

Application of the ENBIPRO Software Code for the Simulation of a Novel IGCC Plant with CO₂ Capture

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Abstract

The purpose of this work is to present a thermodynamic cycle calculation software and its potential in the simulation of novel electricity generation cycles integrating CO₂ sequestration. The software code ENBIPRO (ENergie-BIlanz-PROgram) is a powerful tool for heat and mass balance solving of complex thermodynamic circuits, calculation of efficiency, exergetic and exergoeconomic analysis of power plants. The software code models all pieces of equipment that usually appear in power plant installations and can accurately calculate all thermodynamic properties (temperature, pressure, enthalpy) at each node of the thermodynamic circuit, power consumption of each component, flue gas composition etc. The code has proven its validity by accurately simulating a large number of power plants and through comparison of the results with other commercial software [1].

Following a detailed presentation of the software code, ENBIPRO is used for the evaluation of a novel concept dealing with the carbonation-calcination process of lime for CO₂ capture from coal fired power plants compared to integration of CO₂ capture in a typical Integrated Gasification Combined Cycle power plant. In the novel concept, coal is gasified with steam and lime. Lime absorbs the CO₂ released from the coal, generating limestone. The produced gas can be a low carbon or even a zero carbon (H₂) gas, depending on the ratio of lime added to the process, and can be used for electricity generation in state-of-the-art combined cycles, generating almost no CO₂ emissions or other harmful pollutants. The limestone is regenerated in a second reactor where pure CO₂ is produced, which can be either sold to industry or sequestered in long term disposal areas. Results from thermodynamic simulations dealing with the most important features for CO₂ reduction are presented concerning both technological options. The operating characteristics as well as the main figures of the plants heat balances are included.

Introduction

According to the third assessment report of the Intergovernmental Panel on Climate Change (IPCC), most of the observed global warming over the last 50 years is likely to have been due to the increase in greenhouse gas concentrations in the atmosphere. In identifying strategies for mitigation of climate change, it is concluded that combinations of multiple technologies in all sectors must be considered [2]. Among these, CO₂ sequestration holds an important position. In this context, the integration of CO₂ sequestration concepts in power generation schemes is currently a field of intensive study.

In the frame of CO₂ capture and sequestration in power plants, this paper contributes to the investigation of a new pre-combustion concept, which is based on CO₂ removal during coal gasification by means of CaO. This technology implies the production of a low-carbon fuel gas in one reactor by integrating all the processes, namely gasification, CO shift and CaO carbonation, in a single step. The performance of the Combined Cycle power plant is evaluated by using the software code ENBIPRO.

Nomenclature

ASU: Air Separation Unit

CC: Combined Cycle

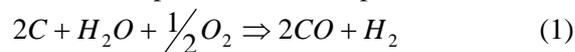
G: Gasifier

GT: Gas Turbine

HP: High Pressure
 HRSG: Heat Recovery Steam Generator
 IGCC: Integrated Gasification Combined Cycle
 IP: Intermediate Pressure
 LHV: Lower Heating Value
 LP: Low Pressure
 NG: Natural Gas
 R: Regenerator
 RH: Reheater
 SH: Superheater
 ST: Steam Turbine
 TEG: Tri Ethylene Glycol

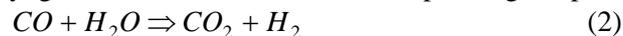
Technology Description

In the frame of CO₂ pre-combustion capture, coal is gasified in order to produce the synthesis gas, which is mainly a mixture of H₂ and CO. In the conventional coal gasification process, coal enters the gasifier with steam and oxygen or air, in a high temperature and pressure atmosphere. The products of conventional gasification are syngas and a solid ash waste product [3]. This process is described by the following reaction



In reality, the synthesis gas contains also CO₂ and CH₄. Since coal gasification is an endothermic reaction, part of the coal is burned to supply the heat needed and to produce CO and CO₂. In the conventional process coal enters the reactor, which operates at a temperature above 1273 K [3].

