

SNG Worked Example for the TEA Guidelines for CO₂ Utilization



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Foreword

Climate change is one of the largest challenges of our time. It is proven that excess amounts of carbon dioxide that humanity has added to the atmosphere plays a key role, and left unaddressed, this will alter ecosystems and fundamentally change life as we know it. Under the auspices of the UN Framework Convention on Climate Change and through the Paris Agreement, there is a commitment to keep global temperature increase to well below two degrees Celsius. Meeting this goal will require a variety of strategies including increased renewable power generation and broad scale electrification, increased energy efficiency, and carbon-negative technologies. Carbon-negative technologies serve two purposes, as a climate mitigation tool near term, and to create a new carbon economy that recycles carbon over the long term- balancing emissions of still essential industrial sectors such as cement and steel. Overall, carbon-negative technologies are a valuable strategy in an overall portfolio of approaches to stabilize the atmospheric carbon dioxide concentration at a level that supports human life on Earth.

Increased attention is being paid to the notion that carbon dioxide can become a valuable resource instead of being a waste product with severe negative consequences to the earth's climate. New technologies, new use cases, interest from the investment community, and growing legislative support poise the use of a carbon dioxide feedstock as a viable economic and societal opportunity.

But not all that glitters is gold! Thorough assessment of the environmental and economic benefits of new technologies is paramount prior to deployment. Transparent and consistent life cycle assessments and techno-economic assessments must provide unbiased information to decision makers to enable sound decisions on investments, deployments, and public support for such.

International demand from government bodies, industry, investors, non-profits, and researchers for harmonized approaches to conduct life cycle assessments and techno-economic assessments for carbon dioxide utilization led us to coordinate and fund an international effort to develop and disseminate Guidelines for TEA & LCA for CO₂ Utilization. First published in 2018, these Guidelines have found widespread attention and use and have recently been updated (<http://hdl.handle.net/2027.42/162573>). A growing list of case studies, and worked examples, is made available to illustrate how to use these Guidelines.

We hope that this case study will be useful to you and we will be grateful for any feedback!

April 2021, Volker Sick, Global CO₂ Initiative

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Abbreviations and symbols

Abbreviations

AACE	Association for the Advancement of Cost Estimating
CAPEX	Capital expenditure
CEPCI	Chemical Engineering Plant Cost Index
CHP	Combined heat and power
EI	Environmental impact
ETS	Emissions trading scheme
HHV	Higher heating value
HRC	Hot-rolled coil
LHV	Lower heating value
MRR	Monitor and reporting regulation
MW	Megawatt
OPEX	Operational expenditure
PEM	Polymer electrolyte membrane
SNG	Synthetic natural gas
TRL	Technology readiness level

Latin symbols

C_i	Cost of equipment i	
D_i	Minimum diameter of equipment i	[m]
E	Activation energy	[cal/mol]
f	Correction factor	
H_i	Height of equipment i	[m]
h_i	Depth of component i	[m]
K	Equilibrium constant	

k	Pre-exponential factor	
M	Exponent for cost calculation	
n	Exponent for rate expression	
N	Number of certain elements	
P	Annual profit	M€/y
p	Pressure	bar
Q	Thermal energy flow	MJ _{th} /s
r	Reaction rate	
T	Temperature	[°C]
t	Time	[s]
u_{s,i}	Settling velocity in equipment i	[m/s]
W	Power	MW _e
Z	Equipment-specific constant	

Chemicals

CH₄	Methane
CO₂	Carbon dioxide
H₂	Hydrogen
MEA	Monoethanolamine
N₂	Nitrogen
O₂	Oxygen

Greek symbols

η	Efficiency of power plant	[%]
ρ_i	Density of phase i	[kg/m ³]

Super- and subscripts

e	Electric
in	Inlet
kd	Knockout drum
l	Liquid phase
M	Material
out	Outlet
T	Temperature
th	Thermal
v	Vapor

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Executive summary

To meet the high demand for natural gas globally, synthetic natural gas (SNG) can be produced as a substitute for natural gas derived from fossil fuels. Nevertheless, the traditional SNG production process is highly carbon-intensive. In the framework of the Power-to-Gas concept, production of SNG can occur via hydrogenation of CO₂, which can be captured from industrial sources. As a result, the reliance of SNG production on fossil fuels can be reduced and, subsequently, associated CO₂ emissions can be controlled.

The goal of the present study is to assess the technical viability and economic feasibility of producing SNG via CO₂ hydrogenation. Additionally, to prepare for integrating the techno-economic analysis (TEA) with a life-cycle assessment (LCA), the challenges and pitfalls of such integration are also discussed. The TEA in this study was carried out mainly from a research & development perspective. The production cost for SNG based on carbon capture and utilization (CCU) is estimated and key cost drivers are identified. The combined indicator of CO₂ abatement cost is also estimated as a quantitative indicator for assessing the TEA and LCA results.

The methanation plant is assumed to be located next to an iron & steel plant in Germany, from which the CO₂ feedstock for producing SNG is by means of MEA-based chemical absorption technology, while the hydrogen (which is produced via electrolysis using surplus electricity) is purchased from a production facility located 250 km away. The output capacity of the methanation plant is 148 MW. Aspen Plus software was used for process modelling and data were taken from the literature.

Through discussions, it was found that setting the system boundaries was a central challenge for aligning the TEA and LCA. While LCA tends towards encompassing the full life cycle of products (cradle-to-grave or -gate), it is not necessary to include the upstream and downstream processes to conduct a TEA in the present study. The information on upstream processes is reflected in the characteristics of the input flows entering the product system. Setting identical system boundaries for TEA and LCA would require solving problems of multi-functionality, which can be very challenging for TEA when the market for the products to be analyzed is still uncertain. To align inventories, the relevant environmental parameters (e.g., CO₂ emissions) should be documented in addition to the technical and economic parameters. For calculating CO₂ abatement cost, system expansion can be used to account for the reduced CO₂ emissions, or the CO₂ feedstock can be regarded as negative emissions.

The results show that the SNG production cost for the analyzed product system is 0.0748 €/MJ and the minimum selling price is 0.271 €/kWh. The production cost is more than 10 times greater than that of the benchmark product (coal-based SNG). The selling price of SNG produced by the proposed system is also significantly higher than that of natural gas in the German market. The CO₂ abatement cost, as a combined indicator of TEA & LCA, was calculated as 0.75 €/kg_{CO2}. Sensitivity analysis reveals that the hydrogen purchase price represents the most significant uncertainty for the analyzed system. At a 95% confidence interval, the estimated production cost ranges between 0.065 and 0.173 €/MJ_{SNG}. Current legislation of the European Union Emissions Trading Scheme (EU ETS) is found to be inapplicable to the product system investigated. Thus, the analyzed CCU system cannot benefit from the emissions trading scheme. To drive CCU-based SNG forward in the future market, it is essential to reduce the production cost of hydrogen.

Technical summary

GOAL	CCU product	Synthetic natural gas (SNG) as a fuel		
	Intended application and reasons for study	What is the economic performance of SNG production via CO ₂ hydrogenation within a renewable power-to-gas context? What is the environmental impact of the methanation plant in terms of CO ₂ emissions?		
	Brief description	CO ₂ is captured via a chemical absorption system from an iron & steel plant, H ₂ is imported, and subsequently SNG is produced via thermochemical synthesis.		
	Intended audience	TEA practitioner		
	Commissioners and assessors			
	Limitations of study	<ul style="list-style-type: none"> Based on literature data H₂ production, storage, and transport are not analyzed within the system boundary Low TRL for CO₂ methanation process 		
SCOPE	System boundary	Gate-to-gate		
	Benchmark system	Coal-based SNG production		
	Plant size	148 MW		
	Functional unit	The production of 1 MJ of SNG as a fuel		
	System elements and technology maturity	System elements	Technology maturity	
		Carbon capture via chemical absorption	TRL 9	
	Methane synthesis	TRL 4		
Assessment indicators				
INVENTORY	Data sources	<input type="checkbox"/> Primary sources <input checked="" type="checkbox"/> Secondary sources <input type="checkbox"/> Stoichiometric data	<input checked="" type="checkbox"/> Process-modelling-based data <input type="checkbox"/> Mixed sources <input type="checkbox"/> Other (please specify)	

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	Energy sources (select all that apply)	<input checked="" type="checkbox"/> Grid mix <input checked="" type="checkbox"/> Power station <input type="checkbox"/> Wind <input type="checkbox"/> Solar	<input type="checkbox"/> Nuclear <input type="checkbox"/> Hydro <input type="checkbox"/> Future (see timeframes) <input type="checkbox"/> Other (please specify)
	Base year	2019	
	Currency	Euro	
	Location	Germany	
	Plant life time	25 years	
	CO ₂ sources and price (if applicable)	Not applicable — capture included within boundary	
	H ₂ sources and prices (if applicable)	Purchased H ₂ with a price of 6.5 €/kg	
CALCULATION OF INDICATORS	Energy consumption per functional unit	Electricity: 0.03 MWe/MW _{SNG} Steam: 0.2 MJ/MJ _{SNG}	
	CAPEX per functional unit	0.012 €/MJ _{SNG}	
	OPEX per functional unit	0.0737 €/MJ _{SNG}	
	Price per functional unit	0.0748 €/MJ _{SNG}	
INTERPRETATION	Sensitivity analysis main factors	H ₂ price, operating hours/yr, reactor cost, steam price, total CAPEX	
	Uncertainty manipulated variables	H ₂ price, operating hours/yr	
	Main conclusions	<ul style="list-style-type: none"> The SNG production cost of the analyzed product system was estimated as 0.0748 €/MJ or 0.269 €/kWh. The minimum selling price is 0.271 €/kWh. The production cost is more than 10 times greater than that of the benchmark product (coal-based SNG). Considering the natural gas market in Germany, the selling price 	

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		<p>of SNG produced in the proposed system is also significantly higher.</p> <ul style="list-style-type: none">• CO₂ abatement cost (calculated as combined indicator of TEA & LCA) is 0.75 €/kgCO₂.• Sensitivity analysis reveals that hydrogen purchase price represents the most significant uncertainty for the analyzed system. At a 95% confidence interval, the production cost ranges between 0.065 and 0.173 €/MJ_{SNG}.• Current EU ETS legislation is found to be inapplicable to the product system investigated, and therefore brings no benefits for the CO₂ abated.
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1 Introduction


Methane, a main component of natural gas, can be used in energy-intensive applications [1]. Worldwide, the demand for natural gas is expected to increase in coming years [2]. Therefore, synthetic natural gas (syngas: SNG), which is primarily comprised of methane, is of great interest as means of establishing a sustainable energy supply. SNG can be used as feedstock in the chemical industry and, more commonly, as a fuel for automobiles, heating, electricity generation, etc. [3]. Traditionally, SNG is produced from fossil fuels. As a core part of the power-to-gas (PtG) concept, production of SNG via hydrogenation of carbon oxides (CO, CO₂), i.e., the Sabatier reaction [4], displays greater potential to tackle climate change and a promising link to carbon capture and utilization (CCU) [5]. The process of producing SNG is generally termed methanation, which is commonly used in the ammonia industry to remove the carbon monoxide component from syngas. More recently, this technology has gained attention as a means of producing a natural gas substitute from coal gasification [6].

