

Article

# Design and Assessment of an IGCC Concept with CO<sub>2</sub> Capture for the Co-Generation of Electricity and Substitute Natural Gas

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**Abstract:** The focus of this work is on the modeling and the thermodynamic evaluation of an integrated gasification combined cycle (IGCC) for the co-production of electricity and substitute natural gas (SNG). At first, an IGCC with CO<sub>2</sub> capture for electricity generation is analyzed. Coal-derived syngas is conditioned in a water gas shift unit (WGS), and cleaned in an acid gas removal system including carbon capture. Eventually, the conditioned syngas is fed to a combined cycle. A second case refers to a complete conversion of syngas to SNG in an integrated commercial methanation unit (TREMP™ process, Haldor Topsøe, Kgs. Lyngby, Denmark). Due to the exothermic reaction, a gas recycling and intercooling stages are necessary to avoid catalyst damage. Based on a state-of-the-art IGCC plant, an optimal integration of the synthetic process considering off-design behavior was determined. The raw syngas production remains constant in both cases, while one shift reactor in combination with a bypass is used to provide an adequate H<sub>2</sub>/CO-ratio for the methanation unit. Electricity has to be purchased from the grid in order to cover the internal consumption when producing SNG. The resulting heat and power distributions of both cases are discussed.

**Keywords:** co-production; IGCC; Methanation; substitute natural gas

## 1. Introduction

The global energy use is rapidly increasing in all forms, including electrical power, liquid fuels and natural gas. Coal is still a reliable and relatively inexpensive primary energy resource for most industrialized countries. In 2012, coal accounted for 30% of the global primary energy supply [1]. According to projections by the U.S. EIA [2], the total primary energy demand will increase by 56% by 2040, while the share of natural gas will grow by 64% (reference year 2010). The focus of current research in this area lies on advanced concepts for the integration of multiple energy sources and the generation of several products. Coal-fired concepts resulting in polygeneration are a promising technology as the co-generation of electricity, liquid fuels and SNG (synthetic natural gas or substitute natural gas) is associated with several economic and ecological advantages. The diversity of products allows a decoupling of the production from the corresponding demand. Synthetic products could serve as a long-term chemical storage based on their high energy density. Therefore, polygeneration concepts also offer a solution to the energy storage problem.

Coupling the production of materials and energy from coal outperforms stand-alone concepts by tightly integrating multiple processes into one system using synergies [3,4]. Moreover, operating the plant in a flexible way is linked to monetary benefits. The types of feedstock and products are determined by the market price and demand. Compared to the separate generation of the same products, polygeneration offers a higher robustness towards market fluctuations due to the fact of having access to several markets. Generally, a particular motivation for the production of SNG is the existing infrastructure for its distribution through natural gas pipelines.

The principle of catalytic methanation was discovered in 1902 by Sabatier and Senderens when a mixture of CO and H<sub>2</sub> was converted to CH<sub>4</sub> over a metallic catalyst [5]. Table 1 presents the main chemical reactions that are related to the methanation process. The predominantly negative values of the standard enthalpy of reaction  $\Delta H_r$  indicate a highly exothermic reaction, which resulted in the development of several cooling and process designs. According to Seglin and Gould [5], these reactions keep their exothermic character over a wide temperature range of 300–1000 °C. Assuming chemical equilibrium, the composition of the product, and thus all quality characteristics of the SNG, depends on the number of equilibrium stages, reaction conditions, and the composition of the supplied syngas.

**Table 1.** Main methanation reactions [3,5,6].

| Reaction  |                             | $\Delta H_r$ (kJ/mol) |    |
|---|-----------------------------|-----------------------|----|
| CO + 3H <sub>2</sub> ↔ CH <sub>4</sub> + H <sub>2</sub> O                 | CO methanation              | −206.28               | R1 |
| CO <sub>2</sub> + 4H <sub>2</sub> ↔ CH <sub>4</sub> + 2H <sub>2</sub> O   | CO <sub>2</sub> methanation | −165.12               | R2 |
| CO + H <sub>2</sub> O ↔ H <sub>2</sub> + CO <sub>2</sub>                  | Water-gas shift reaction    | −41.16                | R3 |
| C <sub>2</sub> H <sub>4</sub> + 2H <sub>2</sub> O ↔ 2CO + 4H <sub>2</sub> | Hydration of ethene         | +210                  | R4 |
| 2H <sub>2</sub> + 2CO ↔ CH <sub>4</sub> + CO <sub>2</sub>                 | Hydration of CO             | −247                  | R5 |
| 2CO ↔ C + CO <sub>2</sub>   | Boudouard reaction          | −173                  | R6 |
| 2H <sub>2</sub> + C ↔ CH <sub>4</sub>                                     | Hydrogasification           | −74                   | R7 |
| CH <sub>4</sub> + H <sub>2</sub> O ↔ CO + H <sub>2</sub>                  | Steam reforming             | +206                  | R8 |