In order to produce a carbon-free or a low-carbon fuel gas (mainly H₂), the water gas shift reaction should take place. According to this reaction, CO is converted into CO₂ and H₂. This reaction is exothermic. In the standard process, the syngas enters another reactor with operating temperature below 673 K [3].



The CO₂ can be captured from the produced fuel gas by using lime sorbent (CaO). This reaction, which is also exothermic, occurs at about 1100 K and produces CaCO₃ [3].



The next step is the regeneration of CaCO₃ to release the captured CO₂ and to produce CaO, which will be consequently reused to remove the CO₂ from the fuel gas.

According to the technology described in this paper, the above-mentioned reactions take place in a single reactor. This process is being integrated in a new concept for power plants for the production of H₂ from carbonaceous fuels. The overall reaction is exothermic and, as a result, there is no requirement for direct coal combustion within the gasifier to produce heat for the coal gasification process. The fuel gas mixture that is produced by the integration of the reactions has a high hydrogen concentration. The basic flow sheet of the process is illustrated in Fig. 1 below.

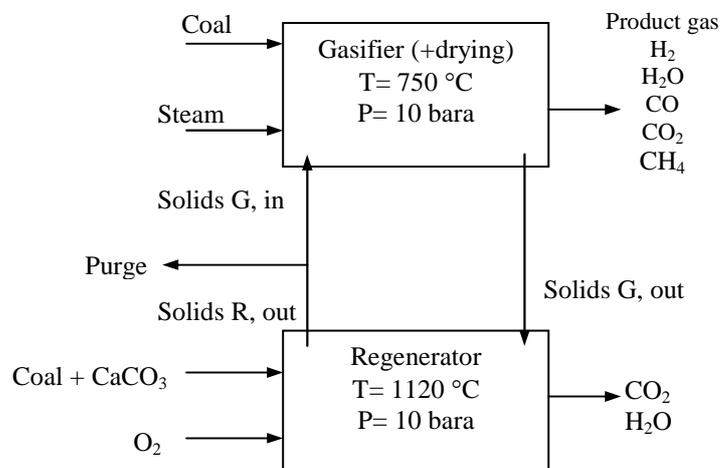


Figure 1: Process flow sheet.

Two fluidized beds can be used as the two main process units, namely the gasifier and the regenerator [4, 5, 6]. The operating pressure of both reactors is 10 bara while the temperature is 750 °C and 1120 °C respectively. In the calcinator, the reverse calcination occurs at higher temperatures and the sorbent is regenerated. Due to the exothermic CO₂ absorption by CaO, the overall reaction in the gasifier can be adjusted to be slightly exothermic, resulting in minimized energetic losses. The produced fuel gas is hydrogen rich, while the regenerator product gas consists mainly of CO₂ and H₂O. The solids that exit the gasifier are CaO, limestone, lignite ash, CaS, gypsum and char (C that has not reacted in the gasifier). On the other hand, the solids that exit the regenerator are CaO, ash and gypsum. The feasibility of the process has been demonstrated by the experimental work conducted for the CO₂ acceptor gasification process [6], the only difference being that they did not produce pure CO₂.

Extra energy is required from the regenerator, which is provided by the combustion of the char that exits the gasifier and an additional fuel flow. This energy includes the sensible heat required from the solids that exit the gasifier at 750 °C and enter the regenerator, which operates at 1120 °C plus the reaction heat of the CaCO₃ (make-up CaCO₃ plus CaCO₃ in the gasifier outlet solids). For the combustion of the char and the regenerator fuel, pure O₂ instead of air is used. In this way, air nitrogen is avoided. As a result, the regenerator product gas contains mainly CO₂ and H₂O and is ready to be compressed for transportation and storage after being cooled down to near ambient temperature and passed through solids removal filters. Cryogenic air separation is used as the most suitable technology, a process capable of producing high flows of high-purity oxygen [7].

