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Techno-Economic Evaluation of Different Scenarios for Carbon Capture and Utilization Concepts for Steel Mill Off-Gases#

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ABSTRACT

The focus of this study is to conduct a techno-economic evaluation of a chemical production plant that utilizes carbon-, nitrogen- and hydrogen-containing steel mill off-gases as a material feedstock. The chemical products analyzed are acetic acid, ammonia, methanol, and urea, all of which, except ammonia, are classified under the carbon capture and utilization (CCU) concept. In order to support the investment decision-making process, a superstructure optimization model is employed, which includes the main technical plants (e.g. reactors, storages and separators) and plant layout decisions (e.g. the choice between two reactors). To determine the impact of future developments, five scenarios are considered, focusing on environmental, technical, and economic key factors for the target operational year of 2040. The scenario-dependent optimization results represent the optimal CCU concept with the highest net present value (NPV) for a German steel plant in Duisburg in 2025. These results, including the chemical plant layout with selected chemicals and plants, demonstrate that different scenarios can lead to significant changes in the NPV and chemicals produced and subsequently exported. The results of this study can be utilized as a foundation for investment decisions.

Keywords: carbon capture and utilization, steel mill off-gases, techno-economic evaluation, renewable energy, superstructure optimization

NOMENCLATURE

Abbreviations	
AA	Acetic acid
ABS	Absorption plant
AEL	Alkaline water electrolysis plant
BAU	Future scenario for business-as-usual
BFG	Blast furnace gas
BOFG	Basic oxygen furnace gas
CHP	Combined heat and power plant
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CO	Carbon monoxide
COG	Coke oven gas
Crisis	Future scenario for energy crisis
H2, H_2	Hydrogen
H2-Max	Future scenario for positive hydrogen
Market	Future scenario for positive economy
MEM	Membrane separation plant
MILP	Mixed-integer linear programming
MeOH	Methanol
N_2	Nitrogen
NG	Natural gas
NH3	Ammonia
NPV	Net present value
P1 – P4	Decision points for plants
PEM	Proton exchange membrane electrolysis plant
PSA	Pressure swing adsorption plant
R1 – R4	Decision points for chemicals
RE-Max	Future scenario for positive renewable energy developments
RV	Residual value
UR	Urea

1. INTRODUCTION

The energy-intensive steel industry is responsible for 5-7 % of CO_2 emissions in Germany [1, 2]. This is mainly due to the blast furnace steelmaking process, which uses coal as the conventional energy source. To mitigate these CO_2 emissions, three promising concepts are under discussion for the German industry [3].

The first concept involves direct reduced iron production using hydrogen as the primary energy source. However, integration of this concept into existing conventional blast furnace plants is impractical and requires significant amounts of renewable green

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hydrogen, which is currently unavailable. The second mitigation concept is carbon capture and storage (CCS) of the carbonaceous off-gases from the blast furnace route. While CCS addresses the problem of CO_2 emissions by transferring them to long-term storage options, Germany currently lacks suitable options for storing these large quantities of CO_2 [4]. The third mitigation concept is the CCU concept. Here, off-gases from the steel production, which are currently used thermally and subsequently emitted as CO_2, are instead used to produce valuable chemical products. This reduces CO_2 emissions but leads to a significant demand for hydrogen from renewable energy sources. As a result, a sector coupling industry is emerging between the steel, energy and chemical sectors.

This paper examines the investigation and evaluation of CCU concepts under different future scenarios. A generic superstructure-based mixed-integer linear programming (MILP) optimization model is employed to ensure the economically optimal chemical plant layout, design capacities and operations. MILP is a widely used approach in scientific research to determine the optimal solution for a given objective [5–7]. Previous studies have employed the MILP approach to evaluate the production of methanol (MeOH) or dimethyl ether from specific off-gases [5]. However, chemical products such as acetic acid (AA), ammonia (NH3), and urea (UR) have not been evaluated in the existing literature with all three types of off-gases from a conventional steelmaking plant. The off-gas amounts and concentrations from the analyzed plant site are taken from [8]. The off-gases are blast furnace gas (BFG, high amounts of nitrogen (N_2), carbon monoxide (CO) and CO_2), basic oxygen furnace gas (BOFG, high concentration of CO) and coke oven gas (COG, high concentration of H_2). In addition, previous works have not considered various future developments of key factors, such as changes in market prices, market volumes of products or raw materials, or technical plant parameters on the optimal plant layout. These key factors and future developments are summarized in five scenarios from [9], which serve as input data for the MILP model to evaluate the economically optimal CCU concept. The goal of this study is to determine and evaluate the chemical plant layouts with corresponding economic key performance indicators for each scenario.

