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Integrated gasification combined cycle (IGCC) process simulation and optimization

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ABSTRACT

The integrated gasification combined cycle (IGCC) is an electrical power generation system which offers efficient generation from coal with lower effect on the environment than conventional coal power plants. However, further improvement of its efficiency and thereby lowering emissions are important tasks to achieve a more sustainable energy production. In this paper, a process simulation tool is proposed for simulation of IGCC. This tool is used to improve IGCC's efficiency and the environmental performance through an analysis of the operating conditions, together with process integration studies. Pinch analysis principles and process integration insights are then employed to make topological changes to the flowsheet to improve the energy efficiency and minimize the operation costs. Process data of the Texaco gasifier and the associated plants (coal preparation, air separation unit, gas cleaning, sulfur recovery, gas turbine, steam turbine and the heat recovery steam generator) are considered as a base case, and simulated using Aspen Plus®. The results of parameter analysis and heat integration studies indicate that thermal efficiency of 45% can be reached, while a significant decrease in CO_2 and SO_x emissions is observed. The CO_2 and SO_x emission levels reached are 698 kg/MWh and 0.15 kg/MWh, respectively. Application of pinch analysis determines energy targets, and also identifies potential modifications for further improvement to overall energy efficiency. Benefits of energy integration and steam production possibilities can further be quantified. Overall benefits can be translated to minimum operation costs and atmospheric emissions.

1. Introduction

Strong dependency on crude oil and natural gas and the associated price and supply chain risk increase the need for efficient utilization of existing non-renewable energy sources (*e.g.*, coal, natural gas, nuclear power, etc.) (Kavouridis & Koukouzas, 2008). The emission of different pollutants, especially green house gases, may urge the environmental regulations to be a strong driver for new developments, in particular for decision makers that regulate the energy policies of states and regions. In this context coal has to be considered as energy source for power generation because of its availability and relatively wide geographic distribution. These developments include coal based electric power technologies, where the integrated gasification combined cycle (IGCC) is an alternative to pulverized coal (PC) combustion systems (Descamps, Bouallou, & Kanniche, 2008; Karg, Haupt, & Zimmermann, 2000; Park et al., 1999; Zheng & Furinsky, 2005), as they obtain higher efficiencies and better environmental performance (Jay, Lynn, Jeff, & Massood, 2002; Minchener, 2005; Ordorica-Garcia, Douglas, Croiset, & Zheng, 2006; Park et al., 1999). In comparison with modern coal combustion technologies (pulverized coal combustion (PCC), fluidized bed combustion (FBC), supercritical and ultra-supercritical technologies), IGCC systems are characterized by lower SO_x and NO_x emissions, comparable vapor organic carbon (VOC) emissions, 20% less CO_2 emissions and use of 20–40% less water. They operate at higher efficiencies, thus requiring less fuel and producing less emission (Zheng & Furinsky, 2005). Commercially available IGCC power plant technologies produce substantially smaller volumes of solid wastes (∼1/2) than the new conventional coal plants (Shilling & Lee, 2003). Furthermore, IGCC solid wastes are less likely to cause environmental damage than fly ash from conventional coal plants because IGCC ash melts in the gasification process (Shilling & Lee, 2003).

IGCC has higher fuel flexibility (biomass, refinery residues, petroleum coke, etc.) and generates multiple products (electricity, hydrogen and chemicals like methanol and higher alcohols) and by-products (sulfur, sulfuric acid, slag, etc.) (Jay et al., 2002). In addition, IGCC technology has the potential for CO_2 sequestration

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(Minchener, 2005; Ordorica-Garcia et al., 2006). Before CO_2 can be sequestered it must be captured as relatively pure CO_2 from power plants and other sources. In IGCC, as coal is not combusted, the relatively small volumes of synthesis gas (syngas) are easier to clean up than the much larger volumes of flue gases at coal combustion plants (Descamps et al., 2008).

Ongoing research activities focus on IGCC thermal efficiency, including cost related aspects and environmental performance indicators. A higher energy conversion efficiency leads to a better use of the coal resource and contributes to the reduction of greenhouse gases and other pollutants.

Apart from design considerations, IGCC performance depends on numerous integration options and can be improved by process optimization. These considerations include (Christopher & Zhu, 2006):

- Gas turbine air extraction to the air separation unit (ASU).
- Increase the gas turbine power.
- High and low temperature heat recovery.
- Steam generation conditions.
- Utility balance.
- Co-production or polygeneration including steam, hydrogen, and other products.
- Optimization of operating conditions, etc.

This paper presents an optimization scheme for IGCC through process simulation and sensitivity analysis of the key operating parameters. Then, a heat integration scheme is presented for different sections of the process. Finally, pinch analysis is performed for the overall process.

2. Gasification based energy conversion system options

Although there are many available technologies, this paper refers to the power generation schemes based on the combined gas turbines and Rankine cycles (Polyzakis, Koroneos, & Xydis, 2008).

There are three technologies for IGCC, classified according to the gasifier configurations and the flow geometry (Minchener, 2005):

- Entrained flow gasifiers, in which pulverized coal particles and gases flow concurrently at high speed. They are the most common option for coal gasification.
- Fluidized bed gasifiers, in which coal particles are suspended in the gas flow, and therefore coal feed particles, are mixed with the particles undergoing gasification.
- Moving bed gasifiers, in which gases flow relatively slowly upward through the bed of coal feed. Both concurrent and countercurrent technologies are available, but the former is more commonly used.

