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Scenario Development for Evaluating Carbon Capture and Utilization Concepts Using Steel Mill Exhaust Gases with Linear Optimization Models †

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Abstract: Utilizing exhaust gases from the steel mill generation to produce chemicals presents a promising avenue for carbon capture and utilization (CCU) concepts. Employing a model-based mathematical approach, specifically mixed-integer linear programming (MILP), enables the identification of optimal production concepts. To evaluate the long-term feasibility under uncertain future conditions, the construction of hypothetical scenarios to depict possible future states is necessary. This study introduces novel and tailored scenarios for a specific CCU concept aimed at producing methanol, ammonia, urea and/or acetic acid from steel mill exhaust gases by the year 2040 to enhance decision-making processes for identifying the optimal concept. These scenarios provide comprehensive insights into potential future conditions, spanning technical, economic and ecological domains. Unlike prior studies that focus on individual key factors, this approach involves analyzing the interactions of 24 identified key factors within the investigated CCU concept. The method yields five distinct scenarios: (1) Business as Usual (*BAU*), (2) CO_2 Reduction and Renewable Energy Target (*RE-Boom*), (3) Technical Improvement and Market Booming (*Market-Boom*), (4) Energy and Market Crisis (*Crisis*) and (5) Hydrogen Booming (*H2-Boom*). These five scenarios can be directly integrated into MILP models, enhancing the significance of the optimization results for identifying the optimal CCU concept.

Keywords: carbon capture and utilization; steel mill exhaust gases; renewable energy; scenario development

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1. Introduction

The impact of human-induced climate change is evident in the 1.1 °C increase in global surface temperatures, with industrial emissions of carbon dioxide (CO_2) being a significant contributor [1]. To reverse this trend, it is necessary to take actions aimed at reducing CO_2 emissions in the future.

The steel industry is one of the main contributors to CO_2 emissions, accounting for approximately 27% of global industrial CO_2 emissions [2] and 5–7% of the total CO_2 emissions worldwide [3,4]. Its substantial environmental impact underscores the pressing need for effective mitigation strategies within this sector. Previous research has highlighted numerous strategies for mitigating or eliminating CO_2 emissions in existing industrial [5,6] and specific steelmaking processes [4,7–9].

One promising pathway in the steel industry involves the replacement of fossil coal, traditionally used as the reducing agent in iron ore reduction, with renewable energy sources such as hydrogen and/or electricity [7]. This strategy, known as carbon direct avoidance (CDA), seeks to diminish the initial reliance on carbon as an energy carrier [10,11]. However, it is noteworthy that a drawback of CDA lies in its inapplicability for retrofitting existing plant sites adhering to the conventional blast furnace steelmaking route, coupled with the substantial quantities of renewable energy required for implementation. Another promising pathway extends downstream from the production plant and involves the implementation of the carbon capture and storage (CCS) strategy [12]. This strategy focuses on capturing carbon emissions post-production, followed by their secure storage [13]. The captured CO_2 is transported through dedicated pipelines or ships [13], subsequently sequestered within geologically deep formations, including but not limited to, deep geological formations, saline aquifers and previously depleted oil and gas reservoirs [12–15]. CCS faces challenges related to effective carbon storage in underground geological formations, primarily due to the need for substantial local infrastructure and secure underground storage facilities, which are essential to accommodate the significant quantities of CO_2 involved in the industry [14,15]. In this paper, we investigated another promising pathway for reusing carbon and other components (like nitrogen) from exhaust gases. In the literature, the strategy for utilizing carbon is referred to as carbon capture and utilization (CCU) [12,14,16] or as integrated carbon capture and conversion (ICCC) [17,18]. Both strategies center around the utilization of CO_2 as a feedstock. Typical applications of these strategies include the production of chemicals, syngas or fuels, as well as mineral carbonation, enhanced oil recovery and direct utilization, such as in the food industry [16,17]. CCU focuses on the reuse of CO_2 in specific applications, whereas ICCC adopts a more comprehensive approach that integrates CO_2 utilization across various sectors, aiming to derive economic benefits from the conversion. However, in this paper, we specifically explore the CCU concept for chemical production using steel mill exhaust gases, including the production of gasoline, polymers and fertilizers [19].

The exhaust gases originating from blast furnaces, coke ovens and basic oxygen furnaces contain significant quantities of carbon monoxide, carbon dioxide, methane, hydrogen and nitrogen. These gases serve as primary raw materials for chemical production. Hydrogen (H_2) is recognized as the limiting reactant in this process, requiring the introduction of external supplements, such as renewable energy (RE), to increase its quantity [9]. Considering these factors, it is imperative to establish a symbiotic relationship between the steel industry and the energy sector, recognizing that such collaboration is essential for assessing the hydrogen supply limitations identified in this process.

Numerous recent studies have primarily emphasized the techno-economical aspects of CCU approaches within the steel industry [4,20,21]. Commonly employed technologies for the extraction of CO_2 from these exhaust gases and their subsequent utilization in the CCU approach include chemical or physical absorption and membrane processes [22–25]. Typical chemical products that can be synthesized from steel mill exhaust gases are methanol [21,26–28], higher alcohols [29,30] or urea [31–33].

To evaluate the long-term feasibility and determine the optimal configuration of the CCU concept, the application of mixed-integer linear programming (MILP) is a commonly employed scientific methodology, as demonstrated by prior research [8,21,34]. For this reason, a model-based mathematical approach with MILP is recommended to evaluate the long-term feasibility of the system [35]. The objective of the MILP model is to find the optimal production pathway, which includes selection of technologies, design and time-dependent operation conditions. However, it is important to note that these models face challenges in acquiring comprehensive information necessary for robust decision-making processes concerning the plant network (Section 2). MILP models are particularly suited for addressing uncertainties in future conditions, requiring the construction of hypothetical scenarios to depict potential future states. In these scenarios, a spectrum of future developments related to key factors in the political, economic, social, technological, ecological and legal (short: PESTEL) domains can be taken into account [36,37]. To find and select the key factors for this system and develop these specific scenarios in a transparent and consistent way, there are several scenario approaches discussed in the literature [38–41].

Kosow et al. [38] identify three primary approaches in this field: trend extrapolation, which overlooks interactions between key factors; systematic formalized approaches, which consider interactions between key factors; and creative narrative approaches, which emphasize intuitive projections of key factors. Scenarios in the literature can vary in their definitions and development methods, making it essential to establish a clear definition at the outset.

In this study, a scenario is defined as a specific part of the future by considering relevant key factors rather than a comprehensive picture. Integrating individual factors shapes the domain of shared development for all these aspects. The expanding slice of future developments of these key factors is described with the scenario funnel in Figure 1.

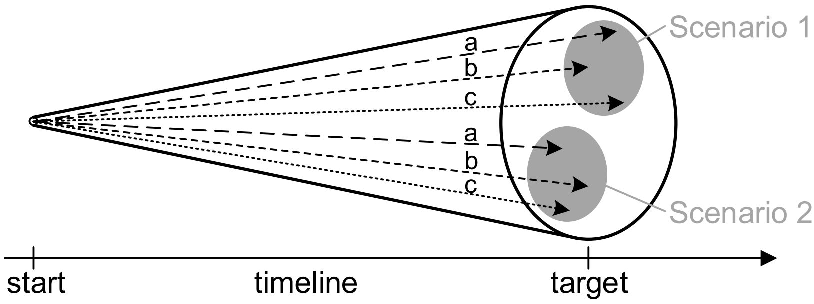

Figure 1. Scenario funnel for representing the developments of three exemplary key factors (a, b and c) in two scenarios from a start time to a target time (adopted and modified from [42]).

Different scenarios in Figure 1 portray diverse future possibilities right from the beginning. To achieve this, potential projections of various key factors (a, b and c) are chosen and bundled into scenarios. It is important to clarify that the term 'projection' should not be conflated with a 'forecast', which asserts the actual probability of occurrence. Instead, it represents a hypothetical construct, implicitly alluding to the potential for alternative futures [38].

