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Contribution to a standardized economic and ecological assessment methodology for e-fuel production in Germany

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Techno-economic and ecological analysis of synthetic fuel production requires a consistent set of assumptions to ensure comparability. The proposed methodology was developed to assess any e-fuel production globally under various local conditions. It includes standards concerning the methodology and cost calculations for individual process stages, along with electricity, H₂, heat, and CO₂ supply. With the presented approach, net production costs, production efficiencies, and the global warming potential can be compared. In this work, the basic assumptions for e-fuel-production in Germany are shared and illustrated with a simplified example.

KEYWORDS

comparability, energy-transition, techno-economic analysis, life cycle assessment, power-to-x process, standardizing

1 Introduction

The transport sector worldwide still does not meet international obligations to become climate neutral. One of the countries lagging behind its set goals is Germany. In 2021, the German transport sector contributed 19.4% of country's greenhouse gas (GHG) emissions ([German Environment Agency, 2022](#)). In order to reach the maximum target of 85 Mt CO₂ equivalents by 2030, emissions need to be reduced by approximately 79 Mt CO₂ equivalents compared to 2020. Moreover, other European countries also have a long way to go to achieve net zero emissions in the transport sector, as depicted in [Figure 1](#).

In order to explore pathways for the de-fossilization of the transport sector at both national and global levels, the German Federal Ministry for Economic Affairs and Climate Action (BMWK) launched the initiative "Energy Transition in the Transport Sector: Sector Coupling through the Use of E-Fuels (EiV) in 2017, with a total funding of 99 M€ and 16 projects ([BMWK, 2017](#)). Since each project started with its own goals to address a certain part of the transport sector, there was no guarantee that their analysis—concerning costs for environmental impacts—would be comparable. To identify the most promising pathways for the short, mid, and long term, these pathways needed to be assessed technically, economically, and ecologically. In this study, a standardized methodology and a framework of basic assumptions, based on previous

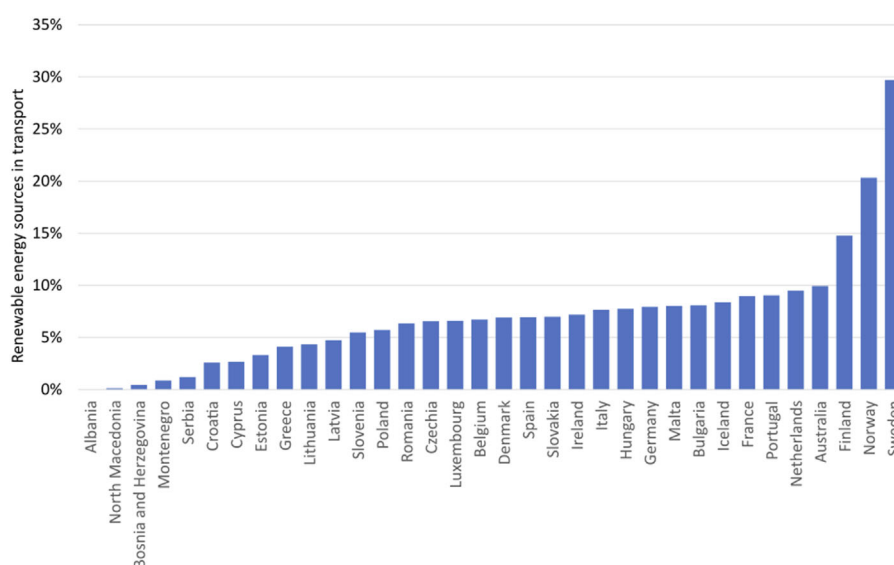


FIGURE 1
Share of renewable energy in the transport sector of selected European countries (adapted from (Eurostat, 2019)).

work (Albrecht et al., 2017), were developed. This was carried out by the authors within the additional project “Accompanying Research on the EiV” (BEniVer) (Energiesystem-Forschung, 2021).

A comparable analysis of power-to-x (PtX) production routes is only possible if the underlying assumptions and methodologies are consistent and clearly reported. However, due to different levels of detail and differing assumptions, this is often not the case, as illustrated by the following examples.

In the absence of all *technical* information, the reproduction of results is limited. In Gorre et al. (2020), information on the catalyst used for methanation is missing. Furthermore, the compressors are only defined by their share of total energy consumption. The target purity of the product is not reported, as is also the case in Moiola and Schildhauer (2022) for their methanol synthesis. Tremel et al. (2015) provided neither a flow diagram nor simulation data. Furthermore, information on the thermodynamic model used, the purity of the product, and the reactor model is missing. Adnan and Kibria (2020) also did not specify product purity. Even though many economic values in Gorre et al. (2019) are listed in a very good manner, failing to mention the product’s purity and assuming that both different electrolysis technologies and different methanation processes have only “minor technological differences” makes their technical insights questionable.