In general, all metals of the eighth transition group of the periodic table catalyze methane synthesis. Due to their availability and price stability, catalysts based on nickel are commercially used. The catalysts can be operated over a wide range of temperature and pressure (250–750 °C, 1–80 bar), wherein the methanation is promoted at low temperatures and high pressures. Concerning load flexibility, thermal energy needs to be supplied to the reactors when the SNG production pauses, to maintain the catalyst activation temperature, thus enabling a faster start-up. Below a temperature of 250 °C, the catalysis is disrupted due to the low activation energy. However, the catalyst begins to sinter above 750 °C [7]. For providing a high conversion of CO, and accordingly a high concentration of CH<sub>4</sub> in the product stream, a H<sub>2</sub>/CO ratio of about 3:1 is required. Since a cleaned syngas typically has ratios of 1:3 to 2:1 [8] depending on the conditions of the gasification, a water-gas shift unit (WGS) is required to convert part of CO to H<sub>2</sub> according to reaction R3 in Table 1. The adjustment of the gas composition is described by the feed gas module M, which is defined in the following:

$$M = \frac{x_{H_2,in} - x_{CO_2,in}}{x_{CO,in} - x_{CO_2,in}} \quad (1)$$

A feed gas module M of three is recommended for maximum methane yield [3–5,8–11]. Since the requirements of the syngas composition are different for the gas turbine and the methanation process, adjustments are necessary in the WGS. Further information is given in Section 3.

The absorption of the heat of reaction by process steam in an adiabatic reactor is not possible as long as the mole fraction of each CO and CO<sub>2</sub> is well above 2.5 mole-% [10]. Typically, the treated syngas has a CO fraction above 20 mole-% and other temperature control systems are required. The majority of the methanation processes has its origin in the 60s and 70s of the 20th century [8].

Today, different reactor configurations are available. All concepts can be grouped into two categories depending on whether they use a fixed-bed or a fluidized-bed reactor. Kopyscinski *et al.* [6] present a detailed overview of existing methanation processes. In commercial applications, mainly fixed-bed reactors are used because of the high abrasion of the costly catalyst in fluidized beds. The TREMP™ (Topsøes recycle energy efficient methanation process (developed by the Danish Company Haldor Topsøe, Kgs. Lyngby, Denmark) became of particular interest since a stable long-term behavior at high conversion rates was proven [12]. The process describes a series of equilibrium-limited fixed-bed reactors (three to four stages) including intermediate gas cooling and a recirculation of the product stream from the first reactor outlet. A serial arrangement is favored based on the exothermic nature of the methanation process in conjunction with insufficient axial and radial heat dissipation when using multiple fixed bed reactors at pressures between 25 and 40 bar. The partial conversion limits the amount of released heat and thereby the adiabatic temperature within the reactors. Recycling the product stream around the first reactor as well as cooling each product gas to around 300 °C leads to a shift of the equilibrium towards higher CH<sub>4</sub> concentrations.

Other studies focused on the single production of SNG derived from coal or biomass gasification [13–16]. Li *et al.* [17–19] used some of the generated SNG for combustion in a combined-cycle process to co-produce electricity. Buttler *et al.* [7] proposed a concept using electrolysis in addition to the water gas shift reactor to produce SNG and electricity. Work using only heat from the SNG production path to generate steam, which is expanded in a steam turbine without using a gas turbine, has been presented by Karellas *et al.* [20]. A cogeneration process for SNG and electricity based on fluidized-bed gasification was analyzed by Bu *et al.* [21]. In their study, electricity was co-produced by recovering heat from the SNG unit. Only few studies focused on integrated concepts for the co-production of SNG and electricity. The integration in these systems is limited to heat integration by recovering heat from the methanation reactors, to produce power as a by-product. However, these studies consider a coproduction only under design conditions. This study analyzes two cases. The design case (BASE Case) deals with a common integrated gasification combined cycle (IGCC) process that produces only electricity. In contrast to other research, the second case considers a co-production of SNG and electricity under off-design conditions and analyses their impact on the heat integration.

Based on a low-cost IGCC concept producing only electricity, the TREMP is implemented to convert syngas coming from the gas-cleaning unit to high-quality SNG. First, the effect of the process and design parameters, such as the number of reactor stages, on the SNG quality has been examined. The heat and power distributions for the BASE Case and the SNG Case are further discussed.

## 2. Assumptions, Methodology and Simulation

The process simulations are undertaken using AspenPlus® 7.1 (Aspen) [22] and Epsilon® Professional 10.03 (Epsilon) [23]. The TREMP unit and the IGCC units, except the steam cycle, are modelled using Aspen. The material properties derive from the NIST database. The equilibrium conditions within the reactors are determined by minimizing the Gibbs free energy using the RGIBBS (Gibbs Reactor)-Model. Kopyscinski *et al.* give the process parameters of the TREMP [5]. The integration of the methanation unit and the resulting design adjustments require a different heat integration scheme. The temperature profiles and the heat demand of subsystems form two sets of boundary conditions for designing the steam cycle of both cases.

In Epsilon, the steam cycle was modeled using the IAPWS-95 (International Association for the Properties of Water and Steam) property method, while, for the gases that are used at the hot side of the heat exchangers, the method “Real Gases” was used. This method includes precise calculations of the thermodynamic properties of pure components, but for mixtures, ideal mixture properties are employed. The pinch temperatures in the counter-current heat exchangers depend on the state of the cooled and heated fluids. Regarding the off-design characteristic of heat exchangers, the calculation of the heat transfer coefficients results from the heat transfer coefficients of the design mode multiplied

by a correction factor that is determined with the aid of one or more characteristic lines. The correction by these lines represent the change of the heat transfer coefficients of the hot and cold side caused by the change of the flow regime.

