

# Carbon chain analysis on a coal IGCC - CCS system with flexible multi-products

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## ABSTRACT

A carbon chain analysis is applied to assess a complex energy conversion system with CO<sub>2</sub> Capture and Storage (CCS). A coal integrated gasification combined cycle, with CCS, which co-produces electricity and liquid fuels (IGCC-LF-CCS) is taken as a case study. A process simulation method is used to estimate the technological data, and balance the heat and electricity for the whole system. Carbon and energy flows are calculated to evaluate the mass conversion efficiency and the energy efficiency. The results show that in the case in which one third of the coal is allotted to synthesize liquid fuels, globally 60 % carbon is captured for storage, 19 % carbon is transferred to liquid fuels, 19 % carbon is emitted to the atmosphere as CO<sub>2</sub>, while the remaining carbon is discharged as solid waste. For the energy flow, 28.1 % of total higher heating value of coal is converted into the liquid fuels. The net electricity efficiency is 20.7 % accounting for the power demands by air separation, CO<sub>2</sub> capture and compression. Three scenarios with different ratio of resource to produce electricity and liquid fuels with or without CCS have been studied and compared. This work will provide useful information for the coal resource utilization with CCS in a carbon-constrained world.

**Keywords:** Carbon chain, IGCC, CCS, liquid fuel, carbon flow, energy flow

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# 1. Introduction

Large scale CO<sub>2</sub> Capture and Storage (CCS) has been considered as one of the most promising ways of mitigating anthropogenic CO<sub>2</sub> emissions and reducing the carbon intensity of the electricity sectors and other industries, like steel, cement and bulk chemicals producers. It is undoubted that carbon sequestration is one of the few options that would allow the use of fossil energy without the threat of dangerously altering the Earth's climate system. Even great efforts and investments are being made by many nations to increase the share of renewable energy in the primary energy supply and to foster conservation and efficiency improvements, addressing climate change concerns during the coming decades will likely require significant contributions from CCS[1]. However, current research has also revealed a lot of pending issues around CCS, such as energy penalty[2, 3], high investments[2, 4], and unknown environmental impacts[5-7], which had become big barriers to commercialization of CCS technologies. Great efforts from both academic institutes and industrial companies have been focused on the solutions to resolve the 3E problems (high Energy penalty, high Economic costs and possible Environmental impacts) which are caused by the deployment of CCS. For example, new modes of combustion for power system, such as pre/oxy-combustion[8], IGCC[9], exhaust gas recirculation[10], membrane WGS reactor[11, 12]; energy-saving CO<sub>2</sub> capture solvents and technologies, such as KS-1 solvent, Econamine FG<sup>+SM</sup>, ionic liquids, zeolitic imidazolate frameworks, membrane etc.[3, 8, 13, 14]; and also new concepts and technologies for CO<sub>2</sub> transport and storage[15], as well as the key issues for scaling up from megatons to gigatons[1].

Even though CCS are new facilities without enough industrial reliability compliance test until now, the necessary components of a CCS system are in commercial available and use today. The technologies for CCS are then rather well known. However, there is no CCS industry today because the components do not currently function together in the manner required for large-scale CO<sub>2</sub> reduction. Therefore, one of the challenges for CCS to be considered as commercial is to integrate and scale up these components[1]. Thus understanding the behavior of complex energy conversion systems with CCS as a whole chain is important before the commercialization of the CCS technologies. This behavior includes economic, technical, environmental and social acceptance issues caused by CCS. One of the important advantages is that many opportunities of energy saving and cost lowering might be found by taking the whole system into account to retrofit the current components or optimize future facilities.

Several works have been down around the concept of chain analysis. A methodology for CO<sub>2</sub> chain was proposed to take the joint impact of several parameters into account and support a systematic evaluation of the potentials of a CO<sub>2</sub> chain. It is an effective tool to assess the behavior and provide important information for decision makers, industries, investors, the public and also the researchers engaged in the technological developments of CCS[16, 17]. The similar concepts were proposed, such as European value chain for CO<sub>2</sub>[18], CO<sub>2</sub> value chain[19], CCS chain[20]. Some applied cases have been studied, such as the value of flexibility in the CCS chain of coal-fired power generation with post combustion carbon capture[21]. K. Damen et al. also proposed a chain analysis method (called CCS chain) to compare energy production costs and CO<sub>2</sub> avoidance costs in a consistent matter, taking electricity and hydrogen production systems as case study. The system boundary of this method was extended and both a spatial and a temporal dimension were considered. The spatial dimension encompasses the infrastructural design to connect energy extraction, conversion, and end-use markets and CO<sub>2</sub> sources with storage reservoirs. The temporal dimension is related to the time frame considered for implementation, i.e., relatively short term and long-term chains [22, 23]. These methods mainly expected

to give the techno-economic performances along the CO<sub>2</sub> chain, but did not investigate the detailed carbon conversion and energy utilization along the chain inside of the system.

Considering carbon is the most important element in complete CCS china, not only existed in CO<sub>2</sub>, but also in raw source, fuel gases, flue gases, liquid fuels with different chemical valencies which show different physical and chemical performances. Thus, the flow of carbon element (direction and amount) in the whole system could be helpful for understanding the efficiencies of mass conversion and energy utilization of a complex system. Hence, in this work, a carbon chain analysis is applied to assess a complex integrated system including CO<sub>2</sub> production, capture, transport and storage, focusing on the efficiencies of carbon conversion and energy utilization. The advantages of the method are: 1) obtaining a more comprehensive chain from resource to CO<sub>2</sub> storage and utilization considering the viewpoint of the whole carbon life cycle; 2) being able to compare energy efficiency and CO<sub>2</sub> emission in a consistent matter as they can differ strongly among technologies and primary resources; 3) knowing the CO<sub>2</sub> emissions over the entire chain which give an indicate on the 'climate neutrality' of de-carbonized electricity and chemicals / products; 4) understanding how the change of a single technology influences the whole carbon chain; 5) providing insight into the trade-off between CO<sub>2</sub> reduction and energy consumed. However, due to the system complexity of CO<sub>2</sub> emitting industries with CCS facilities, a comprehensive carbon chain analysis faces a lot of challenges, such as the definition of the integrated framework of the chain, suitable boundaries, multi-disciplinary, component assessment, technological parameters, data collection and verification, and so on.