Several methanation concepts, such as fixed-bed and fluidized-bed methanation processes, have been developed, [4, 6]. Currently, several commercial SNG plants are in operation worldwide, including GOBIGAS in Sweden, Great Plains Synfuels in the US, and several recently built SNG plants in China [4, 7]. In addition, a few commercial plants are under construction and some pilot-scale plants also exist. However, these commercial plants are all CO methanation projects in which SNG is produced from either coal or biomass [4].

At the beginning of the 21st century, research into CO₂ methanation processes has gained more attention due to growing awareness of climate change. CO₂ methanation projects are mostly seen in Germany, which has committed to transforming its energy system to a 100% renewable-based system [8]. Under the concepts of carbon capture and utilization (CCU) and power-to-gas (PtG), green hydrogen (which is produced by electrolysis via renewable electricity) is used to convert CO₂ (captured from industrial flue gases) into SNG, which can contribute to tackling global climate change and effectively store surplus electricity from wind or solar power [9]. As a substitute for natural gas, an advantage of SNG is that it can be injected into the existing gas grid for distribution to end users and thus no additional infrastructure needs to be constructed. Studies have reported on producing SNG from industrial CO₂ [10, 11].

This study assesses the technical and economic performances, in the German context, of a CCU methanation plant that produces SNG using CO₂ and hydrogen. The CO₂ is captured from a reference iron & steel plant while the hydrogen is produced via electrolysis from renewable electricity. The study also discusses the pitfalls and challenges for the integration of TEA & LCA from a TEA perspective. The CO₂ abatement cost is used as an indicator to demonstrate a quantitative combination of TEA and LCA results.

2 Goal definition

 Reference to TEA Guidelines V1.1

A checklist of items to be included in each section of the report is encompassed in **Chapter B.8, Reporting of the Guidelines 1.1**, which for the goal is as follows:

Goal of the study

- State goal, study context, and the reasons for the study
- State the intended application and target audience of the study
- State commissioners and authors of the study
- State limitations in the applicability of the study
- State the analyzed scenarios and their conditions

2.1 Goal of the study


The goal of the study is to assess the technical viability and economic feasibility of producing synthetic natural gas (SNG) via CO₂ hydrogenation on-site at a steelmaking plant. The study estimates SNG production cost and identifies key cost drivers. The techno-economic analysis (TEA) in this study is conducted mostly from a research & development perspective.

In addition, the present study aims to identify pitfalls for the integration of TEA & LCA of CCU systems. Therefore, discussions are presented throughout the worked example with regard to the potential challenges for combining the two estimation approaches. The discussions are mostly based on Section A.5 of the existing TEA Guidelines V1.1 [12]. To enable quantitative comparison of the TEA and LCA results, a combined indicator (CO₂ abatement cost) is calculated.

The worked example is intended for public use and to demonstrate how the TEA Guidelines V1.1 [12] can be used to conduct TEA for CCU processes and products.

2.2 Assessment scenario

In the base case scenario of the study, the CO₂ feedstock is captured from an integrated iron and steel plant, while H₂ is transported from an external production site. In addition to the base case, alternative scenarios are examined, which are presented in the interpretation phase.

 Reference to TEA Guidelines V1.1


Guideline B.3 discusses how to define assessment scenarios. Alternative scenarios can either be defined during the initial phase of goal definition or when the goal is refined via iteration after key parameters have been identified in the interpretation phase. For the present study, the latter approach is applied, as key factors are unknown initially, which is common in most cases.

2.3 Goal alignment of TEA & LCA

The respective goals of TEA and LCA are different by nature. Therefore, the goal for a combined assessment should cover all three aspects, i.e., technology, economics, and environment. In addition, the same set of assessment scenarios shall be used in both TEA and LCA if a high level of alignment is required.

In this study, the goal is not limited to only examining the techno-economic feasibility. The CO₂ emission—as an indicator of environmental impacts—is also included in the goal as an initial step of combining TEA with LCA. The alignment of TEA and LCA should start from the very beginning of a combined study (goal definition phase).

3 Scope

 Reference to TEA Guidelines V1.1

Checklist of items to be included in the scoping report:

Scope of the study

- State products of applications, functional units, and reference flows
- For corporate-perspective TEAs, state at least one customer group and their needs
- State elements and boundaries of product system in a graphical scheme; If relevant, state reasons for excluding upstream processes
- State benchmark products and systems
- State technology maturity for system elements and the overall product system
- State the selected indicators and assessment methods, including data availability associated with technology maturity
- Document remaining inconsistencies, if any

3.1 Product application and functional unit

SNG can be used as feedstock in the chemical industry and, more commonly, as a fuel or energy storage carrier for automobiles, heating, electricity generation, etc. [3]. SNG can be injected into the existing natural gas grid and then distributed for heating and electricity generation.

In this study, SNG is considered as a fuel product that is used primarily on-site for the production of steel. Therefore, the connection to the national gas grid and subsequent costs are not considered in the scope of this study. Energy is the basis for comparison, and 1 MJ of SNG is used as the functional unit. 1 MW of SNG can be referred to as the reference flow. The methanation plant is designed to achieve a production capacity of $\approx 150 \text{ MW}_{\text{th}}$.

3.2 System elements and boundary

Previous studies [13, 14] show that a typical integrated iron and steel plant has multiple point sources of CO₂ emissions. In the base case scenario, the CO₂ source is the flue gas from the lime production plant in a reference iron and steel plant located in Germany. The proposed CO₂-based methanation plant is assumed to be located next to the iron & steel plant. A conventional MEA-based chemical absorption technology is used to capture CO₂ from the flue gases. Hydrogen, which is produced via electrolysis using renewable power, is transported via truck trailer.

The elements and system boundary are displayed in Figure 1. The studied system consists of three major elements:

1. MEA-based carbon capture system, capturing CO₂ from a reference iron & steel plant;
2. A methanation unit producing SNG;
3. Utility (water, steam, etc.).

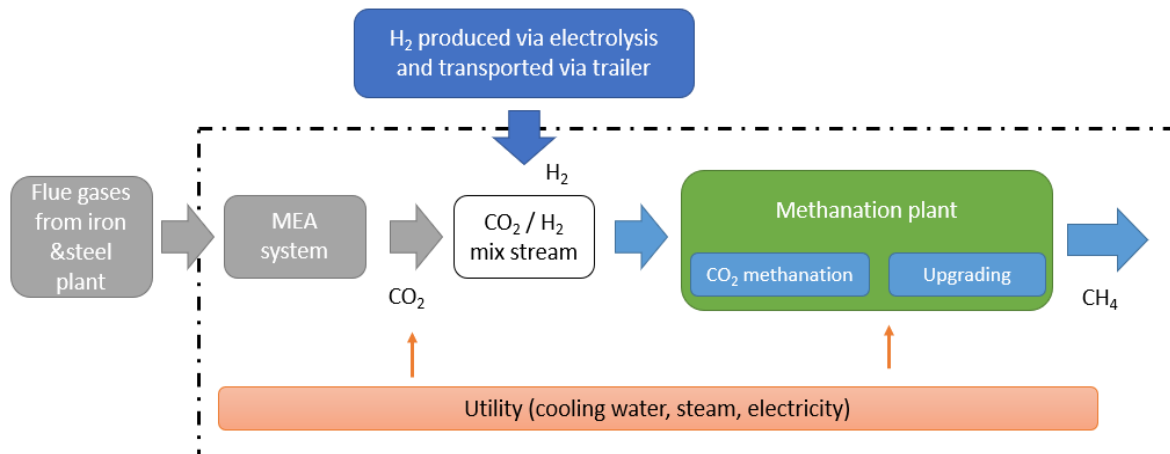



Figure 1 System elements and boundary of the studied methanation process

3.3 Benchmark system and product

As introduced, the mainstream technology for producing SNG is based on a CO methanation process. The coal-to-SNG and biomass-to-SNG technologies are mostly based on this process. Although proposals for converting biomass to SNG have attracted substantial attention in recent years, the technology remains in the development phase [4, 7, 15]. The benchmark system used in the present study is a conventional coal-to-SNG plant in which the production process is based on catalytic CO methanation in adiabatic fixed-bed reactors. In general, the production process consists of a series of processing units including air separation, gasification of coal, gas cleaning, methanation, and gas upgrading [4, 6].

Since Germany currently has no commercially operational coal-to-SNG plants [4], monetary values representing the US context (converted into euro values) will be used for comparison. The US is a pioneer in commercializing the coal-to-SNG concept. The Great Plains Synfuels Plant (North Dakota, US), as the first-of-its-kind, remains the only coal-to-SNG plant in the US. It was commissioned in 1984 and presently has an average output capacity of 1500 MW [4]. In addition, the natural gas is also considered as a benchmark product, as the SNG is essentially a substitute for it. The World Energy report, Outlook for Natural Gas [16], shows that natural gas consumption will continue to increase by 1.6% per year until 2040. In 2019, the price of natural gas in Germany for industrial use (*annual consumption 10^5 to under 10^6 GJ*) was 0.026 €/kWh_{th}, and for households (*annual consumption 20 to 200 GJ*) was 0.06 €/kWh_{th} [17].

