Simultaneous Design of a Coal Pyrolysis and Combustion Cogeneration Process.

Tomás Saldarriaga Villa[a]

Diego Andrés Acosta Maya[b]

[a] *Process Engineering Student, EAFIT University, Medellín, Colombia*
[b] *Advisor, Process Engineering Department, EAFIT University, Medellín, Colombia*

Abstract

In this project a Coal pyrolysis and combustion co-generation process was designed per raw materials and energy generation restrictions (i.e., 20 to 30 kTon/yr of Coal and maximum electricity generation of 10 MW.) Process equipment as pumps, furnaces, compressors, heat exchangers, gasifiers and packed absorption columns were designed per heuristics and engineering standards. In addition, their costs were estimated. DWSIM simulation was conducted by creating a hypothetical compound per ultimate and proximate coal analysis and its combustion by Gibbs reactors was attained. With the simulation, a Plackett-Burman design of experiments (PB DOE) was performed taking into account air to coal mass flow ratio, gasifier temperature, absorbers' solvent mass flowrate, energy recovery boiler superheated steam temperature and pressure, and syngas compressor discharge pressure, as factors and electricity generation as response resulted in ca. 25 kW to 31 kW improvement. The most influential factors in the PB were detected by a Bayes discrimination model R package were the syngas compressor discharge pressure. However, raw material availability did not fulfill electricity generation needs of 10 MW (ca. 25 kW for the base case and 31 kW for the optimized case were obtained) and compared to standard coal cogeneration plants (100-1000 MW) did not turn out to be economically viable. Although the technical feasibility was possible, process equipment was not within standard sizes for turbines nor the energy recovery boiler. We deem possible to explore further this matter under more raw materials availability favorable conditions.

1. Introduction

Colombia has large amounts of natural resources. Sinifaná coal basin is located at the southwest of the department of Antioquia in Colombia. This is a set of coal mines that hosts the mine El Túnel de Bellavista exploited by local miners. The mine produces 2,500 Tons of coal per month mainly used for steam generation in the metropolitan area of Medellín and eastern Antioquia. Unfortunately, this coal is not used for the carbo-chemistry industry, exports, nor pyrolysis nor gasification processes to produce heat for energy through synthesis gas (syngas) where coal has better economic potential. Coal pyrolysis and combustion for a cogeneration plant design, simulation and optimization is pursued in this work. The financial and technical viability of the project are explored, and the results compared to other cogeneration plants that produce electricity from coal.

Although Antioquia is not a department that stands out for coal extraction compared to other departments in Colombia, its local coalfield, the Sinifaná coal basin, has a territory of 236 km^2 with approximately 225 million tons of coal available for exploitation. Antioquia's coal production ranges between 100,000 and 500,000 Tons per year [1]. El Túnel de Bellavista mine produces 30,000 tons/year of coal [2] and it is only used in local industries for steam generation in boilers (e.g., textiles, paper, beer, foundry plants and brick production) [3]. This project explores the combustion of this coal source for pyrolysis/gasification to produce electricity in a cogeneration process.

Unfortunately, coal exports are not viable for Antioquean coal because of its low-quality properties compared to coal extracted from other mines from the country (i.e., quality standards required for coal export cannot be guaranteed) and competitive disadvantages (i.e., other coal mines in the country are closer to ports and shipment cost is much lower) [3]. Coal use in the carbo-chemistry industry is a promising alternative for production of steel, tars, fertilizer, etc. that does not require sophisticated technology. Furthermore, coal by-products can be obtained from what is left of from coal combustion [4].

Internationally, coal will continue to be an important source of affordable energy [6] and, from a national perspective, the generation of electric energy from thermal processes represent 28,4% [7] of the electricity demand in Antioquia (i.e., In 2021 forecasted to be 9,601GWh and for 2022 forecasted to 9,776GWh [8].) These facts show valid reasons to study the design of an electric energy cogeneration process that exploits coal locally produced in Antioquia.