An integrated framework consisting of four sessions (resource conversion, CO<sub>2</sub> capture, CO<sub>2</sub> transport and CO<sub>2</sub> storage) is constructed. The model-based method with process simulation tool is used to estimate the technological data and process parameters. Energy and carbon flow analysis based on the detailed simulation results are used to look into the performance of the whole system. A coal Integrated Gasification Combined Cycle (IGCC) process with CCS which co-produces electricity and liquid fuels (IGCC-LF-CCS) is taken as a case study. The rationale of choosing this case is as follows. As coal is a carbon-intensive but abundant primary energy, the coal industry has been focusing on the development of cleaner and less carbon intensive technologies, such as the IGCC to produce electricity[24], synthesize liquid fuels or natural gas to partly mitigate the tensions of crude oil and gas markets. However, one of the main barriers faced by a coal industry is that the CO<sub>2</sub> emission per kW of electricity or per kg of synthesized fuel or chemical products from coal is much higher than in scenarios using crude oil as the feedstock. Recently, the IGCC with CCS has been evaluated as one of the high potential alternatives to at the same time produce electricity and liquid fuels and capture CO<sub>2</sub>[3, 25], while understanding this process deeply will be important for the future mitigation of global warming in the coal industry. Another key point is that synthesizing transport fuels from coal has become a possible option to limit shortages on the oil market and have a flexible supply. For example, one of typical technologies from coal to liquid fuel is the Fischer-Tropsch process which is relatively mature and developed by Sasol<sup>®</sup>[26].

## **2. Methodology and case study**

### ***2.1 Carbon chain description***

The carbon chain in this work combines energy resource, specific electricity, steam, liquid fuels / chemicals production technologies, power plant, and a dedicated infrastructure for CCS. The whole chain encompasses infrastructures designed to connect the energy extraction, conversion, end-use markets and CO<sub>2</sub> sources with storage

reservoirs with respect to the whole carbon life cycle, as show in Fig. 1. Among the six sub-systems, resource conversion, CO<sub>2</sub> capture, transport and storage are key sub-systems whose influences dominate the whole economic and environmental performances caused by CCS activities compared with the traditional power sector and other industries. In addition, various mature and emerging technologies (in sub-systems 2, 4, 5 and 6 of Fig. 1) will provide options to minimize the possible influences of CCS on the industries. Relatively, the resource extraction in itself is often considered to have a limited influence on the global warming. In the market sub-system, many products and goods will finally be consumed and will then cause CO<sub>2</sub> emission during their use. However, at least now, it seems that there is no good way to capture the CO<sub>2</sub> produced from products (chemicals, liquid fuels etc.) consumption in the market and residential sectors. Thus in this work, we will not investigate in detail the resource extraction and market sub-systems but mainly focus on the sub-systems 2, 4, 5 and 6.

