

SIMULATION OF IGCC TECHNOLOGIES: INFLUENCE OF OPERATIONAL CONDITIONS (ENVIRONMENTAL AND FUEL GAS PRODUCTION)

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Resumen

La Gasificación Integrada con Ciclo Combinando (IGCC) es una de las tecnologías de generación de potencia más promisorias para el aprovechamiento de recursos energéticos como carbón y biomasa. Los altos beneficios ambientales y la alta eficiencia de conversión energética diferencian a esta tecnología de las empleadas tradicionalmente. El comportamiento de una planta IGCC es afectada por diferentes aspectos tecnológicos y operacionales, como son el tipo de gasificador, el agente gasificante, el rango del carbón, las condiciones ambientales y la demanda de potencia. Considerar todo este conjunto de variables obstaculiza el proceso de análisis y diseño de esta clase de tecnologías, haciendo necesario el uso de programas de simulación termodinámica, como Hysys y GateCycle. En este trabajo, se realizaron simulaciones en Hysys para determinar la composición del gas de síntesis obtenido a partir de diferentes tecnologías de gasificación, cinéticas de reacción, agentes gasificantes y tipos de carbón. Estas composiciones de gas fueron empleadas para establecer el comportamiento y eficiencia de un Ciclo Combinado mediante el uso del programa GateCycle, bajo diferentes condiciones de ambientales de operación. Los resultados obtenidos muestran el comportamiento para diferentes tecnologías IGCC bajo diferentes condiciones atmosféricas y de operación, y tipo de carbón.

Palabras Clave: Gas de síntesis, IGCC, Simulación termodinámica.

Abstract

Integrated Gasification Combined Cycle (IGCC) is one of the most promising technologies for power generation; the environmental benefits and the higher energy conversion efficiency distinguish it from traditional coal generation technologies. IGCC performance is affected by different technological and operational aspects, e.g. gasification technologies, gasifier agent, coal rank, environmental conditions, and power demand. This group of conditions hinders the assessment process and conduces necessarily to the use of thermodynamic simulation tools. In this work thermodynamics analysis simulations were conducted in Hysys and GateCycle. Simulations in Hysys were carried out for different gasification technologies, kinetic reactions, gasifying agents and coal types. Syngas composition and lower heat values were calculated for the all different conditions and had been loaded into GateCycle in which Combined Cycle efficiency were studied for different environmental conditions. Results show behavior for IGCC technologies at different places according to its environmental and operational conditions, and coal rank.

Keywords: Synthesis gas, IGCC, Thermodynamic simulation.

1. INTRODUCTION

Thermodynamic simulations are used to estimate general behavior of gasification plants as function of available energetic resources as well operational and environmental conditions. Commercial software is used to do these simulations (Bassily,2007; Zheng y Furinsky,2005)). Through this software is possible to analysis different generation capacities and its behavior under different air, fuel, nitrogen, oxygen, steam and water flow rates. Besides, it is possible to scale up equipments involved in power generation cycles by means of accuracy energy and mass balances. Additionally, thermodynamic simulations can help to establish kinetics behavior of complex phenomena presented in gasification process. Syngas composition is achieved by the knowledge of raw fuel composition used, environmental conditions and kinetic reactions, which are function of reactor pressure and gasification technology.

GateCycle software is used in this work for thermodynamic simulation of power generation combined cycle; meanwhile Hysys software is used for the simulation of gasification process over different commercial available technologies. Below it is presented the methodology used for thermodynamics simulation of IGCC plants, as well the results obtained through Hysys and GateCycle interaction. Results for gasification simulation were obtained at different environmental conditions, coal rank and gasifier configurations (i.e. fluidized bed, fixed bed and entrained flow gasifiers). These results were loaded into GateCycle model and IGCC performance was evaluated taking into account gasification behavior, as well as energy efficiency of Combined Cycle at different operational conditions (i.e. atmospheric pressure, temperature and relative humidity).

2. SIMULATION OF GASIFICATION TECHNOLOGIES

The gasification process can be regarded as the most important process in an IGCC plant because it is responsible for providing the syngas that will be used in a combined cycle power generation process after it has been cleaned. The productivity and efficiency of an IGCC plant depends greatly on the gasification technology employed. The selection of the technology

to be used is carried out by conducting a detailed study of the advantages and disadvantages of one compared to the other, always keeping in mind the power level to be produced, the type of the carbonaceous material and the gasification medium (air, oxygen); as well as other factors of particular interest.

Depending on the flow of the gasification medium and the carbonaceous material, gasifiers can be divided into the following three types: entrained bed, fluidized bed (bubbling or circulating) and fixed (or moving) bed. Depending on the power level to be produced, these gasification processes can be classified as being of a large size (entrained bed), a medium size (circulating fluidized bed) or a small to medium size (fixed bed) (Bassily,2007).

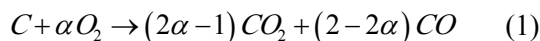
The gasification process involves a series of reactions that due to their endothermic nature require a considerable amount of heat that is provided by the combustion reactions that occur because of the presence of oxygen, making this process autothermic in its characteristics. The reactions that occur in this process are heterogeneous and homogenous, the first being heavily dependent on the nature of the carbonaceous material. For this reason, a great deal of relative experimentation is involved in determining reactivity, which in turn implies that there are great difficulties when it comes to the simulation of the gasification process.