One significant drawback of the procedure is argued to be the rapid reduction of the CO₂-capture capacity of CaO after a number of cycles, due to difficulties in its continuous reactivation. The calcination process results in the loss of the suitable pore volume in the lime-based sorbent, reducing significantly the carbonation capacity [8, 9]. Due to the absorbent decay, a flow of solids from the outlet of the regenerator should exit the system. The CaO that leaves the system by the purge stream is compensated by the make-up CaCO₃ flow in the regenerator.

Simulation of CC fired with the low-C fuel

In order to mode the novel concept, a natural-gas fired single-shaft Combined Cycle plant of 400 MW net electric power production has been used as the backbone of the simulation. The cycle consists of one F-class gas turbine, one steam turbine and a triple-pressure heat recovery steam generator. The gas turbine exhaust gas enters the Heat Recovery Steam Generator (HRSG), which operates at three pressure water/steam levels (HP, IP and LP) with three drums respectively. Steam from the high-pressure superheaters (HP SH) enters the HP steam turbine (HP ST). From the outlet of the HP ST it is mixed with steam from the IP SH and enters the boiler to be reheated. Consequently, it is admitted to the IP ST. The steam from the outlet of the IP ST is mixed with steam from the LP SH and enters the LP ST. Finally, from the outlet of the LP ST it enters the condenser.

Water w. %	50.9
Ash, w. %	6.77
C, w. %	29.2
H, w. %	2.00
N, w. %	0.47
O, w. %	9.44
S, w. %	1.22
LHV (kJ/kg)	9785

Table 1: Lignite ultimate analysis

H ₂ , vol. %	65.81
CH ₄ , vol. %	12.94
CO ₂ , vol. %	0.98
CO, vol. %	3.21
H ₂ O, vol. %	15.73
N ₂ , vol. %	1.33
LHV (kJ/kg)	35419

Table 2: Fuel gas composition

The lignite ultimate analysis that is used for the modelling of the process is shown in Table 1 below. In this case, due to the high water content of the lignite, no extra steam is needed. The composition and the LHV of the low-carbon fuel gas that is produced by the process are shown in Table 2. The equilibrium based mass balance of the dual fluidized bed process for the production of a low-C fuel is based on the following assumptions:

Gasifier

- The gasifier operates at 10 bara pressure
- The temperature is 750 °C
- Char to the regenerator is 20% of the carbon input to the gasifier
- Due to the high moisture content of the coal, no additional steam is required for the gasification
- Coal is not pre-dried before entering the gasifier

Regenerator

- The regenerator pressure is 10 bara
- The temperature is 1120 °C
- Char and coal are burned with pure oxygen produced by a cryogenic ASU
- The excess oxygen for char and coal combustion is assumed to be 2%.
- The fresh limestone and the oxygen are preheated up to 600 °C by the product gas of the regenerator (1120 °C) and the fuel gas (750 °C)
- The purge rate is 12.7 % (Purge flow/ Solids R, out flow)

For the production of 19.40 kg/s of fuel gas, which is the flow needed for the simulated combined cycle power plant, 71.06 kg/s of lignite with the given composition enter the gasifier. This lignite supply quantity corresponds to 20.75 kg/s carbon. 20% of this carbon does not react and enters the regenerator with the flow of solids exiting the gasifier (flow Solids G, out in fig. 1). The char flow and an extra lignite flow of 21.93 kg/s are burned with 31.83 kg/s of pure oxygen produced by the cryogenic ASU.

The main results of the simulations are illustrated in Table 3, where the net efficiency is based on the fuel gas heat input and not on the heat input of the lignite that is consumed for production of the fuel gas.

Power & Efficiency	Combined Cycle fired with low-C fuel gas
GT Power Output (MW)	253.916
ST Power Output (MW)	138.231
Block Net Electric Output (MW)	390.289
Block Net Efficiency (%)	56.8

Table 3: Simulation results of low-C fuel gas fired Combined Cycle power plant.