2. METHODS AND MODELING FRAMEWORK

A comprehensive description of the developed and utilized modeling framework can be found in [10]. A brief overview of the superstructure optimization framework is presented in Fig. 1 above.

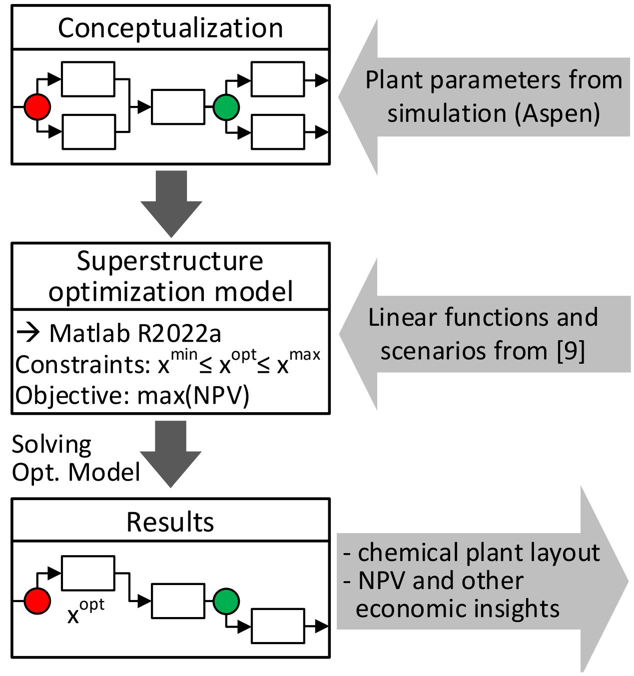

Fig. 1 Modeling framework for the superstructure optimization approach with decision points.

In the first step of Fig. 1, the generic CCU concept is developed with all possible interconnections between the plants for mass and energy flows and plant layout investment decision points. All plants are parameterized with simulation using AspenPlus. Plant parameters include conversion rates, efficiencies and specific energy demands. After conceptualization, a time-dependent superstructure optimization model is implemented in Matlab R2022a. All implemented functions are linear or linearized and the model is parameterized with different scenarios from [9]. After solving the optimization model, the results demonstrate the investment decisions for the optimal plant layout with design capacities and produced amounts of chemicals with the maximized NPV.

3. GENERIC CCU CONCEPT AND SCENARIOS

3.1 Conceptualization and plant parameterization

The generic CCU concept developed in this work is depicted in Fig. 2. On the left side, natural gas (NG) can be imported to produce power and/or heat for the CCU concept in an already installed combined heat and power (CHP) plant. The CHP can also be operated with excess off-gases of BFG, BOFG and COG. The incoming BFG goes to a shift plant to convert the CO with water to CO_2. The reacted CO_2 is separated from the shift gas and enters the methanol (MeOH-R) and/or the urea (UR-R) reaction pathway (decision R2). From COG, the hydrogen can be separated (H_2 intern) in a pressure swing adsorption (H2-PSA) or membrane (H2-MEM) plant (decision P1).

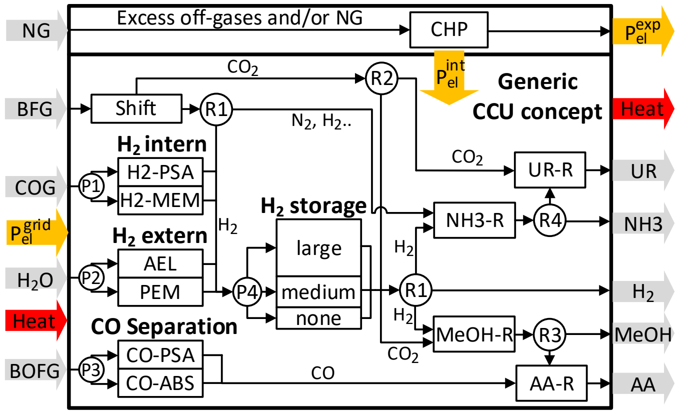

Fig. 2 Generic CCU concept with mass flow interconnections between plants including investment decision points as superstructures. Decision points are for plants (P1-P4) and reaction pathways (R1-R4).