Each option has advantages and drawbacks. Shell and Texaco entrained flow gasifiers are used in nearly 75% of the gasification plants throughout the world that use coal to produce electric power (Minchener, 2005). They are the most versatile type of gasifiers as they can use both solid and liquid fuels and operate at high temperature to ensure high carbon conversion and a syngas free of tars and phenols (Zheng & Furinsky, 2005). In this work the Texaco process has been selected.

3. IGCC process description

The IGCC process model is developed for a Texaco gasifier with radiant/convective cooling system. The simplified process flow diagram is shown in Fig. 1. The coal (Illinois #6, Table 1), is crushed and mixed with water to produce a slurry (35.5%, w/w) and is pumped into the gasifier with oxygen. The gasifier operates in a pressurized, down flow entrained design and gasification takes place rapidly at temperatures higher than 1200 °C (Zheng & Furinsky, 2005). The raw fuel gas produced is mainly composed of H_2, CO, CO_2 and H_2O. The coal's sulfur is primarily converted to H_2S and small quantities of COS (intermediate component). This raw fuel gas leaves the gasifier at 1370 °C along with molten ash and a small quantity of unburned carbon.

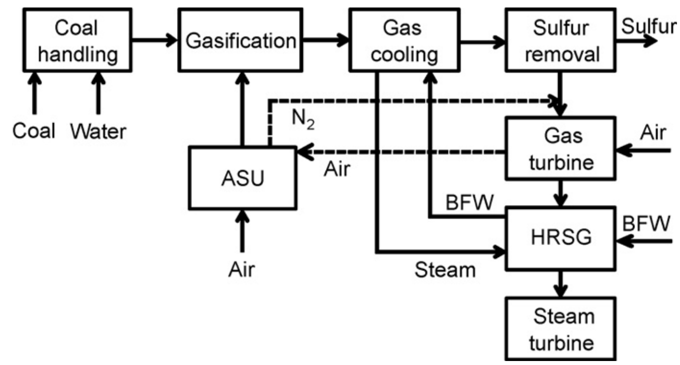

Fig. 1. Simplified diagram for IGCC [15].

The gas/molten solids stream enters a radiant syngas cooler (RSC) and convective syngas cooler (CSC) sections. In the Texaco design, the mix of gas/solids from the gasifier enters a radiant syngas cooling (RSC) system where cooling to approximately 815 °C is accomplished by generating a high-pressure steam. A convective syngas cooling (CSC)/gas scrubbing system cools the raw fuel stream to about 150 °C (27.5 bars) by generating additional steam. It uses a gas scrubber and a low temperature gas cooling/heat recovery section to reduce the raw fuel gas stream to 40 °C, prior to entering a cold gas cleaning unit (CGCU) for sulfur removal. Claus/SCOT sulfur recovery section is used to recover sulfur from the sour gas. Then, the clean syngas drives a gas turbine after being combusted in the combustion chamber of the gas turbine. The heat from the gas turbine exhaust is used to generate superheated steam in the heat recovery steam generator (HRSG). The generated superheated steam drives a steam turbine, producing additional power.

The data for the air separation unit (ASU), the steam cycle and the power block are listed in Table 2. Most of the data are taken from a report of the Process Engineering Division of the American Energy Institute (Shelton & Lyons, 2000). The missing data relating to operating conditions and range of operating variables are retrieved from the literature (Booras & Holt, 2004; Christopher & Zhu, 2006; Osama, Akira, & Yoshinori, 2002; Polyzakis et al., 2008; Sugiyama et al., 2005).

Table 1
The composition of Illinois #6 coal fed to the slurry process (HHV = 27.12 MJ/kg w/w% or 30.51 MJ/kg w/w% dry).

	w/w (%)	w/w (%, dry)
Proximate analysis		
Moisture	11.12	
Ash	9.70	10.91
Volatiles	34.99	39.37
Fixed carbon	44.19	49.72
Ultimate analysis		
Moisture	11.12	
Carbon	63.75	71.72
Hydrogen	4.50	5.06
Nitrogen	1.25	1.41
Chlorine	0.29	0.33
Sulfur	2.51	2.82
Ash	9.70	10.91
Oxygen	6.88	7.75

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Table 2
Data for the simulation of the power block and ASU.

Process section	Parameters	Values
Air separation plant (ASU)	Inlet air pressure	19 bars
	O_2/N_2 pressure	40.7/23.2 bars
Turbine of GT	Power	272 MW
	Pressure ratio	17.63
	Inlet temperature	1416 °C
	N_2 injection	55%
	Isentropic efficiency	92.2%
GT compressor	Pressure ratio	8.08
	Isentropic efficiency	59.4%
Steam cycle (3 pressure level)	Turbine pressure	124/23.6/2.4 bars
	Isentropic efficiency	90%
	Superheat temperature	565 °C
	Exhaust LP turbine	0.05 bar
	HRSG stack temperature	125 °C

4. Methodology

In this work, sensitivity analysis and process integration are applied in order to improve the efficiency and the environmental performance of the process. The analysis is interpreted by linking Aspen Plus® with MS Excel™, thereby directly accessing the required parameters from Aspen Plus® for calculation of the performance indicators.

The performance indicators used are either economic (efficiency) or environmental (emissions). Thermal efficiency, cold gas efficiency and carbon conversion efficiency are among the economic indicators while emission levels of CO_2, SO_2 and NO_x per unit of net power output are the environmental indicators (Christopher & Zhu, 2006; Sugiyama et al., 2005). Cold gas and carbon conversion efficiencies are measures of performance of the gasification section. However, the thermal efficiency is an indicator of efficiency of the overall process.