Results of the process

The block net efficiency of the Combined Cycle power plant coupled with the system for the production of the carbon-free fuel gas is affected by the following power consuming processes:

- Lignite gasification and CO-shift reaction. The lignite heat input to the gasifier produces the low-carbon fuel gas, which has a slightly lower energy content. In the case studied, 1 kg of lignite with LHV 9785 kJ/kg produces 0.273 kg of fuel gas, which has an LHV of 35419 kJ/kg, which equals to 9670 kJ. Due to high H₂ concentration of the fuel gas, a diluent should be added in order to limit the flame temperature and, consequently, the NO_x production. In the present analysis, however, no NO_x control has been accounted for.
- Compression of the low-C fuel gas to 30 bara in order to be supplied to the gas turbine.
- Fuel required for the regeneration process. For 1 kg of lignite that enters the gasifier, about 0.31 kg of lignite is consumed in the calcinator to cover the needs for the regeneration.
- Compression of the regenerator product gas up to 110 bara for transportation and storage.
- Air separation for the production of oxygen for the nitrogen free combustion of fuel and char in the calcinator.
- Oxygen compression up to 10 bara to enter the regenerator
- Pumping of the water for the intermediate cooling during the compression of CO₂ and the air that enters the Air Separation Unit.

Regarding the case studied, the fuel gas heat input of the power plant is 687.15 MW. Consequently, the low-carbon fuel gas that is consumed by the combined cycle plant is 19.4 kg/s. The lignite input to the gasifier is 71.06 kg/s, which equals to 695.32 MW. In addition, 21.93 kg/s of lignite are consumed by the

CaCO₃ regeneration process. This equals to a total (gasifier and calcinator) lignite consumption of 909.91 MW.

The compression of the fuel gas from 10 bara to 30 bara occurs in one step. The fuel gas is assumed to be at 120 °C and the compressor's isentropic efficiency 0.85. The power consumed for this process is 1.28MW.

As far as the CO₂ compression is concerned, three steps with intermediate cooling are required: 10-30 bara, 30-58 bara and 58-110 bara. The fact that the CO₂ rich gas exits the regenerator at 10 bara pressure decreases considerably the CO₂ compressors power consumption. The CO₂ is cooled before each step to 20 °C and the condensed water is removed. At 58 bara pressure and 20 °C the CO₂ is in the liquid state [9]. The compression power that is consumed is 19.32 MW. The isentropic efficiency ratio of the CO₂ compressors is assumed to be 0.85.

It is proposed that in order for CO₂ to be of transportation quality, almost all the water content in the gas should be removed due to corrosion issues and the hydrate precipitation, which can block the transport pipelines. Water condensation with cooling water is not enough, since not all the water in the gas is removed. At the pressure level of 30 bara, the gas enters the TEG unit (Tri Ethylene Glycol) where the remaining water is almost completely absorbed [10].

Cryogenic air separation can provide high purity oxygen in a large scale. Even oxygen purities of 99.7 % are available with this technology. In the case studied, pure O₂ is assumed to enter the regenerator for the combustion of char and lignite. As a result, the ASU power consumption calculations are made for the 99.7 % purity case. For 32.47 kg/s of O₂ (81307.42 Nm³/h) that are needed for the combustion of char and lignite with O₂ excess 2%, 142.90 kg/s (402689.7 Nm³/h) of air enter the Air Separation Unit. The air enters the ASU at 5.85 bara, which is the pressure of the distillation column for the 99.7 % O₂ purity case [7]. The compression from the ambient pressure up to 5.85 bara occurs in 4 steps with intermediate cooling: 1-1.56 bara, 1.56-2.42 bara, 2.42-3.76 bara and 3.76-5.85 bara. Air is cooled after each step to 20 °C. The compression power that is consumed is about 27.39 MW. The isentropic efficiency ratio of the air compressors is assumed to be 0.83.