The amounts of internal H_2 are unable to meet the high demands of the reaction pathways. Therefore, external hydrogen (H_2 extern) from an alkaline electrolysis (AEL) or proton exchange membrane electrolysis (PEM) plant connected to the grid can be used (decision P2). BOFG has high amounts of CO that can be used in the acetic acid reaction pathway (AA-R) with the Monsanto-Cativa reaction process. The upstream of the AA-R pathway includes a decision point, designated P3, which determines whether to utilize a CO adsorption (CO-PSA) or absorption (CO-ABS) plant. Other decision points in the model include P4, which concerns the storage of H_2 (large = 6 h, medium = 2 h and none = 0 h, based on the maximum H_2 flow from electrolysis), R1 for the reaction pathway methanol and/or ammonia (NH3-R), R3 for methanol and/or acetic acid and R4 for ammonia and/or urea. Plant parameters are extracted from literature data or calculated with process simulations and summarized in [10].

3.2 Superstructure optimization model

The detailed model of the generic CCU concept of Fig. 2 is described in [10]. A brief overview of the modelling and economic assumptions is given below.

3.2.1 Plant constraints

For all i plants, the decision options for installation are modeled. The design capacity limits are derived from the off-gas quantities, the chemical market volumes and the technical plant parameters. Eq. (1) describes the electrical design capacity $P_{\mathrm{el},i}^{\mathrm{des}}$ (in MW) with the upper design limit $P_{\mathrm{el},i}^{\max}$ and the lower design limit $P_{\mathrm{el},i}^{\min}$ with the binary investment decision variable $y_{i,\mathrm{inst}}$.

$$y_{i,\mathrm{inst}} \cdot P_{\mathrm{el},i}^{\min} \leq P_{\mathrm{el},i}^{\mathrm{des}} \leq y_{i,\mathrm{inst}} \cdot P_{\mathrm{el},i}^{\max} \qquad (1)$$

The temporal electric consumption $P_{\mathrm{el},i}(t)$ is constrained by $P_{\mathrm{el},i}^{\mathrm{des}}$ according to Eq. 2. $P_{\mathrm{el},i}(t)$ is calculated from the incoming mass flow $\dot{m}_{i,\mathrm{in}}(t)$ (variable in t/h) and the specific electric input $w_{\mathrm{el},i}$ (parameter in MWh/t) as derived in Eq. 3.

$$0 \leq P_{\mathrm{el},i}(t) \leq P_{\mathrm{el},i}^{\mathrm{des}} \qquad (2)$$

$$P_{\mathrm{el},i}(t) = \dot{m}_{i,\mathrm{in}}(t) \cdot w_{\mathrm{el},i} \qquad (3)$$

Detailed modeling of all plants with and mass and energy balances are in [10].

3.2.2 Network constraints

To illustrate the networks, Eq. 4 describes the constrained electricity network between suppliers (left) and consumers (right) of the generic CCU concept in Fig. 2. Furthermore, mass flow and heating networks (calculated with pinch analysis) are considered.

$$P_{\mathrm{el}}^{\mathrm{grid}}(t) + P_{\mathrm{el}}^{\mathrm{int}}(t) \geq P_{\mathrm{el}}^{\mathrm{exp}}(t) + \sum P_{\mathrm{el},i}(t) \qquad (4)$$

3.2.3 Cost & Revenue constraints

Costs are classified into two categories: operational expenditures (OPEX) and capital expenditures (CAPEX). The CAPEX (in bn €) for plants is modeled with piecewise linearization of the non-linear cost estimation functions from the capacity method with CEPC indices for 2025.

OPEX are calculated annually by summing up the optimized cash flows from the time series (Δt =15 min). For example, the annual power price $OPEX_{\mathrm{el}}$ (in M€/a) is calculated from the grid import $P_{\mathrm{el}}^{\mathrm{grid}}(t)$ and the transient spot market price $c_{\mathrm{el},t}^{\mathrm{grid}}$ (in €/MWh).

$$OPEX_{\mathrm{el}} = \sum P_{\mathrm{el}}^{\mathrm{grid}}(t) \cdot c_{\mathrm{el},t}^{\mathrm{grid}} \Delta t \qquad (5)$$

Other terms for annually OPEX include CO_2 emission allowances for the residual emissions of the steel plant $OPEX_{\mathrm{CO2}}$, heat $OPEX_{\mathrm{th}}$, raw materials $OPEX_{\mathrm{raw}}$ and general plant operating costs $OPEX_{\mathrm{gen}}$ — which include labor, maintenance, overhead, etc. — in Eq. 6.

