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Multi-criteria Scenario Development for Linear Optimization Models Utilizing Carbon-Containing Exhaust Gases

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Abstract:

Using the exhaust gases from the steel mill generation to produce chemicals can be a promising carbon capture and utilization (CCU) concept. Applying the model-based mathematical approach with mixed-integer linear programming (MILP) makes it possible to determine the optimal production pathway. However, the MILP aims the uncertain future to evaluate the long-term feasibility. It requires a hypothetical construction to show possible future states. This study aims to develop scenarios as input data for MILP models, representing a comprehensible future description. The investigation domains are determined as the technical, economical, and ecological perspectives to fulfil the multi-criteria evaluation. The factors from domains are projected qualitatively and quantitatively through objective estimations. The mutual relationships between the factors from the different domains such as the electricity price, Carbon footprint, and technical efficiency are implemented properly. The result is represented as five different scenarios: (1) Business as usual (BAU), (2) CO_2 reduction & RE share target (RE-Boom), (3) Technical improvement & Market booming (Market-Boom), (4) Energy & Market crisis (Crisis) and (5) Hydrogen booming (H_2-Boom). The scenarios depict the meaningfully different condition of the CCU concept with the most consistent and plausible combination of the key factors. Additional remarkable results from this study are the rough estimations of the initial capital and operating expenditures through the independently developed method. Consequently, the generated scenarios can be used for MILP models to promote the transparency and traceability of the further decision-making process.

Keywords:

Carbon Capture and Utilization; Multi-criteria Evaluation; Renewable Energy; Scenario Development.

1. Introduction

This study investigates a CCU concept which couples the carbon-emitting steel industry with the chemical and energy industry [1]. Exhaust gases from the blast-furnace, coke oven and basic-oxygen furnace containing large amounts of carbon monoxide, carbon dioxide, methane, hydrogen, and nitrogen serve as raw materials to produce chemicals. Hydrogen is identified as the limiting reactant. Therefore, external supplements utilizing renewable energy (RE) are required to increase its quantity. The exhaust gas can be used to produce products for different markets like methanol (MeOH), acetic acid (AA), ammonia (NH_3) and urea.

The implication of this concept is in a less developed phase. It is still being determined the technical layout of the plant, profitability, and potential environmental impacts. For this reason, a model-based mathematical approach with MILP is suggested to evaluate the long-term feasibility of the system [2]. The target of the MILP model is to find the optimal producing pathway, which includes technologies, design, and time dependent operation conditions. However, the MILP aims for an uncertain future, so the results are depending on the given future situation. From this perspective, this study aims to develop reliably formulated scenarios as input data for MILP. The optimal pathway is represented differently depending on the scenarios. A scenario is presented as a specific part of the future by considering relevant key factors rather than a comprehensive picture. Combining individual factors forms the space of common development of all these aspects. The expanding slice of future developments is described with the scenario funnel in Figure 1.

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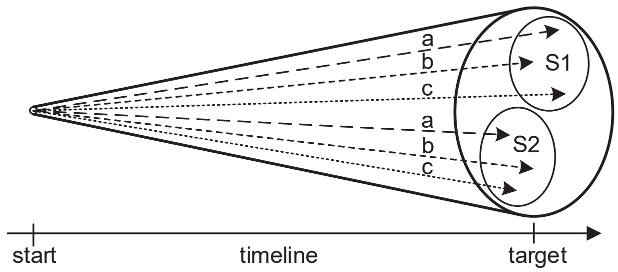

Figure. 1. Scenario funnel for representing the developments from a specific start time to a target time.

Different scenarios in Figure 1, here S1 and S2, now depict the different future possibilities in the target year from the start. For that, the possible projections of the different key factors (a, b, and c) are selected and condensed into scenarios. It should be noted that the meaning of the projection is not identical to the "forecast", which claims the actual probability of the occurrence, but the hypothetical construction to implicitly refer to the possibility of alternative futures [3].

There are some approaches to utilize the scenarios in this CCU context. Here, a short overview of recent contributions and preparatory work in the investigated field is given.

Stießel et al. [4] utilize a single scenario for the target year, 2030. The main target of the research is to identify cross-industrial process concepts of a CCU approach. The authors focus on external influences to formulate the scenarios. The process concept is evaluated in specific desired operating conditions by forcing the factors to be eco-friendly projected. Schlüter et al. [5] investigate a process concept of using steel mill exhaust gases for chemical production in three different operating conditions. The scenarios are developed focusing on the internal technical perspectives. The results are analyzed under time-dependent boundary conditions; thus, the limiting factors for the binding of carbon are identified. Sadlowski et al. [6] discuss the ecological potential of flexible methanol production from steel mill exhaust gases with a MILP model. The authors set up scenarios with three key factors which are external H_2 production, power supply sources and storage capacities. The outcomes are analyzed based on the carbon binding potential for this CCU concept.

In contrast to the concept of recent publications which focusing on a specific perspective to evaluate the CCU approach, the objective from the present work is extended to a multi-criteria evaluation with three different domains. It can be understood as a new and novel approach as the complicated relationships between the different domains are implemented. This approach of scenario development clearly shows the huge difference from the previous studies as it offers more comprehensive future descriptions. In other words, the generated scenarios can be utilized to evaluate the genuine feasibility of the CCU concept with a MILP model.

2. Properties of scenarios for a MILP model

All interconnections for the various technologies and exhaust gas conditions are implemented in the MILP model (e.g., reactors, storages, compressors, separators etc.). The options to be the final products are also set up in the decision point [2]. A detailed description of the model can be found in [6]. The outcome of the model is the optimal pathway, including the selection of technology, products, design and operation of the plants, and it depends on the given future states in form of scenarios.

The generated scenarios from this work can utilized as the input data in a linear optimization model. For that, they involve the special properties which are clearly different from the general scenario development.