The oxygen exits the ASU at about atmospheric pressure and 18 °C. As a result, extra power is consumed for the compression up to 10 bara to enter the regenerator. To compress 32.47 kg of O₂ the power required is 9.95 MW with 0.83 compressors isentropic efficiency.

For the intermediate cooling during the compression of CO₂ and the compression of air before the ASU, the cooling water is assumed to be at 2.5 bara and the power consumption of the cooling water pumps is taken into account for the calculations. The cooling water pumping power consumption for the CO₂ intermediate cooling is 0.44 MW while for the air intermediate cooling it is 0.35 MW.

The simulation results for the Combined Cycle system coupled with the low-carbon fuel gas production system are illustrated in Table 4 below.

Lignite Heat Input (Gasifier and Regenerator) (MW)	909.91
Compression of the fuel gas in order to enter the GT (MW)	1.28
CO ₂ compression (MW)	19.32
ASU (MW)	27.39
Cooling water pumping for CO ₂ and ASU air (MW)	0.79
Oxygen compression (MW)	9.95
Net Power Output (MW)	332.559
Net efficiency (%)	36.55
C entering the gasifier and regenerator (lignite) (mol/s)	2262.76
CO ₂ in the flue gas (mol/s)	431.77
C removal efficiency (%)	80.92
CO ₂ emissions (kg/MWh el)	200

Table 4: Novel concept with lime CO₂ capture - Simulation results.

Energetic and Exergetic analysis of the Combined Cycle

Figures 2 and 3 show the results of the calculations concerning the energy and exergy flow of the combined cycle plant operating at the full load based on the fuel gas produced according to the above mentioned process for the production of a low-carbon fuel. The energy flow calculations are based on the

lower heating value of the low carbon fuel. The energy input of the fuel consists of 100% chemically bound energy. 38.2% of the fuel input energy is transformed into electrical power in the gas turbine. 61.8% of the supplied energy is directed to the heat recovery steam generator. The thermal energy of the flue gas is recovered and an additional 18.6% is converted into electricity by a steam turbine generator. The rest of the input energy is transferred to the environment through the condenser (27.2%) and the flue gas exiting the HRSG (16.0%).