Some approaches involved the constructions of scenarios to evaluate CCU concepts of steel mill exhaust gases. Stießel et al. [43] have crafted a singular scenario, designated for the year 2030, with the principal objective of identifying cross-industrial process concepts for a CCU approach. The authors have predominantly concentrated on external influences to shape this scenario, placing an emphasis on formulating a CCU concept that thrives in specific eco-friendly operational conditions. Within this context, Schlüter et al. [31] have undertaken an investigation into the process concept of utilizing exhaust gases from steel mills for chemical production. This study explores three distinct operating conditions, with a primary focus on internal technical perspectives. The results are subjected to analysis within the framework of time-dependent boundary conditions, thus enabling the identification of the factors that limit carbon binding. Furthermore, Sadlowski et al. [44] delve into the ecological potential of flexible methanol production utilizing steel mill exhaust gases through the application of an MILP model. In their research, they have outlined scenarios underpinned by three pivotal factors: external hydrogen production capacity, power supply sources and storage capacities. Subsequently, the outcomes are scrutinized with a specific focus on the carbon binding potential inherent in this CCU concept. The authors have collectively emphasized the pivotal role that diverse future developments of key factors, such as hydrogen or power prices, have in the evaluation of CCU concepts. This underscores the compelling need for a thorough investigation aimed at establishing consistent scenarios.

Therefore, this study examined scenarios for a particular CCU concept targeting the production of methanol, acetic acid, ammonia and urea from steel mill exhaust gases. This CCU concept and its interaction with future scenarios has not been analyzed in previous research. Our primary goal is to develop different, transparent and consistent scenarios which are suitable as input data for the evaluation using an MILP model. What sets this approach apart from recent publications is its departure from singular perspectives or single scenarios in the assessment of CCU concepts. Instead, a novel approach is introduced, characterized by a comprehensive evaluation spanning various domains of key factors. This innovative scenario development approach distinguishes this work from previous studies, offering a wider and more intricate array of future scenarios. In essence, the scenarios generated here serve as valuable tools for evaluating the long-term feasibility of the CCU concept using an MILP model, making a distinct and noteworthy contribution to the field.

The structure of this work is as follows. Section 2 outlines the key attributes to enable the optimization with an MILP model. In Section 3, we present the comprehensive methodology employed throughout the scenario development process. Section 4 presents the findings and outcomes of our scenario development efforts. The study concludes in Section 5, followed by Section 6, which offers a forward-looking perspective.

2. Scope and Characteristics of Scenarios in an MILP Model

The implications of the CCU concept are currently in a less developed phase, with ongoing determination of the technical plant layout, profitability and potential environmental impacts. As a foundational assumption, it is posited that all interconnections for the various technologies and exhaust gas conditions, such as reactors, storages, compressors, separators, etc., have been integrated into the MILP model, as demonstrated in prior research. The selection of the final products is also established at the decision point [35]. A comprehensive model description for methanol production can be located in Sadlowski et al. [44]. The model's output includes the optimal pathway, encompassing the selection of technology, chemical products, plant capacities and operational strategies. This outcome is contingent upon the provided future states, represented in the form of scenarios.

The scenarios generated in this study enable MILP and serve as input data for a linear optimization model, featuring distinct properties that set them apart from conventional scenario development.

First, the study formulates scenarios based on evaluations across key factors in multiple domains (PESTEL). Considering diverse internal and external influences brings reliable results about the optimal future CCU concept. Secondly, a fixed reference year for the scenarios is established, including the entire operational life span of the CCU concept. However, owing to the intricacy of the MILP model, a reduction in one reference year for evaluating becomes necessary. Thirdly, all considered key factors must exhibit clear quantifiability, either through fixed numerical values or linear mathematical relationships, to ensure the quality of the deterministic optimization results. The exclusion of the challenging-to-quantify political, regulatory and social domains from the PESTEL approach aligns with the premise that unforeseen disturbances during the plant's life span are to be minimized. It is important to note, however, that complete elimination of overlaps between individual key factors and other domains may not be entirely feasible. For instance, certain factors, such as a CO_2 emissions limit, may have direct ecological implications on the concept despite their political/regulatory origin. Lastly, a software-based method examines the individual relationships between these factors. A Cross-Impact Analysis (CIA) is employed to identify the most consistent and plausible combinations of factors for alternative scenarios.

In essence, these unique scenario properties facilitate their utilization within the linear optimization model, ultimately enhancing the reliability and applicability of our approach.

3. Scenario Development Framework and Process

An existing framework for scenario development has been customized to incorporate functionalities specific to the scenarios. This adaptation draws inspiration from a five-phase model introduced by an approach from Gausemeier et al. [39] and an eight-phase model from von Reibnitz [40]. From these influences, a modified generic six-phase model for iterative scenario development is derived, tailored to the specific application of the CCU concept for steel mill exhaust gases. Figure 2 provides an overview of the individual six phases of the modeling framework.

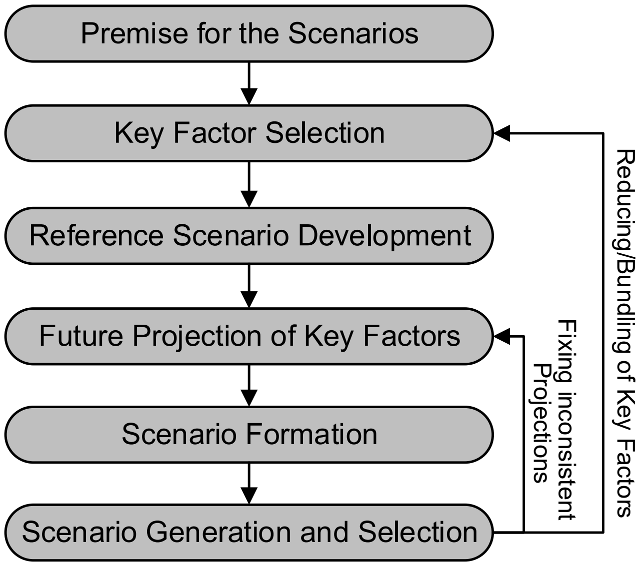

Figure 2. Iterative six-phase scenario modeling framework (author created).

This adapted modeling framework, incorporating both exploratory and quantitative approaches, has been devised to generate the five scenarios within the technological, economic and ecological domains. In the subsequent sections, we will apply the six phases illustrated in Figure 2 to the specific CCU concept.

3.1. Premise for the Scenarios

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 [45,46]
Market boundary	Perfect European market model
Discount rate	2% annually for the whole 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 a 20-year life span—operating from 2030 to 2050. The target year is 2040, the middle of its life span. The maximum generation is restricted under German competition law prohibiting market dominance [46]. The market share-based presumption provides a first indication of dominance where a company's market share exceeds 40 percent [45]. 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 neighbors. 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 life span. 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, the PESTEL domains are suggested in practice [36,37,39]. 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, even leading to a rebound effect [47]. 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 qualitatively rather than as 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 in totally different way. 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 [38]. 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 [38,39]. The factors with a high active sum are selected as key factors out of the 106 influencing factors since they have the biggest influence out of the overall system [40]. This procedure leads to the final 24 key factors to set up further scenario development.

3.3. Reference Scenario Development

The reference scenario, often referred to as the "trend scenario", operates on the assumption that no new measurements will be made by the target year [38,39]. The chosen scenario technique for this purpose is trend extrapolation [38]. This scenario is referred to as "Business as usual" (*BAU*). The current values are derived from well-established and reliable 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 reliable development is unavailable, the assumptions are made through trend analysis. It is carried out by collecting historical data for as long as possible, and past trends are extended to the future [38].

The time series of the electricity price in 2040 are derived from a forecasting model [48]. 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 from historical data from AGORA [49]. The future CF_t is calculated based on the hourly data from 2020 and the varied fraction of RE share in the German grid mix according to Equation (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 3. Figure 3a shows the dimensionless sorted annual CF_t of the year 2020 (RE = 48%) and the projection to reference scenario of 2040 (RE = 85%). Figure 3b 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_{CO_2}/kWh_{el}. Electricity prices are calculated in a similar way.