2.1. Setting up gasification models in Hysys

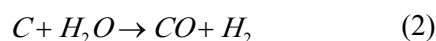
The effects of the operational parameters and the type of coal used on the gasification reaction rate must be known in order to ensure an optimum performance. However, few studies on the reactivity of pressurized coal gasification have been sufficiently thorough, rendering the experimental results difficult to reproduce with the use of simulation schemes obtained from the previously mentioned programs; since reaction rates are highly dependent on the nature of the fuel used, and in the case of coal the difficulty increases due to its particularities.

In this study of the simulation of gasification technologies, several reasonable approximations had to be made in order to consider the reaction systems from a global point of view. Among the many reactions involved in the gasification process, the main determinants of the composition of the syngas obtained are the following:

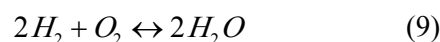
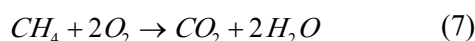
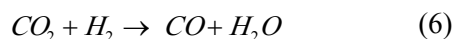
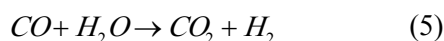
Solid-gas Type Reactions (Heterogeneous)
(Campbell, McMullan y Williams, 2000)



where α is a number between 0.5 and 1.



Gas-gas Type Reactions (Homogeneous) (Campbell, McMullan y Williams, 2000; Treviño, 2003).



The kinetic parameters for reactions (1) to (3) were obtained from the study performed by Harris and Robert (2000), reaction (4) from Niksa and Liu (2004), and those pertaining to equations (5) to (9) from Chejne and Hernandez (2002).

The simulation programs available on the market for IGCC type systems allow for the evaluation of the general behavior of different power generation cycles, making it possible to estimate the consumption level of air, fuel, nitrogen, oxygen, steam and water, among others, in order to achieve a desired level of power generation. In addition to this type of values, the programs allow for the sizing of the selected equipment by employing the knowledge and estimation of certain mass and heat transference rate values obtained previously.

For the gasification process in particular, it is possible to use programs such as Chemcad, Hysys and Aspen which are capable of estimating the final composition of syngas from the use of ideal reactors and the knowledge of the initial composition of the solid fuel. However, due to the complexity of the gasification process this is usually carried out by considering the balance of a reactive system under reasonable suppositions according to multiple bibliographical references (Zainal et al, 2001; Li et al, 2001; Altafini et al, 2003; Deiana et al, 2007); but the various gasifier technologies employed prevent identifying their effects

on the composition of the gas produced. In contrast to the aforementioned studies, De Jong et al (2003), managed to simulate gasification in a fluidized bed by means of a flux reactor model using a subroutine of the Aspen Plus program; in which 353 homogenous reactions, attainable in the gasification process, were involved and the results were very close to those obtained through experimentation. More recently, Zheng and Furinsky (2005), developed simulation schemes with the use of Aspen and Fortran, the latter employed in the gasification process, in order to compare commercial gasifiers made by Shell, Texaco, BGL and KRW. Thus, despite the fact that there are many demonstrative, experimental and various commercial IGCC plants worldwide, even today little is known about some of the variables involved to carry out the simulation process.

Hysys software was used in this project to conduct the simulation of different gasification technologies. For this purpose, several approximations were built up from the theory of chemical reactors (Levenspiel, 1999), allowing the representation of real reactors as a mixture of ideal reactors. In accordance to this, the fluidized bed technology has been modeled as a mixture of recirculating piston fluid reactors (or PFR), as seen in Figure 1, and the entrained bed as two PFR's in a series (Figure 2). The fluidized bed technology has been portrayed as a series of pairs of PFR's in series plus an equilibrium reactor for methanization. In the case of the former, the feeding is limited to only a fraction of the necessary oxidizer, hence allowing the consumption of a portion of carbonaceous material (Figure 3).

The simulation of gasification technologies was performed using simulation schemes (Figures 1 – 3) for five different types of coals available in Colombia. Table 1 shows the characterization for each of the aforementioned coal types and Table 2 presents the feed fluxes for each reactor.

