for West Europe in 1995 is used here.

4) Finally, the LCA results interpretation is realized. As it can be seen in Table.4, biggest normalized impacts are found for marine aquatic ecotoxicity. This fact occurred due to the different compounds emissions during coke production and coal extraction. Fig.1 demonstrates the trend of this impact category due to the substitution of coke by coal. This impact category is heavily influenced by the amount of coke used: the higher the coal fraction the more environmentally friendly electricity production. Second in normalized impact comes the abiotic depletion; once again mostly due to coke production and coal extraction process. However the indicator value is slightly affected due to the substitution of coke using coal. AP and GWP show a similar behavior, the impact category is dominated by simulation results (80%) and the rest is due to raw material extraction process. Another significant result is that all impact categories values diminish by substituting coke to coal.

Impact category	Electricity MIX1	Electricity MIX2	Electricity MIX3	Electricity MIX4
abiotic depletion	1,63E-13	1,64E-13	1,61E-13	1,62E-13
global warming (GWP100)	4,91E-14	4,95E-14	4,98E-14	4,99E-14
ozone layer depletion (ODP)	3,88E-16	3,60E-16	3,07E-16	2,86E-16
human toxicity	3,73E-15	3,56E-15	3,21E-15	3,08E-15
fresh water aquatic ecotox.	5,37E-15	5,10E-15	4,58E-15	4,38E-15
marine aquatic ecotoxicity	2,10E-13	1,99E-13	1,77E-13	1,68E-13
terrestrial ecotoxicity	3,30E-15	3,14E-15	2,83E-15	2,71E-15
photochemical oxidation	3,59E-15	3,47E-15	3,22E-15	3,12E-15
acidification	4,78E-14	4,75E-14	4,66E-14	4,60E-14
eutrophication	2,06E-14	2,06E-14	2,05E-14	2,03E-14

Table 4: Normalized impact assessment results.

4 RESULTS

A validated conceptual model of a co-gasification IGCC power plant has been performed with a very good agreement between model results and ELCOGAS data. Future work will be envisaged to further improve the model simplifications and optimize the process based on economic and environmental considerations.

Differences found between simulated and real data may be caused by a combined effect from several simplifications where this model relies on at this point. Namely, the pyrolisis model that estimates the production of char, nitrogen and sulphur compounds is based on experimental correlations. Char combustion and gasification reactions are also based on experimental correlations. However, these correlations have been taken from the literature and do not exactly correspond to the actual raw material mixtures. ANN results are limited to an interval of variation of gases composition. Also, the combustion of the clean gas is modeled with a Gibbs reactor. According to this LCA, toxicity impacts to humans, fresh water and terrestrial ecosystems are very low; also very low are the impacts to photochemical oxidation (smog formation) and to ozone depletion potential. Most important impacts are found for marine ecosystem damages and for abiotic depletion, these impacts originate from raw material extraction. Cogasification results are used to estimate AP and GWP.

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