The off-design calculation of the steam-turbine output considers off-design isentropic efficiencies based on the nominal efficiencies by means of characteristic curves, which incorporate the change in mass flow rate and change of expansion ratio. The flow characteristic (inlet pressure as a function of the steam flow) of the steam turbine is determined according to Stodola's law [24]. In case of wet steam within the steam turbines, an additional correction of the isentropic efficiency with the aid of the Baumann factor is conducted. The reduction of the heat duty results in lower mass flows, and consequently in lower heat transfer coefficients, taking into account the steam cycle boundary conditions. The decrease of inlet pressures and isentropic efficiencies of the steam turbines simultaneously influences the temperature profiles within the heat exchangers and the isentropic efficiencies of the pumps. The determination of the final off-design variables was performed using an iterative approach. The major assumptions are listed in Table 2. In both cases, the fuel is 50 kg/s bituminous coal (Illinois #6) with a composition (weight %, as-received) of 64.61% C, 4.39% H, 1.39% N, 0.86% S, 7.05% O 12.2% ash and 9.5% moisture. The corresponding higher heating value  $HHV_{ar}$  is 27.07 MJ/kg, while the lower heating value is  $LHV_{ar}$  25.97 MJ/kg. Steady-state operation has been assumed in both cases. An SNG processing concept including drying and compression for pipeline transportation is not considered in this study. The steam cycle has also been modeled in Aspen using the IAPWS-95 steam tables to check the consistency within both programs. The deviations are negligible.

**Table 2.** Major assumptions of the simulation.

| Component/System                                | Unit   | Value      |
|---|--------|------------|
| <i>General</i>                                  |        |            |
| Ambient conditions                              | K, bar | 288, 1.013 |
| Mechanical efficiency of turbo-machinery        | %      | 99–99.5    |
| Electrical generator efficiency                 | %      | 99         |
| Electrical motor efficiency                     | %      | 95         |
| <i>ASU</i>                                      |        |            |
| Electric motor efficiency                       | %      | 98         |
| Outlet pressure HP/LP column                    | bar    | 5.8/1.3    |
| <i>Gasification Island</i>                      |        |            |
| Coal mill electrical demand                     | kJ/kg  | 36         |
| Concentration of slurry to gasifier [25]        | %      | 44         |
| Carbon conversion efficiency [25]               | %      | 98         |
| Heat loss gasifier ( $HHV_{as}$ )               | %      | 0.5        |
| O <sub>2</sub> gasification agent pressure      | bar    | 38         |
| O <sub>2</sub> compressor isentropic efficiency | %      | 85         |
| Gasification temperature                        | °C     | 1250       |
| Radiant cooler raw gas temperature [25]         | °C     | 667        |
| Pressure loss scrubber                          | bar    | 0.3        |
| <i>Water gas shifter</i>                        |        |            |
| HT-shifter inlet temperature [25]               | °C     | 225        |
| LT-shifter inlet temperature [25]               | °C     | 204        |
| Steam demand by outlet mole fraction of CO [26] | %      | 1.9        |
| Pressure loss [25]                              | bar    | 0.3        |

Table 2. Cont.

| Component/System  | Unit    | Value        |
|---|---------|--------------|
| <i>Acid gas removal (AGR)</i>   |         |              |
| Offgas temperature at the inlet   | °C      | 30           |
| LP steam production per kg of H <sub>2</sub> S [27]                                     | MJ/kg   | 29.5         |
| Solvent pumps isentropic efficiency   | %       | 75–85        |
| Solvent/gas mole ratio H <sub>2</sub> S absorber  | -       | 0.2          |
| Solvent/gas mole ratio CO <sub>2</sub> absorber, based on [27]                          | -       | 1.26         |
| Refrigeration compressor isentropic efficiency [28]                                     | %       | 78           |
| CO <sub>2</sub> compressor isentropic stage efficiency [28]                             | %       | 77.2–81.5    |
| CO <sub>2</sub> exit conditions   | °C, bar | 45, 110      |
| <i>Claus plant</i>  |         |              |
| Combustion temperature  | °C      | 1050         |
| H <sub>2</sub> S/SO <sub>2</sub> mole ratio [29]  | -       | 2            |
| <i>Gas turbine system</i>   |         |              |
| Turbine inlet temperature (TIT)   | °C      | 1253         |
| Air compressor isentropic efficiency  | %       | 88.2         |
| Gas turbine isentropic efficiency   | %       | 87.9         |
| <i>TREMP<sup>TM</sup></i>   |         |              |
| Recycle rate  | %       | 70           |
| Recycle-pump isentropic efficiency  | %       | 87           |
| Outlet temperature of product   | °C      | 35           |
| <i>Steam cycle</i>  |         |              |
| Steam-turbine isentropic efficiency HP, IP, LP [30]                                     | %       | 94.2, 96, 89 |
| Isentropic efficiency of pumps  | %       | 85           |
| Condenser pressure  | bar     | 0.035        |
| Pinch-point temperature difference for gas/gas, gas/liquid, liquid/liquid heat transfer | K       | 20, 10, 5    |

### 3. System Design

Two different cases are considered in this study. The BASE case refers to a combined-cycle process for generating only electricity including carbon capture, while in the second case (SNG case), the entire syngas is converted to SNG.

