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Detailed process simulation of pre-combustion IGCC plants using coal-slurry and dry coal gasifiers

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Abstract

The selection of the gasifier in an Integrated Gasification Combined Cycle (IGCC) plant affects both downstream process configurations and net plant efficiency considerably. It is well known that a Shell gasifier using dry coal has lower operating pressure, higher carbon conversion, lower CO_2 production and lower H_2/CO ratio compared to a General Electric Energy (GEE) gasifier using coal slurry. These differences also affect how to configure downstream processes when an IGCC is retrofitted for carbon capture. The net plant efficiency decreases by different extents depending on the gasifier type as shown in the DOE NETL report [1]. The aim of this study is to elucidate how the differences between the two gasifiers correspond to the difference in plant performance without and with carbon capture. To achieve this, detailed process simulations of the two IGCC plants and an integrated Selexol carbon capture unit have been carried out based on literature configurations [1] using the commercial software Honeywell UniSim Design R400[®]. From the analysis of the results an explanation is presented as to why the wet slurry gasifier configuration has a lower net efficiency loss when the carbon capture unit is integrated.

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Keywords: Amine process; MEA; Coal-fire power plant; Process configuration

1. Introduction

IGCC plants can generate power with higher net plant efficiency, ranging from 39 to 42% coal Higher Heating Value (HHV), depending on the gasifier type, compared to pulverized coal fired power plants with a supercritical steam cycle (39% coal HHV). Nevertheless, less attention has been paid to this technology since the increment in plant efficiency is not large enough to justify its economic feasibility due to its high investment cost. Because of the different operation, compared to conventional steam

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cycles, it is easier to implement carbon capture in IGCC plants with a lower loss in net power. Therefore IGCC plants are being considered in order to decarbonise the power sector to meet very stringent targets for carbon emissions reduction. Designs based on 90% carbon capture, IGCC processes with a GEE gasifier have been shown to yield a lower plant efficiency penalty (6%) when compared to PC-fired power plants (11%) [1]. As a result, IGCC processes with pre-combustion capture can accomplish as high as 33% net plant efficiency (coal HHV) while supercritical PC-fired power plants with amine process

have an efficiency of only 28% [1]. Maurstad et al. [2] investigated the quality of the coal used in the gasifier to estimate its effect on IGCC plant efficiency, the net power output, as well as the CO₂ emission per unit of electricity. An IGCC power plant simulation was conducted by Ng et al. considering the different available gasification technologies but incorporating a coal slurry (GEE) gasifier in their work [3]. A more detailed study of the IGCC power plant was presented by Robinson and Luyben [4]. Results were reported on the conventional IGCC power plant as well as the co-generation option of a hybrid IGCC/Methanol plant. They conducted simulations using Aspen Plus® in both steady state and dynamic modes for a power plant with a GEE coal slurry fed gasifier. Moreover, Bhattacharyya et al. [5] reported a steady state simulation of an IGCC power plant presenting their approach on the main areas of the plant. Again, the gasifier considered was GEE. Perez-Fortes et al. [6] implemented an IGCC process simulation using Aspen Plus. Jones et al., [7] focused their study on various process configurations of air separation units for an IGCC power plant, incorporating a GEE-type gasifier. They showed how different configurations of the ASU affect power consumption of this section. Zheng and Furinsky compared different types of gasifiers, including coal slurry and dry coal gasifiers for IGCC power plants, but did not compare directly GEE and Shell gasifiers [8].

IGCC processes show a variation in energy penalty with different types of gasifier. An IGCC process with a Shell gasifier fed by dry coal has 42% net plant efficiency without carbon capture but it ends up with 31% net plant efficiency when integrated with a Selexol process for carbon capture. In this study four process simulations for non-capture and capture IGCC processes incorporating dry-coal and coal-slurry gasifiers using commercial process simulators are presented. The main units of an entire IGCC process include a coal gasifier, syngas cooler, shift reactors, sour stripper, acid gas removal (AGR), gas and steam turbines, heat recovery steam generator (HRSG), elevated pressure ASU, Claus sulphur plant, and CO₂ compression. All the simulations are based on the process configurations in the DOE NETL report [1] of which the data have been assessed by rigorous simulation results. This study will analyse the reasons why there is such a drastic efficiency drop in power generation in the case of a Shell IGCC compared to a GEE IGCC when integrated with the carbon capture unit.