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 European Commission [50] and Bloomberg [51]. H_2 price plays an important role in defining the potential of RE and green electricity. The price is derived from the International Energy Agency (IEA) [52].

The market prices of the chemicals are the biggest part of the revenue. Oxygen as a 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 [53].

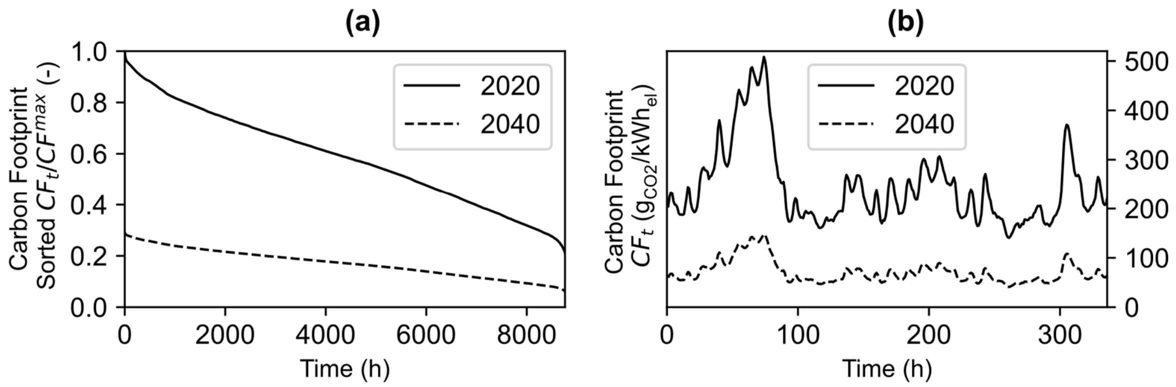

Figure 3. Time series of carbon footprints (CF) for 2020 (48% RE-Share) and *BAU* projection to 2040 (85% RE-Share): (**a**) sorted annual dimensionless CF, (**b**) exemplary two-week period of the CF (adopted and modified from [42]).

The CO_2 emission allowance characterizes the emissions from the steel mill's exhaust gases. At 100%, it represents the endorsement of the existing state, wherein exhaust gas combustion and CO_2 emissions in the atmosphere are accepted without alteration (no Cap). A Cap, such as of 90%, mandates a 10% emissions reduction. In the *BAU* scenario, no adjustments are presumed. However, a reduction in the allowance signals a compulsory decrease in CO_2 emissions, thereby enhancing the CCU potential of the concept.

Table 2 shows the data of the most probable *BAU* scenario. Data from the 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	[54,55]	47.4	EUR /MWh$_{el}$
	b. Natural gas price	31.4	[55]	46.7	EUR /MWh$_{th}$
	c. Coal price	7.5	[55]	11.8	EUR /MWh$_{th}$
	d. H_2 price	3000	[16]	2400	EUR /t
	e. CO_2 certificate price	102	[56]	146	EUR /t
	f. CF and RE share (German grid)	373.4	[57,58]	109.0	g_{CO_2}/kWh$_{el}$
Output	g. CO_2 emission allowance	100	-	100	%
	h. O_2 price	50	[43]	74.3	EUR /t
	i. Methanol price	342.0	[55]	401.6	EUR /t
	j. Urea price	256.3	[55]	428.2	EUR /t
	k. Ammonia price	182.9	[59]	305.5	EUR /t
	l. Acetic acid price	605.9	[59]	711.5	EUR /t
	m. Methanol market vol.	2.2	[55]	3.9	Mt/a
	n. Urea market vol.	4.4	[55]	5.4	Mt/a
	o. Ammonia market vol.	12.5	[55]	15.3	Mt/a
	p. Acetic acid market vol.	1.2	[55]	2.1	Mt/a

Table 2. *Cont.*

Class	Key Factor	Current Value	Source	*BAU*-Value	Unit
Technology	q. Conversion efficiency	1.0	[44,60]	1.0	-
	r. Energy efficiency	1.0	[44,60]	1.0	-
	s. H_2 efficiency	1.0	[61,62]	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)	-	[63,64]	1.0	-
	x. Operating cost	1.0	[63,64]	1.0	-

The target year of the capital expenditure (CAPEX) is set as 2025 following a five-year construction period. The CAPEX is calculated for each plant, including the gas conditioning, external H_2 production and chemical synthesis plants. The calculation is based on the capacity method [63]. 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 [63,64]. The reference data are taken from various techno-economic analysis studies and the C_a is extrapolated to the target year of investing, 2025. It is extrapolated to the 2025 value by applying the chemical engineering plant cost index (CEPCI), as i, to account for the inflation rate. The publication years of the studies are between 2006 and 2021. The 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 Equation (2):

$$C_a = C_0 \cdot \frac{i_a}{i_0} \tag{2}$$

The CAPEX development of the hydrogen production plants is assumed to be lower in the future. According to [65], it is assumed that the CAPEX for alkaline (ALK) and proton-exchange membrane (PEM) electrolysis will be 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 Equation (3), where f is the degression coefficient for the economy of scale for chemical plants with a value from 0.6 to 1.0.

$$C_b = C_a \cdot \left(\frac{S_b}{S_a}\right)^f \tag{3}$$

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 the 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 ${C_b}^{max}$. If there is lower than 10% of ${C_b}^{max}$, it is not worth installing 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 plant for each chemical in *BAU*-scenario

Final Product	S_b^{min}, kg/s	S_b^{max}, kg/s	C_b^{min}, MEUR	C_b^{max}, MEUR	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 the 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 the 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 does not match, an additional sampling point for piecewise linear approximation is considered until it reaches 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 4 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.

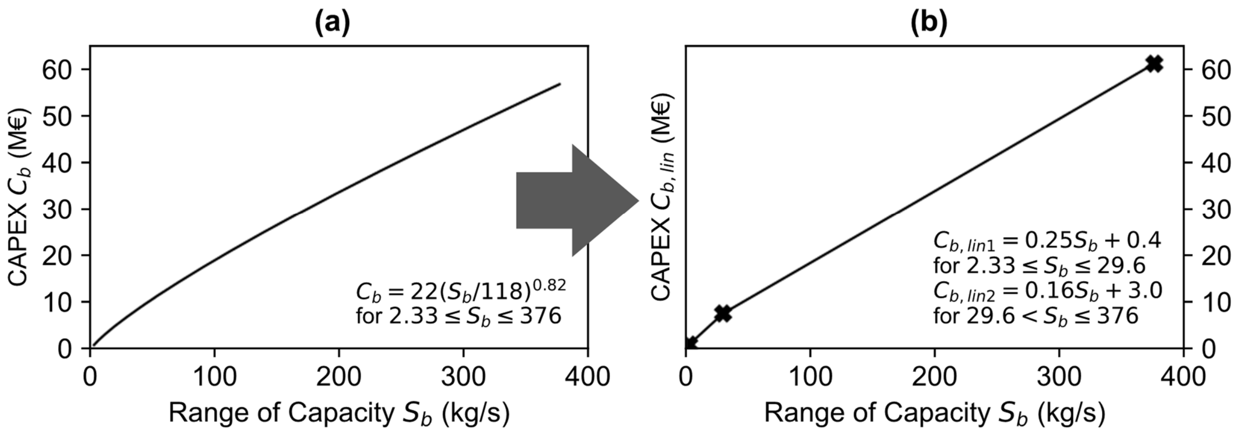

Figure 4. CAPEX functions of WGS plant in *BAU*-scenario: (**a**) cost function through capacity method C_b, (**b**) linearized cost functions $C_{b,lin}$ (adopted and modified from [42]).

Other plants' CAPEX is calculated in a similar way. The maximum relative error is detected in ammonia 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 [66]. The projected OPEX in the *BAU* scenario is estimated to be constant by the target year.