 Reference to TEA Guidelines V1.1

Guideline B.4.4 states that benchmark products and systems shall be selected. The Guidelines introduce two terms: ‘substitute’, which refers to a product that is identical to the benchmark product; and ‘non-substitute’, which refers to a product with different a chemical structure or characteristics. For the present study, SNG is defined as the benchmark product. Although the SNG is mostly comprised of methane, its exact composition may vary from case to case. This is particularly the case since feedstocks for the benchmark system and the analyzed system in the present study are different. The product of the CCU methanation plant is therefore considered a ‘non-substitute’ for the benchmark product, and hence the comparison is based on energy output.

3.4 Technology maturity

The concept of technology readiness level (TRL) is used here to define the technological maturity of the system being analyzed. The individual TRLs of system elements are displayed in Table 1. MEA-based carbon capture technology has been studied for decades and deployed at differing scales. Moreover, it will be used in a commercial-scale project to reduce CO₂ emissions from a cement plant in Norway [18]. Therefore, given its high level of maturity, the process is identified as having a TRL of 9. Regarding the CO₂ methanation process: some projects have been reported as operating at pilot scale [4]. Nevertheless, the conversion process in the present study employs a novel catalyst that, to date, has only reported as operating in a lab environment [19, 20]. Therefore, it is assigned a TRL of 4. It is important to note that the TRL of the overall product system equals the lowest TRL of its constituent process units.

Table 1 TRL for each system element

Process units	TRL
MEA-based carbon capture	9
CO ₂ methanation	4
Overall	4

3.5 Assessment indicators

Technical and economic indicators are selected according to the assessment goals indicated in the goal definition stage. Heat, cooling, and electricity demands are used to assess technical performance. These results can be obtained from process simulations. With respect to economic performance, capital and operational expenditures are selected as assessment indicators. The cost of producing SNG is also calculated in order to analyze profitability. In addition, the cost of CO₂ abated will be used as a combined indicator to integrate TEA and LCA.

3.6 Scope alignment of TEA & LCA

3.6.1 Alignment of system boundary and multi-functionality

The alignment of system boundaries is a major challenge for the integration of TEA and LCA. This study uses a gate-to-gate boundary, whereas LCAs commonly use cradle-to-gate or cradle-to-grave system boundaries. For a CCU system in particular, it is not common for TEA to include upstream processes in the system, whereas LCAs normally include the CO₂ source in the product system in order to analyze the full environmental impacts. Instead, TEA treats the CO₂ flows from the CO₂ source as input flows and assigns relevant attributes to them (*e.g., cost, concentration, etc.*). By doing so, TEA avoids unnecessary complications for system analysis. In this study, the CO₂ source is the iron & steel plant and the CO₂ flow from the lime plant is regarded as an input flow.

As stated in section A.4 of the Guidelines, the decision on whether the TEA and LCA boundaries should be identical depends on the types of integration sought by practitioners. This study calculates combined indicators, which corresponds to the second type of integration, i.e., combined indicator-


based integration. Ideally, identical system boundaries are preferred for TEA and LCA. However, the inclusion of the CO₂ source within the system boundary would lead to problems of multi-functionality. With the inclusion of CO₂ source in the system boundary, the functions of the product system comprise not only the production of SNG but also the main product of the iron & steel plant, i.e., HRC. Consequently, it would be necessary to conduct detailed process modeling and subsequent economic analysis for the CO₂ sources, which introduces unnecessary complexity to the study. Moreover, the production costs need to be allocated to the two products. This could be challenging when the market prices are highly uncertain.

To facilitate combination with an LCA study, the TEA study needs to collect data concerning the environmental impacts of steel and hydrogen production and integrate them into the data inventory. When this is not possible, the CO₂ sources must be included within the boundary by means of a system expansion.

3.6.2 Assessment indicators for combined TEA & LCA

As discussed, this study presents a quantitative integration of TEA and LCA. Therefore, in addition to common indicators of TEA, a combined indicator termed the cost of CO₂ abated is calculated. This combined indicator can reflect both economic and environmental impacts of the analyzed system. Aside from greenhouse gas emissions, other enviro-economic indicators can also be included from the LCA perspective, to broaden the scope of a study, for instance, toxicity indicators of MEA solvents leaking from the capture system, or other wastes. However, since the present study focuses on CO₂ emissions only one combined indicator, i.e., CO₂ abatement cost, is considered.

4 Inventory

 Reference to TEA Guidelines V1.1

Checklist of items to be included in the inventory report:

- Document technological and economic parameters, decisions, and assumptions, where possible based on functional unit and reference flow
- Justify context-specific assumptions and parameters; discuss scale and maturity, as well as temporal, geographic, and regulatory context and related limitations and risks, especially for key inputs such as CO₂, hydrogen, electricity, minerals, fossil feedstocks, or catalysts
- State types and sources of data, including quality and confidentiality
- Report CO₂ capture cost; otherwise, if not available, include a statement on this
- Document characteristics and limitations of data utilized
- Document data in SI units or provide unit definitions
- Document data for each system element independently
- Display economic data collectively

4.1 Types of data and quality control

Process units of carbon capture and CO₂ methanation were simulated using Aspen Plus. Specifications for the units were obtained from the literature. The electrolyte NRTL model was used to simulate the carbon capture process, while the Redlich–Kwong–Soave equation was selected for methanation simulation.

Cost models were established in Microsoft Excel, based on the simulation results. The process- and cost-modelling were completed using secondary data from reports, public databases, and peer-reviewed publications.

4.2 Carbon capture

MEA-based chemical absorption is by far the most mature post-combustion carbon capture technology [21]. The present study uses a model of this technology (see Figure 2) by Markewitz et al. [22]. The MEA solvent and flue gas flow counter-currently in the absorption column; CO₂ is thereby transferred from the flue gas to the amine solvent, forming carbamate or bicarbonate [23, 24]. In the stripping column, the absorbed CO₂ is released by the energy provided by the stripping steam, and a concentrated CO₂ stream is obtained. The MEA solvent, with CO₂ stripped off in the distillation process, is regenerated and sent back to the absorber. The CO₂ stream leaves the top of the stripper and then passes through dehydration and compression units.

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N ₂	vol%	65.88	60.24	71.86	65.52	72.65	69.47
H ₂ O	vol%	6.98	12.58	16.34	6.38	6.9	10.76
CO	vol%	/	/	/	/	0.74	/
SO _x	mg/Nm ³	10	10	10	10	300	10
NO _x	mg/Nm ³	60	30	500	60	200	280
Dust	mg/Nm ³	< 5	< 5	< 5	< 5	< 5	< 5

The absorber and stripper dimensions and operating conditions are shown in Table 3. The dimensions of the distillation column were determined through sizing and rating. Drops in pressure along the heights of the columns were also considered.

Table 3 Dimensions and operating conditions of the MEA-based carbon capture system

Parameter	Unit	Value
Absorber height/diameter	m	20/6
Stripper height/diameter	m	6/3
Pressure of outlet CO ₂ flow	bar	1.8
Temperature of outlet CO ₂ flow	°C	20
Temperature in reboiler	°C	120
Mass flow of CO ₂ feed gas	kg/s	8.2

Given the input data, the technical data of the capture process are displayed in Table 4. The term auxiliary power refers to electricity supply, while the reboiler duty is an indicator of how much thermal energy is demanded. The thermal energy is provided by low-pressure steam in the present study.

Table 4 Technical results of carbon capture process

Parameter	Unit	Result
Auxiliary power	MWe	1.7
Reboiler duty	MW _{th}	29
Cooling duty	MW _{th}	60

4.3 Hydrogen

While most H₂ is presently produced at the site of use, it is worthwhile investigating scenarios in which a national-scale hydrogen supply chain exists, especially in Germany. In light of this, H₂ in the present study is assumed to be imported from a hydrogen production facility located off-site. As the infrastructure for hydrogen supply in Germany is still in development, Reuß et al. [25] estimated the cost of H₂ in their future scenario projected to 2050 for Germany. Their study considered a full hydrogen supply chain covering all phases, including production, storage, and transport, and was therefore utilized as the basis for deriving the price of imported H₂ in the present study.

As defined in the reference studies [25, 26], electrolysis utilizing surplus electricity from the power grid is considered as the hydrogen production technology for this study. The polymer electrolyte membrane (PEM) is assumed to be used. With an outlet pressure of 30 bar, the investment cost for the electrolyzer is 500 €/kW_e [26, 27]. The electricity consumption of electrolysis is 47.6 kW_e/kg_{H₂} [25, 26, 27].

According to the published studies [25, 26], various routes exist for hydrogen transport (see Figure 3). Hence, the cost of purchased H₂ depends on the selected supply chain route. Gaseous H₂ (GH₂) and liquid H₂ (LH₂) are the current state-of-the-art for storage and transport. The present study assumes that the base case scenario employs the following route: H₂ production (electrolysis) > Storage (GH₂ cavern) > Transportation (GH₂ trailer). The cost for purchasing excess electricity generated by wind is set to 0.06 €/kWh_e, and the cost of diesel consumed in transporting H₂ via truck is set to 1.73 €/l [25].

Studies by Reuß et al. [25, 26] provide cost estimates for H₂ associated with different infrastructure technologies that aim to supply hydrogen for fuel cell vehicles in Germany. Therefore, their estimates include the costs of fueling stations, which are not relevant to the present study. After subtracting their estimated cost of fueling stations, the remainder is taken to be the H₂ price for the CCU system analyzed in this study. Sensitivity analysis is described later in this report, to examine the impact of H₂ pricing on economic viability. Further information on the H₂ supply chain is shown in Table 5. All calculations assume a continuous supply of H₂, which can be achieved by establishing a temporary storage system on the site of the CCU plant. However, the unit operation and subsequent costing of such a system is not considered in this study.