First, the scenarios from this study are formulated based on the multi-criteria evaluation. Considering diverse internal and external influences brings reliable results about the technical plant's feasibility, investment decisions, or environmental effects. Secondly, projecting the selected factors from three domains involves the quantitative value in either numeric or linear dependencies to suit the feasibility. The quantitative values are assumed through the independently developed method or mathematically created functions. Finally, the individual relationship between the factors is examined through the software-based method. The cross-impact analysis (CIA) is conducted to find the most consistent and plausible combinations of factors.

3. Scenario development process

An existing method for scenario development is adapted to consider the functions of the scenarios. Based on the scenario technique from von Reibnitz [7]. A modified modelling concept involving the exploratory and quantitative approach is created for generating the five multi-criteria scenarios.

3.1 Premise

Scenario-specific assumptions for further considerations are defined within the premise. The definitions are supplemented by the boundary conditions to form a basis for the scenario development. Table 1 shows a short description of the determined premise.

Table 1. Short overview of the scenario-specific premises.

Parameters	Premise
Time Horizon	25 years (5 years construction + 20 years' operating life span)
Target year	2040 (middle of operating life span)
Maximum generation	40 % of the market volume [8, 9]
Market boundary	European market model
Discount rate	Constant as 2 % annually for life span
Technical parameters	Given from previous studies and project work

The time horizon of the CCU system is estimated as 25 years, with five years of construction and 20 years life span – operating from 2030 to 2050. The target year is 2040, the middle of life span. The maximum generation is restricted under German competition law prohibiting market dominance [9]. The market share-based presumption provides a first indication of dominance where a company's market share exceeds 40 percent [8]. Therefore, the maximum chemical product quantity is 40 percent of its market volume. The overall market assumption in scenario development is based on the system boundaries of and the cross-border trade with European neighbours. The profitability assessment requires the revision of the future cash flows to be compared with the current capital value. The discount rate is assumed to be constant at 2 % annually during the whole amortization period. The technical parameters like possible plant connections, efficiencies, reaction conditions, exhaust gas amounts etc. are given from previous studies, project work and own calculations.

3.2 Key factor selection

First, the domains of influence are determined. For such environmental and energy scenario development, economic, political, ecological, technical, and social influence domains are suggested in practice [10]. However, the social and political influences are excluded from our scenario boundary. The CCU concept can be sensitively affected by adverse social acceptance, which may give policymakers a false sense of security, leading to even a rebound effect [11]. Nevertheless, they are not suitable for our scenario's target. First, the factors from these aspects are often measured in a qualitative approach. For example, political inclination may function importantly in evaluating the feasibility but is formulated qualitative rather than exact values (e.g., left and right orientation). Secondly, the issues depend on subjective assessment. For example, the social acceptance and benefit of CCU concepts can be understood totally different. Based on these reasons, the technical, economic, and ecological domains are determined as the investigation fields' demarcation.

In a first step, 106 internal and external influencing factors from the domains are determined. The importance of the influencing factors is identified through influence analysis. A detailed explanation of the method can be found in [3]. The influence analysis examines the relationships between the factors. All possible pairs of factors are measured on a four-level scale from 0 (no effect) to 3 (strong effect) regarding their mutual impact [10]. As a result, each influencing factor is represented with its active and passive sum. The factors with a high active sum are selected as key factors out of the 106 influencing factors since they have the biggest influence of the overall system [7]. This procedure leads to the final 24 key factors to set up further scenario development.

3.3 Reference scenario

The reference scenario assumes that there will be no new measurements by the target year [10]. The logic is also called "Business as usual" (BAU). The current values are based on well-founded knowledge. Extrapolations in the target years (2040 for operating time and 2025 for investing time) are suggested by a meta-study of different reports about energy and chemical market development scenarios. If a reliable development is unavailable, the assumptions made through trend analysis. It is carried out by collecting historical data as long as possible, and past trends are extended to the future [3].

The time series of the electricity price in 2040 are derived from a forecasting model [12]. This model assumes an energy-only market and calculates the operating plans of the power generation systems. The projected time series of the carbon footprint CF_t for future energy production and RE_t share for 2040 is determined based on the CF_t in 2020 derived with historical data from AGORA [13]. The future CF_t is calculated based on the hourly based data from 2020 and the varied fraction of RE share in the German grid mix according to Eq. (1):

$$CF_{t,2040} = CF_{t,2020} \cdot \frac{(100 - RE_{t,2040})}{(100 - RE_{t,2020})} \tag{1}$$

The exemplary results of the projected time series of the CF_t are shown in Figure 2. Figure 2(a) shows the dimensionless sorted annual CF_t of the year 2020 (RE = 48 %) and the projection to reference scenario of 2040 (RE = 85 %). Figure 2(b) shows an example of a two-week period of the CF_t. The average value for the reference scenario is projected to ca. 110 g_{CO2}/kWh_{el}. Electricity prices are calculated in a similar way.

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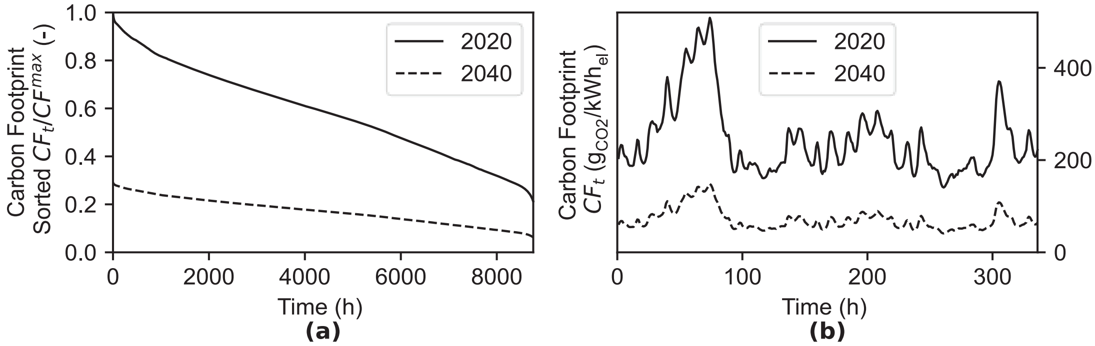

Figure. 2. Time series of carbon footprints (*CF*) for 2020 (48 % *RE*-Share) and BAU projection to 2040 (85 % *RE*-Share): a) Sorted annual dimensionless *CF*, b) exemplary two-week period of the *CF*.