3.4. Future Projection of Key Factors

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 and five depending on the key factor. As mentioned, each projection involves quantified numerical values. If the data from the *BAU* scenario are 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 are 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 are unavailable, they are 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 [52]. 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-the-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 the CAPEX by multiplying itself. The *s-factor* is derived from the water electrolysis' CAPEX as it is available to obtain 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	CAPEX (Current)	CAPEX (*BAU* Scenario)	Future Situation	CAPEX (Future)	Rate *
ALK	1.0	0.86	Pessimistic	1.0	1.16
			Regular	0.79	0.92
			Optimistic	0.72	0.84
PEM	1.0	0.775	Pessimistic	1.0	1.29
			Regular	0.66	0.85
			Optimistic	0.55	0.71

* The rate represents the deviation of future CAPEX from the *BAU* CAPEX and serves as the *s-factor*. A higher *s-factor* indicates greater initial expenditures.

In the *BAU* scenario, the specific CAPEX for ALK and PEM is estimated to decrease 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 a 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 the 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 as 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 systematic formalized scenario technique of cross-impact analysis (CIA) is applied to ensure consistent combinations [38,39]. The CIA analyses the relationships between the key factors and the probabilities of the occurrence of future events by considering their direct and indirect mutual effects [67].

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 in Sections 3.5.1–3.5.4.

3.5.1. CO_2 Reduction and 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
e. CO_2 certificate price	Highly increasing (↑↑)
f. CF and RE share	Highly decreasing (↓↓)
g. CO_2 emission allowance	Highly decreasing (↓↓)
m. Methanol market vol.	Highly increasing (↑↑)
n. Urea market vol.	Highly increasing (↑↑)
o. Ammonia market vol.	Highly increasing (↑↑)
p. Acetic acid market vol.	Highly increasing (↑↑)

The key factors, CO_2 certificate price and *CF* and *RE* share, are forced environmentally 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 and Market Booming (*Market-Boom*)

The 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
h. O_2 price	Highly increasing (↑↑)
i. Methanol price	Highly increasing (↑↑)
j. Urea price	Highly increasing (↑↑)
k. Ammonia price	Highly increasing (↑↑)
l. Acetic acid price	Highly increasing (↑↑)
m-p. Market volumes	Moderately increasing (↑)
q. Conversion eff.	Highly increasing (↑↑)
r. Energy efficiency	Highly increasing (↑↑)
s. Hydrogen efficiency	Moderately increasing (↑)
t. Steel mill energy demand	Highly decreasing (↓↓)
u. Part load range	Highly increasing (↑↑)
v. Dynamic operation	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 *H2-Boom* scenario in Section 3.5.4.

3.5.3. Energy and Market Crisis (*Crisis*)

The *crisis* scenario projects the worst situation from the economic perspective. The concept refers to the current Ukraine conflict with energy and economic crisis. Table 7 presents eight forced factors for the scenario concept.

The factors related to the profitability are all negatively assumed. The prices of raw materials go up immensely, and the 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.

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

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

3.5.4. Hydrogen booming (*H2-Boom*)

The *H2-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
d. H_2 price	Highly decreasing (↓↓)
q. Conversion efficiency	Constant (-)
r. Energy efficiency	Constant (-)
s. Hydrogen efficiency	Highly increasing (↑↑)
u. Part load range (only H_2)	Moderately increasing (↑)
v. Dynamic operation (only H_2)	Moderately increasing (↑)

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

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 analyze 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® v4.52 software is used. In addition, the economic key factors pertaining to the prices and market volumes of the investigated chemicals of acetic acid, methanol, ammonia and urea are bundled into a single key factor. This bundling helps streamline the assessment of the interactions and complexity among these key factors. This judgment is based on the observation that the scenario concepts typically do not entail a direct comparison of the superiority among various projections of the chemicals. Bundling 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 *H2-Boom* are generated.

To select the final and most consistent combination out of the candidate's pool, the Consistency Value (CV) and Total Impact Score (TIS) function as the evaluation criteria [30]. The 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 [67,68]. Based on the scenario selection criteria, the final scenarios are determined. All scenarios have a CV equal to 0 and the highest TIS out of the possible candidates, so they involve the most consistent combination.

4. Results

4.1. Five Final Scenarios

In addition to the comprehensive data presented in Table 9, the scenarios also include time series data for electricity prices and capacity factors, as illustrated in Figure 3. Furthermore, all linearized and scaled CAPEX functions, denoted as C_s, are incorporated within the scenarios. The rationale behind the CAPEX calculations, which are determined post CIA, is elaborated upon below. For a comprehensive view of the different *s-factors* applicable to various hydrogen production plants, please refer to Table 10.

Table 9. Conclusive five scenarios featuring qualitative (QLT) and quantitative (QNT) values for the 24 identified key factors (a–x) of the CCU concept.

Key Factors with Units	*BAU*		*RE-Boom*		*Market-Boom*		*Crisis*		*H2-Boom*	
	QLT	QNT	QLT	QNT	QLT	QNT	QLT	QNT	QLT	QNT
a. Electricity price (EUR /MWh_{el})	(↑)	47.38	(↓↓)	20.66	(-)	41.32	(↑↑) *	72.31	(-)	41.32
b. NG price (EUR /MWh_{th})	(↑)	46.72	(↓↓)	15.68	(-)	31.35	(↑↑) *	69.63	(-)	31.35
c. Coal price (EUR /MWh_{th})	(↑)	11.82	(↓)	5.62	(-)	7.49	(↑↑) *	18.67	(-)	7.49
d. H_2 price (EUR /t)	(↓)	2400	(↓)	2400	(-)	3000	(↑↑)	3900	(↓↓) *	1500
e. CO_2 certificate price (EUR /t)	(↑)	146	(↑↑) *	255	(↑)	146	(↑↑)	255	(↑)	146
f. CF and RE share (g_{CO_2} /kWh_{el})	(↓)	109	(↓↓) *	0	(↓)	109	(↓↓)	0	(↓)	109
g. CO_2 emission allowance (%)	(-)	100	(↓↓) *	80	(-)	100	(-)	100	(↓)	90
h. O_2 price (EUR /t)	(↑)	74.3	(↓)	25.7	(↑↑) *	110.4	(↓↓) *	13.2	(-)	50.0
i. Methanol price (EUR /t)	(↑)	401.6	(↓)	282.4	(↑↑) *	471.7	(↓↓) *	233.1	(-)	342.0
j. Urea price (EUR /t)	(↑)	428.2	(↓)	192.2	(↑↑) *	715.4	(↓↓) *	128.2	(-)	256.3
k. Ammonia price (EUR /t)	(↑)	305.5	(↓)	137.1	(↑↑) *	510.4	(↓↓) *	91.4	(-)	182.9
l. Acetic Acid price (EUR /t)	(↑)	711.5	(↓)	500.2	(↑↑) *	835.5	(↓↓) *	413.0	(-)	605.9
m. Methanol 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. Ammonia market vol. (Mt/a)	(↑)	15.31	(↑↑) *	18.75	(-)	12.5	(↓↓)	7.51	(-)	12.5
p. Acetic Acid market v. (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. H_2 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 (H_2)
v. Dynamic operation (-)	(-)	1.0	(↑)	1.5	(↑↑) *	2.0	(-)	1.0	(↑) *	2.0 (H_2)
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 vary by plant and are presented in Table 10. * Subscripted factors indicate predetermined fixed projections.

Table 10. Scaling factor (*s-factor*) used for projecting future CAPEX of hydrogen production facilities within 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

In Table 10, the qualitative CAPEX projection for both the *RE-Boom* and *Market-Boom* scenarios indicates a decrease (s < 1) because of the CIA. For H_2 supplementation, the CAPEX is projected to show consistent improvement in both scenarios, with a moderate increase tied to the H_2 efficiency projection.

In terms of other components, the s-factor is estimated to be equal to ALK for *RE-Boom* and PEM for *Market-Boom*. It is more likely that *Market-Boom* will experience a greater reduction rate compared to *RE-Boom*, given the assumption of a higher rate of technical improvement in other components within the *Market-Boom* scenario.

The qualitative CAPEX projection for the *Crisis* scenario indicates an increase because of the CIA. Conversely, the CAPEX for the H_2 supplement is determined to exhibit the most adverse development (s > 1). Additionally, the *s-factor* for other components is assumed to be the average value between ALK and PEM projection.