At first sight, one of the most attractive alternatives for coal use from the Sinifaná basin, is in the electricity generation business as it has good thermal properties and generates low emission levels below the maximum allowed by environmental laws [3],[5].

Currently, coal is one of the major energy sources around the world. Since the industrial revolution age to nowadays, coal has played one of the most important roles to satisfy humanity's energy demand. Moreover, coal´s role in underpinning economic and social progress of the world is remarkable [9]. However, in the energy industry, coal exploitation must change because of worldwide concerns about coal's combustion negative environment impact. This has prompted exploration of better coal combustion processes and research about technology development in the efficient use of coal [10].

Nowadays, there are modern procedures of coal gasification that are excellent opportunities to generate energy while minimizing negative environment impact in an economically attractive way [11]. Considering the current energy challenges and environmental problems, some coal-enriched countries have focused on green alternatives to turn coal into a clean energy source for natural synthesis gas for example [12]. Normal coal-fired power plants are based on Rankine's thermodynamic cycle, which generates electric power by producing steam in a boiler and expanding the steam through a turbine connected to an electrical generator [13], but new ideas have been proposed to replace the ancient coal-fired power plants technology approaching a cleaner coal-fired electric power generation. For example, ways of making the use of coal more renewable include (1) supercritical and ultra-super-critical technology in coal-fired plants [14], (2) reducing lifespan of plants from 40 to 30 years to decrease cumulative emission [15], (3) firing coal with biomass in conventional fossil fuel power plants [16], (4) increasing average operation temperature to improve the plants efficiency [17], and (5) special coal power plants designs that include their own system for capturing and disposing of gas emissions [18]. This work studies coal pyrolysis and combustion as a clean alternative to produce electricity.

It is important to mention that studies have estimated that there are over 860 gigatons of proven worldwide coal reserves equivalent to 130 years of continuous and rigorous extraction [19] which roughly doubles oil and natural gas combined reserves [10]. This leads us to conclude that available coal is the main fuel source used for electric power generation. Despite coal's contribution to greenhouse gas emissions world problem, coal is not always equivalent to pollution because current coal-fired power stations produce fewer emissions [9], and the massive global electricity demand indicates that thermal generation and cogeneration plants are still economically attractive. Coal currently supplies approximately a 30% of primary energy and 41% of global electricity generation, with a forecasted increase of 50% by 2030 [20]. To summarize: coal is and will be a most important and efficient long-term exploited resource.

Coal-fired cogeneration plants have been modelled in ASPEN HYSYS [21] and DWSIM [22]. Coal pyrolysis is complex and involves a large number of chemical reactions, mathematical and computational models have tried to predict accurately its actual process [23] and other works have tried to develop kinetic parameters to ease its comprehension [24]. Processes of coal combustion have been modelled due to its different methods and types of coal [25]. Furthermore, optimized simulations have tried to minimize gas emissions of coal combustion [26] and models using syngas have simulated electricity cogenerated efficiently [27].

2. Materials and methods.

Sinifaná coal basin coal was the main raw material of the project. This mineral is a combustible black sedimentary rock with a high amount of carbon and hydrocarbons. Coal is classified as a nonrenewable energy source because it takes millions of years to form. [28] The characteristics and properties of coal from El Túnel de Bellavista mine used in this project and its process simulation are shown in Table 1.

Parameter	Results %p/p
Residual Moisture	12.30
Total Moisture	16.10
Ashes	5.40
Volatile Matter	35.49
Fixed Carbon	43.81
Total Sulfur	0.41
Gross Calorific Value* **(kJ/kg)**	25,083

Table 1. Proximate analysis: Characterization of a coal sample from El Túnel de Bellavista mine. (See Appendix 1)

*Evaluated with the ASTM D5865 / D5865M – 19 method.

The main objective pursued with this specific type of coal was to produce syngas by gasification, mainly composed of carbon monoxide (CO), hydrogen (H_2), nitrogen (N_2) and carbon dioxide (CO_2). This was used to cogenerate electricity by recovering heat from the high temperature of the syngas exiting gasification stream, by generating superheated steam that enters a steam turbine and produces electricity. Syngas cooled stream enters a turbine and generates more electricity. [29]. Due to environmental regulations, syngas processes must have sulfur recovery units (SRU), for disposing substances that come from sulfur (e,g, SO_x), and for capturing CO_2 [30].