#### 3.1. Base Case

The overall system design of the enhanced IGCC with an integrated methanation unit producing SNG is presented in Figure 1 and selected simulation results referring to streams are presented in Table 3. The key subsystems of this concept are a gasifier, an air separation unit (ASU), an acid gas removal (AGR) unit, a gas turbine system and a steam cycle. A General Electric Energy (GEE) oxygen-blown entrained-flow slagging gasifier with a radiant syngas cooler is used to produce syngas at a temperature of 1250 °C and a pressure of 36 bar. The gasifier uses a single-stage, slurry feed design without the need of a coal-drying unit. The slurry feedstock contains 56 weight % coal, which is crushed before it is mixed with recycled water. The syngas temperature is then reduced to 667 °C by producing high pressure (HP) steam through the radiant cooler. Within the gasifier, a heat loss of 0.5% of coal  $HHV_{ar}$  is taken into account. The carbon-conversion efficiency is assumed to be 98%. Oxygen with a 98% of purity is provided by the ASU.

The syngas is further cooled to 177 °C by a water quench which also separates fly ash through scrubbing. The major part of the separated liquid phase is then recycled to the slurry tank. After this cooling section, the syngas enters the water gas shift (WGS) unit (sour shift).

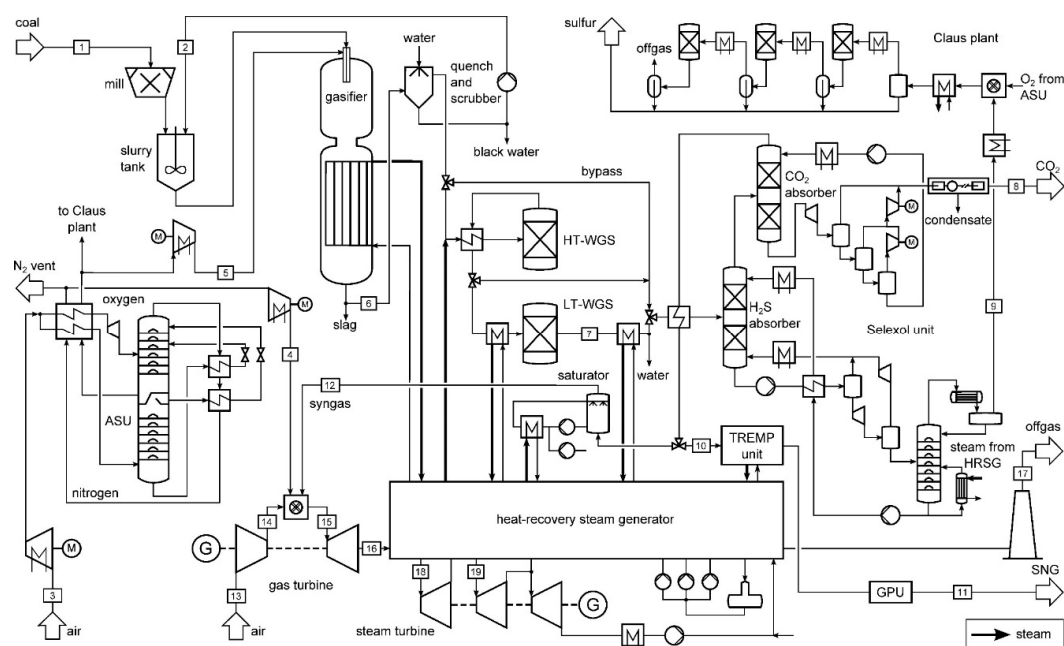


Figure 1. Flow diagram of the overall concept including the BASE and SNG case.

Table 3. Simulation results for selected flows.

| Flow No. | Type                        | Temperature<br>(°C) | Pressure<br>(bar) | Mass Flow<br>(kg/s) |
|----------|-----------------------------|---------------------|-------------------|---------------------|
| 1        | Coal                        | 15.0                | 1.013             | 50.0                |
| 2        | Water                       | 177.3               | 35.7              | 22.0                |
| 3        | Air                         | 15.0                | 1.013             | 164.1               |
| 4        | Nitrogen                    | 126.6               | 26                | 124.1               |
| 5        | Oxygen                      | 93.6                | 38.0              | 40.0                |
| 6        | Raw gas                     | 677.0               | 35.6              | 87.8                |
| 7        | Shift gas                   | 243.9               | 34.4              | 165.2               |
| 8        | CO <sub>2</sub> (BASE case) | 45.0                | 110.0             | 108.0               |
|          | CO <sub>2</sub> (SNG case)  | 45.0                | 110.0             | 70.1                |
| 9        | Acid gas (BASE case)        | 24.9                | 1.3               | 1.3                 |
|          | Acid gas (SNG case)         | 28.9                | 1.3               | 1.3                 |
| 10       | Syngas                      | 19.8                | 34                | 32.3                |
| 11       | SNG                         | 35                  | 26.9              | 32.3                |
| 12       | Syngas                      | 130.9               | 34                | 16.7                |
| 13       | Air                         | 15.0                | 1.0               | 539.9               |
| 14       | Air                         | 426.1               | 19.5              | 539.9               |
| 15       | Combustion gas              | 1253.0              | 19.5              | 680.8               |
| 16       | Exhaust gas                 | 588.6               | 1.1               | 680.8               |
| 17       | Offgas (BASE case)          | 133.2               | 1.02              | 680.8               |
| 18       | Steam (BASE case)           | 597.4               | 168.0             | 246.1               |
|          | Steam (SNG case)            | 450.4               | 129.8             | 62.7                |
| 19       | Steam (BASE case)           | 582.4               | 85.0              | 143.8               |
|          | Steam (SNG case)            | 306.6               | 41.6              | 104.4               |