The CAPEX associated with the H_2 supplement is determined to represent an optimistic future, in line with the H_2 efficiency projection. Unlike the *RE-Boom* and *Market-Boom* scenarios, the concept of *H2-Boom* exclusively concentrates on enhancing hydrogen production, which explains why the *s-factor* is not applied to other plants.

While it may initially appear counterintuitive that the qualitative CAPEX projection decreases through the CIA, this outcome can vary depending on the weight of each influencing factor. In this context, it is plausible that the reduction in CAPEX is primarily driven by the H_2 efficiency factor, given its significant impact on overall CAPEX.

The *s-factor* is applied to the $C_{b,lin}$ function for each individual plant within each scenario to arrive at the ultimate scaled CAPEX functions, denoted as C_s. As an illustrative example, Figure 5 showcases the resulting C_s function for the WGS plant in each scenario.

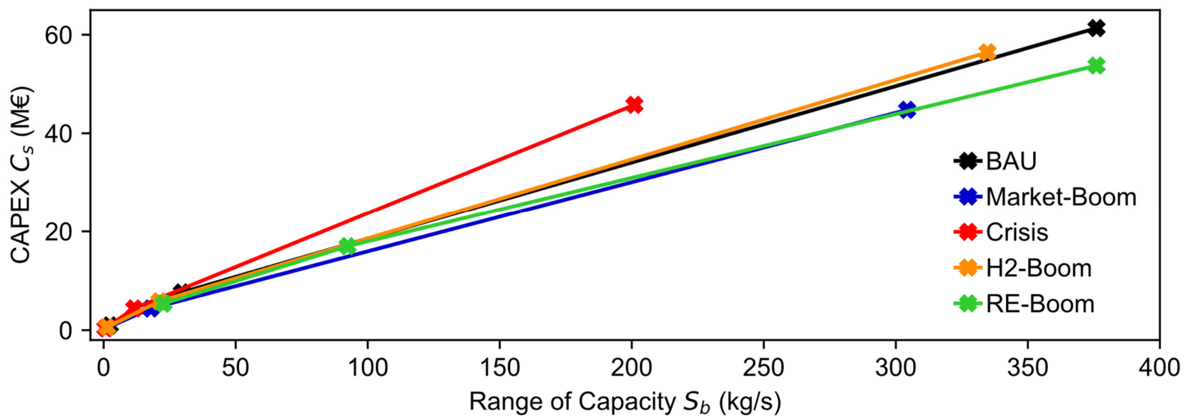

Figure 5. The five linear CAPEX functions C_s, specifically tailored for the Water Gas Shift (WGS) plant within each scenario.

4.2. Evaluation of the Scenarios

All combinations resulting from CIA (Table 9) undergo assessment utilizing three criteria: plausibility, consistency and differentiation. The *BAU* scenario is excluded from the scenario evaluation because it is independently generated through the trend extrapolation method outlined in Section 3.3 (Reference scenario development). Additionally, it is important to note that consistency has already been evaluated as part of the scenario selection process with the CIA, detailed in Section 3.6 (Scenario generation and selection).

4.2.1. Plausibility

The plausibility check for the scenarios involves evaluating whether the scenario combination aligns effectively with the intended concept formulated in Section 3.5 and whether the relationships between the fixed key factors and the remaining key factors are credibly formulated.

The *RE-Boom* scenario portrays a state wherein CO_2 emissions are minimized while the utilization of exhausted gas in the CCU concept is maximized. This conceptual framework effectively aligns with the fixed factors outlined in Table 5. Furthermore, the arrangement of the remaining factors exhibits a coherent structure. Notably, the prices of energy raw materials (factors a to c) undergo a reduction due to the CIA. Given the assumption of a zero CF, it is reasonable to observe a corresponding decrease in energy raw material prices. It is worth highlighting that the impact on the coal price is relatively subdued. This can be attributed to its stronger correlation with steel production, rather than its integration within the CCU concept for chemical production.

The primary focus of the *Market-Boom* scenario revolves around maximizing the economic profitability and technical parameters of the plants. This concept is effectively realized through the optimization of product prices and technical advancements, as detailed in Table 6. In the context of the remaining key factors, an intriguing observation is made regarding the chemicals' market volume. Despite price increments, the CIA indicates a consistent volume for the chemicals market. While this might seem counterintuitive in a typical price–market relationship, it is crucial to understand that this combination arises from the intricate interplay of all key factors in the system, rather than a simple correlation between two factors.

The *Crisis* scenario represents the most adverse situation, characterized by the compulsion of factors outlined in Table 7. Within this scenario, there is a notable discord between the combination of key factors and the intended scenario concept. Specifically, the ecological key factors (f and g) exhibit significant deviations, with substantial increases and decreases, respectively, because of the CIA calculation. These fluctuations are driven by the imposition of steep increases in the prices of energy raw materials. From the perspective of the three domains under consideration, this outcome may appear plausible, echoing a pattern like that observed in the *RE-Boom* scenario. However, this alignment does not resonate with the underlying scenario concept, which is anchored in the ongoing Ukraine conflict. The present abnormal situation has disrupted the typical dynamics within the energy complex. As noted in [69], the price of CO_2 permits surged to a high of 97 EUR /t in 2020, only to plummet to nearly 60 EUR /t after the outbreak of the conflict in 2022. In the year 2023, the price exhibited remarkable volatility, soaring to a historic peak of 105 EUR /t in February, only to subsequently recede to 75 EUR /t by December, as reported in [56]. This fluctuation is highly distinctive and requires further examination to comprehend its unique dynamics. To elucidate this exceptional and fluctuating scenario, it might be beneficial to incorporate considerations related to social or political key factors, such as public acceptance or prevailing political trends. These elements could serve as key determinants in understanding the fluctuation and may contribute to making the retrogressive trend more plausible in the context of the ongoing conflict.

The *H2-Boom* scenario is centered on enhancing overall hydrogen generation, a subdomain within the technical and economic realm. This conceptual framework is effectively realized through the utilization of fixed key factors detailed in Table 8. When considering the remaining key factors, it might appear more plausible for the prices of energy raw materials to decrease rather than remain constant. Under the assumption that H_2 prices experience a reduction and H_2 efficiency undergoes notable advancements, a substantial price drop is anticipated. This is particularly the case when a significant portion of green electricity is utilized, leading to lower market prices and carbon footprints. However, it is essential to note that this study's scenario operates on the premise that a perfect transition to an emission-free system is unattainable by the target year. As indicated in [70], the existing infrastructure imposes limitations on the widespread application of H_2 as an energy source. Germany's current gas supply network, for instance, can accommodate only up to 10% of H_2 by volume in total. The latest developments in German politics suggest a promising future possibility known as the "Wasserstoff-Kernnetz", which could facilitate the transfer of several gigawatt-hours per year of hydrogen within Germany until the year 2032 [71]. Nonetheless, it is apparent that hydrogen plays a progressively significant role within the energy system over time. This becomes evident when comparing it to the *BAU* scenario. In the *BAU* scenario, where the H_2 price decreases at a slower rate than in the *H2-Boom* scenario, there is an assumption of moderate increases in energy raw material prices. Even though H_2, as an energy source, may not bring about an instantaneous transformation of the energy system, it does exert a positive influence on the gradual transition. Consequently, it seems more plausible that the prices of energy raw materials would remain relatively constant within the *H2-Boom* scenario.

4.2.2. Differentiation

The differentiation among the scenarios is evaluated to determine if the generated scenarios portray significantly distinct conditions, thus preventing identical calculation outcomes.

From an economic perspective, the *Market-Boom* and *Crisis* scenarios can be perceived as opposites within the scenario framework. Their key factor combinations are formulated in opposite directions, resulting in divergent economic conditions.

Both the *Market-Boom* and *H2-Boom* scenarios include technical advancements by the target year, leading to similar projections for most elements across different domains. While this may initially appear as a false combination due to their similar situations, it is important to note that their technical concepts differ—*Market-Boom* focuses on overall improvement, whereas *H2-Boom* primarily targets the hydrogen subdomain. Consequently, comparing the results from these scenarios yields notably different outcomes for evaluating the CCU concept.