Incomparable approaches and assumptions in *economic* analysis prevent results from being comparable beyond a given publication. Even though there are good examples of economic analysis, such as for Parigi et al. (2019), Dahiru et al. (2022) stated in their review on techno-economic analysis (TEA) of power-to-X production: “[...] there is not yet any globally accepted method for TEA due to lack of consistency and comparability between different studies.” For instance, Adnan and Kibria (2020) did not report hydrogen costs, annual operating time, or base year for the synthetic methanol production. Schemme et al. (2020) performed an analysis

with a consistent system boundary and the same assumptions for internal comparability. However, e.g., the data for the CO₂ costs and the amount of energy required to extract the CO₂ were taken from different sources and are, therefore, inherently inconsistent. Furthermore, key factors underlying the TEA, such as Lang factor, are missing. Peters et al. (2019) provided no information on plant operating time or capital costs.

Even in *ecological* analysis, data are often neither collected uniformly nor based on the same assumption. In a meta-study of various publications on the life cycle assessment (LCA) of synthetic fuels, Kigle stated, “Despite the large number of publications and normalized LCA standards, comparison of results between different fuels across different studies proves difficult” (translated) (Kigle et al., 2019, p. 7). The GHG emissions for methane fuel, for example, range from just under 200 g CO₂-equivalent km⁻¹ (CO_{2-eq.} km⁻¹) in Wettstein et al. (2018) to 650 g CO_{2-eq.} km⁻¹ in Reiter and Lindorfer (2015). A significant influencing factor is the GHG intensity of the electricity supply and the associated share of the synthetic fuels. Wettstein et al. (2018) considered a photovoltaic (PV) plant as the power source, while Reiter and Lindorfer (2015) assumed the electricity mix. The choice of the system boundary and the functional unit to which the results refer also influences their comparability, as does the process to which any captured CO₂ is attributed (Kigle et al., 2019). The publication of the methodology guideline for LCA of e-fuels was already a step further (Pichlmaier et al., 2021). In addition, Müller et al. (2020) provided a good overview of LCA guidelines. However, an LCA can still be carried out following the standards and yet remain incomparable if the basic assumptions are not defined identically and the methodology is not standardized.

In order to address the issue of non-comparability, a comprehensive summary of the necessary criteria for TEA and LCA was presented by Langhorst et al. (2022). They require that

“the target audience for the study shall be stated,” which seems to imply different qualities of scientific work are acceptable for different audiences. This should not be the case. Due to their focus on using LCA definitions to TEA, the definitions for economic analysis are, sometimes, not sufficient. For instance, in order to define the products, they require stating the intended application. This is not necessary for the calculation of costs and environmental impacts of the production. Even if the intention is to use the application of the product to define its quality, they do not specify the extent to which the application should be described. If, for instance, methanol as fuel for cars is the stated application, it could be used either in an internal combustion engine or in a methanol fuel cell, and the permissible water content could differ significantly between these cases. Similarly, they state that the functional unit of the product should be defined but do not indicate the required level of detail for that definition. For instance, if the functional unit is 1 kg of synthetic natural gas for heating, neither the composition nor the lower heating value is still defined. Natural gas has a lower heating value of 10.42 kWh m⁻³ or 8.87 kWh m⁻³ for natural gas L or H, respective (AG Erdgastechnik, 2019), and for the american market, 10.18 kWh m⁻³ (The Engineering ToolBox, 2003). Even if the functional unit is defined, the results are not comparable unless a standard is established. A more robust approach would be to define the product by its composition (including pressure and temperature). They also omit net production costs (NPCs) as an economic result, focusing instead solely on “profitability,” which highly relies on unknown future market conditions. No one knows what future tax policies will look like or whether demand for one product will exceed demand for another. Currently, there is no established market for renewable fuels. Furthermore, they do not define the methodology of cost calculation. If several analyses are carried out based on their guidelines, different methodologies of cost calculation could be selected. These methodologies can significantly differ, for instance, in the choice of surcharge factors. Without a standardized calculation methodology, the results are not comparable. Finally, their framework allows for varying quality in both input data and analysis. Studies based on different standards are not comparable.

The same applies to Michailos et al. (2018) and Zimmermann et al. (2020) since both are based on Langhorst et al. (2022).