In the BASE case, the syngas is first converted within a high-temperature shift reactor (HT-WGS) at 440 °C and then passes through a low-temperature shift reactor (LT-WGS), which operates at 245 °C. Based on this two-stage design, the CO concentration is significantly reduced. Subsequently, mercury is removed and the shifted syngas enters the AGR unit. H<sub>2</sub>S and CO<sub>2</sub> are captured in a Selexol process. The captured H<sub>2</sub>S exits the regeneration column of the first capture cycle, in which

low pressure (LP) steam is used, and is then sent to a Claus plant. Within the Claus plant, a part of the  $H_2S$  is oxidized to  $SO_2$  and finally condensed to elemental sulfur.

The  $CO_2$  exits the second capture cycle through three flash stages to a multi-stage intercooled compressor to meet the transport conditions of 110 bar and 45 °C. The cleaned syngas exits the AGR unit at 20 °C and 34 bar and yields 96.6 mole-%  $H_2$ . Since this is a considerable amount of  $H_2$ , a dilution with water is used to decrease the firing temperature in the downstream gas turbine system. Additionally, some nitrogen from the ASU is injected into the combustion chamber. The parameters of the gas turbine presented in Table 2 were identified based on the gas turbine SGT5-4000F manufactured by Siemens [31]. Finally, the steam cycle was designed to maximize the produced electricity through the steam turbine. Figure 2 presents the resulting temperature profiles of the heat transfer within the heat recovery steam generator (HRSG) and external sources. The final offgas temperature of the HRSG is quite high.

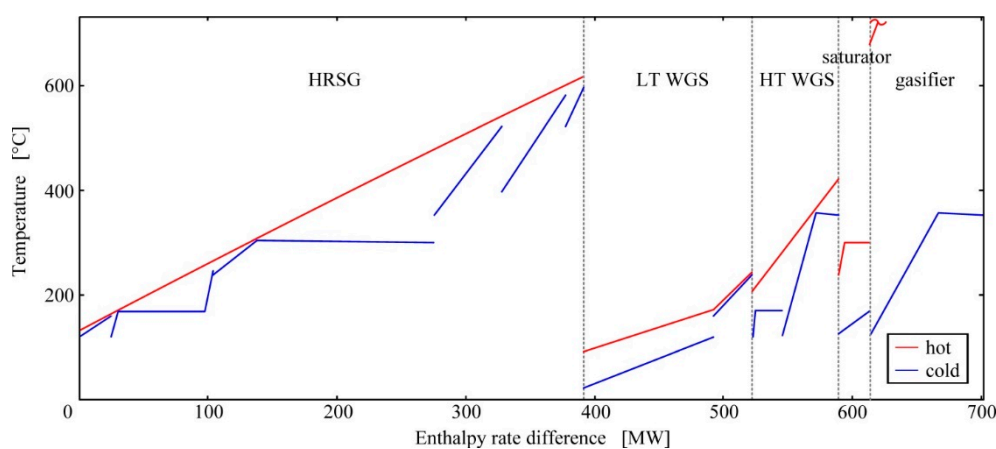
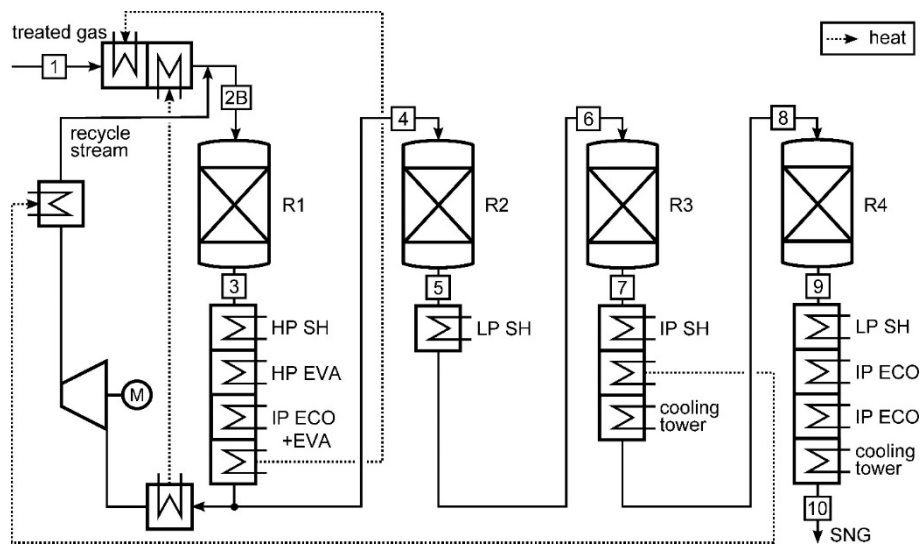


Figure 2. Temperature profiles of the heat transfer within the BASE case.