Conversely, the *RE-Boom* scenario concentrates solely on the independent ecological criteria domain. The combination of key factors within the *RE-Boom* scenario stands out significantly. In essence, this slice occupies a distinct area separate from other scenarios, introducing new criteria for evaluating the feasibility of the CCU concept.

Figure 6 visually illustrates the simplified developmental process and provides a qualitative classification to elucidate the differentiation among the scenarios.

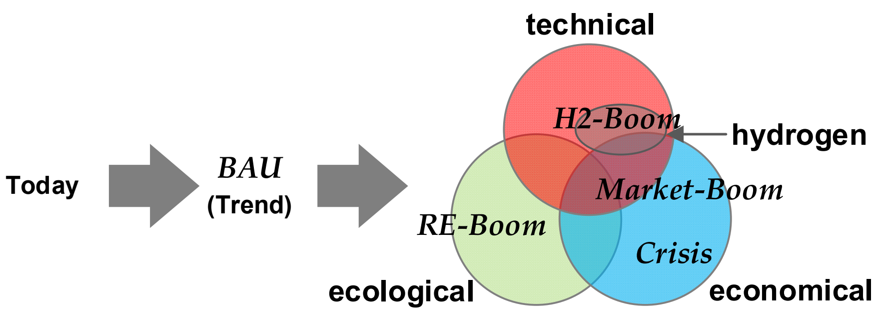

Figure 6. Simplified development and differentiation of scenario concepts illustrated in a Venn diagram.

5. Conclusions

This study aimed to establish coherent, credible and distinct scenarios to serve as input data for MILP models, facilitating the evaluation of the long-term viability of the proposed exhaust gas utilization concept. These five scenarios were created by incorporating both internal and external key factors based on three primary criteria. To construct the Business-As-Usual (*BAU*) scenario, these factors were projected forward to the target years of investment (2025) and operation (2040). Notably, the formulation of initial expenditure was outlined through the assessment of investment costs. A linear approximation approach for the CAPEX functions was employed to ensure compatibility with future use in MILP models while adhering to a maximum error tolerance of 10% from the original nonlinear function.

All 24 crucial key factors were projected into the target years, combining qualitative and quantitative elements to shape a hypothetical future trajectory. This process adheres to an objective methodology that relies on *BAU* scenario data rather than making random predictions. It also incorporates deliberate variations, both exaggerated and conservative, to make the evaluation of the CCU approach more apparent. In instances where *BAU* scenario data were unavailable, quantification was determined based on independently estimated assumptions.

Quantitative projections of investment costs were made possible through the application of a scaling factor (referred to as the "*s-factor*"). This *s-factor*, derived from the water electrolysis CAPEX, ranges from 0.71 to 1.29. It was then applied to other facilities to modulate the amplitude of the CAPEX functions, thereby introducing diverse economic scenarios. An *s-factor* greater than 1 signifies economically unfavorable situations due to higher initial expenditures.

This comprehensive analysis offers novel perspectives on the potential future trends of pivotal key factors, such as electricity prices, the share of renewable energy or the chemicals market trends, as the "Hot potato" key factors.

The concept for each scenario is predetermined prior to the scenario formulation process (Section 3.5). In essence, scenarios are developed based on deliberately specified conditions, resulting in four distinct scenario concepts:

- **CO_2 Reduction and RE Share Target (*RE-Boom*):** This scenario envisions the most favorable ecological conditions, emphasizing CO_2 reduction and a high renewable energy (RE) share.
- **Technical Improvement and Market Booming (*Market-Boom*):** Here, the focus is on achieving optimal economic and technical conditions, with an emphasis on technical advancements and a thriving chemical market.
- **Energy and Market Crisis (*Crisis*):** The *Crisis* scenario represents the most adverse economic situation, depicting a scenario of energy and market crisis.
- **Hydrogen Booming (*H2-Boom*):** This scenario exclusively highlights the most advantageous conditions for hydrogen generation, considering both technical and economic aspects of the plants and market.

These scenario concepts provide a comprehensive spectrum of potential future conditions, each with its distinctive emphasis and perspective.

Based on the predetermined concept, we conduct a cross-impact analysis (CIA) to identify the most consistent combination of key factors within the established conditions. The computed combinations are regarded as highly reliable outcomes. Firstly, in terms of consistency, all scenarios exhibit the desired consistency value (CV) of zero and the highest total impact score (TIS) among the potential candidates. Secondly, determinations of the remaining factors' projections through the CIA calculation are also plausible in describing the scenario concept within the scope of the investigation. Lastly, the results yield significantly different operational conditions that are meaningful. These findings build upon existing evidence of the reliably structured scenarios. The generated scenarios can now be directly applied in a linear optimization model to evaluate the prospective CCU concept.

In summary, the five scenarios we have generated provide a clear portrayal of potential situations for the CCU concept in the target years. These scenarios are founded on a complex interplay of factors from various impact parameters. Importantly, each scenario offers a consistent, plausible and notably distinct combination of key factors.

6. Outlook

In future research, the five scenarios will be applied in the MILP model to identify optimal plant layouts for CCU concepts, including methanol, ammonia, urea and/or acetic acid production from steel mill exhaust gases. The optimization model will determine the best solution, which includes the optimal plant configuration (e.g., methanol or ammonia production), plant size and the operation of the plants. Sensitivity analyses of individual key factors will also be conducted to enhance insights. Therefore, the scenarios will be regularly updated and modified with current data to provide meaningful and accurate results for future investigations.

Furthermore, potential modifications to the scenarios to incorporate political or legal domains or the exploration of alternative scenario development techniques are considered. This methodology can also be extended to include other CCU concepts, such as the analysis of exhaust gases from cement or lime production or the incorporation of additional chemical products like methane, ethene, propylene or polycarbonates, broadening its potential application.

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Nomenclature

C	Capital expenditures (CAPEX) of the plants, MEUR
CF	Carbon footprint of power supply, g_{CO_2}/kWh_{el}
f	Economy of Scale degression coefficient, -
RE	Renewable energy share, %
S	Capacity of the plant, kg/s
s	Scaling factor for investment costs, -
Subscripts and Superscripts	
0	Reference year index 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

References

1. Lee, H.; Calvin, K.; Dasgupta, D.; Krinner, G.; Mukherji, A.; Thorne, P.W.; Trisos, C.; Romero, J.; Aldunce, P.; Barrett, K.; et al. *IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*; Core Writing Team, Lee, H., Romero, J., Eds.; IPCC: Geneva, Switzerland, 2023.
2. Bampaou, M.; Panopoulos, K.; Seferlis, P.; Sasiain, A.; Haag, S.; Wolf-Zoellner, P.; Lehner, M.; Rog, L.; Rompalski, P.; Kolb, S.; et al. Economic Evaluation of Renewable Hydrogen Integration into Steelworks for the Production of Methanol and Methane. *Energies* **2022**, *15*, 4650. [CrossRef]
3. Heidari, A.; Niknahad, N.; Iljana, M.; Fabritius, T. A Review on the Kinetics of Iron Ore Reduction by Hydrogen. *Materials* **2021**, *14*, 7540. [CrossRef] [PubMed]
4. Holappa, L. A General Vision for Reduction of Energy Consumption and CO_2 Emissions from the Steel Industry. *Metals* **2020**, *10*, 1117. [CrossRef]