The calculation procedure to obtain the efficiencies is presented in Eqs. (1)–(5)

$$\eta_t(\%) = \frac{P_{NET}}{M_{Coal} \times LHV_{Coal}} \times 100 \tag{1}$$

where η_t is the thermal efficiency, P_{NET} is the net power output (MW), M_{Coal} is the mass flow rate of coal (kg/s) and LHV_{Coal} is the lower heating value of coal (MJ/kg).

$$P_{NET} = P_{GT} + P_{ST} - P_{AUX} \tag{2}$$

where P_{GT} is the net power output from the gas turbine (MW), P_{ST} is the power output from the steam turbine (MW) and P_{AUX} is the auxiliary power consumption in pumps, compressors, etc. (MW).

$$\eta_{cc}(\%) = \frac{M_{rc}}{M_{ic}} \times 100 \tag{3}$$

where η_{cc} is carbon conversion efficiency, M_{rc} is mass flow rate of the reacted carbon in the gasifier (kg/s) and M_{ic} is mass flow rate of the input carbon to the gasifier.

$$\eta_{cg}\ (\%) = \frac{M_{Syn} \times LHV_{Syn}}{M_{Coal} \times LHV_{Coal}} \times 100 \tag{4}$$

where η_{cg} is cold gas efficiency, M_{Syn} is mass flow rate of syngas (kg/s) and LHV_{Syn} is the lower heating value of the syngas (MJ/kg).

$$LHV_{Syn} = x_{H_2} \times LHV_{H_2} + x_{CO} \times LHV_{CO} + x_{CH_4} \times LHV_{CH_4} \tag{5}$$

where LHV_{H_2}, LHV_{CO}, LHV_{CH_4} are lower heating values of H_2, CO and CH_4 respectively. x_{H_2}, x_{CO} and x_{CH_4} are mass fractions of H_2, CO and CH_4 respectively. The emissions are retrieved from the mass balance of the process performed by the process simulator and normalized by the net power output obtained from the process. Finally, Pinch analysis provides a simple methodology for systematically analyzing chemical processes and the surrounding utility system. Pinch analysis is applied to the process to evaluate the overall standing of the process with respect to the hot and cold utility requirements and explore further potentials of heat integration and energy production.

5. Simulation approaches

The flowsheet has several naturally grouped sections: coal preparation, gasification, gas cooling and cleaning, acid gas removal, gas turbine, HRSG, steam cycle, etc. All these sections were rigorously modeled using Aspen Plus® (Aspen Technology, 2008).

5.1. Physical properties

Process simulation does not alleviate the need for accurate physical property data and models (Agarwall, Li, Santollani, Satyro, & Vieler, 2001; Satyro, Agarwall, Li, Santollani, & Vieler, 2001). This issue becomes particularly important when the product properties have a high impact on the process performance.

Peng–Robinson equation of state with Boston–Mathias alpha function (PR–BM) is used to estimate all physical properties (Aspen Technology, 2008) for the gasification and downstream unit operations. The SOLIDS property option is used for the coal crushing and screening section as it is recommended for size reduction, crushing, grinding, solids separation and cleaning.

The enthalpy model for both COAL and ASH, the non-conventional components, is HCOALGEN and the density model is DCOALIGT (Aspen Technology, 2008). The HCOALGEN model includes a number of empirical correlations for heat of combustion, heat of formation and heat capacity. All other values used were retrieved from the Aspen Plus® database (Table 3).

5.2. Chemical reactions

The chemical reactions involved in the IGCC process are very complex as many components are involved, and there is a network of irreversible consecutive and competitive reactions. The model uses a relatively simple approach to represent the reaction set as some trace reaction products, like CS_2, are not considered. The reactors are modeled with the Aspen Plus® built in models RStoic, RYield and RGibbs.

The RGibbs model is used to simulate gasification of the coal and combustion of the syngas. RGibbs models chemical equilibrium by minimizing Gibbs free energy. However, the Gibbs free energy of coal cannot be calculated because it is a non-conventional component. Therefore, before feeding the coal to the RGibbs block it is decomposed into its element (C, H, O, N, S, etc.). This is done using the RYield model with calculations that are based on the component yield specification. The heat of reaction associated with the decomposition of coal is considered in the coal gasification using a heat stream to carry the heat of reaction from the RYield block to the RGibbs block. The most important coal gasification reactions are given in Eqs. (6)–(8), while the main syngas combustion reactions are shown in Eqs. (9) and (10)

$$C + CO_2 \rightarrow 2CO \tag{6}$$

$$C + H_2O \rightarrow CO + H_2 \tag{7}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{8}$$

$$2CO + O_2 \rightarrow 2CO_2 \tag{9}$$

$$2H_2 + O_2 \rightarrow 2H_2O \tag{10}$$

The RStoic model is used to simulate the COS hydrolysis unit, the Claus and SCOT processes in the sulfur recovery section of the flow-

Table 3
Representative unit operations used in the simulation of the IGCC process.

Unit operation	Aspen plus® model	Comments/specifications
Coal crushing	Crusher	Rigorous simulation of particle size distribution
Coal particles screening	Screen	Rigorous simulation of the separation efficiency of the screen
Coal gasification	RGIBS	Specification of the possible products: H_2O, N_2, O_2, NO_2, NO, S, SO_2, SO_3, H_2, Cl_2, HCl, C, CO, CO_2, CH_4, COS, NH_3, HCN, H_2S
Dust removing	Sep	Simplified simulation of gas/solid separation by fixed split fraction specification together with the temperature drop
Syngas purifying	Absorber, distillation column, RStoic	Rigorous simulation of the H_2S, NH_3 and chloride removal with COS hydrolysis
Syngas combustor	RGIBS	All components may appear in the product stream
Air compressor, O_2 compressor and N_2 compressor	Compressor	Calculates the power required
Boiler	Heater	Simplified simulation of the generation of HP, IP and LP steam in the boiler
HRSG	Counter current multiple stream heat exchanger	Rigorous simulation of the steam cycle with heat recovery of the GT-exhaust
Gas and steam turbines	Compressor	Calculate power produced

sheet. RStoic models stoichiometric reactor with specified reaction extent (or conversion). The stoichiometric equations are given in Eqs. (11)–(17). 95% conversion is considered in these units.