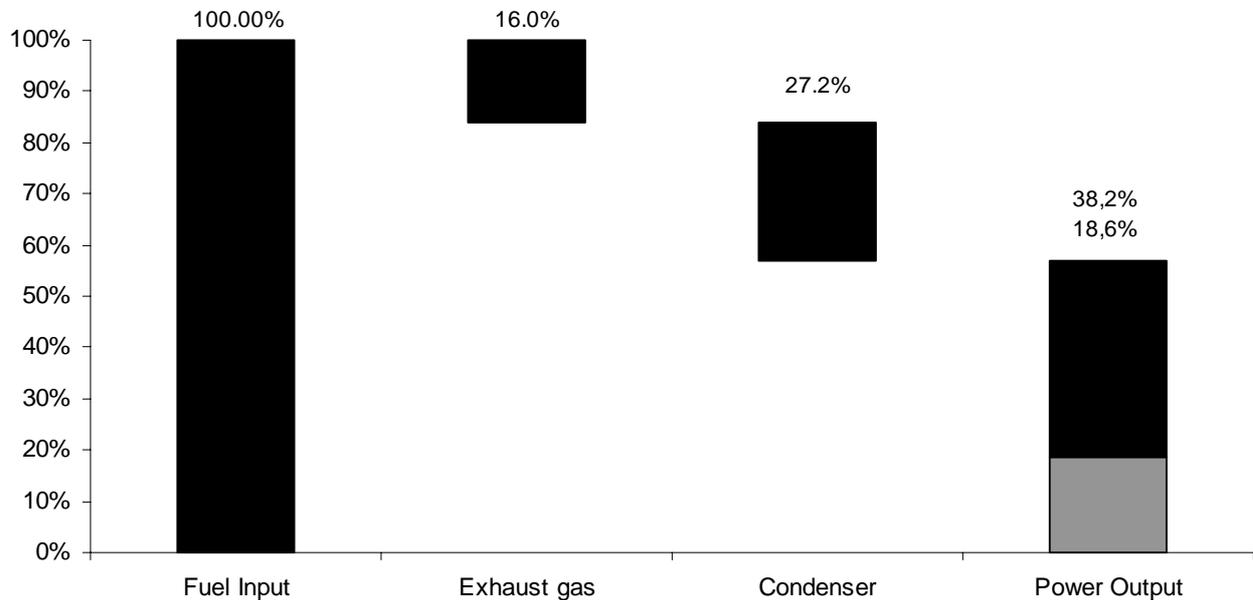


Figure 2: Combined Cycle relative energy flows entering and leaving the process

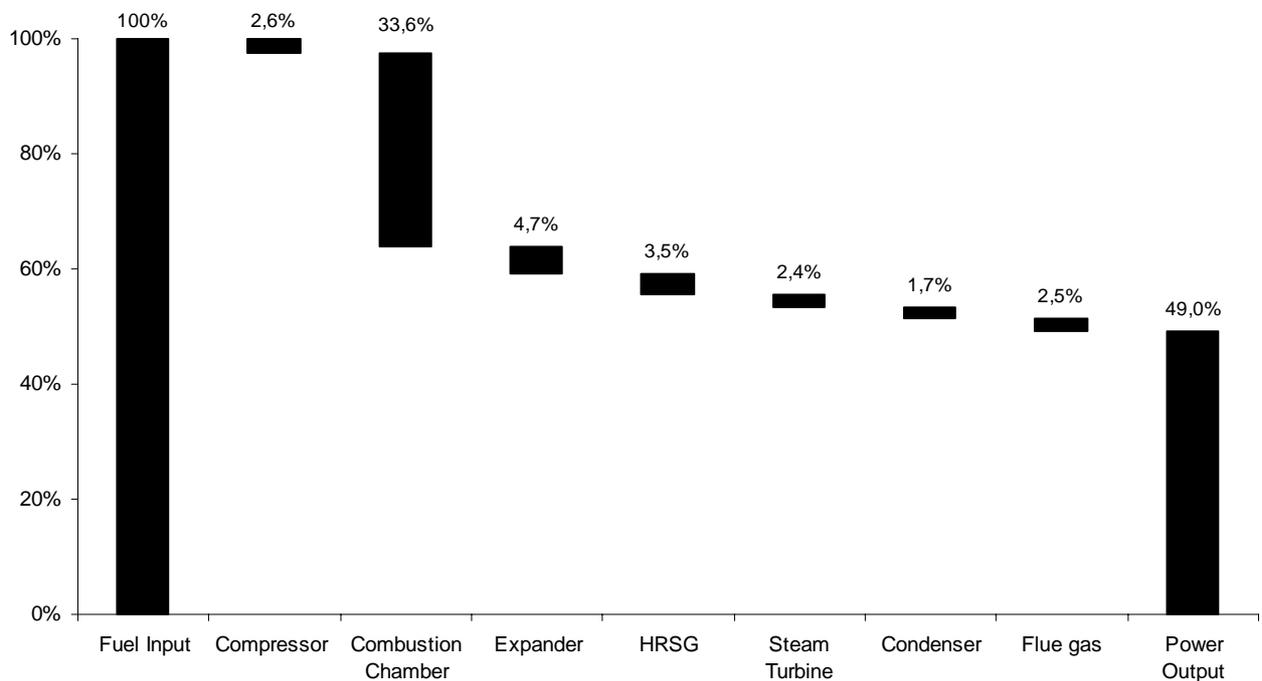


Figure 3: CC relative exergy losses entering the process and losses (with respect to the fuel HHV)