It is necessary to specify fuel prices for natural gas and coal, as well as the CO_2 certificate prices to determine the marginal cost. The prices in the target year are taken from the EU [14] and Bloomberg [15]. H_2 price plays an important role in defining the potential of *RE* and green electricity. The price is derived from the IEA [16].

Market prices of the chemicals are the biggest part of the revenue. Oxygen as by-product from water electrolysis is also considered a part of revenue. The prices are assumed by the trend analysis based on the historical data from 2019 to 2021. Plus, the chemicals' market volumes dramatically affect the size of the plant and expenditure as the maximum generation is regulated by 40 % of the market share limit. They are taken from the IEA [17].

Table 2 shows the data of the most probable BAU scenario. Data from technology domain are shown as relative value (1 = no changes) and are derived from project internal communications and plant development reports. The H_2 generation is a crucial aspect of the system. Therefore, H_2 efficiency, the electricity required to generate the external carbon-free H_2, is considered as a separate factor from the overall energy requirement.

Table 2. Key factors and their values of the reference business-as-usual (BAU) scenario.

Class	Key factor	Current value	Source	BAU-value	Unit
Input	a. Electricity price	41.3	[18, 19]	47.4	€/MWh
	b. Natural gas price	31.4	[19]	46.7	€/MWh
	c. Coal price	7.5	[19]	11.8	€/MWh
	d. H2 price	3000	[16]	2400	€/t
	e. CO2 price	94.5	[4]	135.0	€/t
	f. CO2 certificate price	76.2	[20]	108.8	€/t
	g. CF & RE share (German grid)	373.4	[21, 22]	109.0	g_{CO2}/kWh_{el}
Output	h. O2 price	50	[4]	74.3	€/t
	i. Methanol price	342.0	[19]	401.6	€/t
	j. Urea price	256.3	[19]	428.2	€/t
	k. NH3 price	182.9	[23]	305.5	€/t
	l. Acetic acid (AA) price	605.9	[23]	711.5	€/t
	m. MeOH market vol.	2.2	[19]	3.9	Mt/a
	n. Urea market vol.	4.4	[19]	5.4	Mt/a
	o. NH3 market vol.	12.5	[19]	15.3	Mt/a
	p. Acetic acid (AA) market vol.	1.2	[19]	2.1	Mt/a
Technology	q. Conversion efficiency	1.0	[24]	1.0	-
	r. Energy efficiency	1.0	[24]	1.0	-
	s. H2 efficiency	1.0	[25, 26]	1.0	-
	t. Steel mill energy demand	1.0	-	1.0	-
	u. Part load range	1.0	-	1.0	-
	v. Dynamic operation	1.0	-	1.0	-
Expenditure	w. Investment cost (2025)	-	[27]	1.0	-
	x. Operating cost	1.0	[27]	1.0	-

The target year of the capital expenditures (CAPEX) is set as 2025 following a five-year construction period. CAPEX is calculated for each plant, including the gas conditioning, external H_2 production and chemical synthesis plants. Calculation is based on the capacity method [27]. The CAPEX of a plant C_b and its capacity

S_b is estimated based on the reference CAPEX C_a and its capacity S_a [27]. The reference data is taken from various techno-economic analysis studies and the C_a is extrapolated to the target year of investing 2025. It is extrapolated to 2025 value by applying the chemical engineering plant cost index (CEPCI), as *i*, to account for inflation rate. The publication years of the studies are between 2006 to 2021. Original CAPEX C_0, capacity S_a and CEPCI i_0 for all technical plants and years are used or derived from these studies. The CEPCI value for the year 2025 i_a is determined through trend analysis from the last five years. Therefore, the reference CAPEX C_a is calculated with Eq. (2):

$$C_\mathrm{a} = C_0 \cdot \frac{i_\mathrm{a}}{i_0} \tag{2}$$

The CAPEX development of the hydrogen production plants is assumed to be lower in the future. According to [28], it is assumed that the CAPEX for alkaline (ALK) and proton-exchange membrane (PEM) electrolysis are reduced by 14 % and 22.5 % in next five years, caused by reduced manufacturing costs and assumed technological breakthroughs. Based on the updated C_a to 2025, the C_b is calculated via the capacity method in Eq. (3). Where *f* is the degression coefficient for the economy of scale for chemical plants with a value from 0.6 to 1.0.

$$C_\mathrm{b} = C_\mathrm{a} \cdot \left(\frac{S_\mathrm{b}}{S_\mathrm{a}}\right)^f \tag{3}$$

However, the final S_b of the plant is not determined in the scenario development process. Therefore, the C_b of the individual component is represented as the function within possible installed capacity range of S_b^{min} and S_b^{max}. The C_b^{max} of S_b^{max} is where the exhausted gas utilization is maximized based on the market restriction. It should be noted that the S_b^{max} of each plant is differently estimated depending on the final products due to the varied size of the market volume. C_b^{min} is assumed to be 10 % of C_b^{max}. Lower than 10 % of C_b^{max} it's not worth to install these plants because a significant emission reduction is required for the CCU concept. Table 3 shows the range of S_b and C_b of a water gas shift (WGS) plant for each chemical as an example.

Table 3. Range of S_b (capacity) and C_b (CAPEX) of possible water gas shift plants for each chemical.

Final product	S_b^{min}, kg/s	S_b^{max}, kg/s	C_b^{min}, M€	C_b^{max}, M€	Market volume, Mt/a
Acetic acid	2.33	39	0.88	8.8	2.1
Urea	5.2	86	1.7	17	3.9
Methanol	7.2	120	2.2	22	5.4
Ammonia	22.7	376	5.7	57	15.3

The C_b should be represented in a full range of the plants S_b regardless of the production route. In the case of WGS plant, then, the CAPEX is resulted in the function within the overall range of S_b from 2.33 to 376 kg/s.