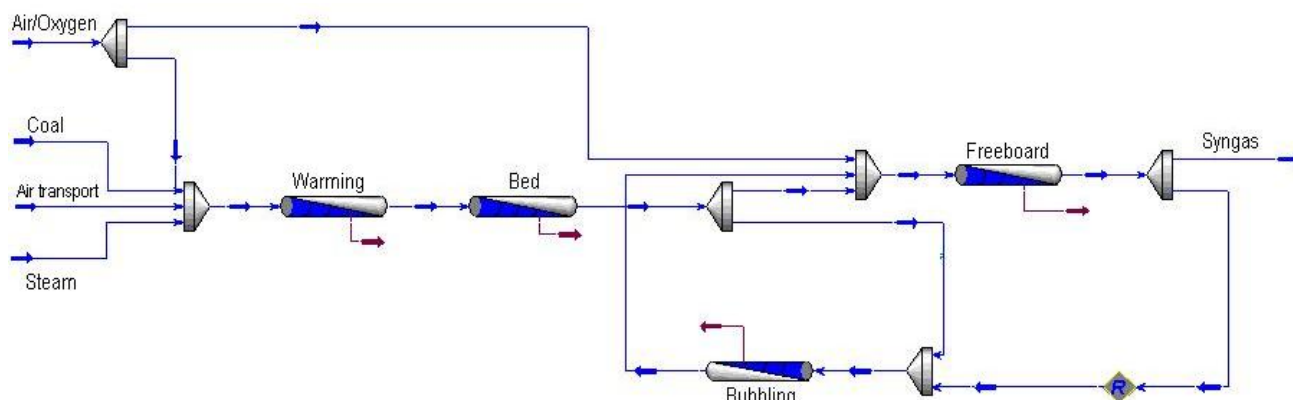


Figure 1. Fluidized Bed Technology Simulation Model

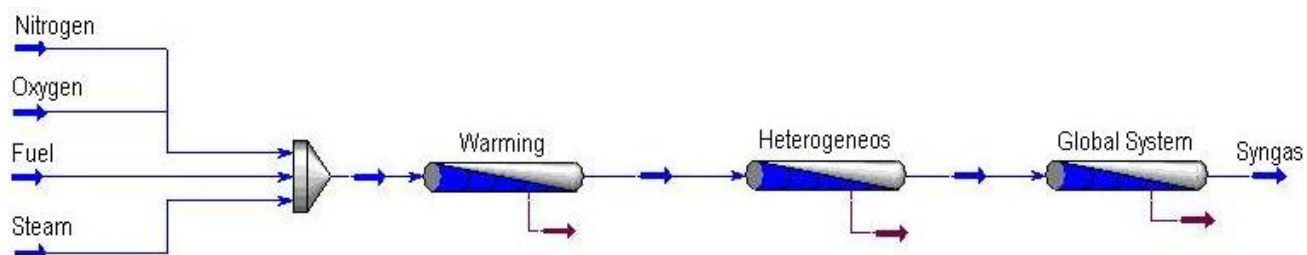


Figure 2. Entrained Bed Technology Simulation Model

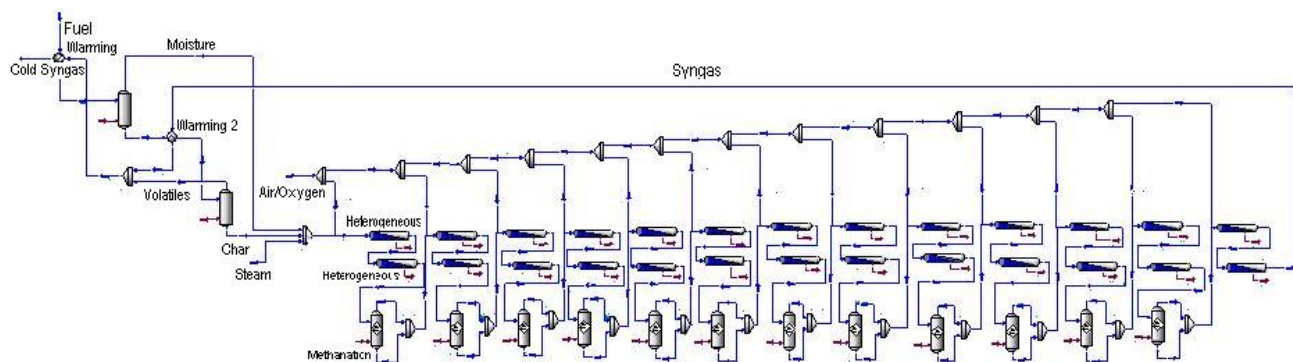


Figure 3. Fixed Bed Technology Simulation Model

Table 1. Elemental analysis coals used for gasification technologies simulation

Species	Case 1	Case 2	Case 3	Case 4	Case 5
C	66.25	69.09	75.54	76.56	71.26
H	3.59	5.14	3.72	5.49	4.84
N	1.37	1.45	2.03	1.60	1.54
O	9.48	9.12	5.96	6.22	5.98
Cl	0.03	0.02	-	-	-
S	0.43	0.655	0.98	0.98	1.16
Ashes	6.94	7.965	16.45	8.77	10.79
HHV (MJ/kg)	26.68	26.147	30.27	31.05	29.21

Table 2. Input data for each gasifier scheme

Gasification Technology	Case	Coal Flux, (kg/s)	Oxygen/Coal, (kg/kg)	Steam/Coal, (kg/kg)
Circulating Fluidized Bed	1-5	9.27	0.608	0.168
	1		0.390	
Entrained Bed	2	24.06	0.187	0.111
	3		0.216	
	4-5		0.234	
Fixed Bed	1-5	92.59	0.381	0.302

2.2 Results and analysis of gasification simulations

Table 3 displays cold efficiency and the composition and higher heat value of the resulting synthesis gas for each gasification technology used on each type of coal reported in Table 1. Several analyses focusing on gasification and the global system were conducted. Gasification in particular has demonstrated, as seen in Figure 4, that the efficiency of the process has a tendency to decrease as the carbonaceous material used as raw material, becomes richer in ashes. This implies that when coal extracted from the Case 3 type zone is used the gasification process is less efficient. The effect of the amount of carbon on the efficiency of the gasification process (Figure 5) and the higher heat value of the synthesis gas produced (Figure 6) were also analyzed, obtaining as a result the nonexistence of a tendency that would allow linking these parameters as a function of carbon content.