$$OPEX_{\mathrm{year}} = OPEX_{\mathrm{el}} + OPEX_{\mathrm{CO2}} + OPEX_{\mathrm{th}} + OPEX_{\mathrm{raw}} + OPEX_{\mathrm{gen}} \qquad (6)$$

Annually revenues REV_{year} of the CCU concept are dominated by the exported chemical products $\dot{m}_{pr}^{\mathrm{exp}}(t)$ (pr = AA, NH3, MeOH and UR), with the corresponding market price c_{pr} (in €/t) and possible revenues through electricity export from the CHP to the grid (Eq. 7).

$$REV_{\mathrm{year}} = \sum \left(\sum \dot{m}_{pr}^{\mathrm{exp}}(t) \cdot c_{pr} + P_{\mathrm{el}}^{\mathrm{exp}}(t) \cdot c_{\mathrm{el},t}^{\mathrm{grid}} \right) \Delta t \qquad (7)$$

3.2.4 Objective function (NPV)

The objective function to maximizes the NPV. The reference state of total thermal utilization of all off-gases with emission of all carbon as CO_2 has an NPV of zero. If an investment is disadvantageous (NPV < 0), the decision is made not to install the CCU concept, so the reference state remains. Conversely, if an investment is beneficial (NPV > 0), the CCU concept with the highest NPV is installed. The NPV is modeled with a discounted cash flow approach, as described by Douglas [11]. All cash flows are discounted with a fixed annual interest rate as q_{I}. The CAPEX is capitalized in the construction period N_{c} in the respective construction year n_{c} with the weighting u_c. In the operating period N_{op}, OPEX and REV are capitalized in the respective operating year n_{op}. It is assumed that all annual cash flows remain constant over time. At the end of the plant life span, all installed plant equipment is sold with a residual value RV_i.

$$NPV = \max\left(-\sum_{n_{\mathrm{c}}}^{N_{\mathrm{c}}}\sum_i CAPEX_i \cdot u_{n_{\mathrm{c}}} \cdot q_{\mathrm{I}}^{n_{\mathrm{c}}} + \sum_{n_{\mathrm{op}}}^{N_{\mathrm{c}}+N_{\mathrm{op}}} \frac{REV_{\mathrm{year}} - OPEX_{\mathrm{year}}}{q_{\mathrm{I}}^{n_{\mathrm{op}}}} + \frac{\sum_i RV_i}{q_{\mathrm{I}}^{N_{\mathrm{c}}+N_{\mathrm{op}}}}\right) \quad (8)$$

Eq. 8 can be simplified to four cumulative discounted cash flow terms for the entire CCU project, including the construction and operation periods (Eq. 9). The assumptions of the objective are summarized in Tab. 1.

$$NPV = -CAPEX - OPEX + REV + RV \quad (9)$$

Tab. 1 Economic assumptions for the objective function.

Symbol	Value [Unit]	Description
N_{c}	5 [a]	Construction period (2025-2030)
n_{c}	0 – 4 [-]	Index from starting year
N_{op}	20 [a]	Plant life span (2030-2050)
n_{op}	5 – 25 [-]	Index from starting year
q_{I}	1,07 [1/a]	7 %/a interest rate
u_{c}	1:2:3:2:1	Share of CAPEX in year n_{c}
RV	25 [%]	25 % of CAPEX [11]

3.3 Scenarios

The scenario development methodology and a detailed description of the five scenarios utilized in this work can be found in a previous paper by Sadlowski [9]. A brief overview of the scenarios is given below.

Five scenarios with different characteristics are employed in the optimization model to gain insight into optimal concepts (layout, economics etc.) due to future changes. The scenario reference year is 2040. All identified key factors with a high impact on the concept are extrapolated to this year. These are 24 key factors from the economic, environmental and technical areas. The key factors include prices for the electricity grid import, CO_2 emission allowances and chemical products (AA, NH3, MeOH and UR), market volumes with export limits, conversion rates, efficiencies, shares of renewable energies in the German grid mix and energy demands of the steel site. A business-as-usual (*BAU*) scenario is created by trend extrapolation of the key factors. Four alternative scenarios are then derived from the *BAU* scenario. For further details on the numerical values and time series, please refer to [9].