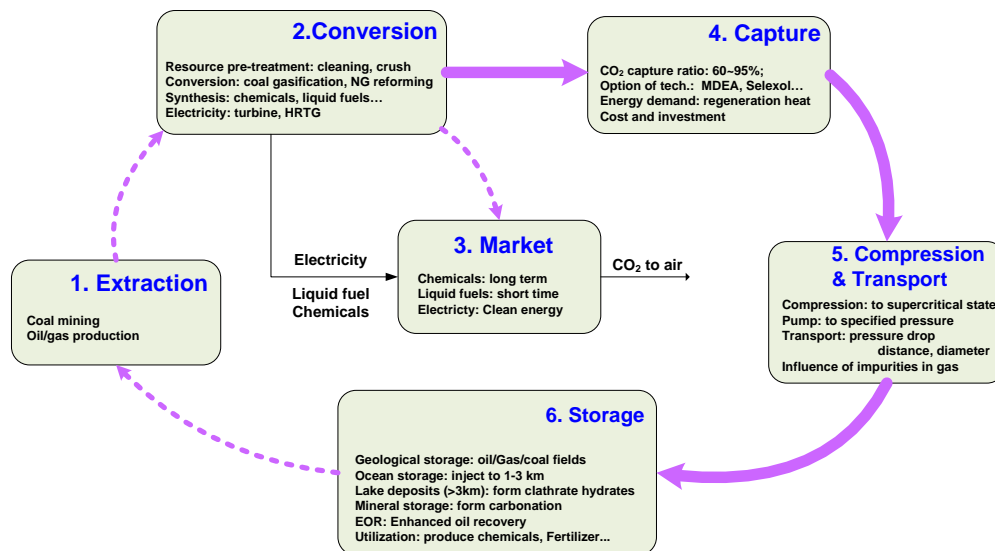


Fig. 1. Carbon chain with respect to the whole carbon life cycle

## 2.2 Method

A carbon chain analysis is applied to assess a complex system which includes the following steps: determination of the system boundary; establishment of the model for each section/unit; key input and output parameters; simulation and data verification; carbon flow and energy flow calculation and assessment. A process simulation software (Aspen Plus) is used to calculate the mass and energy balances of the whole system. The model of each unit in the system is established based on the reactions mechanisms and physical properties. The models and parameters are verified through comparisons with the literature data, industrial data and laboratory data in order to ensure the accuracy and reliability of the simulation results. Based on the simulation results, energy and mass balances, carbon flow and energy flow (HHV-based) can be obtained. The carbon atom utilization efficiency of a unit (or a section, a system) is defined as the percentage of total carbon atom in the useful products (output) to the carbon atom in feedstock (input). The energy efficiency of a unit (or a section, a system) is defined as the percentage of the total useful energy (HHV of the fuel gas, steam, hot water streams, product steams and electricity) from certain unit (or a section, a system) to its total input energy. The CO<sub>2</sub> emission status of the whole system can then be represented. The analysis results can provide a comprehensive status and the level of the energy utilization in the whole system, how and how much of the carbon atoms are converted from one section/unit to another along with the energy flow, and which sections or units might be

the bottlenecks of the energy and mass conversion for the whole system. Hence useful measures and suggestions to reduce the energy consumption of CCS could be obtained and helpful for the possible future deployment of CCS.

### 2.3 Case description

The scheme of the IGCC-LF-CCS case is shown in Fig. 2. It is divided into eight sections: 1) Coal gasification; 2) Heat recovery and steam generation (HRSG-1); 3) Water gas shift (WGS); 4) H<sub>2</sub>S removal and CO<sub>2</sub> capture; 5) Liquid fuels synthesis (F-T Synthesis); 6) Combined heat and power plant (CHP); 7) CO<sub>2</sub> compression and transport, 8) CO<sub>2</sub> storage. The specific technologies of these eight sections have been described in a large body of literatures [2, 15, 22, 23, 27], thus a detailed description will not be given, instead focus will be on some special related features.

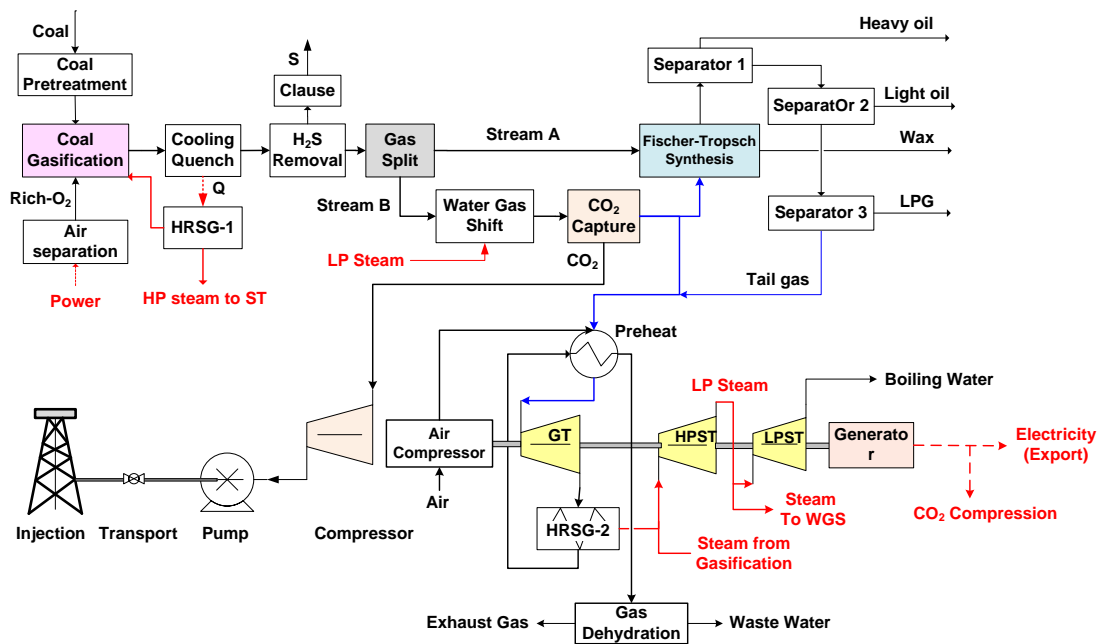


Fig. 2. Scheme of the IGCC-LF-CCS

**Coal conversion.** In Fig. 2, dry coal is introduced to the gasifier via lockhoppers, and oxygen is produced in a cryogenic air separation unit (ASU). Coal, steam and O<sub>2</sub> react in a Shell<sup>®</sup> entrained flow gasifier to produce high temperature syngas. In this paper, it is assumed that the gasification runs about 1540°C and 30 bar, and the carbon conversion is assumed about 99%[24]. Then the HRSG-1 is fed by the hot syngas to recover heat and produce high pressure steam. The specific technological parameters can be obtained from the literature[28-30]. The cold gas is fed to a Selexol<sup>®</sup> acid gas removal unit for desulphurization and further to be converted to elemental sulphur in a Claus plant [2, 31]. The difference between this case and the traditional IGCC is that it is a flexible system in which both liquid fuels and electricity can be produced. The clean syngas stream with low H<sub>2</sub>/CO ratio is divided into streams A and B. The stream A is sent to the F-T synthesis while stream B fed into the two-step WGS to convert CO into CO<sub>2</sub> and improve the yield of H<sub>2</sub>. The related technological parameters and process flowsheet of WGS come from literature[32]. Then the shifted gas is fed into the Selexol<sup>®</sup> unit to extract CO<sub>2</sub> with a CO<sub>2</sub> capture ratio of 95%, and obtain a H<sub>2</sub>-rich gas. A part of this H<sub>2</sub>-rich gas is mixed with stream A to adjust the H<sub>2</sub>/CO ratio of the syngas to be 1.0-2.5 which is a requirement of the F-T synthesis reaction according to the operational conditions and catalysts types. In the F-T synthesis section, the main products are wax, raw diesel oil, raw gasoline, LPG (Liquid Petroleum Gas) and tail gas[25,

26]. The tail gas which is mainly composed of H<sub>2</sub>, CO, low carbon hydrocarbon, CO<sub>2</sub> and so on, is mixed with another part of the H<sub>2</sub>-rich gas and this gas mixture feed the CHP plant. The parameters of the CHP plant come from the literature [2, 29]. The detailed parameters for this section are summarized in table 1. The models and parameters are verified through comparisons with the literature data, industrial data and laboratory data [24, 28-30, 32, 33].