- COS hydrolysis reaction:

$$COS + H_2O \rightarrow CO_2 + H_2S \quad (11)$$

- Claus process reactions:

$$H_2S + 3O_2 \rightarrow SO_2 + H_2O \quad (12)$$

$$2COS + 3O_2 \rightarrow 2SO_2 + 2CO_2 \quad (13)$$

$$2H_2S + SO_2 \rightarrow 3S + 2H_2O \quad (14)$$

- SCOT process reactions:

$$COS + H_2O \rightarrow H_2S + CO_2 \quad (15)$$

$$SO_2 + 3H_2 \rightarrow H_2S + 2H_2O \quad (16)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (17)$$

5.3. Design specifications, calculator blocks and convergence

Simulation is controlled using three FORTRAN routines (calculator blocks) and six design specifications to reduce the number of independent specifications and to adjust automatically those associated variables, *i.e.* the dependent variables are automatically adjusted when independent input variables are modified by the user, a calculator block or a design specification. The main functional relationships (control structures) of the simulation are: the amount of coal input as a function of the gas turbine net power (272 MW), the amount of slurry water as a function of the coal input (35.5%), the makeup water for the steam cycle depends on the temperature of the stack gas (125 °C), the air input to the ASU is determined by the gasifier net duty and air to the gas turbine (GT) combustor is fixed by the combustor net heat duty or the stoichiometric amount of air required. The basic user defined specification is the value of the gas turbine power output which is 272 MW.

Since this is a large and intricate simulation, with ten nested convergence loops, it is very sensitive towards the loop's break points and their initial conditions. To fix the initial conditions, an integration of the practical knowledge of the process and the trial runs of the model are very important. After detailed analysis, a specific computational sequence was set up for the model, and the ranges of initial conditions were established to improve the convergence of the model. The design specs are nested inside tear loops. In doing so, the sequence of the blocks was determined.

5.4. Unit operation models

The most important unit operations represented by Aspen Plus® models are shown in Table 3.

6. IGCC process optimization by sensitivity analysis

The sensitivity of the process for different operating conditions is analyzed. After preliminary analysis, just the variables with a high impact in the results were selected: gasification temperature, combustion temperature, level of N_2 injection and solid concentration of the coal slurry. The main parameters analyzed within each analysis are thermal efficiency based on the low heating value of coal ($\eta_{t(LHV)}$), cold gas efficiency (η_{CG}), carbon conversion efficiency (η_{cc}) and emission levels of CO_2, SO_x and NO_x (Christopher & Zhu, 2006; Sugiyama et al., 2005).

6.1. Effects of gasification temperature

The results in Table 4 illustrate the effect of the gasification temperature (T_{gas}) on the IGCC process performance. The sensitiv-

Table 4
Variation of key process variables to the change in gasification temperature.

T_{gas} (°C)	Coal (kg/s)	Net power (MW)	$\eta_{t(LHV)}$ (%)	η_{cg} (%)	Air:syngas ratio	CO_2 emission (kg/MWh)	SO_x emission (kg/MWh)	NO_x emission (kg/MWh)
1250	44.3	427	36.4	68.3	6.47	784	187	10.3
1300	44.9	431	36.2	67.3	6.32	790	188	10.1
1350	45.8	436	35.9	66.3	6.18	796	189	10.0
1400	46.6	439	35.6	65.3	6.08	800	190	9.80
1450	47.5	444	35.3	64.3	6.01	802	191	9.60
1500	48.4	449	35.0	63.3	5.87	808	192	9.40
1550	49.4	455	34.8	62.3	5.70	814	193	9.20

Table 5
Variation of some key variables with combustion temperature.

T_{comb} (°C)	Coal (kg/s)	$\eta_{t(LHV)}$ (%)	Air:syn	NO_x emissions (kg/MWh)
1250	46.1	35.3	8.58	7.49
1300	45.4	35.7	7.85	8.33
1350	44.8	36.1	7.21	9.18
1400	44.4	36.4	6.64	10.0
1450	44.0	36.6	6.13	10.8
1500	43.8	36.9	5.67	11.5
1550	43.5	37.1	5.26	12.2

ity of the process for the gasification temperature is done under the operational range of temperatures where gasification can take place with slagging of the ash (1250 and 1550 °C) (Zheng & Furinsky, 2005). As the gasification temperature increases, the thermal efficiency decreases due to a decrease in the cold gas efficiency. This decline in cold gas efficiency is due to a rise in the O_2:C ratio in order to combust more carbon to reach high temperature. On the contrary, the total net power increases because the steam turbine power output rises due to a higher amount of the slurry input for the same quantity of gas turbine output. However, the net power output per ton of coal consumed and the thermal efficiency have a decreasing trend.

The CO_2 and SO_x emissions per unit of power output increase due to the rise in the coal consumption for the same level of GT power output. But the NO_x emission per unit of power output drops off very slightly due to a decline in the air:clean syngas ratio, thereby lessening the thermal NO_x formation.