The four alternative scenarios represent different perspectives. In the *RE-Max* scenario, a positive environmental future is assumed, with electricity prices decreasing and prices for CO_2 emission allowances and the market volume of chemical products increasing significantly. This would theoretically allow for the binding of all carbon from off-gases in the chemical products. The *Market* scenario assumes a positive economic and technical future in which product prices rising and market volumes increasing slightly. In addition, the technical efficiencies of plants increase, which should make investments in the concept attractive. The *Crisis* scenario assumes an energy crisis in Europe leading to poor market conditions. Raw material prices, for instance, electricity and hydrogen, increase significantly, and the market volume of products decreases. In the *H2-Max* scenario, specific investment costs for PEM and AEL decrease significantly and technical efficiencies increase.

The five scenarios with completely different characteristics and objectives can be used to identify similarities and differences for an economic CCU concept. They provide an order of magnitude and insight into the most robust CCU concepts. A short overview of the scenarios is presented in Tab. 2.

Tab. 2 Used scenarios from [9].

Scenario	Description
BAU	Business-as-usual, trend extrapolation
RE-Max	Environmental best-case (renewable energy)
Market	Economic best-case (market-booming)
Crisis	Economic worst-case (ongoing energy crisis)
H2-Max	best-case for a hydrogen booming market

4. OPTIMIZATION RESULTS

The MILP models are solved for all scenarios using Gurobi V11 with a MIPGap parameter of 0.1%.

4.1.1 Plant design layouts

The results for the optimal plant layout with all decisions for the five scenarios are shown in Tab. 3.

Tab. 3 Optimal CCU plant layout (points from Fig. 2).

Point	*BAU*	*RE-Max*	*Market*	*Crisis*	*H2-Max*
P1	H2-PSA	H2-PSA	H2-PSA	H2-PSA	H2-PSA
P2	AEL	PEM	PEM	AEL	PEM
P3	CO-PSA	CO-ABS	CO-PSA	CO-PSA	CO-PSA
P4	medium	medium	large	medium	large
R1	both	both	both	MeOH-R	both
R2	both	both	both	MeOH-R	both
R3	AA-R	both	both	AA-R	both
R4	UREA-R	UREA-R	both	none	UREA-R

Tab. 3 shows that for all P decisions (between two different plants) it is always economically advantageous to choose one of the two options. For all R decisions (between two reaction pathways), it depends on the scenario whether it is economically advantageous to choose both options (both), one option (name of pathway), or none of the options (none).

4.1.2 Economics

The NPV including the discounted terms for CAPEX, OPEX, REV and RV from Eq. 9 are shown in Fig. 3.

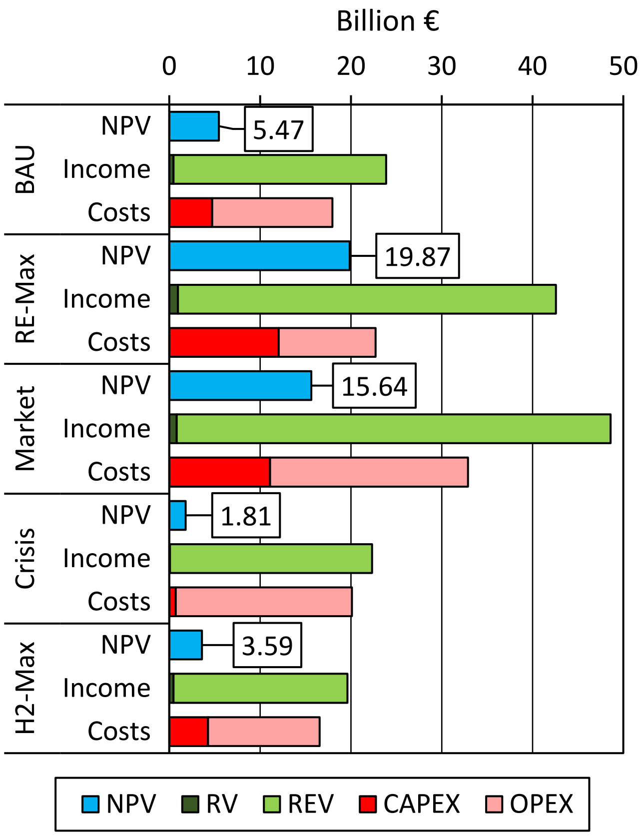

Fig. 3 Net present value (NPV) of the CCU concepts for the five scenarios with cumulative income terms (RV and REV) and cost terms (CAPEX and OPEX) from Eq. 9.