Table 1. Summary of the parameters in CO<sub>2</sub> conversion section

Unit	Parameters
Gasifer	1,540 °C; 30bar; O <sub>2</sub> /Coal (wt): 1; Steam/coal (wt): 0.1
HRSG-1	HeatX-1: Syngas: 1,540 → 600 °C, 30 bar; HP steam: 300 → 560 °C, 120 bar HeatX-2: Syngas: 600 → 102 °C, 30 bar; MP steam: 80 → 470 °C, 46 bar
H <sub>2</sub> S removal	Absorber: 20 °C, 27 bar Desorber: Top: 105 °C, 1 bar; Bottom: 140 ± 5 °C H <sub>2</sub> S removal efficiency: ~96 %
WGS	Stage 1: 450 °C, 25.7 bar; CO conversion: 70 %; Steam/CO: 1.5 (mol) Stage 2: 250 °C, 24.7 bar; CO conversion: 90 %
CO <sub>2</sub> capture	Absorber: Gas: 30 → 7 °C, 25 bar; Solvent: -5 → 10 °C Desorber: 50 °C, 1.05 bar (CO <sub>2</sub> ) CO <sub>2</sub> removal ratio: 95 % CO <sub>2</sub> concentration: 98.5 % (vol)
F-T synthesis	Stage 1: 220 °C, 33.7 bar; CO conversion 61 % Stage 2: 220 °C, 30.3 bar; CO conversion 85 % Feed gas: H <sub>2</sub> /CO ~ 1.5(mol)
CHP	Air compressor: 24 bar Gas turbine: 1,250 → 600 °C; 24 → 1.1 bar High pressure steam turbine: 560 → 470 °C; 120 → 46 bar Middle pressure steam turbine: 470 → 390 °C; 46 → 27 bar Low pressure steam turbine: 390 → 92 °C; 27 → 0.8 bar
Isentropic efficiency	Gas turbine: 91 % Steam turbine: 92 % MP steam turbine: 92 % LP steam turbine: 89 % Compression: 85 % Pump: 75 %

**CO<sub>2</sub> compression.** CO<sub>2</sub> compression is a relatively simple process, but the energy penalty caused by CO<sub>2</sub> compression is high. Indeed, it requires more than half of the total energy penalty caused by CO<sub>2</sub> capture in pulverized fuel power plant, NGCC, IGCC, etc[2]. Thus designing carefully the CO<sub>2</sub> compression process will probably decrease the energy consumption and the cost of CCS remarkably. The optimal mode is that the relatively pure CO<sub>2</sub> from the CO<sub>2</sub> capture section is compressed to be supercritical and then pumped to a specific pressure. Hence, compressors will be used from 1 to 73.8 bar then a pump shall be used from 73.8 bar to the pressure desired (in general 110-150 bar), depending on the requirement of the transport and storage[5]. Purity of CO<sub>2</sub> gas is also a key parameter in the compression process. Low CO<sub>2</sub> concentration needs higher compression power as other highly volatile gases, like N<sub>2</sub>, are pressurized at the same time than CO<sub>2</sub>. For example, the compression power will increase 1.5 % while the CO<sub>2</sub> concentration decreases from 99 % to 97 % based on the simulation with isentropic compression.

**CO<sub>2</sub> transport.** The compressed CO<sub>2</sub> is transported by pipeline to the storage site to inject it into saline aquifer or other available storage ways [22]. In practice, phase changes and pressure conditions of the CO<sub>2</sub> fluid might cause pipeline leakage and raise issues regarding safety and perturbations of normal operation. A few typical problems should be taken into account regarding the CO<sub>2</sub> transport: 1) maintaining minimum pressure along the pipeline above 85 bar; 2) avoiding two-phase flow in pipelines; 3) influence of impurities. High impurities in CO<sub>2</sub> gas will cause high flow velocities due to the lower density and lower storage potential in aquifers [34]. Water content should be less than 500 ppm to avoid the hydrate formation and limit corrosion. For this case, we assumed that a moderate distances of the transport is 500 km which is considered to be both technically and economically feasible[1]. It is assumed that CO<sub>2</sub> is always maintained well above the critical pressure, which therefore requires recompression every 300 km[35]. The pressure drop during the pipeline transport is about 0.06 bar/km[5]. Therefore in this work, the CO<sub>2</sub> flow is only recompressed one time.