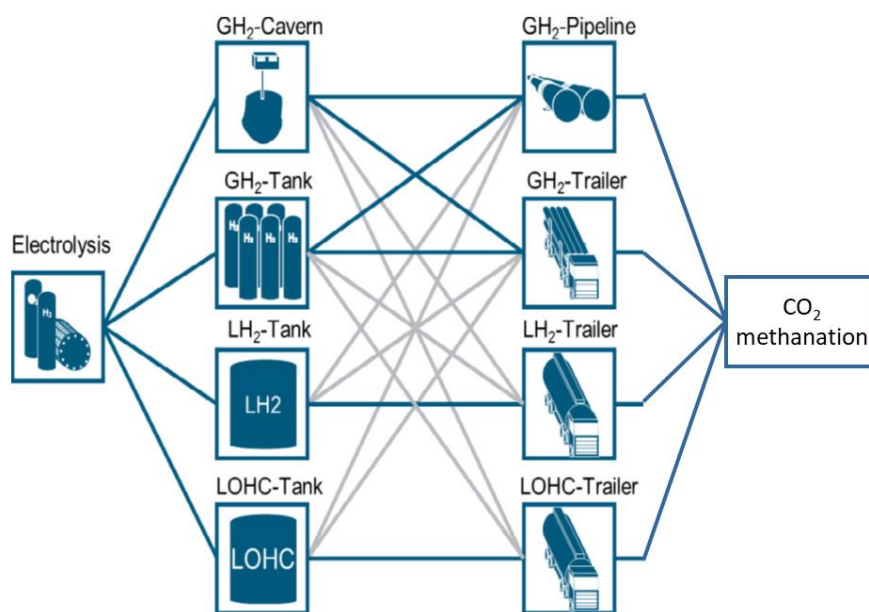



Figure 3 Possible hydrogen supply routes. Source: adapted from Reuß et al. [26]

Table 5 Assumptions and characteristics of imported hydrogen [25, 26]

Parameter	Unit	Value
Production method	/	Electrolysis utilizing surplus electricity
Transport distance	km	250
Storage method	/	GH ₂ cavern
Transport method	/	Truck
Pressure for transport	bar	300
Purity	mol%	99.9
H ₂ cost	€/kg	6.5
CO ₂ emissions	kgCO ₂ /kgH ₂	2.4
Mass flow	kg/s	1.5

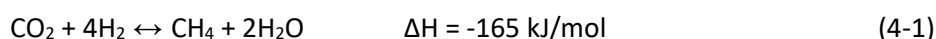
 Reference to TEA Guidelines V1.1

A decision tree for deriving prices for input flows is included in Version 1.1 of the TEA Guidelines (Chapter B.5.3). Three factors must be examined before the price for an input flow is assumed, i.e., technical specification, system boundary, and location.

Specifically, steps for deriving H₂ price are clearly stated in section B 5.5 of the Guidelines. The H₂ price needs to represent the cost of production or a market price. According to the guidance, if H₂ production is excluded from the system boundary, as in the current base case, then H₂ price needs to be collected from a supplier quote or a location-average estimate specific to the production route. The latter approach was chosen for the present study. The estimated cost of H₂ in Germany based on current available technology was used as the imported price. Moreover, the guidance also states that transport and storage need to be reflected in the H₂ price. Hence, the considered transport and storage methods are clearly presented.

4.4 CO₂ methanation

Fewer studies have reported on CO₂ methanation as compared to CO methanation. In the present study, the synthesis process was designed largely based on reported CO methanation technology [28, 29, 30]. An adiabatic fixed-bed reactor was chosen for CO₂ methanation, as these are widely used for commercial coal-to-SNG production [4, 6, 28, 31]. With respect to the CO₂ methanation, two reaction routes are generally considered. One is a linear combination of the reverse water-gas shift reaction and CO methanation. The other reaction route is the direct conversion of CO₂ to methane as shown in the following [32, 33]:



A study by Falbo et al. [19] shows that the latter reaction is dominant over a Ru-based catalyst. Gallandat et al. [20] conducted experiments over Ru/Al₂O₃ and achieved CO₂ conversion rates of up to 99%. Based on those high reported conversion efficiencies, the present study only considers the direct conversion route. The reaction kinetics were analyzed in Aspen Plus software using the Langmuir–Hinshelwood–Hougen–Watson (LHHW) model. The rate expression and kinetic parameters associated with the reaction (4-1) are presented in Table 6.

Table 6 Kinetics of CO₂ methanation over a Ru-based catalyst [19]

Rate expression	Kinetic factor, k [mol/s·g·atm ⁵ⁿ]	Activation energy, E [kJ/mol]	Exponent [n]	α [1/atm]
$r_{\text{CO}_2} = \frac{k}{1 + \alpha P_{\text{H}_2\text{O}}} \left[[P_{\text{CO}_2}^n P_{\text{H}_2}^{4n}] - \frac{P_{\text{CH}_4}^n P_{\text{H}_2\text{O}}^{2n}}{(K_{eq}(T))^n} \right]$	95.43	75.3	0.152	0.91
Equilibrium constant: $K_{eq}(T) = \exp \left[\left(\frac{1}{1.987} \right) \cdot \left(\frac{56000}{T^2} + \frac{34633}{T} - 16.4 \cdot \ln T + 0.00557 \cdot T \right) + 33.165 \right]$				

The process flow diagram of the methanation process simulated in Aspen Plus is shown in Figure 4. As can be seen, the H₂ and CO₂ feedstock gases (H₂:CO₂ ratio of 4:1) are first mixed and then sent to the first-stage reactor. Since the imported H₂ is at higher pressure than that required in the reactor, it is first decompressed using a turbo-expander, which can generate electricity. Meanwhile, the CO₂ stream is compressed to the target pressure. The gas mix enters the reactor and is reacted under adiabatic conditions. Since the reaction (4-1) is exothermic, the temperature of the gas stream at the outlet is higher than that at the inlet. Part of the gas stream exiting the reactor (60%) is recirculated to the inlet, where it is combined with the feedstock gas mix. This recirculation can increase the temperature of the feed gas, thereby moderating the operating temperature inside the reactor. After synthesis, the product stream is cooled, and part of the water content is removed in a flash tank. The final product stream requires CH₄ purity >96 mol% for supply to the natural gas grid [28, 34]. An output of 148 MW is obtained, which is of the same order of magnitude reported for a benchmark system [35].

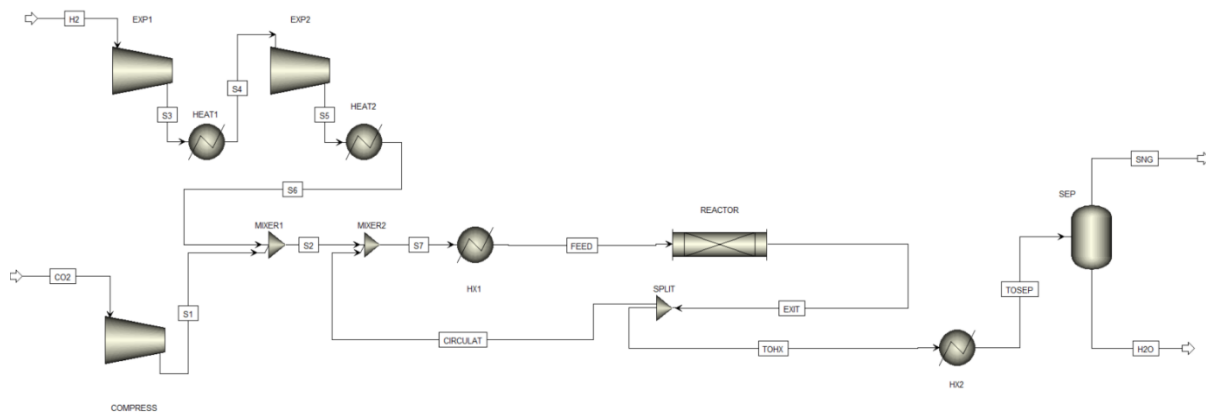


Figure 4 The process flow diagram of CO₂ methanation

Given a similar magnitude of production capacity, the same reactor dimensions and catalysts usage reported by Er-rbib et al. [29] were used for this study, with the difference that the reference study was based on CO methanation. It is assumed that 0.5 wt% Ru/Al₂O₃ catalyst is placed in the reactor. The specific reaction parameters are summarized in Table 7. The resulting technical performance parameters of the methanation process are summarized in Table 8.

To demonstrate a simple example: Only one reactor was modeled for the methanation process in the present study, which is uncommon in practice. For better control of the operating temperature, multi-stage reactors with intermediate cooling are usually adopted, such as those using the Lurgi gasification process [6]

SNG Worked Example for TEA Guidelines
Table 7 Reactor dimensions and operating parameters in the reactor

Parameter	Unit	Value
Reactor type	/	Adiabatic fixed-bed
Tube length	m	10.57 [29]
Inner diameter	m	2.44 [29]
Operating temperature	°C	320 – 813
Pressure	bar	5
Catalyst amount	kg	1500 [29]
Bed voidage		0.4

Table 8 Technical results

Parameter	Unit	Result
Electricity demand	MW _e	3.3
Cooling duty	MW _{th}	47
Output pressure	bar	2
Output temperature	°C	20
Gas composition of product SNG		
CH ₄	wt%	98
H ₂	wt%	0.2
H ₂ O	wt%	1
CO ₂	wt%	0.8
Heating value of product SNG (LHV basis)	MW	148

4.5 Utility

Cooling water, steam, and electricity are required to operate the process units introduced above. Their mass balances and costs must be calculated. Steam is needed to regenerate the MEA solvent in the capture system. In the base case scenario, the steam is assumed to be purchased from an external CHP plant near the methanation plant, and hence no additional transport costs are considered for the purchased steam. The cooling water and electricity are also purchased, and their input prices and climate impacts are summarized in Table 9. The isentropic and mechanical efficiencies for all turbo-expanders, pumps, and compressors used in the CCU project were set at 85%. The make-up rate of cooling water is assumed to be 1 m³/GJ_{th} and the degradation of MEA is assumed to be 1 kg/t_{CO₂}.