If *f* of the component is less than 1 like WGS plant (0.82), the C_b is a root-function. The MILP model requires linearity of C_b and therefore should be revised as a linear approximated function $C_{b,lin}$. The linearized functions maximum relative error tolerance from the original C_b is set as 10 %. If this doesn't match, an additional sampling point for piecewise linear approximation is considered till it reach the <10 % criteria. In the case of the WGS plant, two linear functions are generated with one piecewise sampling point and a maximum relative error of 7.4 %. Figure 3 presents the original C_b function on the left side and the derived piecewise linear functions $C_{b,lin1}$ and $C_{b,lin2}$ on the right for the WGS plant.

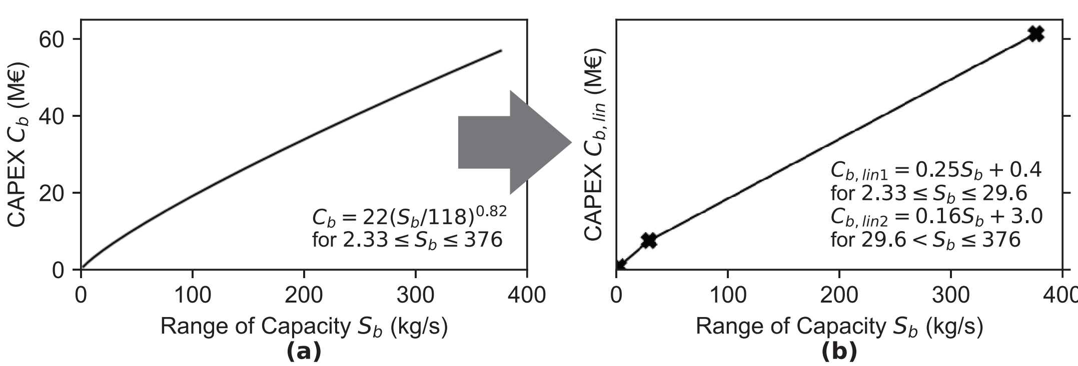

Figure. 3. CAPEX functions of WGS plant: a) Cost function through capacity method C_b, b) linearized cost functions $C_{b,lin}$.

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Other plants CAPEX is calculated in a similar way. The maximum relative error is detected in NH_3 synthesis plant as 9.4 %. The range of CAPEX for each plant, regardless of the production pathway, is generated.

The operating cost (OPEX) is the expenditures incurred in the plant. It considers the variable, fixed, and other costs of the system. The variable costs, including the raw and auxiliary materials, are calculated differently depending on the operating time and final production pathway. The fixed and other costs are structured based on [29]. The projected OPEX in BAU scenario is estimated to be constant by the target year.

3.4 Future projection

Each key factor is projected into the future in alternative states. Qualitative projections are created at first. This includes the possible projections of highly decreasing (↓↓), moderately decreasing (↓), constant (-), moderately increasing (↑) and highly increasing (↑↑). Not all projections make sense (e.g., decreasing projection of CO_2 certificate price) so the number of varied projections differs between three or five depending on the key factor. As mentioned, each projection involves quantified numerical values. If the data from the BAU scenario is available, the projection is based on it. The variation rate from the current value to fixed projection of the BAU scenario is applied to other alternative projections identically.

It should be noted that some key factors involve deliberately exaggerated or passive quantification. The factors that contain exaggerated quantification is the "driving factor". The extreme value of these driving factors brings a clear difference from other projections. On the other hand, the passive quantification is for the case that the value from the BAU scenario is over-predicted. The scenario which involves the projection may cause discord with other elements. Thus, they are quantified at a lower variation rate. Passive quantification makes the combination of the factors more consistent.

If the data from the reference scenario is unavailable, it is quantified based on the independently estimated assumption. For example, the H_2 efficiency has an improving rate of 5 % for projection (↑) and 10 % for (↑↑), according to [16]. The factors, conversion efficiency and energy efficiency, are assumed to be identical in improving rates of H_2 efficiency. It is not plausible to assume that they have greater improvement than external H_2 supplements because these plants are at a state-of-art level.

The investment cost is projected through the independently generated method. A scaling factor, "*s-factor*", is applied to the generated $C_{b,lin}$ function of each plant to switch the range of CAPEX by multiplying itself. The *s-factor* is derived from the water electrolysis' CAPEX as it is available to get reliable data on future development. Plus, it can be compared with the current CAPEX as the f is equal to 1 - It is not affected by the varied size of the capacity. Table 4 presents the assumed CAPEX of ALK and PEM in diverse future situations.

Table 4. Development of specific CAPEX of ALK and PEM water electrolysis in varied situations.

Unit	Current CAPEX	BAU CAPEX	Future situation	CAPEX in future	**Rate**	Unit	Current CAPEX	BAU CAPEX	Future situation	CAPEX in future	**Rate**
ALK	1.0	0.86	Pessimistic	1.0	**1.16**	PEM	1.0	0.775	Pessimistic	1.0	**1.29**
			Regular	0.79	**0.92**				Regular	0.66	**0.85**
			Optimistic	0.72	**0.84**				Optimistic	0.55	**0.71**

* Rate is the variation rate of future CAPEX from the BAU CAPEX, and it functions as the *s-factor*.
* The higher *s-factor* demonstrates the higher initial expenditures.

In the BAU scenario, the specific CAPEX for ALK and PEM is estimated to be decreased to 86 % or 77.5 % by the target year, respectively [28]. In a pessimistic future, the CAPEX is assumed to be constant as the current value. A regular projection assumes 50 % higher decreasing rate of the CAPEX than the BAU scenario. In the optimistic situation, the decreasing rate is doubled by the BAU scenario. The variation rates of future CAPEX from the BAU CAPEX are the *s-factor.* They are applied to all considered plants of the CCU concept depending on the scenario concept and the result of a cross-impact analysis. Through the process, the range of the component's CAPEX is newly assigned for each scenario. Another external H_2 supplement option, methane pyrolysis (MP), is applied an identical *s-factor* with the ALK.