**CO<sub>2</sub> storage.** CO<sub>2</sub> geological reservoirs suited for storage are classified into depleted oil and gas fields, deep saline aquifers and coal beds. The costs for storage are various, depending on the storage location and capacity, the reservoir type and characteristics (pressure, thickness, permeability and depth) and storage rate. For example, an onshore aquifer storage with an injection depth between 1,000 and 2,500 m and a storage rate of 1~2 MtCO<sub>2</sub>/year, costs 3 €/tCO<sub>2</sub> stored; while an onshore gas field will have the same cost for a depth between 2,500 and 3,500 m. Among the storage types, Enhanced Oil Recovery (EOR) and Enhanced Gas Recovery (EGR) technologies are relatively mature and might represent an opportunity to store CO<sub>2</sub> at low cost due to the revenues from extra oil and gas. Tests have shown that the adsorption rate for CO<sub>2</sub> is approximately twice the one for methane, giving EGR the potentials to efficiently displace methane and store CO<sub>2</sub>. Compared with EOR or EGR, the sequestration of CO<sub>2</sub> in deep saline formations does not produce any valuable by-products, but it has other advantages such as important storage capacities, easy access to the most existing large CO<sub>2</sub> point sources and being a relatively mature and safe technology. So far, its monitoring suggests that no CO<sub>2</sub> has currently escaped[15]. Thus it is regarded as a good option for CO<sub>2</sub> storage, at least in a near or middle future. Integration of coal bed methane recovery with a coal-fired electricity generating system can provide an option for additional power generation with low CO<sub>2</sub> emissions [15, 36]. However, this type of storage is still in an experimental phase and the real test data are limited, so the deep saline aquifers are chosen as the storage reservoirs and it is assumed that the depth of the aquifers is 1,000 m.

**Heat and electricity balances.** The electricity produced from the CHP plant provides the power demanded by the CCS, ASU and others drive sets in the whole system. The net electricity production and electricity efficiency are then calculated. In this work, the steam is balanced considering the extraction of steam in the HRSG and the CHP to compensate the one consumed by the steam turbine, the gasification and the WGS. Some key parameters are listed in table 1.

## 3. Results and discussions

### 3.1 Carbon flow analysis

Fig. 3 shows the carbon flow of the IGCC-LF-CCS system. The total carbon in the coal feedstock was assumed to be 100 % (wt).

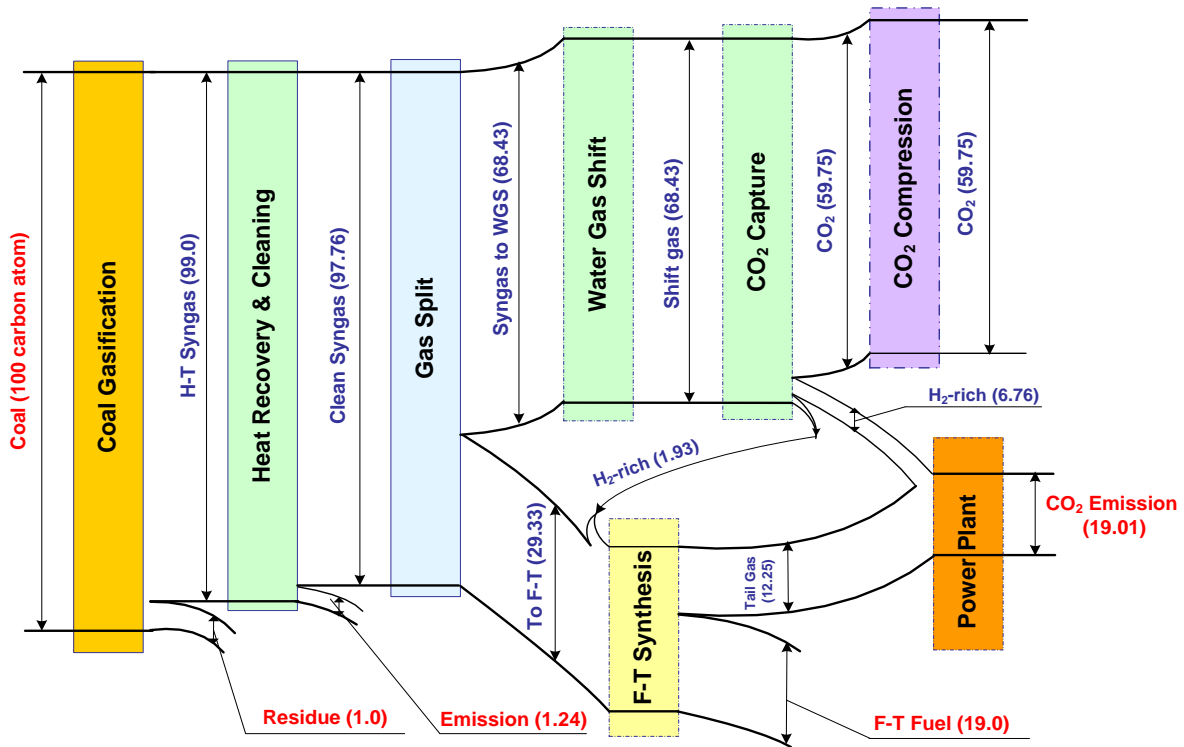


Fig. 3. Carbon flow of the whole IGCC-LF-CCS system

The total carbon in the coal feeds the Shell<sup>®</sup> gasifier which has a carbon conversion efficiency of 99 %. The remaining carbon is discharged as a solid residue; under this shape, carbon is regarded not to cause global warming as it is not in gaseous form. In the section of gas cooling and cleaning, around 1.24 % of total carbon is lost with the discharged waste water containing particles, the dust and the tar are removed from raw syngas. The clean syngas is divided in two parts and 30 % of the total carbon (Stream A, Fig. 2) is sent to the F-T synthesis section. The rest of the clean syngas (Stream B, Fig. 2) is shifted in WGS to produce a H<sub>2</sub>-rich gas (the molar concentration of H<sub>2</sub> increases from 28.8 % to 55.7 %). No carbon loss occurs in the WGS but the carbon is transformed from CO into CO<sub>2</sub>. The shifted syngas is sent to the CO<sub>2</sub> capture section using the Selexol technology to remove 95 % of the CO<sub>2</sub> and get a H<sub>2</sub>-rich gas with around 90 % (mol) H<sub>2</sub>. In order to adjust the H<sub>2</sub>/CO ratio of the gas fed into the F-T reactor to a suitable value, part of the total H<sub>2</sub>-rich gas is extracted to mix it with stream A and obtain a gas mixture with H<sub>2</sub>/CO ratio of 1.5~1.6 which feed the F-T synthesis reactor. 19 % of the total carbon is converted into liquid fuel products.