Table 9 Price and characteristics of imported consumables

Utility	Price	CO ₂ emissions	Reference
Low-pressure steam (140 °C)	12.9 €/MWh _{th}	192 kg/MWh _{th}	CEMCAP [36]
Electricity	0.088 €/kWh	523 kg/MWh _e	BMW _i [37]
Cooling water	0.15 €/m ³		IEAGHG [38]

4.6 Inventory alignment of TEA & LCA

As stated in the TEA Guidelines, technological and economic parameters shall be documented in a TEA report. However, this does not suffice for a combined assessment of TEA & LCA. To make TEA compatible with LCA, the carbon footprints and subsequent climate impacts of all process units within the system boundary must be added to the inventory. In addition, the environmental impacts associated with the input flows should also be documented.

For example, in the base case scenario, the capture system only deals with CO₂ emissions from the lime plant. Given the system boundary defined in Figure 1, CO₂ emissions from the other point sources are not considered and therefore have no impacts on the results of TEA. Apart from the CO₂ sources (iron & steel plant), carbon footprints are also associated with the operation of other units (*e.g.*, the transportation of hydrogen; electricity consumed for methanation and utilities). For alignment of TEA and LCA, all the CO₂ emissions associated with the production of the CCU product ought to be accounted for. Given the system boundary, the technical inventory containing information on CO₂ emissions is presented in Figure 5. It can be seen that all technical flows have been related to the functional unit.

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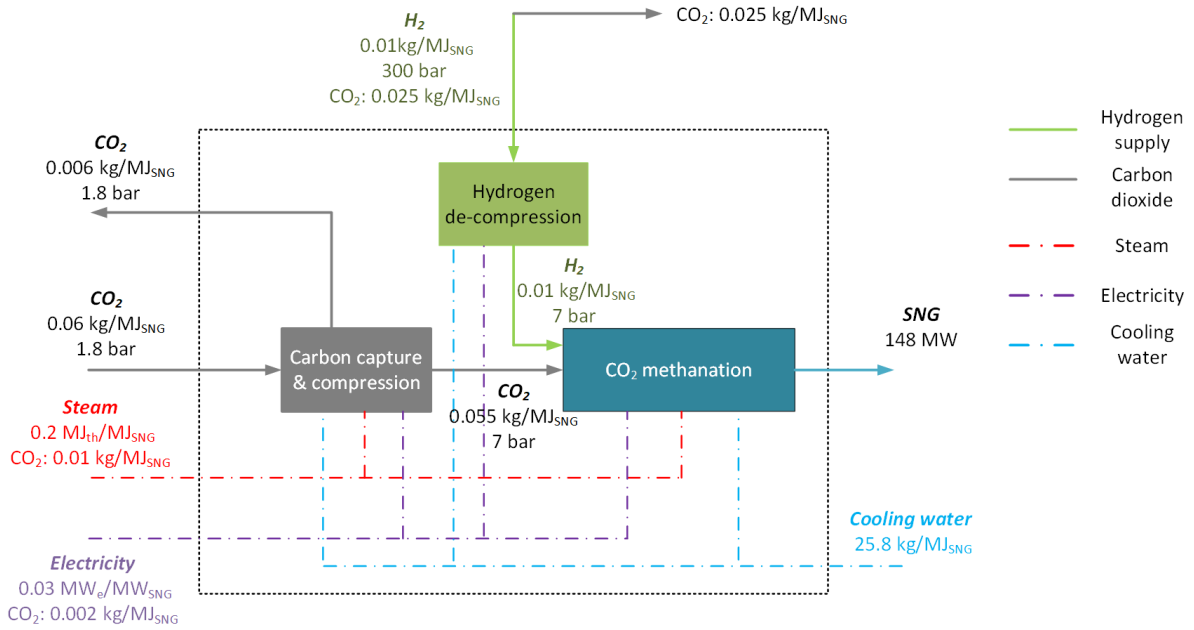



Figure 5 System elements with technical flows for TEA

5 Calculation of indicators

 Reference to TEA Guidelines V1.1

Checklist of items to be included in the inventory report:

- State calculation procedures, including potential additional assumptions and estimates utilized
- Present equations for each indicator applied; For uncommon methods, describe motivation
- State all relevant results for the overall system as well as for each system element individually

The previous chapters have provided all necessary data and assumptions required for techno-economic assessment. This chapter will present the calculated results based on the process simulation and assumptions documented in the inventory.

5.1 Technical indicators

Some major technical indicators for the carbon capture and methanation processes are depicted in Table 10. The indicators presented include CO₂ conversion rate, which is defined as the ratio of the decreased molar flow rate of CO₂ in the reactor divided by the inlet molar flow rate of CO₂. In addition, other indicators, such as specific cooling duty, specific electricity demand, etc., were calculated based on the functional unit. To display the global warming impact, the specific amount of CO₂ abated is also presented as technical data. The indicator is calculated via:

Specific amount of CO₂ abated

$$= \frac{CO_{2in,capture} - CO_{2out,capture} + CO_{2in,H_2} + CO_{2in,steam} + CO_{2electricity}}{SNG\ output} \quad (5-1)$$

Where $CO_{2in,capture}$ represents the mass flow of CO₂ entering the capture system, $CO_{2out,capture}$ is the mass flow of CO₂ leaving the system boundary, CO_{2in,H_2} is the mass flow of CO₂ generated by importing hydrogen, and $CO_{2in,steam} + CO_{2electricity}$ represent the amount of CO₂ entailed by utility in the analyzed system.

The energy efficiency (η_{energy}) of the analyzed system is calculated as the ratio of the energy flow of SNG divided by the total input energy flows on LHV basis:

$$\eta_{energy} = \frac{Q_{SNG}}{W_{electricity} + Q_{steam} + Q_{H_2}} \quad (5-2)$$

The calculated indicators include Wobbe index [11], which is an indicator of the interchangeability of fuel gases. Fuel gases with identical Wobbe indices will yield the same amount of energy regardless of gas compositions. The index is defined as:

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$$Wobbe\ index = \frac{HHV_{SNG}}{\sqrt{\frac{\rho_{SNG}}{\rho_{air}}}} \quad (5-3)$$

Here, HHV_{SNG} is the higher heating value of the product SNG, ρ_{SNG} is the density of the product SNG, and ρ_{air} is the density for air at standard condition (1bar, 0 °C).

Table 10 Technical indicators

Parameter	Units	Value
CO ₂ conversion rate	%	99
LHV	MJ/kg	49.2
Energy efficiency (η_{energy})	%	69.5
Wobbe index	MJ/kg	72.8
Specific amount of CO ₂ abated	kg _{CO2} /MJ _{SNG}	0.017
Specific reboiler duty in the carbon capture system	GJ/MJ _{SNG}	0.196
Specific electricity demand for carbon capture	MWh/MJ _{SNG}	0.004
Specific cooling duty for carbon capture	MJ/MJ _{SNG}	0.4
Specific electricity demand for methanation	MWh/MJ _{SNG}	0.03
Specific cooling duty for methanation	MJ/MJ _{SNG}	0.32

5.2 Basis for cost estimation

5.2.1 Purchased equipment cost

Purchased equipment cost is estimated according to the following equation [39]:

$$C_i = C_B \left(\frac{Q}{Q_B}\right)^M f_M f_P f_T \quad (5-4)$$

where C_i = equipment costs for equipment i of capacity Q ; Q is obtained from the simulation.

C_B = base costs of equipment i of capacity Q_B

M = exponent depending on the type of equipment.

f_M, f_P, f_T = correction factors for the material of construction (M), operating pressure (P), and operating temperature (T).

For separation vessels (absorber, stripper, etc.), the equipment costs are calculated using the method of Turton [40] as there are no reference data available for costs.

$$\log_{10}C_i^\circ = Z_1 + Z_2 \log_{10}(Q) + Z_3 [\log_{10}Q]^2 \quad (5-5)$$

K_n represents the equipment-specific constants while C_i° is the purchased equipment costs in 2001 US\$ at standard condition, and Q refers to the capacity measure. In particular, it is assumed that the reactor for producing syngas can be used for CO₂ methanation reaction because the nature of the reactants is similar [41]

5.2.2 Cost escalation

As cost data are from various studies published in different years, the chemical engineering plant cost index (CEPCI) is used to transform the data and results to be based in the same year:

$$\text{Cost in year A} = \text{Cost in year B} * \frac{\text{CEPCI in year A}}{\text{CEPCI in year B}} \quad (5-6)$$

5.2.3 Estimation of capital expenditure (CAPEX)

The ‘Factor Method’ was adopted for estimating CAPEX in the present study. The breakdown of the CAPEXs for the MEA (direct & indirect costs) is demonstrated in Table 11. The quantifying factor for each element is selected according to relevant literature covering both carbon capture and methanation plants.

Table 11 Breakdown of CAPEX [28, 39, 42, 43]

Elements	Percentage of PEC [%]
Direct costs	
Purchased equipment cost (PEC)	100
Purchased equipment installation	53
Instrumentation and control	20
Piping	40
Electrical	11
Building and building services	10
Yard improvements	10
Service facilities	20
Land	5
Indirect costs	
Engineering	10

Construction expenses	10
Contractor fees	0.5
Contingency	17
Fixed capital investment (FCI) = Indirect cost + Direct cost	
	Percentage of FCI [%]
Fixed capital investment (FCI)	100
Working investment (WI)	15
Start-up cost and initial MEA cost (SUC)	10
CAPEX = FCI + WI + SUC	

5.2.4 Estimation of operational expenditure (OPEX)

The breakdown and quantification methods for OPEX are presented in Table 12. The following equation was used to estimate the operating labor [44]:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (5-7)$$

Here, N_{OL} represents the number of operators per shift, P is the number of processing steps (*e.g.*, transport, distribution, etc.), and N_{np} is the number of non-particulate processing steps (*e.g.*, compression, heating, etc.).