3.5 Scenario formation

Based on the projections of key factors, the actual formation of scenarios takes place. The scenario technique of cross-impact analysis (CIA) is applied to ensure consistent combinations [10]. The CIA analyses the relationships between the key factors and the probabilities of occurrence of future events by considering their direct and indirect mutual effects [30].

A cross-impact matrix is first created, which assesses the conditional probability of specific projections if another future event has occurred according to the seven-level scale from -3 (Strong inhibitory influence) to 3 (Strong promoting influence) [30]. After that, the concept of each scenario is developed. The scenario concepts focus on the state of the specific domain to be improved or regressed or the worst or the best operating situations. Based on the concept of the scenarios, the corresponding factors are fixed in a particular projection to fulfil the determined idea. Four different scenarios, excluding the reference scenario, are created. A brief explanation of the different scenario concept and targets is shown below.

3.5.1 CO_2 reduction & RE share target (*RE-Boom*)

The *RE-Boom* depicts the best condition from the ecological perspective. Table 5 presents seven key factors which are forced to demonstrate the scenario.

Table 5. Forced projections for the ecological optimistic scenario *RE-Boom.*

Fixed factor	Projection	Fixed factor	Projection
e. CO_2 price	Highly decreasing (↓↓)	n. Urea market vol.	Highly increasing (↑↑)
f. CO_2 certificate price	Highly increasing (↑↑)	o. Ammonia market vol.	Highly increasing (↑↑)
g. *CF* & *RE* share	Highly decreasing (↓↓)	p. Acetic acid market vol.	Highly increasing (↑↑)
m. Methanol market vol.	Highly increasing (↑↑)		

The key factors, CO_2 certificate price, and *CF* & *RE* share, are forced environment friendly. The chemicals market volume is fixed to be highly increased to remove the market restriction for more possible CCU production. The CO_2 price is defined to be decreased to reduce the availability of direct CO_2 sales options.

3.5.2 Technical improvement & Market Booming (*Market-Boom*)

Scenario *Market-Boom* set the perfect condition from the economic and technical perspectives. Table 6 shows the eleven fixed key factors to fulfil the scenario concept.

Table 6. Forced projections for the economic optimistic scenario *Market-Boom.*

Fixed factor	Projection	Fixed factor	Projection
h. O_2 price	Highly increasing (↑↑)	r. Energy efficiency	Highly increasing (↑↑)
i. Methanol price	Highly increasing (↑↑)	s. Hydrogen efficiency	Moderately increasing (↑)
j. Urea price	Highly increasing (↑↑)	t. Steel mill energy demand	Highly decreasing (↓↓)
k. Ammonia price	Highly increasing (↑↑)	u. Part load range	Highly increasing (↑↑)
l. Acetic acid price	Highly increasing (↑↑)	v. Dynamic operation	Highly increasing (↑↑)
q. Conversion eff.	Highly increasing (↑↑)		

The key factors related to the revenue are all fixed to be highly increased to maximize the profits. The factors in the technology class are defined to be highly advanced. However, the H_2 efficiency is estimated to be moderately increased to make a clear difference with the *H_2-boom* scenario in section 3.5.4.

3.5.3 Energy & Market crisis (*Crisis*)

Crisis scenario projects the worst situation from the economic perspective. The concept refers to the current Ukraine war and an economic crisis. Table 7 presents eight forced factors for the scenario concept.

Table 7. Forced projections for the negative extreme scenario *Crisis*.

Fixed factor	Projection	Fixed factor	Projection
a. Electricity Price	Highly increasing (↑↑)	i. Methanol price	Highly decreasing (↓↓)
b. Natural Gas price	Highly increasing (↑↑)	j. Urea price	Highly decreasing (↓↓)
c. Coal Price	Highly increasing (↑↑)	k. Ammonia price	Highly decreasing (↓↓)
h. O_2 price	Highly decreasing (↓↓)	l. Acetic acid price	Highly decreasing (↓↓)

The factors related to the profitability are all negatively assumed. Prices of raw materials goes up immensely, and revenue of the products is reduced substantially. Regarding the product's market condition, it is evaluated from the perspective of the supplier. In other words, it is assumed that the chemicals market is in depression, so the supplier must sell the product at a lower price.

3.5.4 Hydrogen booming (*H_2-Boom*)

The *H_2-Boom* focuses only on the best condition of H_2 generation from the technical aspects. Table 8 shows six essential key factors to satisfy the scenario concept.

Table 8. Forced projections for Hydrogen optimistic scenario *H2-Boom*.

Fixed factor	Projection	Fixed factor	Projection
d. H_2 Price	Highly decreasing (↓↓)	s. Hydrogen efficiency	Highly increasing (↑↑)
q. Conversion efficiency	Constant (-)	u. Part load range (only H_2)	Moderately increasing (↑)
r. Energy efficiency	Constant (-)	v. Dynamic operation (only H_2)	Moderately increasing (↑)

H_2 price is assumed to be reduced following a drop in generation cost due to highly increasing manufacturing cost and technology breakthroughs. It aims on the hydrogen subdomain from the overall technical domain.

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3.6 Scenario generation and selection

Based on the formulated cross-impact matrix and the scenario concepts, the CIA is conducted to determine the most consistent combination. It tests all theoretically possible combinations to analyse their contradictions with the framework conditions. However, the generated matrix involves more than a billion possible combinations. The CIA, thus, can only be checked with algorithm-based software support. For this reason, the *ScenarioWizard*® software is used. Plus, the economic factors related to the chemicals (price and market volume) are combined into a single factor to manage the complexity. It is judged by the fact that the scenario concepts mostly do not involve the comparison of the superiority between the chemicals. A merge does not affect the quantitative values for each factor but merely has an identical qualitative projection. As a result, the bundle containing the possible candidates to be a final scenario is generated for each scenario. In our case, eight options for *RE-boom*, five for *Market-Boom*, two for *Crisis*, and fifteen for *H_2-Boom* are generated.