In the CHP section, the H<sub>2</sub>-rich gas is mixed with the tail gas from F-T to be combusted and then passes through a Gas Turbine to produce electricity. The flue gas with low CO<sub>2</sub> concentration (~4 % mol) is emitted to the atmosphere after recovering the heat with HRSG-2, causing the emission of 19 % of the total carbon. Including waste water from the gas cooling and cleaning section, 20 % of the total carbon is emitted to the atmosphere. The real carbon fixed ratio which includes the carbon fixed in the coal gasification residue and other solid wastes, the liquid fuels and the CO<sub>2</sub> capture, is about 80 %. However only ~60 % of the total carbon is compressed and transported to the storage site by pipeline. Compared to the power plant with the post-combustion and pre-combustion of coal or natural gas which generally have a capture ratio between 85 % and 90 % [2], this case has a relatively lower percent of CO<sub>2</sub> captured since a part of the carbon is fixed in the liquid fuel products. Here, the CO<sub>2</sub> emissions contributed by the transport and storage chain, and possible leakage of CO<sub>2</sub> from the storage site are not taken into account.



Looking into the liquid fuel synthesis section, the distribution of the F-T production is shown in Table 2. The yield of fuel products, which is the main preferred product mixture in F-T process, is 26.4 % (wt). The tail gas by-produced which mainly consists of N<sub>2</sub>, Ar, H<sub>2</sub>, CO, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub> and so on, is 20.5 % (wt). It can be sent to the power plant as fuel. The CO<sub>2</sub> and water by-produced are respectively 25.7 and 27.3 % (wt). This means that more than half of the products from the F-T synthesis process are non-valuable products, causing low carbon atom utilization efficiency and high energy consumption (as a large amount of H<sub>2</sub> or hydrocarbon is transformed into waste water during this process). This is why coal based chemical industry is considered to have a high CO<sub>2</sub> emission and high waste water discharge. The main reason is the limitation of the F-T reaction itself as the product distribution follows the Anderson-Schulz-Flory (ASF) polymerizing model [26, 37]. A great technological challenge, for countries with a large share of coal in their primary energy mix, is to improve the catalyst performances and optimize the reaction routes so as to develop much better technologies to avoid this issue.

Table 2 Product yields and distribution of fuel products in F-T synthesis

<b>Product yield (Versus the total feedstock)</b>							
Products	Liquid fuel products	Tail gas	CO <sub>2</sub>	H <sub>2</sub> O			
wt%	26.4	20.5	25.7	27.3			
<b>Distribution of fuel products</b>							
Fuel products	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>4</sub>	LPG*	Gasoline	Diesel oil	Wax
wt%	9.9	4.1	5	25.1	29.7	16.0	10.2

\*: Liquid Petroleum Gas (mainly refers to the C<sub>3</sub> to C<sub>4</sub> hydrocarbon products).

In this work, the liquid products are assumed to be composed of LPG (C<sub>3</sub>-C<sub>4</sub>), raw gasoline (C<sub>5</sub>-C<sub>9</sub>), raw diesel oil (C<sub>10</sub>-C<sub>18</sub>) and wax (C<sub>+19</sub>). The lighter components are taken as fuel gas to the power plant. Indeed, even if CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> and C<sub>2</sub>H<sub>4</sub> are not the desired products, they represent almost 20 % of the fuels produced in the F-T synthesis, as shown in Table 2, with more than half of it due to methanation. Therefore, inhibiting these by-reactions would improve the yield of the objective products.

### 3.2 Energy flow analysis

Fig. 4 shows the energy flow of the IGCC-LF-CCS system. It is assumed that the total Higher Heating Value (HHV) of the coal feedstock material is 100 (MJ/hr)<sup>1</sup>. According to Fig. 4, the HHV of the high temperature raw syngas from the gasifier is 94. The heat losses in this section are mainly due to the residue discharge and the thermal losses in the gasifier and the pipes. In the HRSG-1 section, the high temperature syngas is cooled to produce steam (21.7) send to power plant. The HHV of the low temperature syngas from the HRSG is 81.9, and then decreases to 78.7 after the acid gas removal unit for desulphurization with Selexol<sup>®</sup> technology. 23.6 (HHV) of the clean syngas is transferred to the F-T synthesis section and the remaining is sent to WGS. In the WGS, high pressure boiling water is preheated by the exothermic WGS reaction to finally produce high temperature water (7.8) which is sent to the HRSG-1 to generate high pressure steam then to the steam turbine (ST) in the CHP. The shift gas is sent to the CO<sub>2</sub> capture section to produce H<sub>2</sub>-rich gas. A part of this H<sub>2</sub>-rich gas, with 19.65 (HHV), flows to the F-T section to satisfy the H<sub>2</sub> demand of the F-T reaction, while the rest of the H<sub>2</sub>-rich gas is sent to the power plant. In the F-T synthesis section, the total HHV of the liquid fuel products is 28.09, and the tail gas, with 9.76 (HHV), flows to the power plant. The total energy fed into the

<sup>1</sup> In the rest text of this paragraph, the unit of the values we omitted.

power plant is 67.19, while the electricity output is 26.8 (net value, eliminating the electricity consumed by air compression into the CHP plant). The electricity needed for CO<sub>2</sub> compression, pumping and re-pumping is 1.92. Considering the electricity consumption required by the CO<sub>2</sub> capture, the air separation unit, and the CO<sub>2</sub> compression and transport, the net electricity production in this system is 20.7 % of the total fed coal (HHV). While including the F-T section, the total net energy efficiency of the whole IGCC-LF-CCS chain is 48.8 % of the total fed coal.