While pursuing the gasification alternative for coal use and taking into account coal production in-situ, it was found that this parameter is too low compared to actual coal power plants. However, this project explores an integrated gasification combined cycle (IGCC) technology despite of the low production rate of coal compared to other IGCC plants [31]. A combined cycle in IGCC includes a gas turbine, a heat recovery steam generator and a steam turbine [32]. Studies have shown that IGCC processes obtain higher efficiencies, better environmental performance and produces less SO_x and CO_2 emission than other coal combustion technologies [31].

Process design was based on syngas processes found in the literature [33] and by heuristic rules. Process simulation was performed using open-source software DWSIM sequential modular steady state simulator that comes with two CAPE Open thermodynamic databases, ChemSep and a native thermodynamics package [34]. This simulator was created by Daniel Medeiros and allows user to better understand the behavior of chemical processes at no cost [35].

The design and simulation of a coal pyrolysis/gasification and combustion process shown in this project use: (1) A gasifier and a combustor simulated as a Gibbs Reactors, (2) a compressor to pressurize syngas, (3) two turbines for electricity generation from superheated steam and syngas, (4) absorption columns to dispose of CO2 and SOx, (5) a boiler to generate superheated steam, (6) heat exchangers to decrease syngas temperature and (7) a pump to pressurize water. All equipment design calculations can be found on the appendix.
Peng-Robinson thermodynamics package was used for the simulation as per literature recommendations [31]. Steam Tables were used for the superheated steam generation section, and NRTL for the absorption columns. Validation of these property packages was performed using cases from the literature for each of the unit operations modelled with an error range between 6% and 8% in electricity generation.

Engineering standards were used in the project including National Electric Manufacturers Association (NEMA) for engines and electric generators, ASME Boiler and Pressure Vessel Code (BPVC) for standard vessel dimensions and vessels thickness. Commercial catalogs for turbines and boilers from Siemens and Babcock & Wilcox were reviewed.

For the financial analysis of the process, fixed capital costs and costs of manufacturing without depreciation were estimated by using Turton's correlations [36]. Revenues from electricity sales coupled with the aforementioned costs were used for a discounted and non-discounted cumulative cash flow diagram. All financial estimated were made in $USD.

In terms of the process optimization and due to raw materials and energy generation restrictions, a Plackett-Burman fractional factorial design of experiments was performed with air to coal flow mass ratio, gasifier outlet temperature, energy recovery boiler superheated steam pressure, energy recovery boiler superheated steam temperature, absorption column (K1) solvent flowrate, syngas compressor discharge pressure, and absorption column (K2) solvent flowrate as factors, and kW steam turbine, kW syngas turbine and total kW as response variables.

3. Results and analysis

Process Description – Base case

3.500 kg/h of coal with previous shown specifications and a particle size distribution range between 3cm and 4cm are transported by a conveyor belt into the gasifier hopper and mix with 50 kg/h of air. The gasifier (C1) has 6 m^3 of capacity, operates in atmospheric pressure and the outlet temperature of the main product is 1200 ºC. This gasification produces a lot of waste in form of ash. Then, the hot gas product is cooled by a 25m^2 (heat transfer area for saturated vapor and superheated steam generation) boiler (D1) to produce 530ºC superheated steam at 50 bar by a reciprocating pump (P1A/P2B). The 77 kg/h of superheated steam feeds a steam turbine (A1) that produces 8.96 kW of energy.