2. Process simulation

IGCC processes have been simulated using Honeywell UniSim process flowsheet simulator. Additional tests were performed using BR&E Promax, which was utilized to simulate syngas cooling, the sour stripper, and the Claus sulphur plant. Promax has more accurate thermodynamic models available for these sections, which allows to check the predictions of process performance.

2.1. Gasifier and Syngas Cooler

Carbon conversion is a very important parameter in evaluating a gasifier. A gasifier converts coal into synthetic gas (syngas) by reacting coal with oxygen and water. Given the Illinois No. 6 bituminous coal [1], the carbon conversion is estimated as 98.0 and 99.5 % for GEE and Shell gasifiers, respectively. An Elevated Pressure (EP) ASU produces 95% oxygen from air for its use in the gasifier and the Claus

sulphur plant. The GEE gasifier is operating at 1,316 °C and 5,617 kPa, while the Shell gasifier is operating at 1,618 °C and 4,031 kPa. In this study, it is assumed that 8 reactions take place in the gasifier and the conversion rate of each reaction was adjusted in order to match the mass balance as reported by the DOE NETL [1]. Knowing the reactions and their conversion percentage, a conversion reactor has been utilised to generate a syngas stream having same composition solving the following gasifier reactions.

Reactions in gasifier

 $\begin{array}{l} 2\mathrm{C} + \mathrm{O}_2 \leftrightarrow 2\mathrm{CO} \\ \mathrm{C} + \mathrm{O}_2 \leftrightarrow \mathrm{CO}_2 \\ 2\mathrm{C} + 2\mathrm{S} + \mathrm{O}_2 \leftrightarrow 2\mathrm{COS} \\ \mathrm{C} + 2\mathrm{H}_2 \leftrightarrow \mathrm{CH}_4 \\ \mathrm{S} + \mathrm{H}_2 \leftrightarrow \mathrm{H}_2\mathrm{S} \\ \mathrm{Cl}_2 + \mathrm{H}_2 \leftrightarrow 2\mathrm{HCl} \\ 2\mathrm{H}_2\mathrm{O} \leftrightarrow 2\mathrm{H}_2 + \mathrm{O}_2 \\ \mathrm{N}_2 + 3\mathrm{H}_2 \leftrightarrow 2\mathrm{NH}_3 \end{array}$

The hot syngas generated in the gasifier is cooled in the syngas quench, syngas scrubber and in the heat exchangers used to generate steam generation. At the same time, sour water is condensed out from the syngas by cooling or produced in the syngas scrubber. It is important to estimate the distributions of H_2S and NH_3 into gas and aqueous phases since they will affect the AGR plant operating conditions. In this study, an electrolyte model was utilised in ProMax to obtain accurate predictions of these gas solubilities.

2.2. Water Gas Shift Reactors (WGSR)

In IGCC power plants with carbon capture, the raw gas leaving the gasifier is mixed with shift steam and is sent to two-stage shift reactors: High Temperature Shift Reactor (HTSR) and Low Temperature Shift Reactor (LTSR) in series, releasing the heat of 41 kJ/mole of CO reacted. It should be noted that the same shift conversion rate was assumed in both cases (95.7%) even though the syngas composition is very different, for example lower H_2/CO ratio and lower CO_2 content are obtained in the case of the Shell gasifier. This is a reasonable assumption since in the Shell IGCC, the higher CO and lower CO_2 mole fractions, which favour conversion, are offset by the higher operating temperature as shown in Figs. 1 and 2, which would reduce the conversion. In this simulation, equilibrium reactors were used to let the simulator calculate the conversion rate at the given conditions. The conversion rates obtained were 80% and 79% at HTSR and LTSR, respectively, which correspond to 95.7% conversion overall. The final product passes through a series of coolers where water is knocked out and sent to the AGR unit.