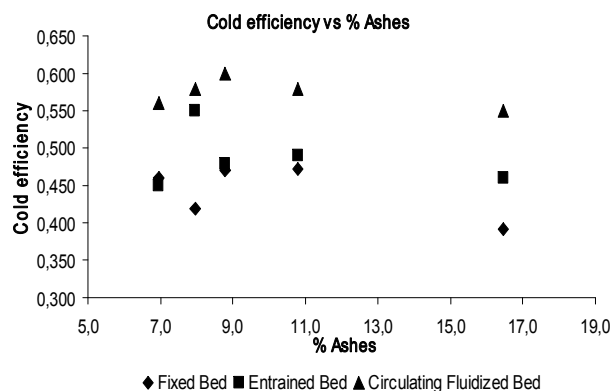


Figure 4. Efficiency variation with ash % in coal

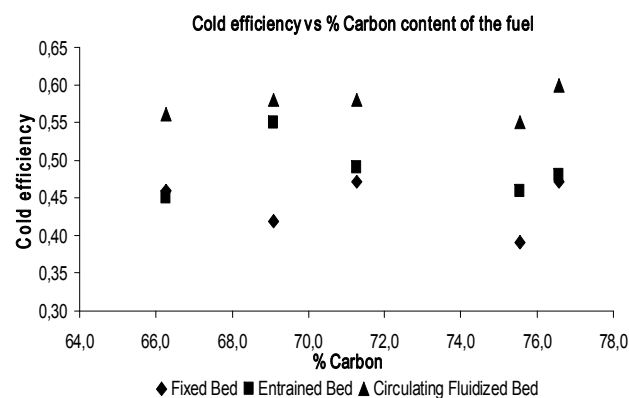


Figure 5. Variation in efficiency with the % of Carbon

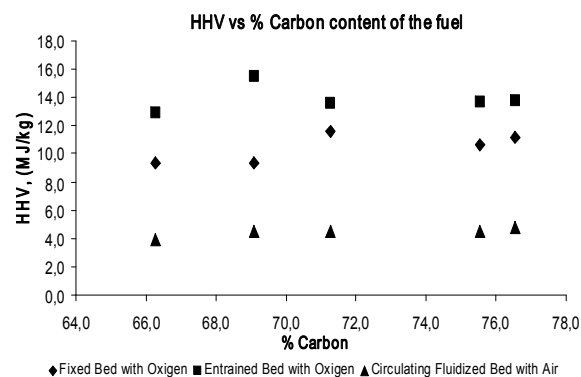


Figure 6. Higher heat value variation of the synthesis gas with the % of Carbon

3. COMBINED CYCLE SIMULATION IN GATECYCLE

Integrated Gasification Combined Cycle (IGCC) is one of the most promising technologies for power generation; the environmental benefits and the higher energy conversion efficiency distinguish it from traditional coal generation technologies. IGCC performance is affected by environmental and operational aspects, including gasification technology, coal rank and environmental condition, among others. In the earlier section it was presented the steps to simulate gasification process with Hysys software. GateCycle software is now used for combined cycle thermodynamic simulation. Initially, the configuration of combined cycle plant is settled up according to regular configurations for this kind of systems. Secondly, the models available in GateCycle for equipments used to develop the diagram of a combined cycle systems (gas and steam turbine, heat exchanger, evaporators, among others) are validated through

comparison between simulation results with available values for a benchmark plant. Finally, gasification technologies and environmental conditions effects over combined cycle behavior are considered by introduction in GateCycle of different syngas composition obtained during gasification simulations with Hysys.

As benchmark plant was used the ELCOGAS plant at Puertollano. This plant has a successfully worldwide industrial behavior and had been widely used as standard reference for the study of new technologies (Campbell, McMullan y Williams, 2000). Puertollano's combined cycle has a 317 MW net capacity (182 MW from gas turbine and 135 MW from steam turbine). Shell gasification technology with pure oxygen is implemented in Puertollano, the flow is ascendant and fuel feed up is dried with nitrogen (Treviño, 2003). Heat recovery steam generator (HRSG) is used to recover heat from exhaust gas turbine gases and from cooling process of raw syngas.

Table 3. Synthesis gas composition obtained through the simulation of different gasification technologies.

Circulating Fluidized Bed								
Case	Specie							
	H ₂	CO	CH ₄	CO ₂	N ₂	H ₂ O	HHV, (MJ/kg)	Cold Efficiency
1	14.48	21.31	0.03	6.22	50.80	7.11	3.90	56
2	17.59	22.09	0.05	4.66	49.30	6.24	4.50	58
3	17.14	22.38	0.06	4.31	50.46	5.54	4.47	55
4	18.39	23.26	0.07	3.47	50.15	4.60	4.78	60
5	17.14	22.40	0.06	4.30	50.47	5.53	4.48	57
Entrained Bed								
Case	Specie							
	H ₂	CO	CH ₄	CO ₂	N ₂	H ₂ O	HHV, (MJ/kg)	Cold Efficiency
1	37.27	55.87	0.00	5.69	1.12	0.00	12.93	45
2	49.42	44.62	0.00	4.69	1.12	0.00	15.51	55
3	39.69	54.55	0.00	4.27	1.50	0.00	13.64	46
4	40.17	54.18	0.00	4.26	1.50	0.00	13.74	48
5	39.59	54.61	0.00	4.34	1.39	0.00	13.61	49
Fixed Bed								
Case	Specie							
	H ₂	CO	CH ₄	CO ₂	N ₂	H ₂ O	HHV, (MJ/kg)	Cold Efficiency
1	36.46	9.82	10.63	32.93	0.79	9.40	9.33	46
2	36.46	9.81	10.63	32.93	0.79	9.40	9.33	42
3	40.30	11.27	12.54	34.62	1.28	0.00	10.67	39
4	45.70	9.20	9.80	29.20	0.75	5.30	11.21	47
5	46.40	9.56	10.50	30.60	0.85	2.14	11.62	47