Later on, the cold gas product is sent to a 0.25m diameter and 1.18m height Pall rings packaged absorption column (K1) to remove the amount of SO_2 with water. The absorption column uses 728 kg/h of pure water as a solvent, and this captures all SO_2 in the gas product producing an acid water which later is delivered to a specialized company that is able to treat these industrial wastes that contain sulfur diluted in water to latter disposal [37].
The sweetened gas product now is mixed again with a small amount of air to be then pressurized (V1) and cooled (W1) to 35 bar and 157ºC, respectively to feed a combustor (C2), the final step of producing syngas at 550ºC. This pressurized hot syngas enters into a gas turbine (A2) that produces 16.9 kW of energy and a 6 bar exhaust, that finally is cooled (W2) into 25ºC to be able to enter in the 0.31m diameter and 2.33m height Pall rings packet absorption column (K2) that is responsible to capture part of the CO_2 produced in the process. The column uses 9050 kg/h of an aqueous mixture of water and caustic soda (5%) as solvent.
Cooling water was used as utility in both W1 and W2. Figure 1 illustrates process diagram.

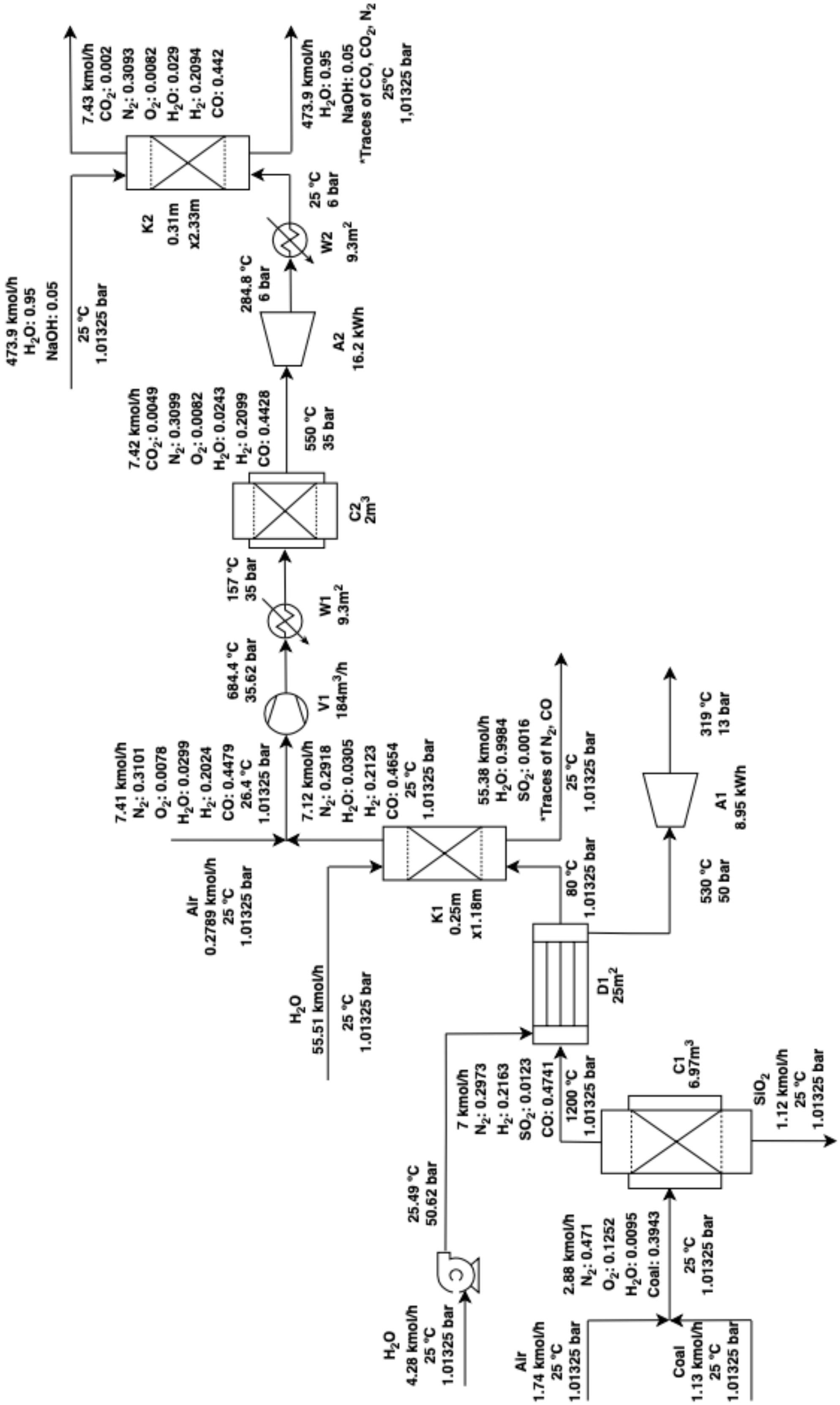

Figure 1. Base case process flow diagram with basic information.

Analysis – Base case

IGCC is a robust technology that provides electricity in orders of magnitudes of 100MW to 1000MW [38]. Compared to other coal cogeneration plants and research projects in the open literature [31], [32], [33], [39], the process discussed here is clearly undersized. Coal mass flow requirements for actual and conventional IGCC plants and processes ranges between 20 and 50 kg of coal per second and greatly exceed the capacity of coal production that the El Túnel de Bellavista coal mine can handle. It is possible to affirm that this process is economically inviable; considering that the coal mass flow of the other plants and processes is in the order of magnitude of tones per process hour, compared to the few kilograms per hour fed to this process. As coal