5. Li, P.; Wang, Y.; Feng, J.; Tan, H.; Li, L. Effect of Carbon-Containing Solid Waste from Calcium Carbide Production on Combustion and Slagging Characteristics of Zhundong Coal Blend. *Combust. Sci. Technol.* **2023**, 1–16. [CrossRef]
6. Wang, B.; Li, S.; Sun, D.; Bian, J.; Zhao, H.; Li, H.; Zhang, Y.; Ju, F.; Ling, H. Emission characteristics of benzene series in FCC flue gas. *Chemosphere* **2023**, *328*, 138561. [CrossRef] [PubMed]
7. Draxler, M.; Schenk, J.; Bürgler, T.; Sormann, A. The Steel Industry in the European Union on the Crossroad to Carbon Lean Production—Status, Initiatives and Challenges. *Berg. Huettenmaenn. Monatsh.* **2020**, *165*, 221–226. [CrossRef]
8. Ghanbari, H.; Helle, M.; Saxén, H. Optimization of an Integrated Steel Plant with Carbon Capturing and Utilization Processes. *IFAC-PapersOnLine* **2015**, *48*, 12–17. [CrossRef]
9. Bampaou, M.; Panopoulos, K.; Seferlis, P.; Voutetakis, S.; Matino, I.; Petrucciani, A.; Zaccara, A.; Colla, V.; Dettori, S.; Annunziata Branca, T.; et al. Integration of Renewable Hydrogen Production in Steelworks Off-Gases for the Synthesis of Methanol and Methane. *Energies* **2021**, *14*, 2904. [CrossRef]
10. Jacobasch, E.; Herz, G.; Rix, C.; Müller, N.; Reichelt, E.; Jahn, M.; Michaelis, A. Economic evaluation of low-carbon steelmaking via coupling of electrolysis and direct reduction. *J. Clean. Prod.* **2021**, *328*, 129502. [CrossRef]
11. Kolbe, N.; Cesário, F.; Ahrenhold, F.; Suer, J.; Oles, M. Carbon Utilization Combined with Carbon Direct Avoidance for Climate Neutrality in Steel Manufacturing. *Chem. Ing. Tech.* **2022**, *94*, 1548–1552. [CrossRef]
12. Hong, W.Y. A techno-economic review on carbon capture, utilisation and storage systems for achieving a net-zero CO_2 emissions future. *Carbon Capture Sci. Technol.* **2022**, *3*, 100044. [CrossRef]
13. Shreyash, N.; Sonker, M.; Bajpai, S.; Tiwary, S.K.; Khan, M.A.; Raj, S.; Sharma, T.; Biswas, S. The Review of Carbon Capture-Storage Technologies and Developing Fuel Cells for Enhancing Utilization. *Energies* **2021**, *14*, 4978. [CrossRef]
14. Regufe, M.J.; Pereira, A.; Ferreira, A.F.P.; Ribeiro, A.M.; Rodrigues, A.E. Current Developments of Carbon Capture Storage and/or Utilization–Looking for Net-Zero Emissions Defined in the Paris Agreement. *Energies* **2021**, *14*, 2406. [CrossRef]
15. Tadjer, A.; Bratvold, R.B. Managing Uncertainty in Geological CO_2 Storage Using Bayesian Evidential Learning. *Energies* **2021**, *14*, 1557. [CrossRef]
16. Ghiat, I.; Al-Ansari, T. A review of carbon capture and utilisation as a CO_2 abatement opportunity within the EWF nexus. *J. CO_2 Util.* **2021**, *45*, 101432. [CrossRef]
17. Chen, J.; Xu, Y.; Liao, P.; Wang, H.; Zhou, H. Recent Progress in Integrated CO_2 Capture and Conversion Process Using Dual Function Materials: A State-of-the-Art Review. *Carbon Capture Sci. Technol.* **2022**, *4*, 100052. [CrossRef]
18. Sun, S.; Sun, H.; Williams, P.T.; Wu, C. Recent advances in integrated CO_2 capture and utilization: A review. *Sustain. Energy Fuels* **2021**, *5*, 4546–4559. [CrossRef]
19. Deerberg, G.; Oles, M.; Schlögl, R. The Project Carbon2Chem®. *Chem. Ing. Tech.* **2018**, *90*, 1365–1368. [CrossRef]
20. Leitner, W.; Franciò, G.; Scott, M.; Westhues, C.; Langanke, J.; Lansing, M.; Hussong, C.; Erdkamp, E. Carbon2Polymer—Chemical Utilization of CO_2 in the Production of Isocyanates. *Chem. Ing. Tech.* **2018**, *90*, 1504–1512. [CrossRef]
21. van Beek, M.; Sadlowski, M. Transient Optimization of Coproduction Systems for Steel and Value-Added Chemicals. *Chem. Ing. Tech.* **2020**, *92*, 1431–1443. [CrossRef]
22. Uribe-Soto, W.; Portha, J.-F.; Commenge, J.-M.; Falk, L. A review of thermochemical processes and technologies to use steelworks off-gases. *Renew. Sustain. Energy Rev.* **2017**, *74*, 809–823. [CrossRef]
23. Ramírez-Santos, Á.A.; Castel, C.; Favre, E. A review of gas separation technologies within emission reduction programs in the iron and steel sector: Current application and development perspectives. *Sep. Purif. Technol.* **2018**, *194*, 425–442. [CrossRef]
24. Luca, A.-V.; Petrescu, L. Membrane technology applied to steel production: Investigation based on process modelling and environmental tools. *J. Clean. Prod.* **2021**, *294*, 126256. [CrossRef]
25. Dunstan, M.T.; Donat, F.; Bork, A.H.; Grey, C.P.; Müller, C.R. CO_2 Capture at Medium to High Temperature Using Solid Oxide-Based Sorbents: Fundamental Aspects, Mechanistic Insights, and Recent Advances. *Chem. Rev.* **2021**, *121*, 12681–12745. [CrossRef]
26. Schlüter, S.; Hennig, T. Modeling the Catalytic Conversion of Steel Mill Gases Using the Example of Methanol Synthesis. *Chem. Ing. Tech.* **2018**, *90*, 1541–1558. [CrossRef]
27. Deng, L.; Adams, T.A. Methanol Production from Coke Oven Gas and Blast Furnace Gas. In *13th International Symposium on Process Systems Engineering (PSE 2018)*; Eden, M.R., Ierapetritou, M.G., Towler, G.P., Eds.; Computer-Aided Chemical Engineering 44; Elsevier: Amsterdam, The Netherlands; Boston, MA, USA; Heidelberg, Germany, 2018; pp. 163–168.
28. Voß, J.M.; Daun, T.; Geitner, C.; Schlüter, S.; Schulzke, T. Operating Behavior of a Demonstration Plant for Methanol Synthesis. *Chem. Ing. Tech.* **2022**, *94*, 1489–1500. [CrossRef]
29. Xu, D.; Wang, Y.; Ding, M.; Hong, X.; Liu, G.; Tsang, S.C.E. Advances in higher alcohol synthesis from CO_2 hydrogenation. *Chem* **2021**, *7*, 849–881. [CrossRef]
30. Peters, M.; Menne, A.; Gielisch, H. Synthesis of Sustainable Fuels and Intermediates from Ethanol and Methanol. *Chem. Ing. Tech.* **2022**, *94*, 1501–1508. [CrossRef]
31. Schlüter, S.; Geitner, C. Simulation of Methanol and Urea Production from Catalytic Conversion of Steel Mill Gases. *Chem. Ing. Tech.* **2020**, *92*, 1403–1415. [CrossRef]
32. Büker, K.; von Morstein, O.; Yildirim, Ö.; Frey, A.; Voss, C.; Geisbauer, A. Practical Aspects of Converting Steel Mill Gases to Chemical Feedstocks. *Chem. Ing. Tech.* **2022**, *94*, 1452–1457. [CrossRef]