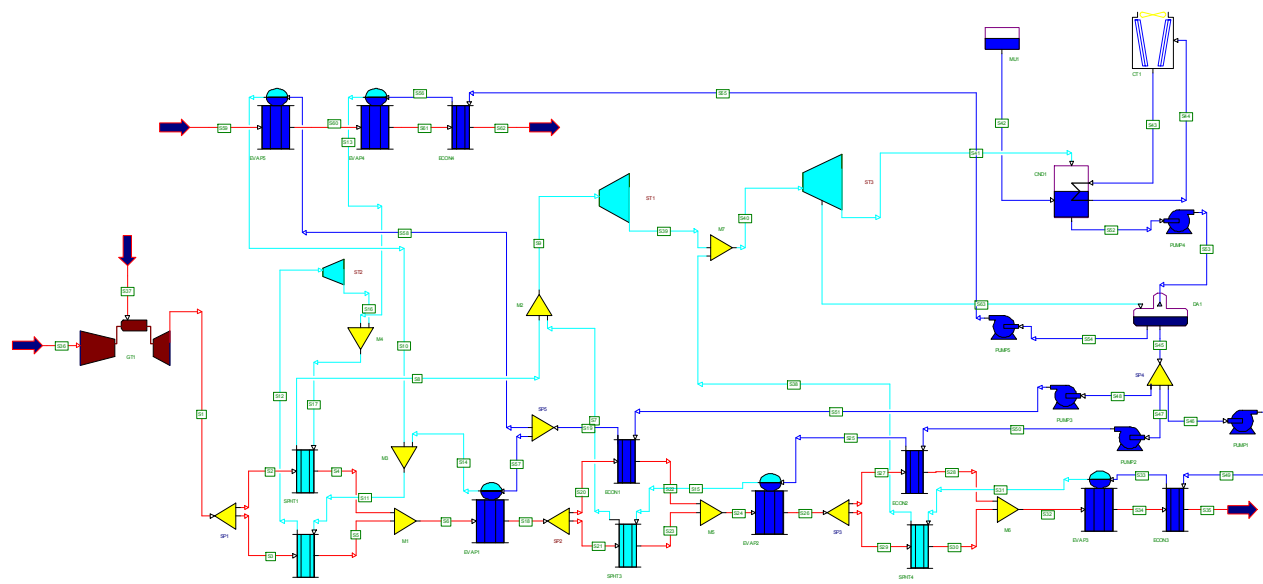


Figure 7. IGGC Gate Cycle's model

GateCycle's model (Figure 7) was developed with the information presented in Table 4. Two syngas streams are used to consider the recover of heat from raw syngas and to feed up gas turbine. In the first one, temperature, pressure and mass flow information is provide for estimation of heat recovery and steam production from the gasification island. The second stream is feed with information related to clean syngas composition as well temperature, pressure and mass flow. This stream passes through gas turbine equipments (i.e. compressor, combustion and expansion cameras) and then combusted gases goes to HRSG equipments (e.g. economizers, heaters and super heaters, and boilers) and steam production and heat recovery are estimated. Finally, the electric power generated is estimated and efficiency and heat rate is evaluated for IGCC analysis behavior.

3.1. Setting up and validations of models

Validation results for models applied in GateCycle are presented below. Turbine syngas fuel flow, pinch temperature (steam-combusted gas) and heat exchanger areas were controlled during IGCC thermodynamics simulations developed. Results obtained were validated by comparison with operational information of Puertollano's plant. Steam, gas and combined cycles power generation data were compared with our own simulations results. Besides, heat rate and efficiency of combined cycle (included coal gasification efficiency) were used to validate our thermodynamics simulations.

In Table 5 both our own simulations results and reported by peers are shown. Relative error for GateCycle simulations are below to 8%. Thus, the strategy implemented in this software was validated and then, is possible to use the methodology developed to analysis other gasification technologies and generation capacities at different operational and environmental conditions.