flowrate is directly proportional to electricity generation, and economic income, there's not enough revenue to repay the fixed capital investment. Additionally, all the equipment for an IGCC plant is considerably high (reactors, turbines and energy recovery systems), that leads into a large fixed capital investment (FCI_L). In this case, more than 4 and a half million were estimated to cover the FCI_L, 1.3 million in working capital and 65,000 of the land cost. Also, in addition to this, it is necessary to invest more than 18 million per year in manufacturing costs (COM_D). This represents a considerably high cost that cannot be recovered with the $34,000/yr income from selling electricity locally (profits estimated using local costs of energy selling [40]). To be able to repay these substantial costs, IGCC technology plants need larger electricity generation magnitudes in actual coal processes [39]. Figure 2 illustrates the negative internal rate of return and the large losses that the project presents, which only improves at the end of its useful life by selling all its equipment having a projected salvage price as 10% of FCI_L. These facts confirm that, although this conceptual design provides an alternative to use coal, the project execution will represent an inevitable economic loss and incapable of being profitable.

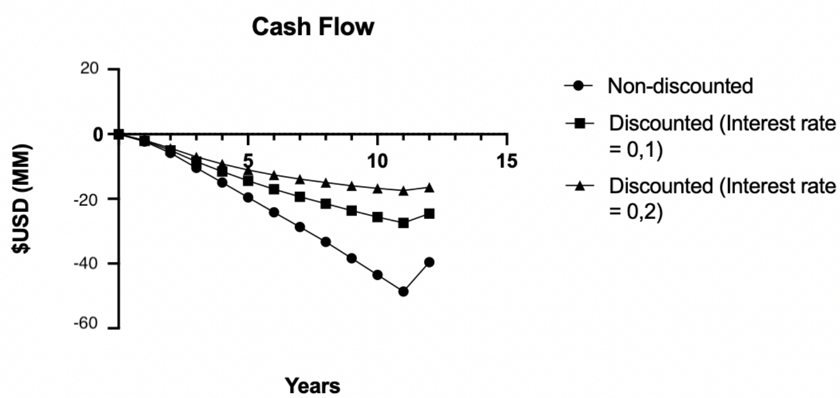

Figure 2. Non-discounted and two interest rated discounted Cash Flow.

However, taking into account that the process designed in this project is based on successful cases from the literature and real cogeneration plants, this project is technically viable since it fulfills its main objective of cogenerating electricity from a specific amount of coal available from the selected mine. Besides, as a modern coal electricity generation plant, it is attractive by its effective SRU and its energy recovery system. Also, methane [41] and/or methanol [42] production is an opportunity to employ the sweetened syngas exhaust (rich in CO and H_2), subproduct of electricity cogeneration.