2.3. Acid Gas Removal (AGR) Unit

A dual-stage Selexol unit has been modelled for H_2S and CO_2 removal in cases 2 and 4 while a singlestage Selexol unit was used for H_2S removal only in the simulations of the non-capture cases. A variety of configurations of the Selexol units can be devised to capture acid gas depending on the levels of impurities in the feed, feed pressure and capture target. In this study, the gas stream from the H_2S concentrator was recycled to the H_2S absorber instead of feeding to the re-absorber. For the dual-stage Selexol, the syngas exiting the H_2S absorber is routed to another absorber for CO_2 removal. While the rich solvent leaving the H_2S column is sent to steam stripper for its regeneration, the solvent leaving the CO_2 absorber is sent to several flash drum stages to recover CO_2 from the solvent at high pressure. This results in a saving of power in the CO_2 compression unit. The clean syngas coming out of the CO_2 absorber is sent to the humidifier in the Shell IGCC and the fuel gas reheater in the GEE IGCC, while the acid gas from the steam stripper is sent to the Claus process to recover the sulphur.

The initial simulations based on the values of the H_2S and CO_2 solubilities in Selexol included in the UniSim Design database led to inconsistent results. This was investigated in detail and new parameter sets for the Henry constant were obtained by regressing experimental data [9, 10].

2.4. Combined Cycle

Two identical advanced F class gas turbines are installed in parallel, each having 232 MWe of net power generation. As it is hard to estimate accurately the performance of this gas turbine due to lack of information, it was assumed that the power generation at the gas turbine would be 464 MWe in total without any further detailed simulation, but all the streams going into or out of the gas turbine are kept to the same conditions as those in the DOE NETL report [1].

The hot flue gas exiting the gas turbine flows through the Heat Recovery Steam Generator (HRSG) to recover the large quantity of thermal energy that it contains. The HRSG is the part of the power plant where steam is generated. The HRSG consists of three sections. The High Pressure (HP) heat exchanger train, the Intermediate Pressure (IP) and the Low Pressure (LP) heat exchanger train. Steam produced in these pressure levels is sent to the HP, IP and LP turbine respectively. The flue gas finally exits the HRSG at 132°C for all the cases investigated and is sent to the atmosphere.

The exhaust gas exits the gas turbine at around 602°C and enters the HRSG where additional heat is recovered until the flue gas exits the HRSG at 132°C. The steam raised in the HRSG is used to generate power by running commercial steam turbines using a 12.4 MPa/566°C/566°C steam cycle in the non-capture case. The flue gas temperature at the exit of the gas turbine is slightly lower at around 567°C in the capture case so the operating condition of the steam cycle is adjusted to 12.4 MPa/538°C/538°C.

3. Comparison between GEE and Shell IGCCs

3.1. Conventional IGCC without Capture

The coal feed rate required to run an IGCC plant is calculated by determining the fuel gas flowrate required to operate its gas turbine. This is fixed when a specific gas turbine model is selected. In the DOE report [1], same gas turbine has been used for all cases, so the energy content of the fuel gas feed should be very close between the two cases even though the H_2 /CO ratio may be quite different.

As expected, the main difference between the two IGCCs comes from the different gasifiers where coal is fed as different phases: a coal-slurry in the GEE gasifier (cases 1 and 2) and a dry coal in the Shell gasifier (cases 3 and 4). The difference of feed, gasifier internal and operating condition gives rise to the different syngas composition and carbon loss to slag. As shown in Table 1, the Shell gasifier has a higher carbon conversion to syngas up to 99.5% and very low CO₂ formation (2%) and high CO yield (H₂/CO = 0.51) at the gasifier outlet. The GEE gasifier has lower carbon conversion rate (98.0%), higher CO₂ yield (15%) and low CO yield (H₂/CO = 0.97). Given the difference of carbon conversion, and CO₂ yield, the Shell IGCC may well need less coal in order to produce a fixed energy flow of fuel gas. The use of different gasifiers in the IGCC plants results in a 3% difference in net plant efficiency between cases 1 and 3. Case 3 shows a lower gross power generation in the steam cycle due to the need to use some steam

as both gasifier and gas turbine diluents. In the two non-capture cases, a single-stage Selexol unit was used to achieve 99.5% removal of H₂S from the syngas.