33. Arvola, J.; Harkonen, J.; Mottonen, M.; Haapasalo, H.; Tervonen, P. Combining Steel and Chemical Production to Reduce CO_2 Emissions. *Low Carbon Econ.* **2011**, *2*, 115–122. [CrossRef]
34. Kenkel, P.; Wassermann, T.; Rose, C.; Zondervan, E. A generic superstructure modeling and optimization framework on the example of bi-criteria Power-to-Methanol process design. *Comput. Chem. Eng.* **2021**, *150*, 107327. [CrossRef]
35. Sadlowski, M.; van Beek, M. *Integration und Strukturelle Optimierung Verschiedener Chemischer Syntheserouten zur Abgasnutzung Bestehender Stahlproduktionsanlagen*; Democratization of the Energy System 7; Internationale Energiewirtschaftstagung (IEWT); TU Wien: Vienna, Austria, 2019.
36. Ioannou, A.; Angus, A.; Brennan, F. Risk-based methods for sustainable energy system planning: A review. *Renew. Sustain. Energy Rev.* **2017**, *74*, 602–615. [CrossRef]
37. Schomaker, R.M.; Sitter, A. Die PESTEL-Analyse—Status quo und innovative Anpassungen. *Der Betriebswirt* **2020**, *61*, 3–21. [CrossRef]
38. Kosow, H.; Gaßner, R. *Methoden der Zukunfts-und Szenarioanalyse: Überblick, Bewertung und Auswahlkriterien*; DIE Studies 39; Institut für Zukunftsstudien und Technologiebewertung: Bonn, Germany, 2008.
39. Gausemeier, J.; Fink, A.; Schlake, O. *Szenariomanagement: Planen und Führen mit Szenarien*; Paderborner Universität: München, Germany, 1996.
40. Reibnitz, U.; von Hammond, P. *Scenario Techniques*; McGraw-Hill: Hamburg, Germany, 1988.
41. Greeuw, S.C.; van Asselt, M.; Grosskunth, J.; Storms, C.; Rijkens-Klomp, N.; Rothman, D.; Rotmans, J. *Cloudy Crystal Balls. An Assessment of Recent European and Global Scenario Studies and Models*; Environmental Issues Series No. 17; European Environment Agency: Copenhagen, Denmark, 2000.
42. Sadlowski, M.; Lim, C.E. Multi-Criteria Scenario Development for Linear Optimization Models Utilizing Carbon-Containing Exhaust Gases. In Proceedings of the 36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems (ECOS 2023), Las Palmas de Gran Canaria, Spain, 25–30 June 2023; Smith, J.R., Ed.; Curran Associates Inc.: Red Hook, NY, USA, 2023; pp. 1363–1374.
43. Stießel, S. Entwicklung eines Referenzmodells zur Multikriteriellen Bewertung von Cross-Industriellen Systemen. Ph.D. Dissertation, Ruhr-Universität Bochum, Bochum, Germany, 2020.
44. Sadlowski, M.; van Beek, M. Ecologic Potential for Flexible Methanol Production from Steel Mill Off-gases. *Chem. Ing. Tech.* **2020**, *92*, 1416–1424. [CrossRef]
45. Polley, R.; Apel, K. The Dominance and Monopolies Review: Germany. Available online: https://thelawreviews.co.uk/title/the-dominance-and-monopolies-review/germany (accessed on 8 December 2023).
46. Bundesministerium der Justiz. Competition Act. Available online: https://www.gesetze-im-internet.de/englisch_gwb/englisch_gwb.html (accessed on 8 December 2023).
47. Vreys, K.; Lizin, S.; van Dael, M.; Tharakan, J.; Malina, R. Exploring the future of carbon capture and utilisation by combining an international Delphi study with local scenario development. *Resour. Conserv. Recycl.* **2019**, *146*, 484–501. [CrossRef]
48. Raths, S.; Koopmann, S.; Müller, C.; Meinerzhagen, A.; Falke, T.; Cramer, M.; Kulms, T.; Beulertz, D. (Eds.) *The Energy System Development Plan*; Blueprints for the New Energy Age 17; Institute of Electrical and Electronics Engineers Inc.: Bonn, Germany, 2015.
49. Agora Energiewende. *German Net Power Generation, Consumption, and Exports*; Agora Energiewende: Berlin, Germany, 2020.
50. European Commission, Directorate General for Energy; European Commission, Directorate General for Climate Action; European Commission, Directorate General for Mobility and Transport. *EU Reference Scenario 2020: Energy, Transport and GHG Emissions: Trends to 2050*; European Commission: Brussels, Belgium, 2021.
51. Henze, V. *Carbon Offset Prices Could Increase Fifty-Fold by 2050. Surging Demand and Unanswered Questions on Supply Could Push Offset Prices to Unsustainable Highs or Ill-Fated Lows*. 2022. Available online: https://about.bnef.com/blog/carbon-offset-prices-could-increase-fifty-fold-by-2050/ (accessed on 17 January 2024).
52. IEA. Global Hydrogen Review 2021: Paris. 2021. Available online: https://www.iea.org/reports/global-hydrogen-review-2021 (accessed on 8 December 2023).
53. IEA. The Future of Petrochemicals: Paris. 2018. Available online: https://www.iea.org/reports/the-future-of-petrochemicals (accessed on 7 August 2022).
54. Fraunhofer ISE. Annual Electricity Spot Market Prices in Germany: Freiburg. 2022. Available online: https://energy-charts.info/?l=en&c=DE (accessed on 8 December 2023).
55. Statistical Office of the European Union. Statistics on the Production of Goods (Prodcom). 2022. Available online: https://ec.europa.eu/eurostat/de/web/prodcom (accessed on 8 December 2023).
56. Trading Economics. EU Carbon Permits: EU CO_2 Certificate Price from 24 February 2023. Available online: https://tradingeconomics.com/commodity/carbon (accessed on 8 December 2023).
57. Prognos; Öko-Institut; Wuppertal Institut. *Towards a Climate-Neutral Germany. Executive Summary Conducted for Agora Energiewende, Agora Verkehrswende and Stiftung Klimaneutralität*; Agora Energiewende: Berlin, Germany, 2020.
58. Umweltbundesamt. Indicator: Greenhouse Gas Emissions. 2023. Available online: https://www.umweltbundesamt.de/en/data/environmental-indicators/indicator-greenhouse-gas-emissions (accessed on 8 December 2023).
59. Procurement Resource. Chemicals Price Trend. 2021. Available online: https://www.procurementresource.com/resource-center/ (accessed on 8 December 2023).

60. Luyben, W.L. *Chemical Reactor Design and Control*; John Wiley & Sons: San Francisco, CA, USA, 2007.
61. Nel Hydrogen Electrolysers. *The World's Most Efficient and Reliable Electrolysers*. 2018. Available online: http://www.silpac.com.cn/download/Electrolysers-Brochure-Rev-C.pdf (accessed on 17 January 2024).
62. IEA. The Future of Hydrogen. 2019. Available online: https://www.iea.org/reports/the-future-of-hydrogen (accessed on 8 December 2023).
63. Towler, G.; Sinnott, R. *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*; Butterworth-Heinemann: Oxford, UK, 2021.
64. Bejan, A.; Tsatsaronis, G.; Moran, M.J. *Thermal Design and Optimization*; A Wiley-Interscience Publication; Wiley: New York, NY, USA, 1996.
65. Zauner, A.; Böhm, H.; Rosenfeld, D.; Tichler, R. Innovative Large-Scale Energy Storage Technologies and Power-to-Gas Concepts after Optimization. Available online: https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5c58ae3ff&appId=PPGMS (accessed on 7 December 2023).
66. Geldermann, J. *Anlagen-und Energiewirtschaft: Kosten-und Investitionsschätzung Sowie Technikbewertung von Industrieanlagen*; Franz Vahlen: Munich, Germany, 2014.
67. Weimer-Jehle, W. *ScenarioWizard 4.4: Constructing Consistent Scenarios Using Cross-Impact Balance Analysis*; University of Stuttgart: Stuttgart, Germany, 2021.
68. Weimer-Jehle, W.; Key Figures Used in the Analysis of CIB Scenarios. Cross-Impact Balance Analysis—Guideline No. 4. 2018. Available online: https://cross-impact.de/deutsch/CIB_d_ScW.htm (accessed on 17 January 2024).
69. Ambrose, T. EU Carbon Permit Prices Crash after Russian Invasion of Ukraine. 2022. Available online: https://www.theguardian.com/environment/2022/mar/02/eu-carbon-permit-prices-crash-after-russian-invasion-of-ukraine (accessed on 17 January 2024).
70. Agora Verkehrswende, Agora Energiewende and Frontier Economics. *The Future Cost of Electricity-Based Synthetic Fuels*; Frontier Economics Ltd.: London, UK, 2018.
71. Fernleitungsnetzbetreiber. Antragsentwurf Wasserstoff-Kernnetz (15 November 2023). Available online: https://fnb-gas.de/wasserstoffnetz-wasserstoff-kernnetz/ (accessed on 8 December 2023).