### 3.2. SNG Case

The gasification island and the ASU are working under the same conditions as in the BASE case. In contrast to the BASE case, the WGS unit consists of only one shift reactor in conjunction with a bypass of the second stage to provide an adequate  $H_2/CO$ -ratio for the SNG-synthesis. The conditioned syngas has a mole composition of 32%  $H_2$ , 11%  $CO$ , 19.5%  $CO_2$  and 36%  $H_2O$  resulting in a feed gas module of  $M = 3.03$  (see Section 1). A smaller stream has to be removed in the AGR unit for  $CO_2$  transport since the  $CO$  shift conversion decreases compared to the BASE case.

Recommendations on the quality and the composition of a syngas fed to the catalytic methanation unit are presented by Gärtner *et al.* [4] and Seglin and Gould [5]. Subsequently, the prepared syngas enters the TREMP unit. Figure 3 shows the flow diagram of the reactor system. First, the syngas is preheated in a heat-recovery system to ensure the catalysis activation temperature after recycled gas is mixed into the main stream. The heat is supplied by cooling the product gas of reactor R1, and it is transported via two internal closed loops. The residual heat from reactor R1 is used to produce HP and intermediate pressure (IP) steam. The produced saturated IP steam is further injected into the raw syngas prior to the WGS unit. The major part of the gas, about 70 weight-%, is recycled to reactor R1. To overcome pressure losses in the recycle, the gas is compressed to a pressure of 34 bar. The  $CH_4$  concentration of the remaining gas increases in the following reactor stages according to the exothermal reaction mechanism presented in Table 1.



**Figure 3.** Flow diagram for the simulated TREMP™ process (SH—superheater, EVA—evaporator, ECO—economizer, HP—high pressure, IP—intermediate pressure, LP—low pressure).

By cooling the product gas of the second reactor, LP steam gets reheated to increase the steam quality at the exit of the LP steam turbine and to increase the thermal efficiency of the bottoming cycle. Moreover, part of this thermal energy is internally shifted to preheat the recycled gas after compression, while another part is cooled by the cooling tower. The product gas of reactor R4 is first cooled by superheating LP steam and then preheating IP and LP steam before the remaining heat is transferred to the cooling tower. Further information regarding the heat integration is given by the temperature profiles in Figure 4. The equilibrium diagram in Figure 5 shows the relationship between the temperature and the CH<sub>4</sub> concentration on a dry basis for the TREMP unit. The black solid line represents the states of complete chemical equilibrium while the horizontal dashed line in Figure 5 is the upper temperature limit for the operation of the catalyst (sintering temperature). Every reactor has a significant contribution to the overall CH<sub>4</sub> conversion, ranging from 8 to 21 percentage points. In comparison to the reactors R1 to R3, the conversion rate of reactor R4 is low. At the outlet of the reactor R3, no CO is left and only methanation over CO<sub>2</sub> takes place. However, the contribution of reactor R4 is important for improving the SNG quality. Recycling the product gas around reactor R1 (point 4) has two advantages. The initial CH<sub>4</sub> concentration increases from point 1 to 2B, and the adiabatic equilibrium temperature is well below the sintering temperature of the catalyst (around 750 °C). In case of no gas recycling, the adiabatic equilibrium temperature of reactor R1 would be above the sintering temperature (Point 2A). In respect to the conversion, an advantageous temperature between 450 °C and 750 °C is achieved.



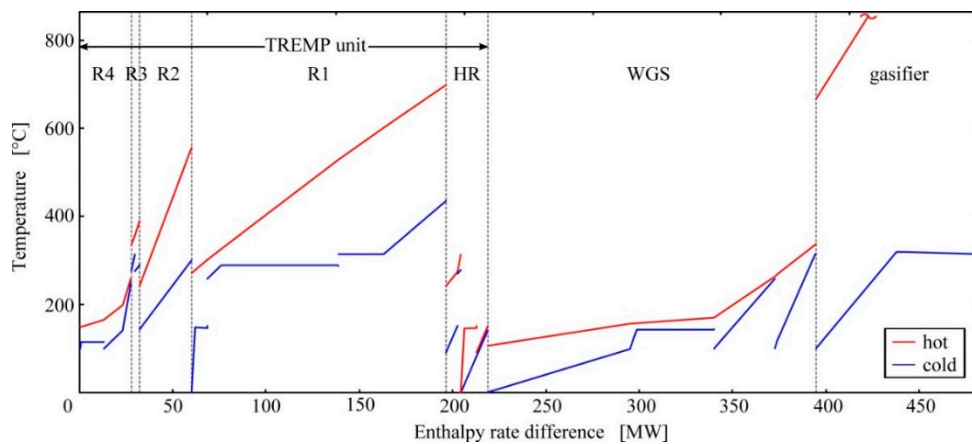


Figure 4. Temperature profiles of the heat transfer within the SNG case.