Table 4. Puertollano's technical specifications (Treviño, 2003)

System	Variable		Value	
Environmental conditions	Temperature [°C]		15	
	Humidity [%]		0.8	
	Pressure		1	
Coal	Flow [kg/s]		29.7	
	LHV [kJ/kg]		22550	
Syngas	Flow [kg/s]		120	
	LHV [kJ/kg]		4242	
Gasfication island	High pressure recovering temperature [°C]	In	800	
		Out	400	
	Middle pressure recovering temperature [°C]	In	400	
		Out	235	
	High pressure steam	Pressure [bar]	126	
		Flow [t/day]	230	
	Middle pressure steam	Pressure [bar]	35	
		Flow [t/day]	23	
	Heat recovery steam generator	Steam	High pressure [bar]	127
			Middle pressure [bar]	35
Low pressure [bar]			6,5	
Exchanger area [m²]		300000		
Combusted gas temperature [°C]		In	535	
		Out	103	
Gas turbine	Power [MW]		182	
	Mass flow air [kg/s]		537	
	Compression		15:1	
	Thermal efficiency [%]		34.6	
Steam turbine	Power [MW]		135	
	High pressure superheated steam	Pressure [bar]	122	
		Temperature [°C]	509	
	Reheated steam	Pressure [bar]	29	
		Temperature [°C]	517	
Air splitter unit	Air flow [kg/s]		80	
Combined cycle	Net power [MW]		317.7	
	Efficiency [%]		47.44	
	Heat Rate [kJ/KWh]		7589	

Table 5. Validation results for Puertollano thermodynamics simulation in Gate Cycle

Variable	Puertollano	GateCycle	Error [%]
Steam cycle net power [MW]	182	197,43	8,30
Gas cycle net power [MW]	135	136,95	1,14
Combined cycle net power [MW]	317.7	334,38	5,25
Combined cycle global efficiency [%]	47.44	49,93	5,25
Combined cycle Heat Rate [kJ/KWh]	7589	7210,6	4,99
Gasification island thermal efficiency [MW]	190	198,2	4,3
Air mass flow [kg/s]	537	503.81	6.18

3.2. Simulation and analysis of combined cycle for different operational conditions

Results for simulations on IGCC plants for five different cases are presented below. The simulations were performed for four types of Siemens gas turbines (Table 6) changing the inlet angle of air on the compressor in two levels (0 and 15 grades angles). The environmental conditions analyzed in the five cases are shown in Table 7. Simulations were developed using the IGCC model developed in GateCycle (Figure 7) and using syngas composition from a Hysys model presented in section 2.2 (see Table 3 and Table 8). The first step was to

evaluate IGCC plants under standard conditions of temperature and pressure (ISO standards, 1 atm, 15 °C, 60 % HR). This initial step permits the resizing of gas turbine air compressor looking to get nominal values on the gas turbine.

Table 6. Gas Turbines tested.

Supplier	Model	Power [MW]
Siemens	V64.3A	71
	V84.2	108
	V84.3	153
	V94.3	222

Table 7. Environmental Conditions

Variables	Case 1	Case 2	Case 3	Case 4	Case 5
Relative humidity (%)	72	67	76	68	80
Ambient Temperature (°K)	301	302	287	300	286
Atmospheric pressure (Kpa)	101	99	74	98	74

Table 8. Syngas characteristics

Case	Entrained Bed		Fluidized Bed		Fixed Bed	
	LHV (kJ/kg)	Temperature (°K)	LHV (kJ/kg)	Temperature (°K)	LHV (kJ/kg)	Temperature (°K)
1	12925	1681	3897	878	9321	384
2	15470	1691	4480	888	9321	384
3	13631	1666	4448	898	10666	476
4	13733	1673	4757	915	11287	450
5	13600	1665	4453	897	11535	473
Efficiency	91%		81%		75.5%	

From the simulations results is possible to observe a series of phenomena inherent to the regions simulated and independent of the type of turbine and technology used for the obtained gas. These phenomena are presented as a greater efficiency of plants in cold areas like in cases 3 and 5 (Figure 8 to Figure 10) regarding the hot zones (case 1, case 2 and case 4) and greater capacity for energy production in areas with air pressure near the atmospheric pressure at sea level like in case 1, 2 and 4 (Figure 11 to Figure 13). The phenomena mentioned are mainly due to environmental factors, which affect the behavior of gas turbines as follows:

- Ambient temperature: Has an impact on the efficiency and power.
- Atmospheric pressure: Has an impact on the power.
- Humidity: Has an impact on the power.
- Damper angle: Has an impact on the efficiency and power.

The energy production capacity of a gas turbine is directly related to the mass flow of air that enters the turbine (Capella y Vasquez, 2000); in turn, the mass flow of air is dependent from atmospheric air density. The air density is influenced in our case by three factors, which are temperature, humidity and pressure. At lower temperatures and higher values on the atmospheric pressure will probably mean an air with higher density, however, the incidence of both phenomena on the density is not in the same proportion, being much more the effect of the incident pressure.

The effect of moisture in the air density is not so crucial like the previous two, but must be consider as it is one factor that affects the performance of turbine. The relationship of the moisture with the density is inversely proportional, that's mean a higher percentage on the relative humidity will mean a lower air density. Temperature, pressure and humidity are among the factors which are determinant by the region where the power plant was evaluated.

However, there are other factors influencing on power plant performance, related to the syngas for each gasification technology and the coal rank. When comparing results for each technology (entrained bed, fluidized bed, and fixed bed), is possible to find greater efficiencies and production capacities in power plants using entrained bed technology, followed by the fluidized bed and finally fixed bed. IGCC's efficiency is direct function of gasification technology efficiency as is summarized in Table 8. Moreover, plants power capacity are function of gas exhaust temperatures during gasification process, thus larger plants power capacities are present when syngas leaves the gasifier vessel at higher temperature. Consequently, power plants using entrained and fluidized bed technologies provides its greater efficient in cold areas due to the effect of syngas and environmental temperatures but fixed bed technology with large capacity gas turbines (153MW and 222MW turbines) present similar values of efficiency in these regions due condition of syngas fuel (higher values for lower heating value).