6.2. Effects of gas turbine inlet temperature (syngas combustion temperature)

The analysis is performed for temperatures (T_{comb}) around the base case (1370 °C) and the results of the analysis can be seen in Table 5. For an increase in T_{comb} between 1200 and 1550 °C, thermal efficiency ($\eta_{t(LHV)}$) boosts by 5%. Along with a rise in $\eta_{t(LHV)}$, the CO_2 and SO_x emissions per unit power output also drop off. This is due to the decline in the level of coal consumption for the same GT power output. But, the NO_x emission rises because of the increase in thermal NO_x formation at higher temperatures. The carbon conversion efficiency, the cold gas efficiency and the O_2:C ratio remain almost constant as they are independent of the combustor operating temperature.

6.3. Effects of level of N_2 injection

As the fraction of N_2 injection to the GT combustor increases:

- The thermal efficiency increases, due to a decrease in the slurry (coal) requirement, as more N_2 is used to drive the turbine.
- The net power output declines because of a decrease in the steam turbine power output owing to the decrease in coal flow, thereby lowering the amount of exhaust gas from the gas turbine.
- The net power output per ton of coal input is enhanced because the coal requirement for the same level of GT output gets reduced.
- The CO_2, SO_x and NO_x emissions lessen due to the decline in the coal consumption and the diluting effect of the N_2 that decreases thermal NO_x formation.

6.4. Effects of solid concentration in coal slurry

With the rise in solids concentration, the O_2:C ratio decreases because of the reduction in required energy to vaporize and superheat water. The syngas heating value increases because less coal is used to supply energy for the gasification. Therefore, there is a boost in the thermal efficiency and the net power output per ton of coal used. The emissions per unit power of CO_2, SO_x and NO_x slightly increase because of the small decrease in the total net power, owing to decline in the steam turbine power output. The steam produced in the HRSG is minimized as the coal consumption drops off. This is because a relatively small amount of coal is utilized to produce the 272 MW of electricity from the gas turbine thereby lowering the GT exhaust feed to the HRSG.

6.5. Simultaneous analysis of the effects of level of N_2 injection and syngas combustion temperature

The thermal efficiency increases almost linearly with the increase in the combustor temperature for all levels of N_2 injection to the combustor (Fig. 2). Therefore, the power augmenting effect of the N_2 flow is greater than its diluting effect in the combustor. No trade-off between these two effects was found.

N_2 injection level of 98% is the upper bound on the total amount of N_2 available for injection, as venting is inevitable and N_2 can be used as a coolant in the gas turbine. Therefore 98% of N_2 injection to the combustor operating at the highest pos-

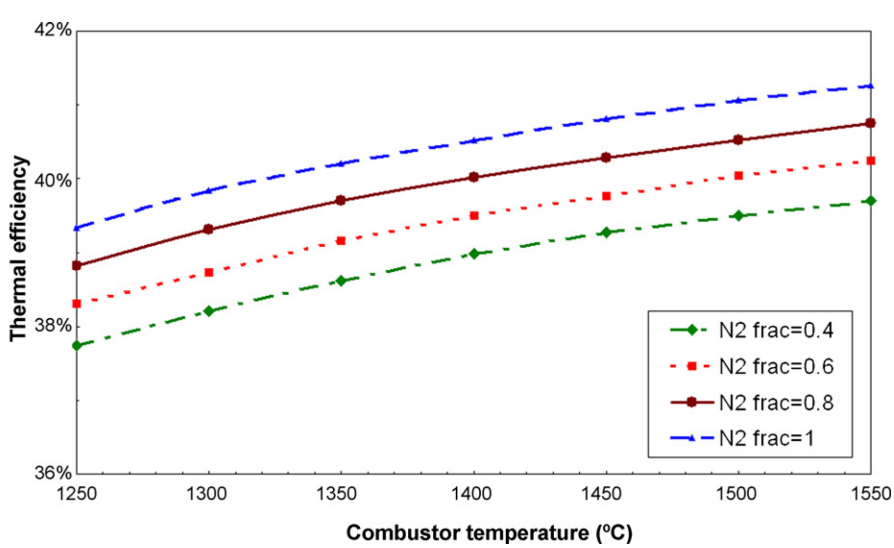

Fig. 2. Effects of simultaneous variations of the level of N_2. injection and combustor temperature on thermal efficiency.

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sible temperature (depending on the turbine inlet temperature specification) produces power with relatively high thermal efficiency.

7. Heat integration

With the aim of improving thermal efficiency and environmental performance, the effects of heat integration of the gasifier and GT combustor are analyzed. The result is supplemented by heat integration of air separation unit (ASU) and gas cleaning unit. With the objective of evaluating the overall process utility consumption and further potential of heat integration and energy production, pinch analysis is applied to the process.

7.1. Heat integration of the gasifier and the GT-combustor

In this analysis, the gasifier is heat integrated with the GT-combustor. The level of integration is optimized by varying the oxygen and air requirements of the gasifier and combustor, respectively. As the gasification reaction is endothermic, its net heat duty is kept zero, *i.e.* adiabatic operation, so that no external heat is added to the system, except from the combustor. Basically the gasifier gets heat for gasification from the combustion of part of the carbon feed. But, this results in a decline in the thermal efficiency because the heating value of the syngas is reduced. In this analysis, the objective is to minimize the amount of carbon burnt by supplying external heat to the gasifier from the combustor because the reaction in the combustor is exothermic.