Fig. 3 shows the economic efficiency as NPV for the year 2025 of the optimal CCU concepts for all five scenarios. Depending on the scenario, the order of magnitude ranges from one to tens of billions of euros.

5. DISCUSSION

The plant layout decisions from Tab. 3 are discussed first. For internal hydrogen separation (P1), adsorption (H2-PSA) is a better option than membrane (H2-MEM) in all scenarios. For external H_2 production with electrolysis (P2), AEL is the best option in the *BAU* and Crisis scenarios. For the *RE-Max*, *Market* and *H2-Max* scenarios, PEM is a better option than AEL electrolysis. For CO separation from BOFG (P3), the adsorption plant (CO-PSA) is recommended for all scenarios except *RE-Max*. H_2 storage is an economically advantageous option in all scenarios and varies between medium and large size. In all scenarios except *Crisis*, both reaction pathways are selected for methanol and ammonia (R1). All scenarios with ammonia production also include a downstream production of urea from the feedstocks NH_3 and CO_2 (R1 = R2). In the *BAU*, *RE-Max* and H2-max scenarios, all ammonia produced is converted to urea and subsequently exported with revenues (R4 = UREA-R). In the *Market* scenario, both urea and ammonia are exported. In the *Crisis* scenario, only the product acetic acid is exported with the feedstocks MeOH and CO. The decision point R3 is between producing methanol and/or acetic acid with subsequent export. Therefore, in all five scenarios, it is economically advantageous to export acetic acid because R3 is at least positive for acetic acid (AA-R). In the *RE-Max*, *Market*, and *H2-Max* scenarios, it is also economically advantageous to export methanol (R3 = both). In addition to the results of Tab. 3, in the *Crisis* scenario internal H_2 and CHP electricity are exported with revenues. Thus, all five scenarios show different patterns of optimal plant selection (P points) and export of chemical products (R points).

As shown in Fig. 3 ,the highest NPV and therefore the best economic case is the *RE-Max* scenario with almost 20 billion €, followed in descending order by the *Market*, *BAU*, *H2-Max* and *Crisis* scenarios. All scenarios show that the residual value (RV) does not have a significant impact on the income compared to the whole plant life span revenues from the exported chemicals .

In the *Crisis* scenario, only a small chemical plant layout is built compared to the other scenarios, which is reflected in the low CAPEX. This is due to the fact, that it is economically more advantageous to sell H_2 from the off-gases and electricity from the CHP than to produce chemical products with high production costs.

In the *RE-Max* and *Market* scenario, the economic and technical developments (market prices, efficiencies etc.) are favorable to produce high quantities of CCU products from the off-gases. Therefore, the revenues over the 20-year production period are more than 40 billion € and most of the carbon from BFG can be captured and bounded in the chemical products of acetic acid and urea. These scenarios have the highest potential for economic CO_2 reduction with CCU in the future.

The *BAU* and *H2-Max* scenarios are of similar magnitude in terms of costs and revenues. The reason for the higher NPV in the *BAU* scenario is the higher market volume of the chemical products compared to the *H2-Max* scenario. The effect of reduced investment costs for the electrolysis in the *H2-Max* scenario does not have a significant positive impact on the NPV.

6. CONCLUSIONS

The results of the analysis demonstrate that the CCU concept is economically advantageous in all five scenarios studied. This is evidenced by the fact that the net present value is positive and exceeds the reference state of total combustion of the off-gases. The most valuable product is acetic acid, which is exported profitably in all scenarios. Four scenarios allow for the profitable export of urea, three permit the export of methanol, and only one allows for the profitable export of ammonia due to the lack of economic benefit from carbon capture. The optimal concept differs significantly in each scenario, indicating that future developments in technical, economic and environmental key factors will have a significant impact on the design and economics of the concept. The net present value in 2025 ranges from about 1.8 billion € in the negative energy crisis scenario to 20 billion € in the scenarios with positive renewable energy development and ideal market conditions.

The developed model can be utilized to illustrate the preliminary economic viability of a chemical production plant for CCU concepts from steelmaking off-gases. To obtain a more comprehensive understanding, additional scenarios can be investigated, sensitivity analyses can be conducted (e.g. variations in individual key factors such as electricity prices, hydrogen costs, CO_2 allowance prices or chemical product prices) or interactions with the higher-level power grid can be examined.

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