The exergy method shows how the performance of a system differs from the ideal cycle, to what extent each component contributes to this difference and what can be done to design better, less irreversible systems. As can be seen in Figure 3, the exergy flow decreases much more rapidly than the energy flow, as exergy destruction occurs in each component. The presented flows, in percentage, are derived from the division of the exergy flow by the exergy of the fuel (HHV). Each flow shows the exergy change because of

heat, mass or work transfer as well as because of exergy destruction by irreversibilities. The largest source of exergy destruction is the combustion chamber, in which 33.6% of the supplied fuel exergy is lost. The exergy destruction in the compressor and the gas turbine and the steam turbine has been calculated equal to 2.6% and 4.7% and 3.5% respectively. The exergy losses because of heat transfer in the heat recovery steam generator have been estimated to about 3.5%. The relative exergy flows leaving the combined cycle plant without further utilisation for electrical power production are represented by the exergy losses of the condenser and the flue gas (1.7% and 2.5%). The amount of the exergy input (HHV) which is leaving the process as electrical power is presented on the last bar and is equal to 49%.

Discussion of physical absorption process effect on IGCC efficiency

Coal gasification technology is applied in IGCC systems. Coal gasification processes usually operate with pure oxygen and water vapour and the synthesis gas contains CO and H₂. As mentioned above, in order to precipitate the CO₂ before the combustion of the synthesis gas, the CO is converted into CO₂ and H₂ through an exothermic reaction known as ‘CO shift’ or ‘water shift’ reaction. After the conversion, the synthesis gas consists mainly of H₂ and CO₂. The advantage of these systems regarding the CO₂ sequestration concept is that the gas volume to be treated is small while the CO₂ partial pressure is high enough, allowing the physical absorption CO₂ capture technique to be an effective and efficient alternative [11].

According to the physical adsorption technology, carbon dioxide is adsorbed physically in a solvent. Henry’s Law dominates this process, which means that the absorption is pressure and temperature dependent. The CO₂ capture have better results in high partial pressures and low temperatures allowing high levels of separation with high purities of CO₂ [11]. The amount of energy required is low.

Physical Absorbents that can be used for the CO₂ removal from the produced fuel gas are:

- Methanol- Rectisol
- n-methyl-2 pyrrolidon (NMP)
- dimethyl-ether-polyethylene-glycol (DMPEG)- Selexol
- Propylene carbonate

In Table 5 below, the efficiency penalty of a coal fired IGCC power plant with pre-combustion CO₂ capture is illustrated [12]. The CO₂ capture system includes the shift reactor and physical absorption with Selexol. The oxygen required for the process is produced by a cryogenic ASU. The CO₂ is assumed to be compressed up to 110 bara for transportation and storage.

	IGCC original	IGCC with CO₂ capture
Plant size (MW el)	776	676
Net efficiency (%)	43	34
CO ₂ emissions (kg/MWh el)	763	142

Table 5: Efficiency decrease of IGCC with CO₂ physical absorption using Selexol.

Conclusions

The IGCC system with CO₂ capture during coal gasification with CaO provides an optimized process for the production of a low-carbon fuel gas from coal. The integration of coal gasification, CO shift reaction and CO₂ capture in one single reactor is a promising technology which is expected to result in decreased energy and efficiency penalties compared to the IGCC with pre-combustion CO₂ capture with physical absorption by means of Selexol. However, due to the fact that this pre-combustion concept is new, further investigation should be conducted regarding the process flow and process units of such a system. Further considerations of the IGCC with integrated gasification/CO₂ removal process include the thermodynamic optimization as, for example, the recovery of the high energy content of the fuel gas that exits the gasifier and the waste gas that exits the regenerator. Taking into account that both streams should be cooled down to near ambient temperature, the sensible heat could be integrated in the water/steam cycle of the combined cycle power plant. The study, including the energetic and exergetic analysis of the Combined Cycle utilizing the low-carbon fuel gas produced by the process, has been supported by the thermodynamic cycle calculation software ENBIPRO (**EN**ergie-**BI**llanz-**PRO**gram).

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