With the increase in the level of heat integration, the net power output increases, but the net power per ton of coal consumed increases until it reaches a maximum (Fig. 3a). The decrease in the O_2:C ratio with the increase in the level of integration has a positive effect on the thermal efficiency at first, because it favors the gasification reaction (compared with the combustion reaction) and increases the cold gas efficiency. Then, with further decrease in the O_2:C ratio, the carbon conversion efficiency and, in turn the cold gas efficiency, start to decrease (Fig. 3b), thereby lowering the thermal efficiency. The air requirement in the combustor also decreases as the net heat duty of the combustor increases. This is to minimize the heat absorbed by the excess air, to maintain the operating temperature. The maximum in Fig. 4 represents an optimal trade-off between these two opposing scenarios.

7.2. Heat integration of the air separation unit (ASU) and the gas cleaning unit

The oxygen stream from the ASU to the gasifier is heat integrated with the condenser of the amine regenerator (condenser regeneration) in the gas cleaning unit. This is proposed due to the availability of high quality heat from the amine regenerator unit.

Fig. 4 shows a similar trend: the maximum is shifted to the left and the efficiency is improved. The maximum efficiency is

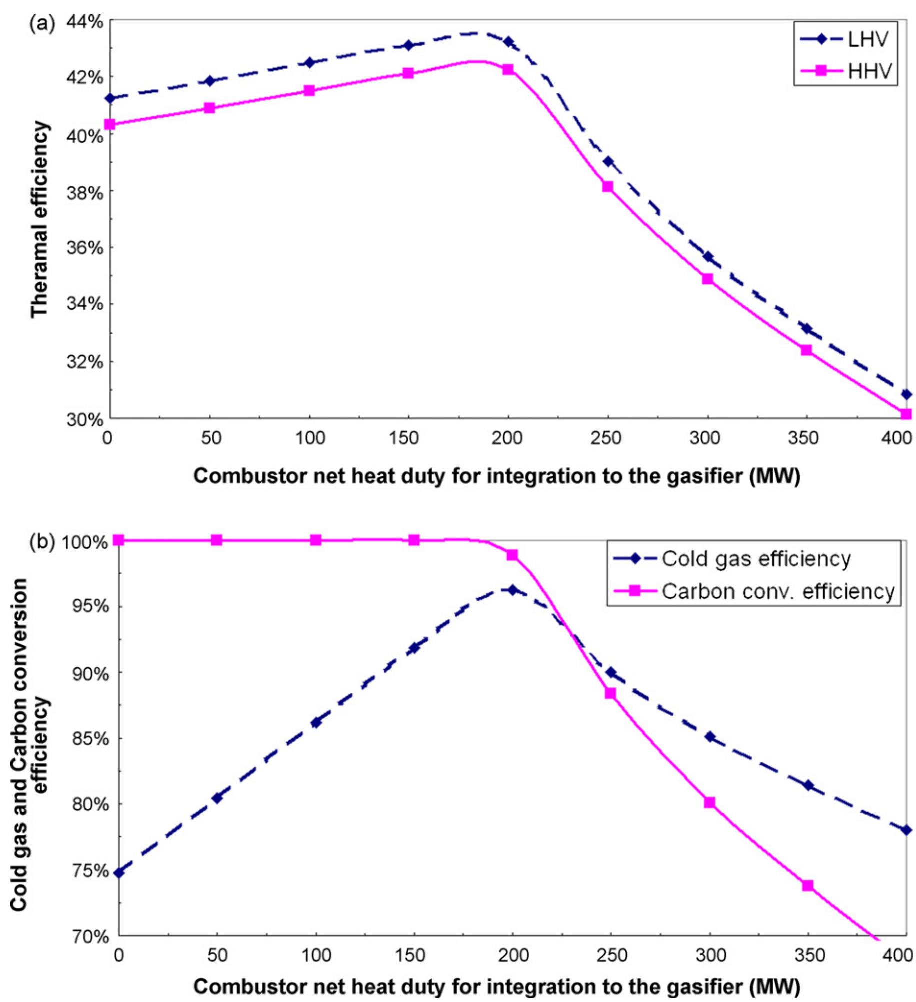

Fig. 3. (a) Dependence of thermal efficiency on heat integration of GT-combustor and gasifier. (b) Dependence of cold gas efficiency and carbon conversion efficiency on heat integration of GT-combustor and gasifier.

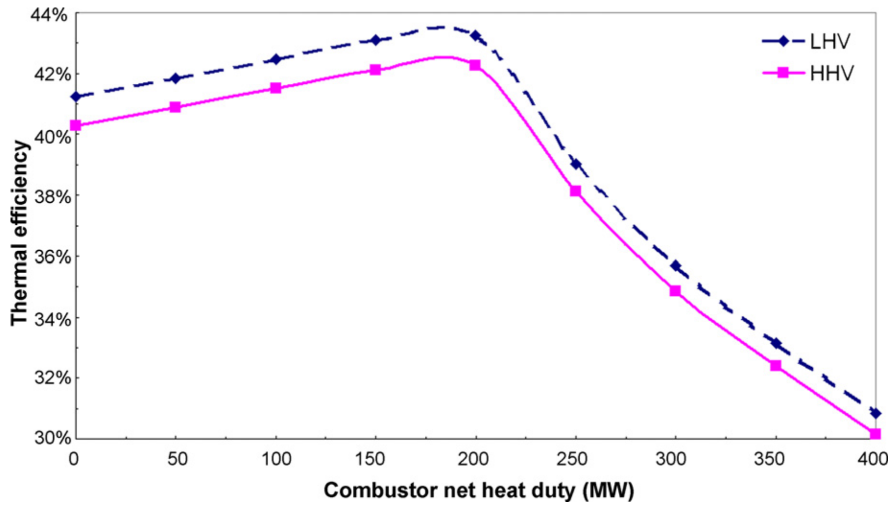

Fig. 4. Combustor and gasifier integration for the case of ASU and gas cleaning units heat integration.