To perform a TEA and LCA of renewable fuels, the balance limit, assumptions, and assessment methodologies must be standardized and consistent. In this work, we provide a defined methodology for TEA and LCA that is specific enough to allow for comparable results yet flexible enough to assess various production paths and scenarios. The aim is to facilitate comparability among various studies on PtX production in a fair and unbiased manner. In Table 1, a set of all necessary assumptions for a single methodology of TEA and LCA is presented, with example values for German production in 2018. Forecasted values for the years 2030 and 2045 are also included. The methodology can be applied to any other location, plant size, operating hours, or manufacturing process by adjusting a few input parameters (see Table 1 and Section 4.5) and is, therefore, generally valid not only for e-fuels but also for PtX processes worldwide (see also Garcke (2024)).

For explanatory purposes, an oversimplified example process is presented at the end of this publication. A realistic analysis of the

given process using the methodology presented in this study can be found in Rahmat et al. (2023).

Even though the energy transition includes production, logistics, retrofitting, acceptance, and utilization, only production is considered in this study. Other aspects are planned to be published by the project BEniVer.

2 Methodology

The following section describes the methodology that can be used for the standardized technical, economic, and ecological analysis of PtX products. Figure 2 shows the general production pathway of PtX products with easily comparable balance limits.

The process starts with the supply of H₂, which is usually produced using electricity. Since electricity usually constitutes the highest share of NPCs, establishing a valid base for the electricity price is crucial. In Section 3.2, the cost data and the environmental impact of the electricity are listed. For more details, see SI chapter 3. H₂ is itself a PtX product. To improve storage capability and/or to enable desired applications, another reaction partner can be added to hydrogen in a synthesis process. These could include, for instance, CO₂ or N₂, both of which must be purified beforehand. After synthesis, further purification of the product might be necessary. Within a PtX plant, heat, electrical power, and materials should be integrated to improve efficiency. Depending on the location of the PtX plant, it might even be possible to use waste heat locally, e.g., for district heating.

There are two preferable balance limits: either electrolysis and CO₂/N₂ purification are included within the boundary, allowing the entire PtX route to be compared, or—if the focus of comparison is the synthesis processes itself—CO₂/N₂ and H₂ can be treated as educts, leaving their production and purification outside the balance limit. In order to compare this approach, the costs and environmental impacts of the respective streams must be set equal. For the case of H₂ and CO₂, see Sections 3.3, 3.4, respectively.

To analyze a PtX process from both a techno-economic and a techno-ecological perspective, the procedure presented schematically in Figure 3 can be carried out.

In the *first step*, the technical basis of the process is defined to enable the setup of a detailed process simulation. Whenever possible, this step should be carried out with the participation of industry partners since they possess detailed knowledge of the process. Further information can be collected through literature research. In the *second step*, a detailed process simulation is created in order to identify existing dependencies in the production process and estimate the minimum equipment requirement. The simulation is optimally validated together with industrial partners. In the *third step*, the calculation of the cost data and environmental impact and the analysis of technical key performance indicators (TKPIs) are carried out. This step is executed on the basis of the technical analysis, literature data, databases, and generally accepted calculation methods. In the *fourth step*, key parameters are analyzed, and in the *fifth step*, the results can be communicated back to project partners in order to further optimize the process, if possible.

TABLE 1 Minimal base assumptions with example values for a German PtX plant.

	Example value	Explanation
General		
Country	Germany	Basis for other assumptions
Year	2018	All input data given and available No effects of SARS-CoV-2 and war in Ukraine
	2030	Medium-term German political goal. Forecasts with uncertainties
	2045	Long-term German political goal Per definition: "all energy is renewable." Forecasts with uncertainties
Balance limit	Figure 2	Electrolysis in comparison or excluded?
Plant size	"Small-scale:" 3 MW _{el}	Experimentally validated assessment
	"Large-scale:" 300 MW _{el}	No experimental validation available yet. Approach: scale up of experimental results Still too small for large-scale production
Location	"Brownfield"	Refinery/chemical complex assumed for the lowest NPC. Disclose if selected otherwise
NPC/GWP Allocation of multiple product streams	Energetic allocation: LHV	Disclose if selected otherwise
Technical		Select and disclose consistent material properties
LHV Hydrogen	33.3 kWh kg ⁻¹	RP-Energie-Lexikon (2022)
LHV Methanol	5.5 kWh kg ⁻¹	Ausfelder and Dura (2018)
Redundancies	No	Lowest NPC. Might not be applicable in all cases
Plant decommissioning	No	Depending on assumed lifetime
Heat transfer coefficients	Supplementary Table S8	VDI-Wärmeatlas (VDI, 2013) Disclose other sources
Educt and product purities	Supplementary Table S5	Possible reason for deviation in results
Operating conditions	Process-dependent	Disclose validation
Construction materials	Supplementary Table S6	Disclose if other materials are used
Process simulation assumptions	Depending on process	Disclose equations of state, reaction rates, pressure losses, etc.
Economic		
Currency	€ ₂₀₁₈	To account for inflation: disclose the year of analysis
Interest rate	5%	IRENA (2021)
Calculation methodology	Peters et al. (2004), Albrecht et al. (2017)	
Cost factors	Supplementary Table S1–S2	
Annual operation time	8,000 h/a	Downtime for maintenance assumed
Lifetime plant	20 years	cf. Schemme et al. (2020), Schorn et al. (2021), and Kramer et al. (2018)