Hence, analyzing the size of the process equipment and comparing them to other actual cogeneration equipment, this process fits in what can be considered a coal mini-cogeneration plant, the process simulation that exposes conceptual design can be found in appendix. To be able to cogenerate electricity with an IGCC or a similar technology, larger operating flows and equipment are needed.

In terms of process technology, this project is also in disadvantage compared to the guide processes in literature because these ones count with air separation units (ASU). This process unit separates atmospheric air into its primary components, air and oxygen by fractional or cryogenic distillation, membranes or pressure swing absorption methods [43]. By having availability of pure oxygen, the pyrolysis and gasification process is more efficient and syngas quality is better [33]. However, the implementation of an ASU increases the fixed capital investment, which in this process is already considerably high. This can be considered another restriction for the project because investors are not able to implement ASU by its elevated cost

However, all the design, simulation and economic analysis of the coal pyrolysis, gasification and combustion process to cogenerate power provided in this document can be scaled-up to make it economically feasible for other processes by having a higher coal mass flowrate and hence, having more electricity generation capacity.

Optimized case.

Taking into account coal availability, electric energy and investment restrictions, optimization options were limited and a PB DOE approach was chosen. By using RStudio and BsMD package [44], for Bayesian screening and model discrimination, the optimum conditions for the process were determined. Table 2 shows, a series of runs changing process variables levels between determined values that were used to maximize the response variables (1) Y_1: kW generated in the steam turbine, (2) Y_2: kW generated in the syngas turbine and (3) Y_3: kW generated in the whole process. An R script ran in RStudio was used to analyze the PB DOE and can be found in the Appendix.

Run	X_1	X_2	X_3	X_4	X_5	X_6	X_7	Y_1	Y_2	Y_3
1	55	1400	85.62	650	1000	50	600	13.7	15.7	29.3
2	50	1400	50.62	650	1000	50	473.9	10.5	19.5	30.0
3	50	1200	85.62	530	1000	50	600	11.5	19.5	31.0
4	55	1200	50.62	650	727.73	50	600	10.5	19.9	30.4
5	50	1400	50.62	530	1000	35	600	9.0	16.9	25.9
6	50	1200	85.62	530	727.73	50	473.9	11.5	19.5	31.0
7	50	1200	50.62	650	727.73	35	600	10.5	16.9	27.4
8	55	1200	50.62	530	1000	35	473.9	9.0	16.9	25.9
9	55	1400	50.62	530	727.73	50	473.9	9.0	19.5	28.4
10	55	1400	85.62	530	727.73	35	600	9.0	16.9	25.9
11	50	1400	85.62	650	727.73	35	473.9	10.5	17.7	28.2
12	55	1200	85.62	650	1000	35	473.9	10.5	17.7	28.2
Base Case	50	1200	50.62	530	727.73	35	473.9	9.0	16.9	25.9

Designation	Process variables	Unit
X_1	Air to coal flow mass ratio.	kg/h / kg/h
X_2	Gasifier outlet temperature.	°C
X_3	Energy recovery boiler superheated steam pressure.	bar
X_4	Energy recovery boiler superheated steam temperature.	°C
X_5	Absorption column (K1) solvent flowrate.	kg/h
X_6	Syngas compressor discharge pressure.	bar
X_7	Absorption column (K2) solvent flowrate.	kmol/h
Y_1	kW steam turbine	kW
Y_2	kW syngas turbine	kW
Y_3	Total kW	kW

Table 2. (A) – Top. PB DOE runs. (B) – Bottom. Factors and response variables.

BsMD package analyzes the data and produces Bayes plots in which the most significant process variables stand out above the others with the largest posterior marginal probability. Figure 3 summarizes the results of 12 different runs by performing a posterior marginal probability analysis in which the most significant factors display the highest marginal probability. In this case the probability that none of the factors are significant is the largest for Y_1 and Y_2 (higher than 95%) and of the order of 20% for Y_3. Factor X_6 is most significant for Y_3. In order to find the optimized case, the run with the largest amount of electricity generated in the process was chosen.