To select the final most consistent combination out of the candidate's pool, the Consistency Value (CV) and Total Impact Score (TIS) function as the evaluation criteria [30]. TIS means the sum of the impact scores of all selected scenario variants. The CV is the parameter to evaluate if the chosen combination of the factors is consistent. In the case of a positive or zero CV, the combination is accepted as consistent [30]. Based on the scenario selection criteria, the final scenarios are determined. All scenarios have the CV equal to 0 and the highest TIS out of the possible candidates, so they involve the most consistent combination.

4. Results

4.1 Final scenarios

Table 9. Final five scenarios with qualitative (QLT) and quantified values (QNT) for the 24 key factors (a - x).

Key factors with units	BAU		RE-Boom		Market-Boom		Crisis		H2-Boom	
	QLT	QTY	QLT	QTY	QLT	QTY	QLT	QTY	QLT	QTY
a. Electricity price (€/MWh)	(↑)	47.38	(↓↓)	20.66	(-)	41.32	(↑↑)*	72.31	(-)	41.32
b. NG price (€/MWh)	(↑)	46.72	(↓↓)	15.68	(-)	31.35	(↑↑)*	69.63	(-)	31.35
c. Coal price (€/MWh)	(↑)	11.82	(↓)	5.62	(-)	7.49	(↑↑)*	18.67	(-)	7.49
d. H2 price (€/t)	(↓)	2400	(↓)	2400	(-)	3000	(↑↑)	3900	(↓↓)*	1500
e. CO2 price (€/t)	(↑↑)	135.0	(↓↓)*	61.2	(-)	94.5	(↓)	76.1	(↑)	112.9
f. CO2 certificate price (€/t)	(↑)	108.8	(↑↑)*	190.5	(↑)	108.8	(↑↑)	190.5	(↑)	108.8
g. CF & RE share (g_{CO2}/kWh_{el})	(↓)	109	(↓↓)*	0	(↓)	109	(↓↓)	0	(↓)	109
h. O2 price (€/t)	(↑)	74.3	(↓)	25.7	(↑↑)*	110.4	(↓↓)*	13.2	(-)	50.0
i. MeOH price (€/t)	(↑)	401.6	(↓)	282.4	(↑↑)*	471.7	(↓↓)*	233.1	(-)	342.0
j. Urea price (€/t)	(↑)	428.2	(↓)	192.2	(↑↑)*	715.4	(↓↓)*	128.2	(-)	256.3
k. NH3 price (€/t)	(↑)	305.5	(↓)	137.1	(↑↑)*	510.4	(↓↓)*	91.4	(-)	182.9
l. Acetic Acid price (€/t)	(↑)	711.5	(↓)	500.2	(↑↑)*	835.5	(↓↓)*	413.0	(-)	605.9
m. MeOH market vol. (Mt/a)	(↑)	3.85	(↑↑)*	13.36	(-)	2.2	(↓↓)	1.1	(-)	2.2
n. Urea market vol. (Mt/a)	(↑)	5.39	(↑↑)*	25.97	(-)	4.4	(↓↓)	2.64	(-)	4.4
o. NH3 market vol. (Mt/a)	(↑)	15.31	(↑↑)*	18.75	(-)	12.5	(↓↓)	7.51	(-)	12.5
p. Acetic Acid market vol. (Mt/a)	(↑)	2.1	(↑↑)*	3.42	(-)	1.2	(↓↓)	0.6	(-)	1.2
q. Conversion efficiency (-)	(-)	1.0	(↑)	0.95	(↑↑)*	0.9	(-)	1.0	(-)*	1.0
r. Energy efficiency (-)	(-)	1.0	(↑)	0.95	(↑↑)*	0.9	(-)	1.0	(-)*	1.0
s. H2 efficiency (-)	(-)	1.0	(↑)	0.95	(↑)*	0.95	(-)	1.0	(↑↑)*	0.9
t. Steel mill energy demand (-)	(-)	1.0	(↓)	0.9	(↓↓)*	0.8	(-)	1.0	(-)	1.0
u. Part load range (-)	(-)	1.0	(↑)	1.5	(↑↑)*	2.0	(-)	1.0	(↑)*	2.0 (H2)
v. Dynamic operation (-)	(-)	1.0	(↑)	1.5	(↑↑)*	2.0	(-)	1.0	(↑)*	2.0 (H2)
w. Investment costs s-factors (-)	(-)	1.0	(↓)	var[1]	(↓)	var[1]	(↑)	var[1]	(↓)	var[1]
x. Operating cost (-)	(-)	1.0	(↓)	0.75	(↓)	0.5	(↑)	1.5	(↓)	0.75

[1] Scaling factors (s-factors) for investment cost calculations are plant-dependent and shown in Table 10.
* The factors with subscript * denote the predetermined fixed projection.

Additional to Table 9, with all numerical values, the scenarios additional includes the time series for electricity price and *CF* (Figure 2) plus all linearized and scaled CAPEX functions C_s. The explanation for CAPEX, which is determined after CIA, is given below. Table 10 shows different s-factors for all hydrogen production plants.

Table 10. Scaling factor *(s-factor)* to estimate future CAPEX of hydrogen production plants for the scenarios.

Scenario	ALK	PEM	MP	Other components
BAU	1.0	1.0	1.0	1.0
RE-Boom	0.92	0.85	0.92	0.92
Market-Boom	0.92	0.85	0.92	0.85
Crisis	1.16	1.29	1.16	1.23
H2-Boom	0.84	0.71	0.84	1.0

The qualitative projection of CAPEX for the *RE-boom* and *Market-boom* are calculated to be decreased ($s < 1$) through the CIA. The CAPEX of the H_2 supplement is determined to be regularly improved for both scenarios following the projection of H_2 efficiency, moderately increasing. Regarding other components, the *s-factor* is estimated to be identical to the ALK for *RE-boom* and the PEM for *Market-boom*. It is more plausible that *Market-Boom* has a bigger reduction rate than *RE-Boom* as the technical factors of other components is assumed to be improved at a higher rate in *Market-boom*.