Composition	GEE gasifier	Shell gasifier
Ar	0.0079	0.0097
CH_4	0.0010	0.0004
СО	0.3442	0.5716
CO_2	0.1511	0.0211
COS	0.0002	0.0007
H_2	0.3349	0.2901
H_2O	0.1429	0.0364
H_2S	0.0073	0.0081
N_2	0.0089	0.0585
NH ₃	0.0017	0.0033
O_2	0.0000	0.0000
SO_2	0.0000	0.0000
Total	1.0000	1.0000

Table 1. Syngas composition at the gasifier outlet in case of Illinois No.6 Bituminous coal gasification [1].

3.2. IGCC with 90% Carbon Capture

In case of retrofitting a pre-combustion capture unit to an IGCC power plant, it can be expected that additional fuel would be fed to the gasifier in order to operate the same gas turbine. This is because the heating value of the fuel gas will be reduced due to exothermic shift reaction so more coal should be fed to the gasifier to compensate the heat loss. However, the increments of fuel in the two cases are different as shown in Table 3. The syngas from the Shell gasifier contains less CO_2 and more CO than that from the GEE gasifier but both syngases experience the same 95.7% shift conversion rate as explained in 2.2. This means that the absolute amount of CO being converted to CO_2 is greater in the Shell IGCC system as shown in Figs. 1 and 2. Therefore, more fuel should be added to the coal feed and the difference of heat input between the two cases is almost equivalent to the difference of heat of reaction generated in the shift reaction. In addition, the different H₂ and CO recovery in the AGR units between the non-capture and capture cases would also affect the coal input increment.

One obvious change in the Shell IGCC with carbon capture is the need to cool down the raw syngas by quench water instead of syngas recycle. In case 3, the syngas recycle reduces the syngas temperature to 885 °C, which facilitates the operation of the syngas cooler at a lower temperature. In case 4, however, the syngas is cooled by water quench, which sacrifices most HP steam generation but has the syngas enriched with water. This change is beneficial in that the amount of shift steam injection can be drastically reduced to a level similar to the steam usage in the GEE IGCC. The amount of water quench and its temperature is fixed so that the syngas at the syngas scrubber is saturated with water at 200 °C. Use of more water could not increase the water content in the syngas scrubber since saturation is achieved. The amount of water at the syngas scrubber is higher in the Shell IGCC even at very similar temperatures since the total pressure is very different.



Figure 1.Schematic diagrams of the GEE gasifier, syngas scrubber, and shift reactors in (a) non-capture (case 1) and (b) capture (case 2) mode [1]. Syngas Recycle



Figure 2.Schematic diagrams of the Shell gasifier, syngas scrubber, and shift reactors in (a) non-capture (case 3) and (b) capture (case 4) modes [1].

Plant Performance (kWe)	GEE IGCC without capture (Case 1)		GEE IGCC with capture (Case 2)		Shell IGCC without capture (Case 3)		Shell IGCC with capture (Case 4)	
	NETL	This work	NETL	This work	NETL	This work	NETL	This work
Thermal Input,kWth	1,674,044		1,710,780		1,547,493		1,617,772	
Power summary								
Gas turbine power	464,300	464,000	464,010	464,000	464,030	464,000	463,630	464,000
Steam turbine power	298,920	298,974	274,690	274,698	283,990	283,996	229,925	229,950
Syngas Expander	7,130	7,282	6,260	6,339	-	-	-	-
Total power generation	770,350	770,256	744,960	745,037	748,020	747,996	693,555	693,950
Total Auxiliaries	130,100	130,759	189,285	197,657	112,170	111,397	176,420	189,180
Net Power	640,250	639,497	545,936	547,380	635,850	636,599	517,135	504,770
Net power plant efficiency (HHV), %	38.2	38.2	32.5	32.0	41.1	41.1	32.0	31.2

Table 2. Comparison of DOE NETL[1] data and simulation of cases 1-4.