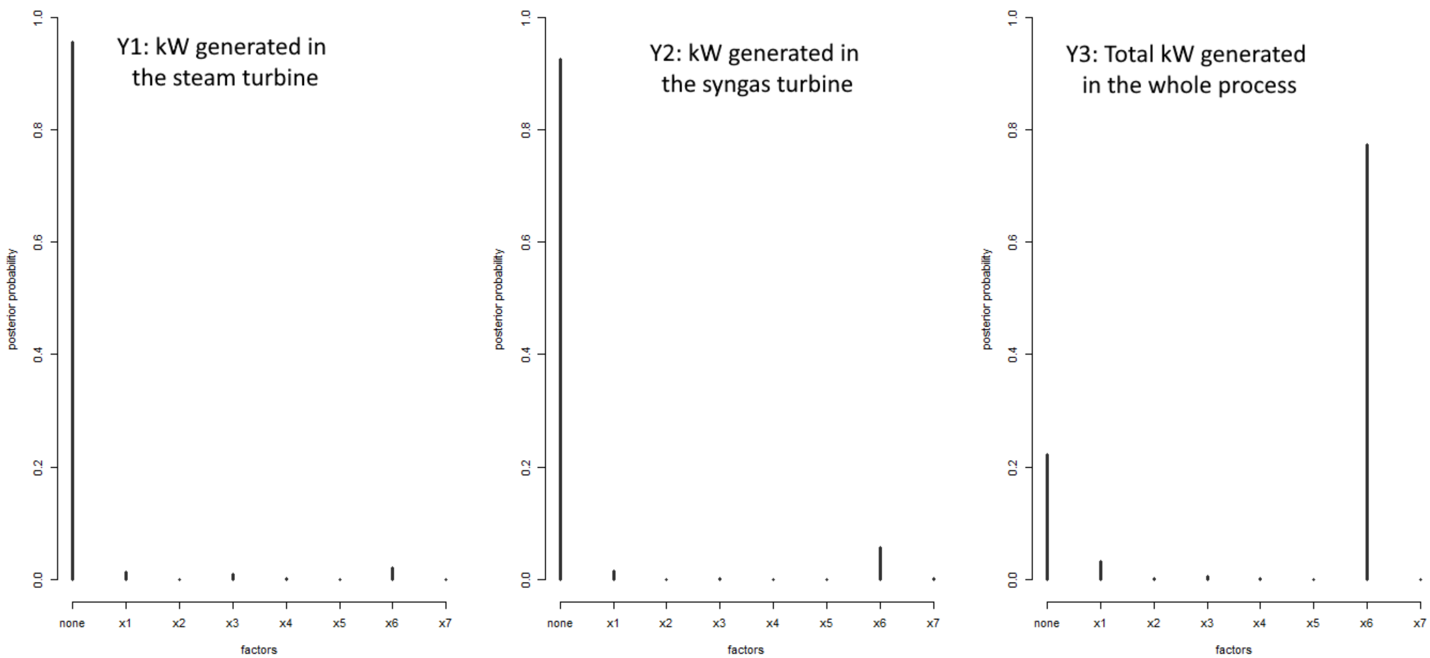

Figure 3. Posterior probability vs process variables.

As it can be seen in the previous plots, the process variables that have a larger bar are the ones that higher impact in the response variables. Analyzing all three plots, X_6 (compressor discharge pressure) is the variable that contributes the most for the electricity maximization by increasing the kW produced in the process. This result makes sense since the syngas compressor discharge pressure is the process variable that control the inlet pressure of the main turbine, the syngas turbine. Varying the compressor discharge in a range selected by Siemens common commercial turbines [45], the pressure difference generated in the syngas turbine can increase, hence the work generated by this turbine is larger and therefore, the electricity generation is also larger.

X_1 (air to coal flow mass ratio) is another variable that affects the response variables but much less compared to X_6. In spite that the oxidizing agent is important in the coal gasification/pyrolysis process, having to use air, is not most efficient and negatively impact the whole process.