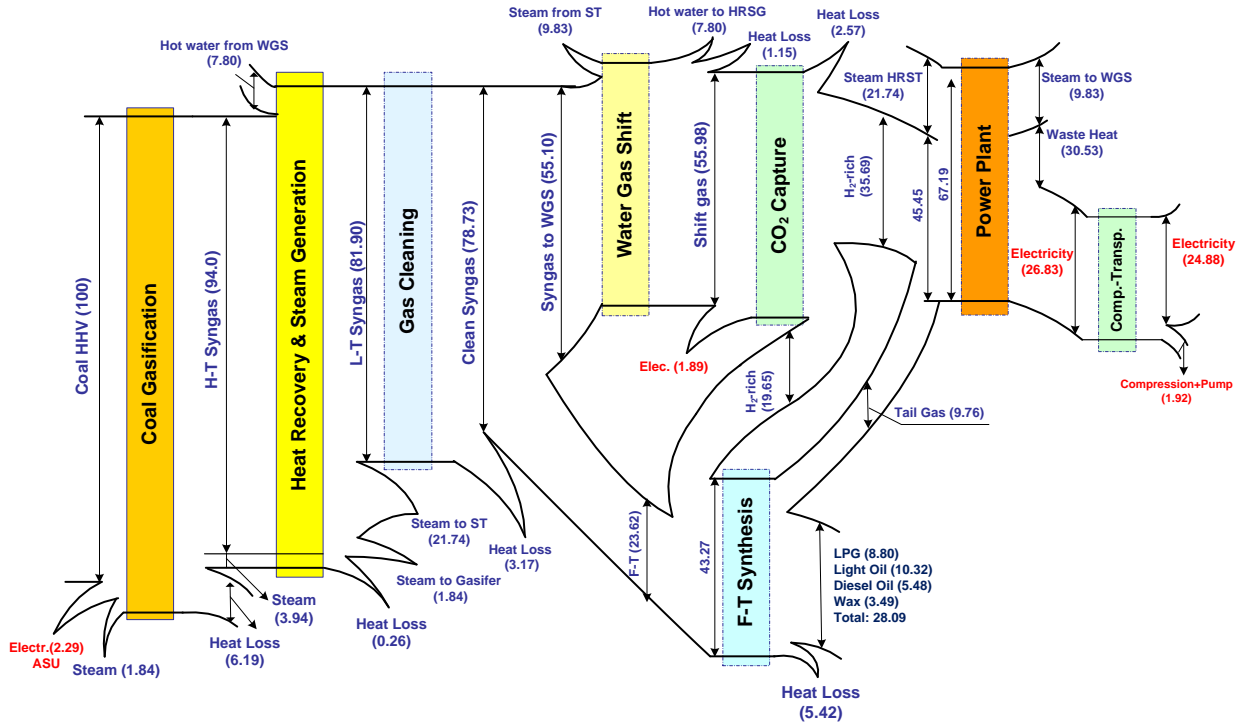


Fig. 4. Energy flow of the whole IGCC-LF-CCS system

### 3.3 Energy efficiency of each section

The energy efficiency ( $\eta_s$ ) of each section along the carbon chain is shown in Fig. 5. Here,  $\eta_s$  is defined as the percentage of total useful energy (HHV of the fuel gas, steam, hot water streams, product streams and electricity) from a certain section to its total input energy. The total efficiency of gasifier is 94 % with the high temperature raw syngas (1,540 °C, 30 bar), but after recovering the heat from the hot syngas, the HHV energy efficiency of cold syngas to coal decrease to 81.9 % (~100 °C). In the heat recovery and steam generation section, the total energy efficiency is nearly 99% due to the heat transfer efficiency is not considered. The efficiency of the CO<sub>2</sub> capture section is 95 % and the energy losses are mainly due to the electricity used by the Selexol technology. The highest energy loss is in the power plant due to the thermodynamic limitation of the conversion from heat to power. In the F-T synthesis section, the efficiency of the total section is 87.5 %, thereinto from syngas to liquid fuel is 67.5 %. The figure of the energy efficiency of each section provides an overview of the energy utilization of the whole process.