Table 3. Energy penalty in simulation cases.

Source of energy penalty	GEE	IGCC	Shell IGCC		
Source of energy penalty	Energy change	Energy penalty	Energy change	Energy penalty	
Heat input increase, kW _{th}	36,736	_	70,279	_	
Gas turbine, kW _e	0	0.60 %	0	1.30 %	
Sweet Gas Expander, kWe	-943	0.06 %	_	_	
Steam Turbine, kWe	-24,276	1.80 %	-54,046	4.14 %	
Gross Power Generation, kWe	-25,219	2.46 %	-54,046	5.44 %	
Auxiliary Total, kWe	66,898	3.74 %	77,783	4.50 %	
Total , kWe	-92,117	6.20 %	-131,829	9.94 %	

As shown in Fig. 2, the syngas temperature is allowed to decrease below the COS hydrolysis temperature as long as the water content is more than what is required in the reaction in case 3. But, in case 4, the syngas temperature should be kept higher than 200 °C until it enters the shift reactor since the amount of water quench was determined as the amount of water needed in the syngas when it is saturated with water at 200 °C.

The quench water should be heated to achieve the correct steam content but maintain the syngas temperature at a sufficiently high temperature. Part of the quench water should be heated by the hot flue gas in the HRSG. As a result, this energy consumption gives rise to the significant drop in power generation at steam cycle as shown in Table 2. This process change is not needed in the GEE IGCC since the raw syngas is already saturated with water by the water quench taking place inside the gasifier. This leads to a reduced drop in power generation in the steam cycle.

Table 2 shows that the results of this work have efficiency drop which are 0.5 to 0.8% larger that what reported by the DOE [1]. In the DOE report [1], it was assumed that 100% H₂ can be recovered at the dual-stage Selexol unit, but it is more likely that a small amount of H₂ would be lost in both the steam stripper sour gas and the CO₂ product. In this study, the H₂ solubility in the Selexol solvent was taken into account and the dual-stage Selexol processes were designed such that they can recover 99.4% H₂ from the

AGR feed H₂. At the same time, the operating conditions have been selected to meet 99.5% H₂S removal, 90% overall carbon capture defined as *(Carbon in CO₂ product)* \div *(Carbon in the coal – Carbon in the slag)* \times 100, and around 10ppm sulphur in CO₂ product. The overall net plant efficiency is reduced because of the higher power consumption in the AGR unit predicted in this study.

The energy penalty relating to carbon capture in both gasifier cases was summarised in Table 3. As explained above, the Shell IGCC would experience higher energy penalty than the GEE IGCC since more fuel should be fed to the gasifier to overcome the loss of the heat flow in the shift reaction. Also higher loss in the steam turbine can be explained by the use of water quench instead of syngas recycle in cooling down the syngas temperature.

4. Conclusions

The Shell IGCC has a far better plant efficiency than the GEE IGCC in case of the non-capture case due to its high carbon conversion and low CO_2 yield. However, the syngas of the Shell IGCC using dry coal has a lower water content than that of the GEE IGCC using coal slurry, which makes the implementation of the WGS sections very different and results in a drop in net plant efficiency of 10%. To avoid this drastic plant efficiency drop, it is worth considering how to improve the carbon capture rate in the AGR unit without significant increase in its power consumption in order to reduce the shift conversion given the target to achieve 90% carbon capture rate overall. This can improve the net plant efficiency in the Shell IGCC by saving coal consumption.

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