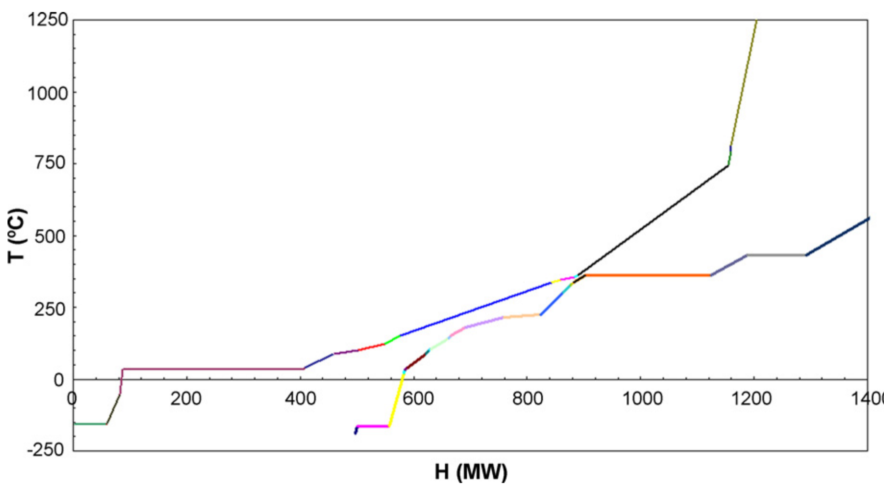

Fig. 5. Hot and cold composite curves for IGCC with dT_{min} = 15 °C.

reached at a combustor duty of 150 MW (a value that differs from the 200 MW found in the previous case) due to the further decrease in the O_2:C ratio as the O_2 inlet temperature to the gasifier increases. Therefore, it is possible to minimize the oxygen requirement by heating the inlet oxygen to the gasifier using process heat. This modification increases the overall efficiency, as less energy is used in the ASU to compress oxygen and air.

7.3. Pinch analysis

Pinch analysis is performed to compare the energy consumption of the optimized model with the energy consumption of the process analyzed at a certain fixed pinch approach temperature. The hot and cold composite curves for the process are constructed with a minimum approach temperature of 15 °C (Fig. 5). From these curves, the total net heating and cooling requirements of the process when designed optimally can be identified on each of the hot and cold ends. Also, the total amount of heat recovery that can be achieved within the process can be determined by the overlap-area between the two curves. These values are known as energy targets. The problem table algorithm is used to construct the grand composite curve (Fig. 6). From this curve, the hot energy target is indicated as 225 MW with a temperature level of more than 440 °C (this is the case when all hot requirements are added by only one utility). On the other hand, the cold utility target is 450 MW, at a temperature lower than −160 °C. Pinch temperature is at almost 380 °C. Fig. 6 shows some potential schemes for improving the energy efficiency of the overall basic design. For example, instead of utilizing an external hot utility, an exhaust steam from steam turbines at a temperature level close to 440 °C can be used to fulfill the heat-

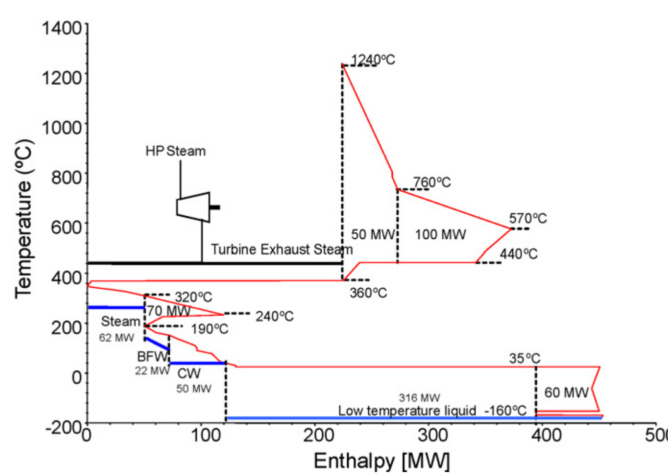

Fig. 6. Grand composite curve with δT_{min} = 15 °C.

ing requirement. On the cooling energy requirement, a possible scheme of utility placement is also suggested in Fig. 6. For this scheme, saturated steam at 230 °C can be produced with a flow rate of 123 ton/h. The heat load on boiler feed water BFW preheating will be 22 MW. Then, the rest of cooling utilities will be provided by cooling water with a cooling duty of 50 MW, and a refrigerant medium at a temperature of −160 °C at a load of 312 MW.

As for heat integration opportunities, the composite curve provides details of how much and at what level these energies are available, *e.g.*, above the pinch temperature two heat sources are available in excess of 50 and 100 MW at temperature levels of 1240–760 and 760–570 °C, respectively. On similar manner, excess heat sources below the pinch can heat cold processes or streams that require energy; *e.g.*, heats of 70 and 60 MW at temperature intervals of 320–240 and 30 °C, respectively, are available.

Comparing the utility requirements of the optimized process and the process at the pinch point, the hot utility consumption efficiency is calculated to be 94% and that of the cold utility efficiency is 97%. These values show that the optimized process operates nearly at the pinch point.