Qualitative projection of CAPEX for the *Crisis* scenario is calculated to be increased through the CIA. The CAPEX of the H_2 supplement is decided to be the worst development (s > 1). The *s-factor* of other components is assumed as the average value of ALK and PEM.

The CAPEX of the H_2 supplement is determined to be the optimistic future under the projection of H_2 efficiency. The *s-factor* is not applied to other components as the concept of the *H_2-boom* focuses only on the H_2 improvement, so it clarifies the difference with the *RE-boom* and *Market-boom*. It may look illogical that the qualitative projection of CAPEX is calculated to be decreased through the CIA. However, the result of the CIA can be varied depending on the weight of the influence. It is plausible that the CAPEX reduction is mainly because of the H_2 efficiency factor, as it has a more significant impact on the CAPEX.

The s-*factor* is multiplied to $C_{b,lin}$ function for individual plants of each scenario to reach the final scaled CAPEX functions C_s. Figure 4 presents the derived C_s function of the WGS plant for each scenario as an example.

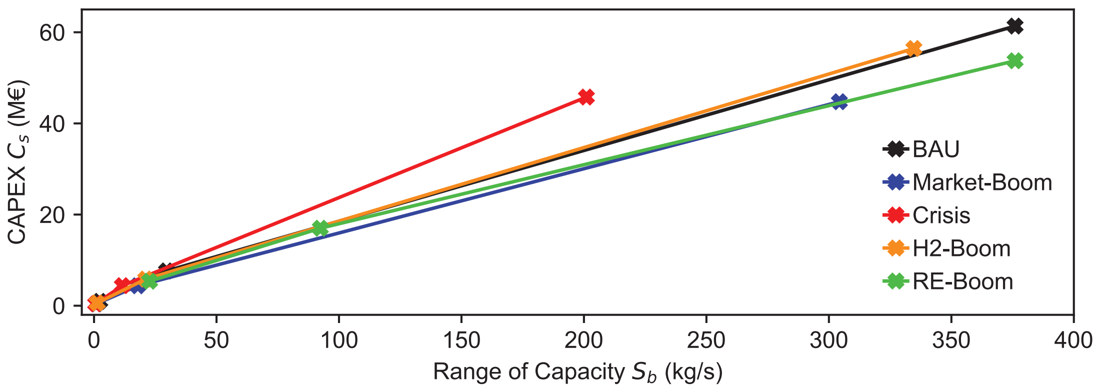

Figure. 4. The five developed linear CAPEX functions Cs of the water gas shift plant for each scenario.

4.2 Scenario evaluation

All combinations from CIA (Table 9) are evaluated based on the three criteria: plausibility, consistency, and differentiation. The BAU scenario is not part of the scenario evaluation due it is generated by the independent method (3.3 Reference scenario). Plus, consistency is already measured in the scenario selection process (3.6 Scenario generation and selection).

4.2.1 Plausibility

Plausibility check of the scenarios is assessed if the combination of the scenario is well matched with the aimed concept and the relationship between the fixed factors and the remaining factors are plausibly formulated.

Scenario *RE-boom* depicts the condition that minimizes the CO_2 emission and simultaneously maximizes the quantity of used exhausted gas. The concept is well satisfied with fixed factors from Table 5. The combination of remaining factors is also well structured. Significantly, the prices of energy raw materials (factors a. to c.) are decreased by the CIA. As the *CF* is assumed to be 0, it is plausible that the prices are decreased accordingly. However, the coal price is less affected as it relates more to steel production.

Main idea of *Market-boom* is the maximization of profitability and technical performance. The concept is well fulfilled by optimizing the product price and technical development in Table 6. Among the remaining factors, the chemicals market volume is resulted to be constant by the CIA even if the prices are incremented. It may

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look illogical in general price and market relationship. However, the generated combination results from all factors' mutual interaction, not a pair of two factors. It is plausible to assume that the chemicals market volume is resulted to be constant because of other factors' indirect influences.

The *Crisis* represents the worst situation with the forced factors from Table 7. A discord between the combination of the key factors and the scenario concept is identified. The ecological factors (f. and g.) resulted in highly increased and decreased, respectively, through the CIA calculation as the prices of energy raw materials are forced to be highly increased. It is plausible from the perspective of three considered domains, like the case of *RE-Boom.* However, it does not align with the scenario concept, which refers to the ongoing Ukraine conflict. The current abnormal situation decouples the general relationship of the energy complex. According to the [31], the price of CO_2 permits reached a high of 97 €/kWh_{el} in 2020. After the start of the conflict in 2022, the price dropped to almost 60 €/kWh_{el}. It is reported as the biggest crash since 2014. To elaborate this unique situation, social or political aspects (e.g., acceptance or political trends) should be included. It may function as a "joker", making the retrogress trend plausible.

H_2-boom scenario focuses on the improvement of the overall H_2 generation, a subdomain in the technical and economic field. The concept is fulfilled with the fixed factors from Table 8. Regarding the energy raw materials from the remaining factors may look more plausible to be reduced rather than constant. Assuming that the H_2 price is reduced and the H_2 efficiency is notably advanced, a significant price drop is expected. It is particularly true if a high proportion of green electricity is used, leading to low market prices and *CF*. However, the scenario from this study assumes that the perfect transition to an emission-free system is impossible by the target year. According to the [32], the existing infrastructure has limited application regarding H_2 as an energy source. Germany's current gas supply network can tolerate only 10 % of H_2 by volume in total [32]. However, it is also evident that H_2 gradually contributes to the energy system, simultaneously. It becomes obvious by comparing it with the BAU scenario. As the H_2 price in the BAU scenario decreases at a lower rate than *H_2-boom*, the energy raw materials prices are assumed to be moderately increased. So, even if H_2 as the energy source cannot change the energy system in a flash, it positively influences the gradual transition. Consequently, it is more plausible that the prices of energy raw materials will be constant for *H_2-Boom*.