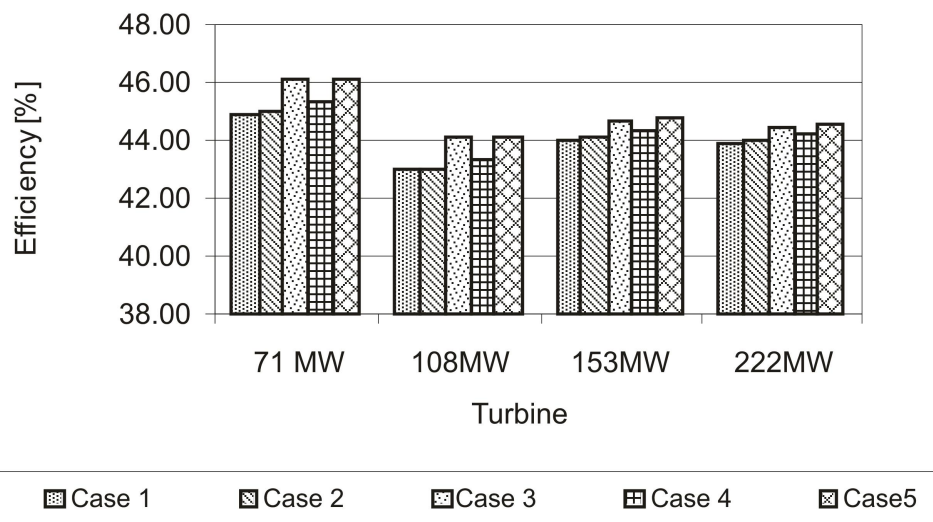


Figure 8. Efficiency for IGCC plants against gas turbine type – Entrained flow gasifier

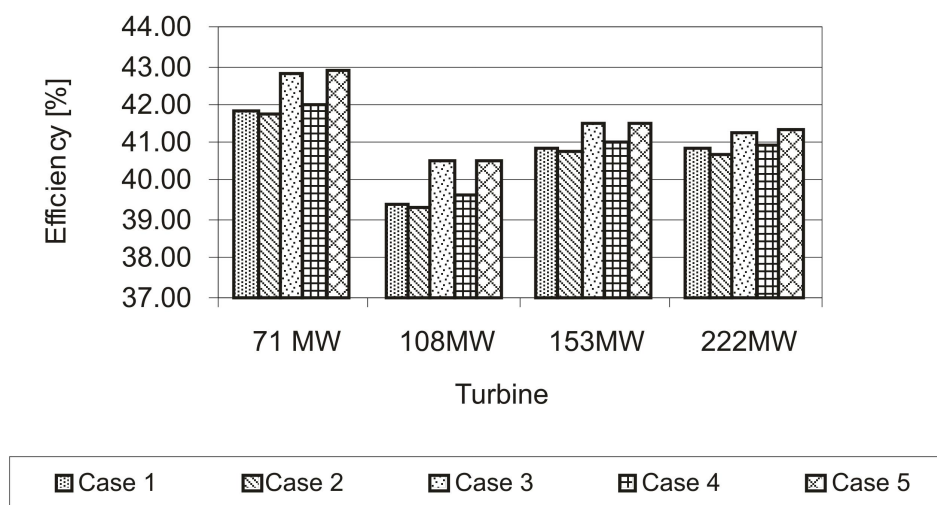


Figure 9. Efficiency for IGCC plants against gas turbine type – Fluidized bed flow gasifier

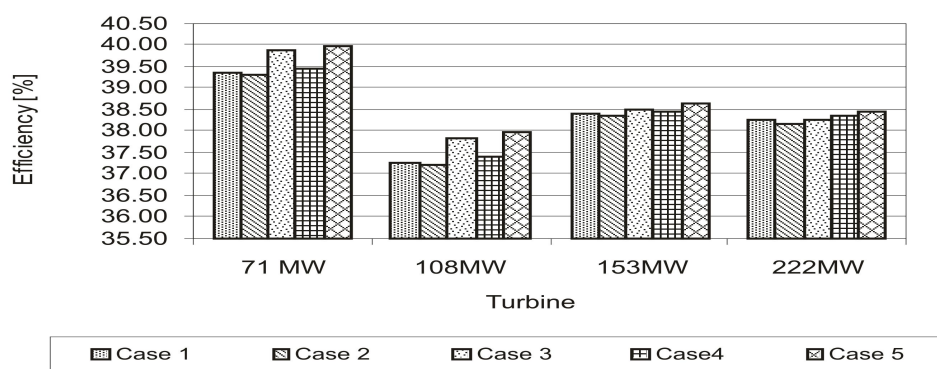


Figure 10. Efficiency for IGCC plants against gas turbine type – Fixed bed flow gasifier