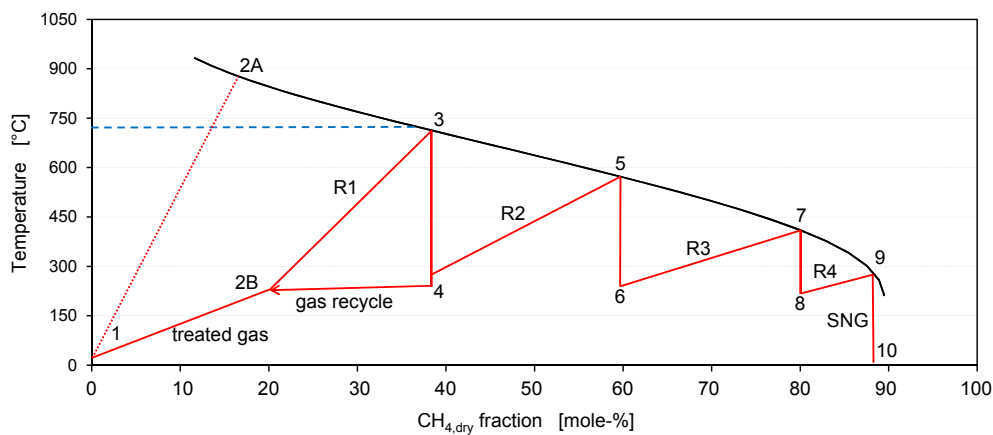
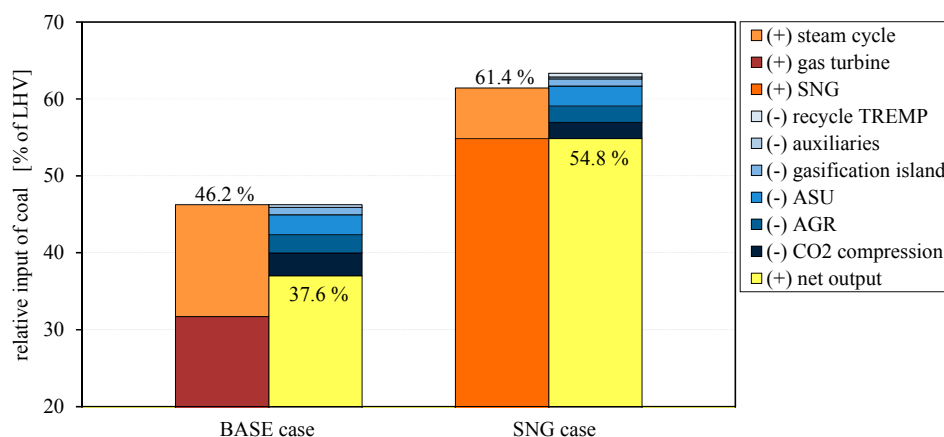


Figure 5. Equilibrium curve of the four-stage TREMP at 27 bar.

When approaching a temperature below 240 °C, the reaction breaks down. The SNG product consists of 47 mole·% CH<sub>4</sub>, 47 mole·% H<sub>2</sub>O, some N<sub>2</sub> and a trace of H<sub>2</sub>. Condensing the water in a downstream gas-processing unit would result in a CH<sub>4</sub> mole fraction of 88% (see Figure 5). The *LHV* of the SNG is 43.2 MJ/kg, while the *HHV* is 48.0 MJ/kg. The TREMP unit as feed-in gas to the grid provides a mass flow of 16.5 kg/s SNG.

#### 4. Results and Discussion

The performance of both cases is presented in Figure 6. The gas turbine system and the steam turbine produce electricity that is partly consumed by various internal subsystems. The steam cycle consists of steam turbines and pumps at three pressure levels (HP, IP and LP). Regarding the ASU, the consumption considers mainly the air compressor. The gasifier includes the compression of oxygen, some pumps as well as the work required for coal milling. In the AGR unit various pumps, the refrigerant compressor and a recycle compressor are taken into account. Moreover, an electrically driven multi-stage compressor is used to provide the pressure for the CO<sub>2</sub> transportation. Despite its small share in internal consumption, the recycle compressor of the TREMP is presented as a separate block. Auxiliaries include components such as coal and slag handling, ASU and AGR auxiliaries, cooling tower fans and auxiliaries used for the gas turbine system and the turbo-machines within the steam cycle.



**Figure 6.** Overall efficiency and power distribution of the analyzed cases.

The key parameters of the steam cycle subsystem are presented in Table 4. The overall net efficiency for the BASE case is 37.6%, while it is 54.8% for the SNG case based on the *LHV* of coal. The corresponding efficiencies based on the *HHV* of coal are 36.1% and 52.6%, respectively. The gas turbine accounts for 69% of the gross output in the BASE case. Accordingly, 31% of the gross output is generated by the steam cycle. 20% of the gross electricity output is consumed internally, mainly by the ASU, the AGR and the CO<sub>2</sub> compressor system. In both cases, the electricity consumption of the ASU amounts to approximately 2.6% of the coal input based on the *LHV*.