4.2.2 Differentiation

The differentiation between the scenarios is assessed if the generated scenarios depict the meaningfully varied condition to prevent further calculation results in an identical outcome. *Market-Boom* and *Crisis* scenarios can be understood as the antipodes in the scenario funnel from the economic point of view. The combinations of all the factors in both scenarios are formulated oppositely. They offer different situations in terms of economic conditions. Both, *Market-Boom* and *H_2-Boom,* involve technical improvement by the target year. Because of the similar relationship between the factors, most other elements from the different domains resulted in similar projections. It may be considered a false combination because both slices depict a similar situation. However, the technical concept of these scenarios is distanced - *Market-Boom* for overall improvement, but *H_2-Boom* for mainly H_2 subdomain. Thus, comparing the results from the scenarios bring clearly different results to evaluate the CCU concept. Finally, the *RE-Boom* concentrates on the sole independent domain, the ecological criteria. The combination of *RE-Boom* is conspicuously different. In other words, the generated slice is sketched at a totally distanced area from other scenarios, so it can offer new criteria to evaluate the feasibility of the CCU concept. Figure 5 presents the simplified development process and a qualitative classification to elaborate the differentiation of the scenarios.

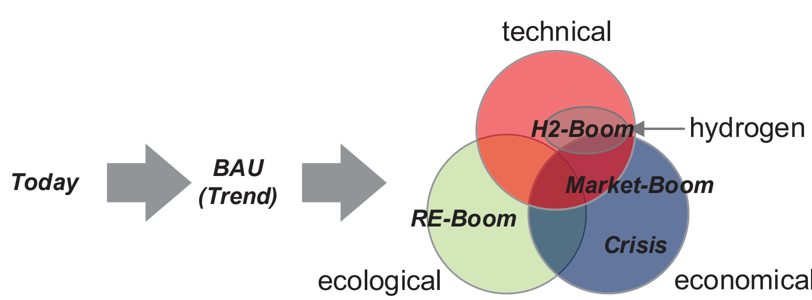

Figure. 5. Simplified development and differentiation of the scenario concepts as a Venn diagram.

5. Conclusion and Outlook

This research aimed to build up consistent, plausible, and meaningfully different scenarios as input data for MILP models to evaluate the long-term feasibility of the desired exhausted gas utilization concept. The generated five scenarios involve internal and external key factors from three main criteria. To build up the BAU scenario, they are extrapolated to the target years for investing (2025) and operating (2040). Especially, the formulation of the investment cost offers a rough sketch of the initial expenditures. A linear approximation method for CAPEX functions is applied to be suited for the later use in MILP models. It fulfils the criteria for a maximum error tolerance of 10 % from the original nonlinear function.

All 24 key factors are qualitatively and quantitatively projected into the target years to construct the hypothetical future development. The process is carried out in an objective methodology, utilizing the BAU scenario data rather than forecasting the random value. It also involves exaggerated or passive projection so that further evaluation of the CCU approach becomes more evident. If the data from the BAU scenario is unavailable, then the quantification is determined based on independently estimated assumptions. The investment costs are quantitatively projected by applying a scaling factor (*s-factor*). The *s-factor* is derived from the water electrolysis CAPEX and ranges from 0.71 to 1.29. It is applied to other plants to switch the amplitude of CAPEX functions and offering varied economic situations. An s-*factor* greater 1 is represents economically unfavourable scenarios due to higher initial expenditures. This compositional work provides new insight into the probable future development of the "Hot-potato" factors - such as the electricity price, RE share, or the chemicals market.

The concept of each scenario is determined in advance of the scenario formulation. In other words, the scenarios are developed based on the deliberately specified condition. Four scenario concepts are generated: 1. CO_2 reduction & RE share target (*RE-Boom*), 2. Technical improvement & Market booming (*Market-Boom*), 3. Energy & Market crisis (*Crisis*), and 4. Hydrogen booming (*H_2-Boom*). The *RE-Boom* depicts the best condition from the ecological perspective. The *Market-Boom* set the perfect condition from the economic and technical perspective. The *Crisis* projects the worst situation from the economic domain. Finally, the *H_2-Boom* focuses only on the best condition of H_2 generation from the technical and economic aspects.

Based on the predetermined concept, the CIA is carried out to find the most consistent combination of the key factors within the fixed condition. The calculated combinations are considered highly reliable consequences. First, regarding consistency, all scenarios have the desired CV and the highest TIS out of the possible candidates. Secondly, the determinations of the remaining factors' projections through the CIA calculation are also plausible to describe the scenario concept within the investigation domains. Finally, the results also offer meaningfully different operating conditions. These results build on existing evidence of the reliably structured scenarios. The generated scenarios can now be directly utilized in a MILP model for the CCU approach.

In conclusion, the generated five scenarios represent a comprehensible description of the possible situation of the CCU concept in the target years based on a complex network of factors from different impact parameters. All scenarios have consistent, plausible, and meaningfully different combinations of the key factors. Consequently, the optimal solutions for utilizing the exhausted gas are calculated by the MILP optimization model in varied ways depending on the scenarios. It promotes the transparency and traceability of the further decision-making process of the CCU concept.

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Nomenclature

C Capital expenditures of the plants, M€

CF Carbon footprint, g/kWh

f Degression coefficient, -

RE Renewable energy share, %

S Capacity of the plant, kg/s

s Scaling factor, -

Subscripts and Superscripts

0 Index for reference year of data source

a,b Index for reference year (2025) before (a) and after (b) scaling with degression coefficient

lin Linearized function

min/max Minimum and Maximum value

s,t Index for scenario number and time series

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