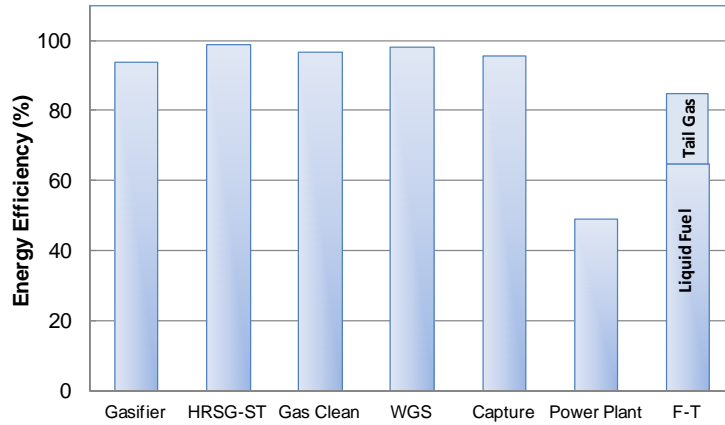


Fig. 5. Energy efficiencies of each section along the carbon chain

### 3.4 Analysis of products distribution

Three scenarios were simulated to compare the influence of the liquid fuel production on the energy utilization efficiency, and the CO<sub>2</sub> captured and emitted from the whole system, as shown in Fig. 6. The unit of each data is shown in the figure. In these three scenarios, the percentage of syngas sent to the F-T synthesis to produce liquid fuels is respectively 0 %, 30 % and 50 %. It indicates that when increasing the ratio of syngas sent to the F-T synthesis, the HHV extracted from coal as electricity produced from the CHP with and without CCS decreases. It is worth noting that as the CO<sub>2</sub> is captured from the syngas after the WGS unit, the amount of CO<sub>2</sub> captured decrease when more syngas is sent to the F-T synthesis (as less syngas is sent to the WGS unit). The CO<sub>2</sub> emissions increase with the ratio of syngas sent to the F-T synthesis because more tail gas is produced and then sent to the CHP where capturing from the exhaust gas (~4 % of CO<sub>2</sub> in flue gas) is uneconomic. Therefore, one can obtain a qualitative comparison and the trade-off between the different coal utilizations depending on the energy efficiency and the CO<sub>2</sub> captured and emitted.

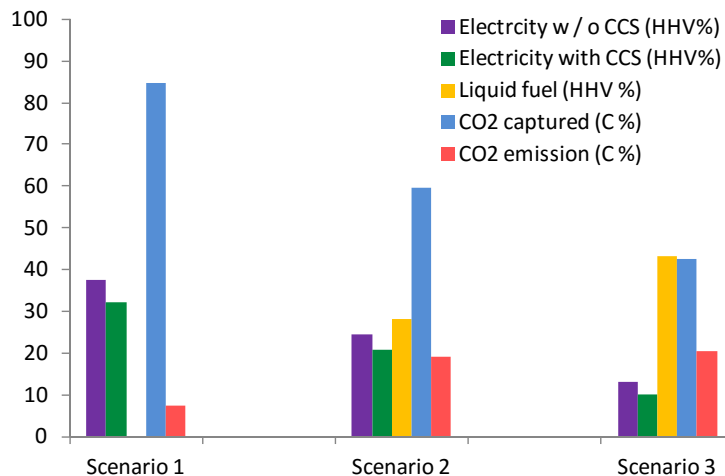


Fig. 6. Analysis on the ratio of syngas sent to the F-T synthesis

## 4. Conclusions

Systemic research and efforts to find solutions to the problems of high energy penalty, high economic costs and possible environmental impacts caused by the deployment of CCS are now considered as an important area. The carbon chain analysis is a relevant and useful method for such complex systems with numerous mass and energy streams. In this work, the carbon chain analysis was used to investigate carbon and energy flows along the whole carbon chain of a flexible process using coal to produce both liquid fuels and electricity with CCS. This work also included a study of the carbon utilization and energy efficiencies. The flexible process with numerous mass and energy streams consists of resource (coal) conversion, CO<sub>2</sub> capture, CO<sub>2</sub> transport and CO<sub>2</sub> storage.

For the specific scenario in which about 30 % of the resource is used to produce liquid fuel products, the carbon conversion efficiency in a coal gasifier is 99 %. Globally 60 % carbon is captured and compressed for transport and storage, 19 % carbon is transferred to liquid fuels, and 19 % carbon is emitted to the atmosphere as CO<sub>2</sub>. Regarding the energy efficiency (HHV %) of each products, 28.1 % of total fed coal is converted into liquid fuels, and totally 26.8 % to electricity. The net electricity production represents 20.7 % of the HHV of the total coal feed when accounting for the power demands by air separation, CO<sub>2</sub> capture, CO<sub>2</sub> compression and transport. The total energy efficiency combining both electricity and liquid fuels for the whole IGCC-LF-CCS chain is 48.8 %. Another important result is the high quantities of CO<sub>2</sub> and waste water produced in the process of coal to liquid fuel products, which is one of the disadvantages of routes of coal to liquid fuel/chemical products. This is also a great challenge for countries with a large share of coal in their primary energy mix.

Analysis of products distribution using three scenarios with different liquid fuels and electricity production ratio with or without CCS has been carried out. A comparison and trade-off between the different coal utilizations depending on the energy efficiency and the CO<sub>2</sub> captured and emitted can provide useful information for the coal resource utilization with CCS in a carbon-constrained world.

Considering the whole carbon chain proposed in this work, focuses was mainly on the resource conversion, CO<sub>2</sub> capture, compression and transport, but closing the loop in Fig. 1 and understanding the whole system, would require knowledge about the possible synergy between CO<sub>2</sub> storage and energy resources extraction. For example, enhanced coal-bed gas with CO<sub>2</sub> injection can probably increase the economic performance of CCS. Further investigation and detailed analysis on energy efficiency, environmental effects as well as risks should be studied intensively. Another issue is that the energy flow method used in this work can give a clear vision of the energy sources and sinks, as well as the energy efficiency and heat losses, but the quality of the energy cannot be represented. Thus exergy (available energy) analysis which can indicate the energy loss as a result of internal or external irreversibilities should be applied in future work. Economic evaluation and environmental impact as well as risk assessments along the carbon chain should be addressed too, and will provide a more comprehensive insight on the potentials and problems of deployment and commercialization of the CCS technologies.

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## Abbreviations

ASF, Anderson-Schulz-Flory; ASU, Air Separation Unit; CCS, CO<sub>2</sub> Capture and Storage; CHP, Combined Heat and Power Plant; EGR, Enhanced Gas Recovery; EOR, Enhanced Oil Recovery; F-T, Fischer-Tropsch; HRSG, Heat Recovery and Steam Generation; IGCC, Integrated Gasification Combined Cycle; LF, Liquid Fuels; HHV, Higher Heating Value; LPG, Liquid Petroleum Gas; NGCC, Natural Gas Combined-Cycle; WGS, Water Gas Shift;

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