It can be said that X_3 (superheated steam pressure) has a very low incidence in all three scenarios. However, since the energy recovery boiler superheated steam pressure defines the inlet steam turbine pressure, this process variable does have some incidence due to the pressure gradient that occurs in the steam turbine.

As a final result of the PB DOE, the best from the new 12 cases increases the electricity generation from 25 kW to 31 kW. Although the PB DOE method improves the base case, there is no actually substantial improvement in the process. Further, the financial analysis of the improved case only rises the revenues in approximately 3.5% that isn´t enough to repay fixed capital costs as in the base case. The PB DOE parameters and files can be found in the appendix.

4. Conclusions.

A conceptual design, simulation, and optimization of a syngas from coal pyrolysis/gasification and combustion process was performed for a 25kW IGCC technology plant. DWSIM process simulation using Peng-Robinson and NRTL thermodynamics property packages, was used to model the process. The resulting process was not profitable due to its low coal mass availability and electricity generation that made payback impossible. On the other hand, technical feasibility for the process was verified as an alternative for El Túnel de Bellavista coal mine located in Angelópolis, Antioquia.

Coal combustion was simulated by Gibbs reactors to produce hot syngas. Energy from cooling coal combustion syngas at 1200ºC exiting the gasifier was recovered by producing superheated steam with an aquo-tubular boiler and generating electricity with a steam turbine. Also, electricity was generated by using a syngas turbine. Absorption columns sweetened the syngas in two different process stages capturing SO2 and CO2 to fulfill environmental regulations.

Process optimization was performed with a Plackett Burman Design of Experiments to maximize net electricity generation that increased from 25kW to 31kW. For future projects, it is advised to set aside restrictions and scale-up the design and process simulation to find the process conditions that make the project profitable.

5. Appendix.

Table x. Additional documents included within the project degree.

Name	Autorship	File type	Google drive link
Characterization of a coal sample from El Túnel de Bellavista mine.	Universidad Nacional de Colombia	.pdf	https://is.gd/rQJZ0w
SimulationParametes	Tomás Saldarriaga Villa	.docx	https://is.gd/J8sFaN
Base Case	Tomás Saldarriaga Villa	.dwxmz	https://is.gd/J8sFaN
COAL PROCESS	Tomás Saldarriaga Villa	.png	https://is.gd/J8sFaN
Coal	Tomás Saldarriaga Villa	.json	https://is.gd/J8sFaN
Coal	Tomás Saldarriaga Villa	.dwcsd2	https://is.gd/J8sFaN
PFD_BaseCase	Tomás Saldarriaga Villa	.png	https://is.gd/XdEQ6Q
CASE 3	Tomás Saldarriaga Villa	.dwxmz	https://is.gd/J8sFaN
RScriptPBDOE	Tomás Saldarriaga Villa	.R	https://is.gd/XdEQ6Q
Design_A.Column_K1[46]	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_A.Column_K2 [46]	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Boiler	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Gasifier [47][48]	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Heat_Exchanger_W1	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Heat_Exchanger_W2	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Pump	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Steam_Turbine	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Syngas_Compressor	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA
Design_Syngas_Turbine	Tomás Saldarriaga Villa	.xlsx	https://is.gd/fofWHA

Non-Discounted Cash Flow	Tomás Saldarriaga Villa	.png	https://is.gd/e69zYO
Discounted Cash Flow (IR=0.1)	Tomás Saldarriaga Villa	.png	https://is.gd/e69zYO
Discounted Cash Flow (IR=0.2)	Tomás Saldarriaga Villa	.png	https://is.gd/e69zYO
COSTS	Tomás Saldarriaga Villa	.xlsx	https://is.gd/e69zYO
Plackett-Burman	Tomás Saldarriaga Villa	.xlsx	https://is.gd/XdEQ6Q
SpecSheet_A1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_A2	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_C1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_D1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_K1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_K2	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_P1AP2B	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_V1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_W1	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1
SpecSheet_W2	Tomás Saldarriaga Villa	.png	https://is.gd/3g8my1

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