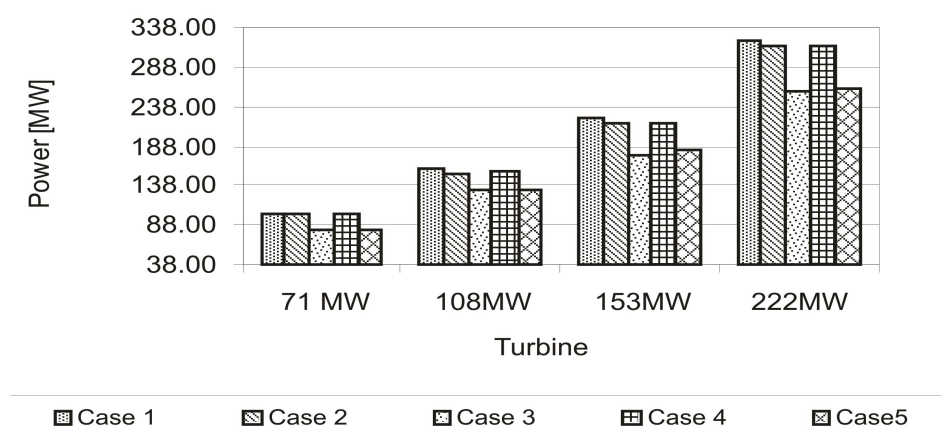


Figure 11. Power plant against turbine type- Entrained flow

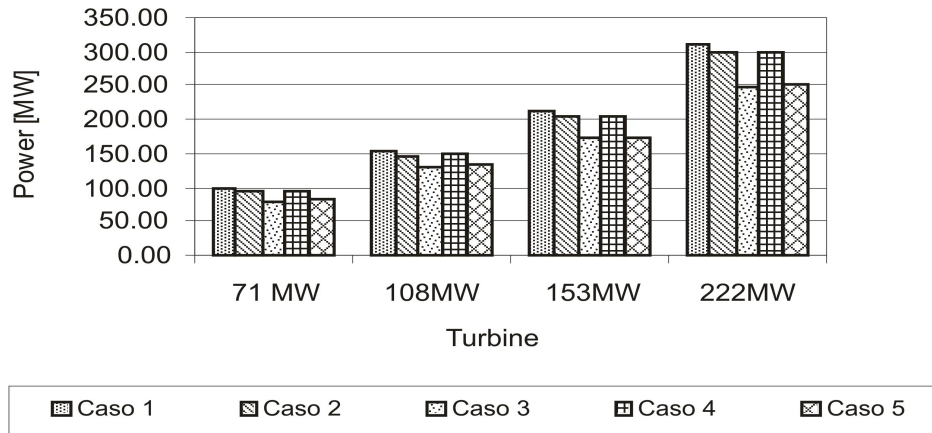


Figure 12. Power plant against turbine type- Fluidized bed flow

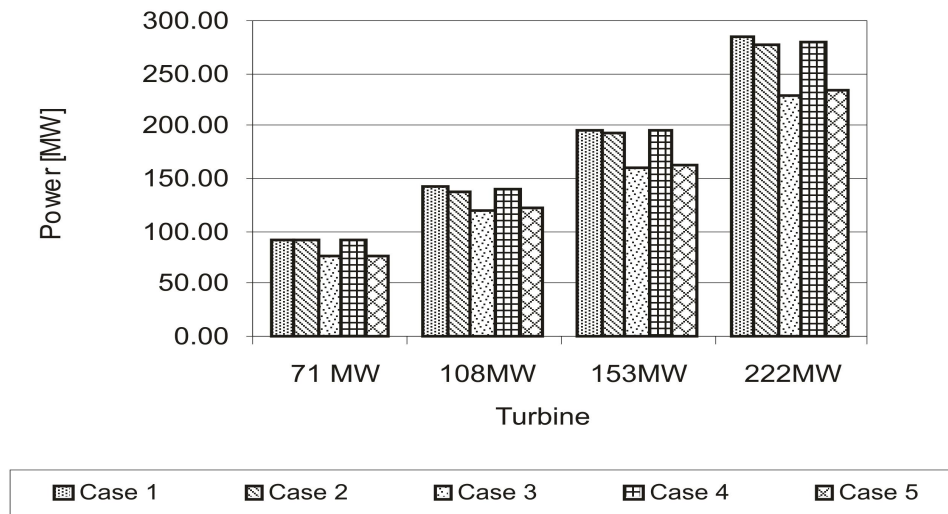


Figure 13. Power plant against turbine type- Fixed bed flow

4. CONCLUSIONS

The Hysys software is an adequate tool for simulating the gasification process. This is of great importance as it makes possible to estimate the performance and composition of syngas using different coals, thus constituting a database for the study of the technical viability before making a decision on the selection and construction of an integrated gasification combined cycle power plant. It is evident that the composition of the carbonaceous material being fed, the technology and the parameters of operation greatly influence the composition of the syngas produced in the gasification process. It was found that the less appropriated coal was that used in Case 3, regardless of the technology employed for its evaluation. This is largely due the amount of ash in this coal.

The IGCC plants with greater capacity and higher net cycle efficiency are the entrained bed technology. Plants with the larger capacity of energy production are those located in regions next to the sea level (Case 1, Case 4). Entrained and fluidized bed plants present their greater efficiency in areas like those in case 3 and case 5. Fixed bed technology with high capacity gas turbines (153MW turbines, 222MW) are not affected significantly in their efficiency by the impact of weather conditions in regions.

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