Table 12 Breakdown of OPEX [39, 45]

Elements	Quantification method
Variable costs	
Imported hydrogen	Unit price × demand
Cooling water	Cooling water make-up [m^3/GJ] × Cooling duty [GJ] × cooling water costs
Catalyst	1000 €/kg × annual usage [46]
Electricity	Electricity costs [€/MWh] × Consumption
MEA make-up	MEA cost × MEA degradation
Steam	Unit price × demand
Fixed costs	
Local taxes	2% of FCI

Insurance	1% of FCI
Maintenance (M)	4% of FCI
Operating labor (OL)	No. of shifts × 45 €/h·shift
Supervision and support labor	30% of OL
Operating supplies	15% of M
Laboratory charges	10% of OL
Plant overhead cost	60% of (M + OL + S)
General expenses	
Administrative costs	15% of OL
Distribution and marketing	0.5% of OPEX
R&D costs	5% of OPEX

$$\text{OPEX} = \text{Variable costs} + \text{Fixed costs}$$

5.2.5 Basics and assumptions for the calculation of economic indicators

Some assumptions were made for the estimation of CAPEX, OPEX, and other indicators (see Table 13). A discounted cash flow approach was used in this study for financial valuation. The depreciation period was set to 15 years, which is identical to that set for a coal-to-SNG study [31]. The salvage value is set to zero, which assumes that any such value is offset by decommissioning expenses.

To determine the minimum selling price of SNG, net present value (NPV) was calculated via the following formula:

$$NPV = \sum_{n=1}^{25} (CF / (1 - i)^n) - \text{total capital cost} \tag{5-8}$$

Here, *CF* is annual cash flow. Given a tax rate of 40% and calculated depreciation cost (*d*), the profit (*P*) can be estimated via:

$$P = (CF - 0.4d) / (1 - 0.4) \tag{5-9}$$

As the technology readiness level of the analyzed system is low and the market for the CCU SNG is not clear, it is not possible to predict future cash flows and thus calculate NPV. Instead, the minimum selling price of SNG was calculated with NPV set to zero.

Table 13 Assumptions for economic estimation

Parameter	Unit	Value
Location		Germany
Base year		2019
Project lifetime	year	25
Exchange rate	€/US\$	1.11 [47]
Discount rate	%	8
Tax rate	%	40
Debt term	year	10
Construction period	year	1
Operation time	hr/y	8000
Degradation rate of MEA	kg/tCO ₂	1
MEA make-up cost	€/kg	2.3
Depreciation period	year	15 [31]
Salvage value	€	0

5.3 Economic indicators

Based on Equation 5-1, the total cost of purchased equipment was estimated to be 13.8 M€. The economic consideration for each piece of equipment can be found in the Appendix A. A breakdown of purchased equipment costs is presented in Figure 6. It can be seen that the largest contributor to total equipment cost is the reactor (37.4%), which is the core component of SNG production, followed by the absorber (16.1%) and heat exchangers (16%).

Based on the equipment costs, CAPEX and OPEX were calculated using the ‘factor method’ and the results are shown in Table 14. The sum of annualized CAPEX and OPEX leads to the total annual cost of 318.2 M€/y. Notably, OPEX is much higher than annualized CAPEX. A breakdown of OPEX is shown in Figure 7. The purchase of hydrogen accounts for the vast majority (i.e., 89.5%) of OPEX.

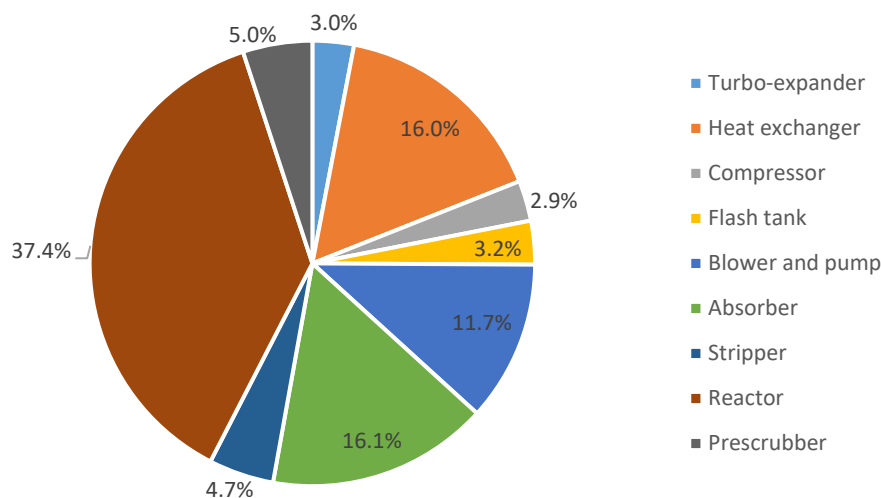


Figure 6 Breakdown of purchased equipment cost

Given the calculated CAPEX and OPEX, the production cost of SNG was calculated and is shown in Table 14. The minimum selling price was also calculated, based on assumptions. In addition, the production cost of SNG in the analyzed system are compared with the economic indicators of benchmark products (see Table 15). Since no commercial-scale coal-to-SNG project has been reported operating in Germany or Europe, the reference cost of the benchmark system is taken from a study based in the US. [31, 35]. The cost values were translated to euros values in 2016. The results suggest that the production cost of the proposed system is more than 10 times greater than that of the benchmark system. The selling price of the SNG produced by the proposed system is also significantly higher than the price of natural gas in Germany in 2019.

Table 14 Economic indicators

	Unit	Carbon capture	CO ₂ methanation	Total
Equipment cost	M€	5.6	8.2	13.8
CAPEX	M€	21.5	30	51.5
Annualized CAPEX	M€/y	1.8	2.5	4.3
OPEX	M€/y	8.1	306	314.1
Production cost of SNG	€/MJ			0.0748
	€/kWh _{th}			0.269
Minimum selling price	€/MJ			0.0754
	€/kWh _{th}			0.272

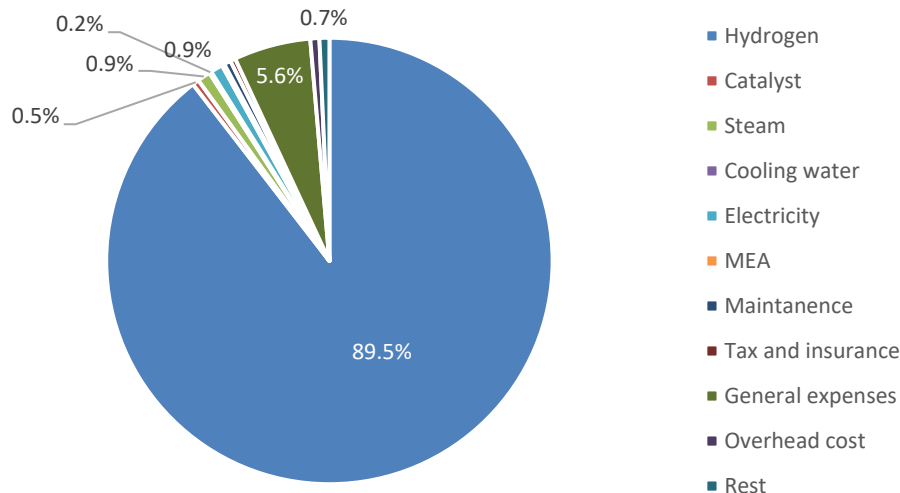


Figure 7 Breakdown of OPEX

Table 15 Comparison of economic assessment indicators with published data

Indicator	Present study	Coal-to-SNG [31, 35]	Natural gas [17]
Output capacity	148 MW	293 MW	
Production cost	0.269 €/kWh _{th}	0.027 €/kWh _{th}	
Production cost per functional unit	0.0746 €/MJ	0.0076 €/MJ	
Selling price	0.271 €/kWh _{th}		Industry: 0.026 €/kWh _{th} Household: 0.06 €/kWh _{th}

5.4 Combined indicator for TEA and LCA

The cost of CO₂ abatement (C_{abated}) is a commonly used indicator for integrating TEA and LCA. In the present study it is calculated via:

$$C_{abated} = \frac{C_{CCU} - C_{ref}}{EI_{ref} - EI_{CCU}} \quad (5-7)$$

Here, C_{CCU} and C_{ref} represent the production costs in the CCU and benchmark systems, respectively, while EI is environmental impact. For this study, the impact is embodied in the form of CO₂ emission intensity.

Calculating the amount of CO₂ abated by the studied system is more easily done from an LCA perspective. In order to do this, the system boundary must be expanded to include the CO₂ source as shown in Figure 8. Given this expanded boundary, the CO₂ emission intensity of the product system was calculated to be 1.943 kg_{CO2}/MJ_{SNG}. To compare this with the benchmark SNG system, the system

SNG Worked Example for TEA Guidelines

expansion approach from LCA (see Guidelines C4.3) was used. Both the reference iron & steel plant without carbon capture and benchmark SNG system should be included in the system boundary (see Figure 9). Doing so guarantees that the studied and benchmark product systems result in the same functions. The reference benchmark coal-to-SNG system is reported to emit 0.075 kg of CO₂ per 1 MJ of SNG produced. As a result, the CO₂ emission intensity of the benchmark system is 2.035 kg_{CO2}/MJ_{SNG}. The C_{abated} was calculated to be 0.73 €/kg_{CO2}.

As mentioned in the preceding chapters, it is uncommon for TEA to conduct system expansion as it is usually necessary to maintain consistent system boundaries. The system expansion described above can only be used to quantify emissions. The production costs are still based on the boundary prior to expansion. In other words, no TEA is conducted for the expanded boundary. Another solution to calculating CO₂ emission intensity without system expansion is to regard the CO₂ feedstock as representing negative emissions, which in this case is -0.017 kg_{CO2}/MJ_{SNG}. Consequently, the same result is obtained for C_{abated}.

To summarize, the system expansion approach from LCA, can be used to calculate the CO₂ emission intensity (environmental impacts). This method is straightforward and helps provide practitioners with a comprehensive overview of all emissions. However, this is approach uncommon, and sometimes impossible for TEA when the emission data for the CO₂ source are incomplete. In such cases, this can be resolved by treating the CO₂ feedstock as negative emissions.