8. Conclusions

A base case of integrated gasification cycles has been simulated using Aspen Plus®. Sensitivity of the process for different operating variables was then studied. As result of this analysis, thermal efficiency (LHV) as high as 45% was attained, and the corresponding CO_2 and SO_x emissions were 698 kg/MWh and 0.15 kg/MWh, respectively. This result corresponds to a gasification temperature of 1250 °C, a combustion temperature of 1550 °C, 98% of N_2 injection to the GT combustor, and a slurry solid concentration of 80%. For the practical application of this improvement, other considerations like the capacity of the equipment and its cost, the flowability of the slurry at the high level of solids concentration have to be considered.

Heat integration of the gasifier and the combustor revealed that the best value of the combustor heat duty for the integration is around 200 MW. However the analysis for the heat integrated case of the ASU and the CGCU shows that the best value of the combustor net duty for the integration is 150 MW. The latter case is preferred because the thermal efficiency is higher due to lower power consumption in the ASU compressors. According to the results shown in Figs. 3a, b and 4, it is advisable to operate at combustor net heat duties slightly below the optimum value in order to avoid a significant loss in the efficiency during operation.

The optimum design of the gasification cycle was further analyzed according to pinch analysis principles. The analysis was able to provide further opportunities of heat integration above and below the pinch temperature. Multiple utilities levels can be used for minimum operation costs. Also steam can be produced by the excess heat available, leading to reductions in atmospheric emissions.

Nomenclature

ASU	air separation unit
BFW	boiler feed water
CGCU	cold gas cleaning unit
CSC	convective syngas cooler
FBC	fluidized bed combustion
GT	gas turbine
HRSG	heat recovery steam generator
IGCC	integrated gasification combined cycle
LHV_i	lower heating value of component *i* (MJ/kg)
M_i	mass flow rate of component *i* (kg/s)
PC	pulverized coal
PCC	pulverized coal combustion
P_{AUX}	auxiliary power consumption (MJ)
P_{GT}	gas turbine net power (MJ)
P_{NET}	net power output (MJ)
RSC	radiant syngas cooler
T_{comb}	syngas combustion temperature (°C)
T_{gas}	coal gasification temperature (°C)
x_{CH_4}	mass fraction of CH_4 in syngas
x_{CO}	mass fraction of CO in syngas
x_{H_2}	mass fraction of H_2 in syngas

Greek symbols

η_t	thermal efficiency (%)
η_{cc}	carbon conversion efficiency (%)
η_{cg}	cold gas efficiency (%)

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2009.04.007.

References

Agarwall, R., Li, Y.-K., Santollani, O., Satyro, M. A., & Vieler, A. (2001). Uncovering the realities of simulation. Part I. *Chemical Engineering Progress*, *97*, 42.

Aspen Technology. (2008). *Aspen Plus® 2006 reference manual*. Cambridge, MA: Aspen Technology Inc.

Booras, G., & Holt, N. (2004). Pulverized coal and IGCC plant cost and performance estimates. In *Proceedings of the gasification technologies conference* Washington, USA,

Christopher, H., & Zhu, Y. (2006). Improved system integration for integrated gasification combined cycle (IGCC) systems. *Environment Science and Technology*, *40*, 1693–1699.

Descamps, C., Bouallou, C., & Kanniche, M. (2008). Efficiency of an integrated gasification combined cycle (IGCC) power plant including CO_2 removal. *Energy*, *33*, 874–881.

Jay, A. R.-B., Lynn, M. M., Jeff, W. H, & Massood, R. (2002). An environmental assessment of IGCC power systems. In *Proceedings of the nineteenth annual Pittsburgh coal conference*.

Karg, J., Haupt, G., & Zimmermann, G. (2000). Optimized IGCC cycles for future applications. In *Proceedings of the gasification technologies conference* San Fransisco, CA.

Kavouridis, K., & Koukouzas, N. (2008). Coal and sustainable energy supply challenges and barriers. *Energy Policy*, *36*, 693–703.

Minchener, J. (2005). Coal gasification for advanced power generation. *Fuel*, *84*, 2222–2235.

Ordorica-Garcia, G., Douglas, P., Croiset, E., & Zheng, L. (2006). Technoeconomic evaluation of IGCC power plants for CO_2 avoidance. *Energy Conversion and Management*, *47*, 2250–2259.

Osamu, S., Akira, Y., & Yoshinori, K. (2002). The development of advanced energy technologies in Japan IGCC: A key technology for the 21st century. *Energy Conversion and Management*, *43*, 1221–1233.

Park, T. J., Kim, J. H., Lee, J. G., Hong, J. C., Kim, Y. K., & Choi, Y. C. (1999). Experimental studies on the characteristics of entrained flow coal gasifier. *Energy Conversion Research Department Korea Institute of Energy Research*.

Polyzakis, A. L., Koroneos, C., & Xydis, G. (2008). Optimum gas turbine cycle for combined cycle power plant. *Energy Conversion and Management*, *49*, 551–563.

Satyro, M. A., Agarwall, R., Li, Y.-K., Santollani, O., & Vieler, A. (2001). Uncovering the realities of simulation. Part II. *Chemical Engineering Progress*, *97*, 64.

Shelton, W., & Lyons, J. (2000). Texaco gasifier base cases PED-IGCC-98-001, US Department of Energy. *Process Engineering Division*, 1–52.

Shilling, N. Z., & Lee, D. T. (2003). IGCC—Clean power generation alternative for solid fuels. *PowerGen Asia*.

Sugiyama, S., Suzuki, N., Kato, Y., Yoshikawa, K., Omina, A., Ishii, T., et al. (2005). Gasification performance of coals using high temperature air. *Energy*, *30*, 399–413.

Zheng, L., & Furinsky, E. (2005). Comparison of shell, Texaco BGL and KRW gasifiers as part of IGCC plant computer simulations. *Energy Conversion and Management*, *46*, 1767–1779.