**Table 4.** Characteristic data of the steam cycle for both cases.

|                           | Unit | BASE Case | SNG Case |
|---------------------------|------|-----------|----------|
| live steam pressure HP    | bar  | 168.0     | 129.8    |
| live steam pressure IP    | bar  | 85.0      | 41.6     |
| live steam pressure LP    | bar  | 7.7       | 5.9      |
| live steam temperature HP | °C   | 597.4     | 450.4    |
| live steam temperature IP | °C   | 582.4     | 306.6    |
| live steam temperature LP | °C   | 119.1     | 317.4    |
| mass flow                 | kg/s | 246.1     | 187.1    |
| heat input                | MW   | 549.9     | 297.1    |
| heat output               | MW   | −203.4    | −166.1   |
| generated electricity     | MW   | 192.7     | 90.2     |

As presented by Buttler *et al.* [7], the reactors must stay at the activation temperature range during standstill to reduce the start-up time. In this study, the heat that needs to be provided was not considered in the BASE case. The overall SNG product amounts to 16.5 kg/s corresponding to 712 MW based on the *LHV*. The electricity generated by the steam turbine amounts to only 11% of the common energy equivalent gross output of the two products. Haldor Topsøe presented a heat recovery of about 20% for the TREMP unit based on the heating value of the syngas [12]. In this study, a heat recovery of 25% is obtained based on the *LHV* corresponding to 22% based on the *HHV*. The gas turbine does not operate in the SNG case since the entire syngas is converted to SNG in the methanation unit. Consequently, no water needs to be provided for the saturation of the syngas, resulting in a decreasing of the heat output of the steam cycle in the SNG case (see Figure 4). To cover the internal consumption, additional electricity has to be purchased from the grid. The efficiencies of the SNG case do not include the import of electricity. The internal consumption slightly decreases for the SNG case. On one hand, additional work for compression is required by the gas recycle of the TREMP, while on the other hand, less work is required for the CO<sub>2</sub> compression caused by a decreasing CO<sub>2</sub> concentration of the syngas entering the TREMP unit.

In both cases, the share of internal consumption of the CO<sub>2</sub> compressor, the ASU and the AGR unit amounts to more than 90%. Hence, the electrical consumption of the gasification island, the auxiliaries and the TREMP recycle compressor are of minor importance. Although the reaction within the TREMP unit is exothermal, the released thermal energy cannot fully substitute the heat that is supplied by the HRSG in the BASE case. A full integration of the heat released by the reactors of the TREMP unit is not possible due to a surplus in low-temperature heat supply. In particular, the low-temperature heat from reactors R3 and R4 cannot be integrated into the steam cycle due to a similar temperature profile of the WGS. Hence, only 83% of the available thermal energy from the TREMP unit can be integrated. Compared to the BASE case, 51% of the heat transferred in the HRSG can be substituted in the SNG case. Therefore, the total mass flow of steam decreases in the SNG case. Based on the released thermal energy from the methanation unit, 28% are recovered as HP steam, 41% as IP steam, 22% as LP steam and 9% is used for internal heat recovery. In both cases, IP steam needs to be provided to the water quench, scrubber and the WGS unit. In accordance to the Stodola law, the HP and IP live steam parameters decrease since the supplied heat decreases disproportionately, because it is related to the total mass flow. However, the live steam temperature of the LP steam turbine increases. In the off-design case the isentropic efficiencies for the IP and LP steam turbines are reduced to 95.3% and 89.2%, respectively. As a result, the electrical power generated by the steam turbine decreases significantly.

The overall net efficiency of the coal-to-SNG process is 54.8%. A straight thermodynamic comparison of the two analyzed cases is not feasible due to the production of different products. The overall net efficiency decreases by 1%–2%-points when including the import of electricity from the grid as well as an SNG gas-processing unit using a multi-stage compressor for transportation at 80 bar. Chandel and Williams [32] present overall net efficiencies ranging from 44.6% to 49.4% (based on *HHV*) using lignite in different types of gasifiers for the co-production including carbon capture. Li *et al.* [17–19] found an overall efficiency of 59% to 65% (based on *LHV*) for their proposed cogeneration system by using some part of the SNG from the TREMP in a combined cycle. The study of Karellas *et al.* [20] showed an overall efficiency of 66.5% to 69% (based on *LHV*) when the heat of the methanation unit was used for electricity generation in a steam cycle. In contrast to this study, no import of electricity is considered there.

## 5. Conclusions

This study presents an energetic analysis for an IGCC concept including carbon capture and producing SNG and electricity based on two characteristic cases. The overall net efficiency for the BASE case producing only electricity is 37.4% while it is 54.8% for the SNG case (based on the *LHV*). In the SNG case, an additional 1.9% of electricity related to the coal input based on the *LHV* has to be purchased from the grid to cover the internal consumption.

The released thermal energy by the methanation unit is not sufficient to produce enough steam for generating electricity. Additionally, the low-temperature heat cannot be fully integrated into the steam cycle. The waste heat from the TREMP unit is mainly recovered by producing HP and IP steam. Further investigations could be conducted for improving the heat integration scheme, e.g., by using a mixed integer non-linear optimization algorithm. In the next step, an exergy, economic and exergoeconomic analysis [33] will be performed to improve the understanding of the overall process. As a long-term task, other units (e.g., a methanol production unit) can be integrated into the IGCC concept to increase the product diversity.

**Author Contributions:** Max Sorgenfrei conceived and designed the simulation for a conventional IGCC. Timo Blumberg set up the simulations for the methanation unit and the steam cycle and implemented both to obtain the meta simulation. Timo Blumberg and Max Sorgenfrei analysed the data and elaborated the results. The paper was written by Timo Blumberg and revised by Max Sorgenfrei and George Tsatsaronis.

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