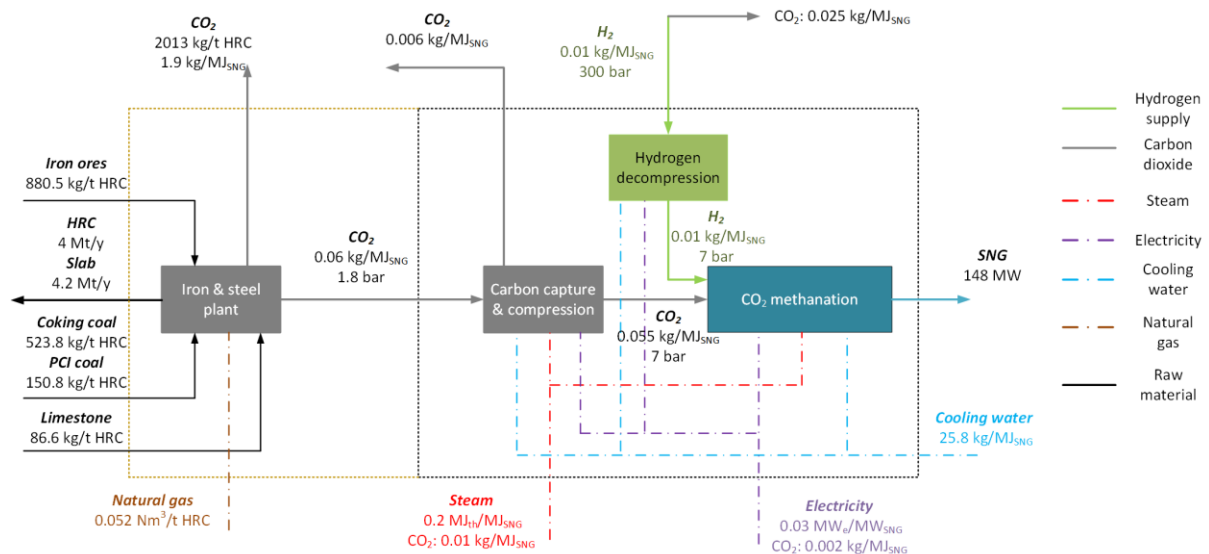


Figure 8 Expanded system boundary

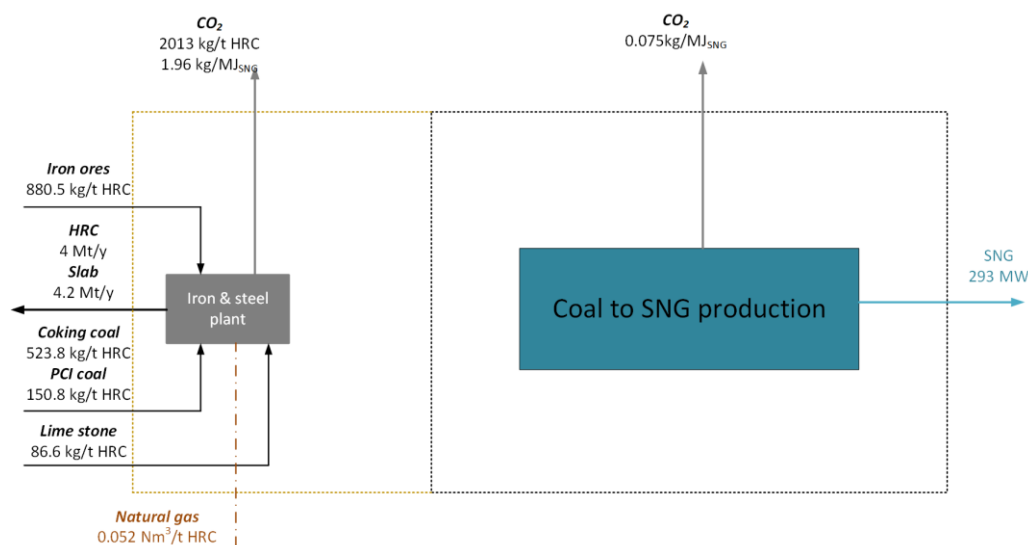



Figure 9 Benchmark system with system expansion


 Reference to TEA Guidelines V1.1

Guideline A.4 discusses the definition of combined indicators and, in particular, how to calculate the cost of CO₂ abated. Lower abatement cost indicates higher economic efficiency of the analyzed CCU system. This approach is applied because key factors are initially unknown, which is common in most cases.

5.5 CO₂ regulation

The impact of CO₂ regulation was not considered in the present study, as it is found that current schemes such as the European Union Emissions Trading Scheme (ETS) are not applicable to the analyzed CCU system. The Monitor and Reporting Regulation (MRR) of the ETS indicates that, at present, only technologies for long-term geological storage of CO₂ (i.e., carbon capture and storage, CCS) qualify for the EU ETS. Although proposals have been brought forward to amend the scope of the ETS to include CCU technologies, any changes to the legislation will still focus on the CCU pathways that are able to store CO₂ permanently (e.g., mineralization) [48]. For CCU products that will lead to re-emission of CO₂, such as chemical products and fuels, the jurisdiction of the CO₂ trading scheme will require further examination. A broader system boundary is likely necessary in order to analyze the environmental impacts of CCU-based chemical and fuel products.

6 Interpretation

 Reference to TEA Guidelines V1.1

Checklist of items to be included in the inventory report:

- Describe uncertainty and sensitivity of the results
- Provide conclusions, presenting the whole spectrum of criteria relevant for decision making
- Discuss limitations
- State recommendations, if any

6.1 Sensitivity and uncertainty analysis

6.1.1 Local sensitivity analysis

In this section, a local sensitivity analysis was carried out to investigate the impacts of several parameters on the production costs. The expense of hydrogen makes up most of the OPEX. Therefore, it was chosen as the first parameter to be investigated. In addition, the effects of CAPEX, reactor cost, operating hours per year, and steam price were also investigated. These parameters were varied across a range of $\pm 30\%$, based on which a tornado chart was plotted (see Figure 10)

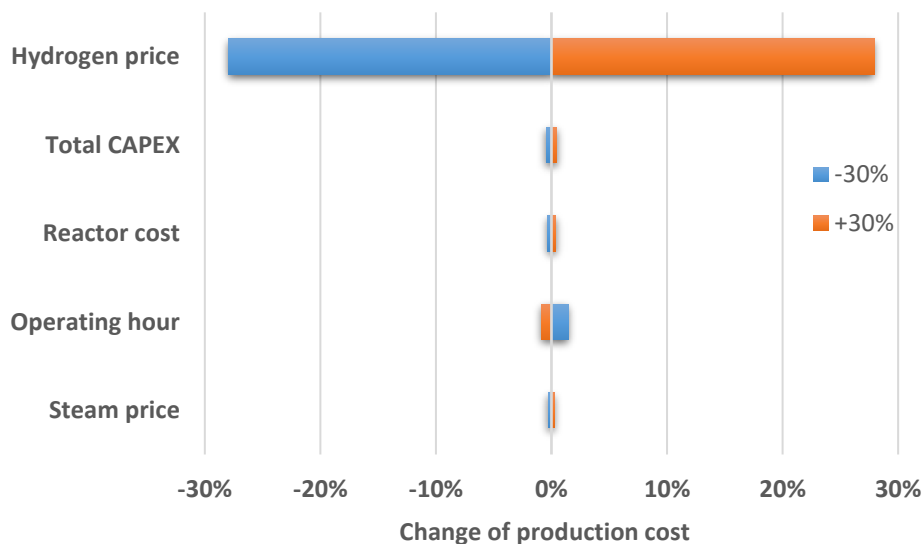


Figure 10 Sensitivity analysis

It can be observed from Figure 10 that hydrogen price has a far more pronounced impact on production cost than any other factors. The results indicate that varying the hydrogen price by $\pm 30\%$ would lead directly to around $\pm 28\%$ change in overall production cost. In comparison, the same $\pm 30\%$ range that was tested for the other parameters has much less influence on production cost. Only the change in operating hours leads to a variation of more than 1% in the production cost. Hence, hydrogen price is the factor exerting by far the greatest influence on the output of the analyzed system. Note that, in practice, +30% operating time is not feasible as it already exceeds the maximum

yearly operating time. Therefore, this scenario is only included to illustrate the mathematical (rather than practicable) change in the output values.

6.1.2 Uncertainty analysis

The accuracy of the analysis is expected to be within AACE class 4 [49], i.e., a preliminary estimate based on limited cost data and design details. In addition, the sensitivity analysis identified hydrogen price as a source of significant uncertainty for the system.

The Monte Carlo method was used to conduct an uncertainty analysis. Since the sensitivity analysis shows that the hydrogen price and operating hours input variables have more noticeable effects on the outputs than the other variables, they were selected for the simulation. According to the estimates of Reuß et al. [26], hydrogen price ranges from approximately 5.5 €/kg to 16 €/kg depending on the supply pathways. Meanwhile, annual operating hours are considered for the range 5600 h to full-time operation (8760 h/year). Triangular distributions were assigned to the two variables with the values used in the base case scenario considered to be most likely to occur. The output variables tend to be normally distributed. The effects of the two input variables on SNG production cost are depicted in a cumulative distribution plot (see Figure 11). The mean value of the distribution is 0.118 while the standard deviation was calculated to be 0.034. At a 95% confidence interval the production cost ranges between 0.065 and 0.173 €/MJ_{SNG}.

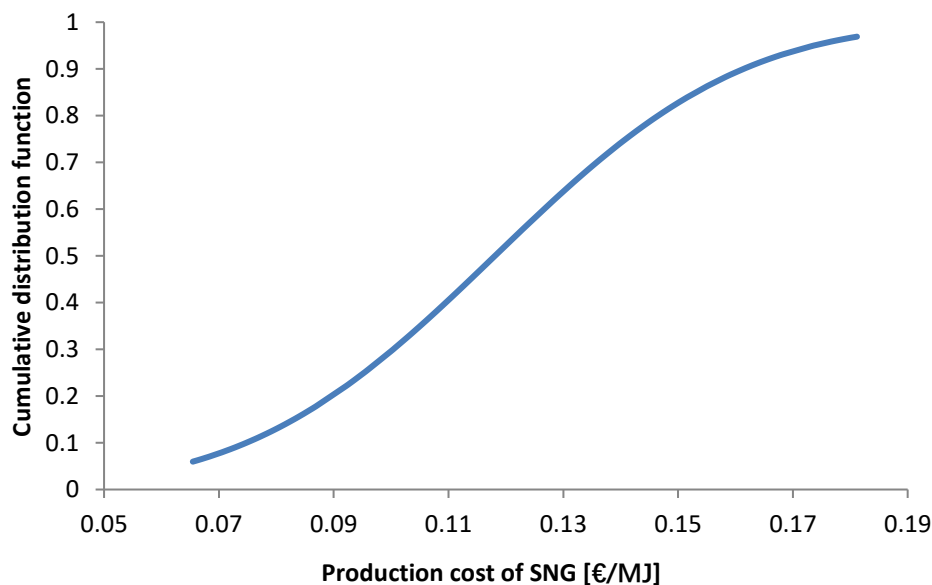


Figure 11 Uncertainty analysis for the production cost of SNG

Reference to TEA Guidelines V1.1

Based on the sensitivity and uncertainty analysis: Variables that introduce high levels of uncertainty should be targeted in order to improve their data quality (using an iterative approach), and otherwise should be documented. For this study, the highly variable data on hydrogen price leads to a significant uncertainty in the system. However, the data quality cannot be further improved at present because, to date, they can only be obtained from predictive studies.

6.2 Scenario analysis

As discussed above, the cost of hydrogen has a significant impact on the economic assessment. Henceforth, different scenarios with respect to H₂ supply routes are investigated in this section. In the base case scenario, the hydrogen is assumed to be supplied in the form of gaseous H₂. A cavern storage method is used, and the hydrogen is transported to the CCU plant via truck. In this section, two alternative supply chains, which have also been studied by Reuß et al. [25, 26], are considered. In alternative scenario 1, H₂ is still supplied in the gaseous form but via pipeline. In alternative case 2, liquid hydrogen, which has a higher density than its gaseous form, is provided to the production site via truck. The characteristic data regarding the two alternative supply routes are reported in the study of by Reuß et al. [26] and summarized in Table 16.

Table 16 Characteristics of alternative scenarios [26]

	Base case scenario	Alternative scenario 1	Alternative scenario 2
H ₂ form	Gas	Gas	Liquid (-252 °C)
Storage	Cavern	Cavern	Cryogenic tank
Delivery	Truck	Pipeline	Truck
Price [€/kg _{H2}]	6.5	5.5	7
CO ₂ emission [kg _{CO2} /kg _{H2}]	2.4	1.2	0.52

Given the data shown in Table 16, the total annual costs for alternative scenarios 1 and 2 were calculated to be 273.2 M€/y and 341.4 M€/y, respectively. The economic indicators for the alternative scenarios are shown in Figure 12. It should be noted that the pre-treatment units for liquid H₂ need to be modified, as the temperature and pressure differ in these scenarios.

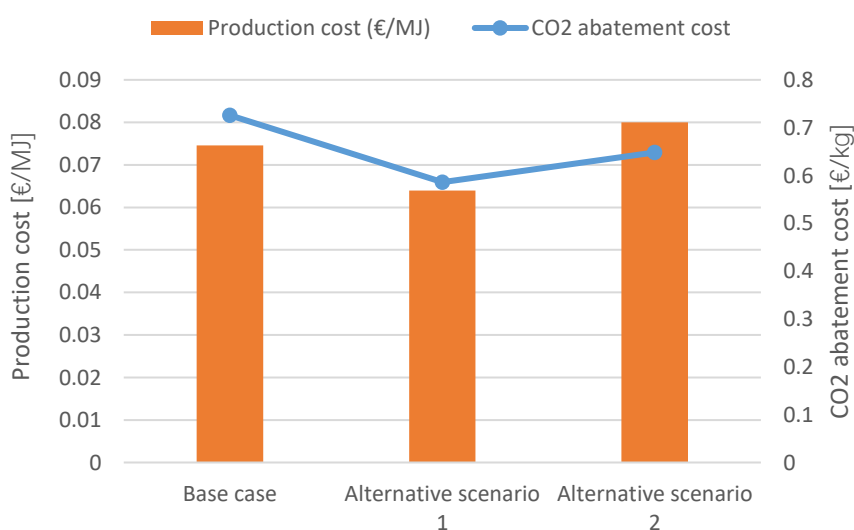


Figure 12 Production costs and CO₂ abatement costs for the alternative scenarios

SNG Worked Example for TEA Guidelines

Alternative scenario 1 results in the lowest costs for both production and CO₂ abatement. Transport via pipeline provides a cheaper feedstock of hydrogen. In comparison, alternative scenario 2 leads to higher production cost than the base case because: the cost of hydrogen is higher; and additional equipment costs are also incurred in converting liquid hydrogen to the reaction condition. Nonetheless, the CO₂ abatement cost in case 2 is lower than the base case scenario because the inherent CO₂ emission derived from the transport of liquid hydrogen is notably lower.

7 Summary and conclusion

The report has investigated the technical and economic viability of producing SNG via a CO₂ hydrogenation process, which was subject to rigorous simulation in Aspen Plus modeling software. In the process, CO₂ feedstock is captured from an iron & steel plant next to the methanation installation, while hydrogen, which is produced via electrolysis using surplus electricity, is purchased from a production site located 250 km away. The output capacity of the methanation plant is 148 MW.

The SNG production cost of the analyzed product system was estimated to be 0.0748 €/MJ (= 0.269 €/kWh), with a minimum selling price of 0.0754 €/MJ (= 0.271 €/kWh). The estimated SNG production cost is more than 10 times that of the benchmark product (coal-based SNG). As compared to the natural gas market in Germany, the selling price of SNG produced by the proposed system is also significantly higher. CO₂ abatement cost was estimated as 0.75 €/kg_{CO₂}, as a combined indicator of TEA & LCA. Sensitivity analysis reveals that variability in hydrogen purchase price is the source of greatest uncertainty for the analyzed system. At a 95% confidence interval, the production cost ranges between 0.065 and 0.173 €/MJ_{SNG}. Current EU ETS legislation is inapplicable to the product system investigated and therefore brings no benefits for the CO₂ abated. To drive CCU-based SNG forward in the future market requires significant reduction in hydrogen production cost, and the extension of legislation concerning CO₂ emission allowances to include more CCU technologies.

With respect to the potential integration of the present TEA with an LCA, it is found that the main challenge involves setting appropriate system boundaries. In the present study, conducting a TEA does not require the inclusion of upstream and downstream processes related to the production processes, whereas in contrast LCA is more likely to favor a cradle-to-gate or -grave boundary. In TEA, information on upstream processes can be attached to input flows that enter product systems. If identical system boundaries are set for TEA and LCA, a challenge for TEA is solving multi-functionality, which can be very challenging when the potential markets for the products analyzed are highly uncertain. To align inventories, relevant environmental parameters (e.g., CO₂ emissions) should be documented in addition to the technical and economic parameters. When calculating CO₂ abatement cost, system expansion can be used to account for the reduced CO₂ emissions, or else the CO₂ feedstock can be regarded as negative emissions.

Appendix A Cost data

Table A. 1 Cost data and considerations for purchased equipment cost [39, 44, 50]

Equipment	Capacity measure [Unit]	Base size Q_B	Base costs C_B [US\$ ₂₀₁₀]	Material	f_M	f_P	f_T	Exponent
Shell-and-tube heat exchanger	Area [m ²]	80	3.28×10^4	CS	1.9	1	1	0.68
Compressor, incl. motor	Power [kW]	250	9.84×10^4	CS	1	1	1	0.46
(Large) Centrifugal pump, incl. motor	Power [kW]	4	9.84×10^3	CS	2.4	1	1	0.55
Scrubber (incl. random packing)	Volume [m ³]	0.1	4.92×10^3	CS				0.53
Reactor	Flow rate [kg/s]	57.9	10^6 (€ 2005)	SS (high grade)	3.4	2.1	1	0.67
Turbo-expander	Power [kW]	Equation (5-2)		SS (high grade)	3.4	1	1.9	
Distillation column (Tower + packing)	Volume [m ³]	Equation (5-2)		SS (high grade)	3.2	1	1	

CS: carbon steel

SS: stainless steel

Table A. 2 Coefficients used in the equation (5-5)[44]

Equipment	Capacity measure [Unit]	Z_1	Z_2	Z_3
Tower	Volume [m ³]	3.4974	0.4485	0.1074
Packing	Volume [m ³]	2.4493	0.9744	0.0055
Turbo-expander	Power [kW]	2.7051	1.4398	0.1776

Appendix B Sizing of column

Towler and Sinnott [51] have provided a series of formulae to estimate the sizes of gas–liquid separators. The diameter of a vessel D_i is calculated according to:

$$D_i = \sqrt{\frac{4 V_i}{\pi u_{s,i}}} \quad (\text{C.1})$$

where V_v is the vapor flowrate and $u_{s,i}$ the settling velocity for vapor droplets. The settling velocity for knockout drums $u_{s,kd}$ is estimated as:

$$u_{s,kd} = 0.07 \sqrt{\frac{\rho_l - \rho_v}{\rho_v}} \quad (\text{C.2})$$

while the settling velocity for a scrubber ($u_{s,c}$) is estimated by the following equation:

$$u_{s,c} = (-0.171l_t^2 + 0.27l_t - 0.047) \sqrt{\frac{\rho_l - \rho_v}{\rho_v}} \quad (\text{C.3})$$

where ρ_l and ρ_v are the liquid and vapor flow density, respectively; l_t is the tray sizing, for which 0.5 m is used.

The vessel height H_i is determined as:

$$H_i = \frac{3}{2} D_i + 0.4m + h_l \quad (\text{C.4})$$

wherein the liquid depth h_l can be estimated as:

$$h_l = \frac{4 V_l t_{hold}}{\pi D_i^2} \quad (\text{C.5})$$

where V_l is the liquid flowrate; t_{hold} is the hold-up time in the vessel and is assumed to be 5 mins for all vessels.

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