(Continued on the following page)

TABLE 1 (Continued) Minimal base assumptions with example values for a German PtX plant.

	Example value	Explanation
Working hours	Process-dependent	
Labor cost	41 € h ⁻¹	(Eurostat, 2018, p. 4)
Equipment	Standard equipment	Pumps, heat-exchangers, etc. (Peters et al., 2004)
	Special equipment	Electrolyzer SI: Chapter 4
Transport cost	0 €	Minimal cost. Transport location-dependent
LCOE electricity and source	Table 2; Supplementary Table S10–S14	Highly important for NPC.
H ₂ cost and source	Table 4, Supplementary Table S15–S23	Highly important for the NPC. Define and disclose pressures and qualities
CO ₂ cost and source	Table 6, Supplementary Table S24–S29	Highly important for the NPC. Define and disclose pressures and qualities
Cost of auxiliary materials and by-products	Supplementary Table S5	
Ecological		
Functional unit	1 kWh of electricity 1 kg of hydrogen/1 t of CO ₂	Depending on technology
Impact assessment method	ReCiPe 2016	Huijbregts et al. (2017) Disclose if different method is used
Scope	Cradle-to-gate	Disclose if different scope is used
Impact category	Climate change	Target for climate neutral transport. Further impact categories desirable
GWP impact of:		
Electricity	Table 3, Supplementary Table S14	Values are dependent on assumed location
Produced hydrogen	Table 4	
Extracted CO ₂	Table 6	

2.1 Technical analysis

A validated process model is the basis for all further analysis, not only for PtX processes. Experimentally derived performance maps of reactors and other equipment should be included in a rigorous process flow diagram (PFD) simulation. Commercial software packages like Aspen Plus® provide chemical component properties and thermodynamic methods to calculate their interactions. The user has to assemble and interlink all required units, define the operating points, and set specifications to achieve an overall system performance at the end. For transparency and reproducibility, it is viable to share all necessary data. A good example can be found in Parigi et al. (2019).

In the technical analysis of a PtX-process, the necessary equipment and its specifications—such as sizes, pressures, temperatures, flow rates, efficiencies, exchange rates, energy losses, kinetic models, catalyst degradation, and achievable temperatures—have to be defined. Some of these parameters might

also be technical results, which must be shared transparently. All simplifications and all assumptions should be communicated. For the comparison of technical results, TKPIs are used. For a carbon-based PtX process, the energetic efficiency η_e and carbon efficiencies Y_C (and Z_C) should be calculated as described in the following equations.

Energetic efficiency, η_e , of the fuel production process is calculated as shown in Equation 1:

$$\eta_e = \frac{\sum \dot{m}_{Prod} \cdot LHV_{Prod}}{\sum \dot{m}_{Educt} \cdot LHV_{Educt} + P_{el}}. \tag{1}$$

Here, $\dot{m}_{Prod}$ is the mass flow of the product, and LHV_{Prod} is the lower heating value of the product. They are divided by the mass flows of the educts $\dot{m}_{Educt}$ multiplied with their lower heating values, LHV_{Educt} , and the sum of electrical power inputs P_{el} . In case of the electrolysis being inside the balance limit (as shown in Figure 4), $\dot{m}_{Educt}$ equals 0, and the efficiency is called the “power-to-fuel” efficiency η_{PtF} , as provided in Equation 2. This efficiency is useful in

TABLE 2 German grid electricity-determined retail prices^a (Fette et al., 2020; Kalis and Wilms, 2020; Eurostat, 2023; Bundesnetzagentur, 2021).

	Unit	2018	2030 ^b	2045 ^{b,c}
Cost—electricity purchase				
Annual average from 8,000 h	€ ₂₀₁₈ (MWh) ⁻¹	44.47	65.53	40.10
4,000 cheapest hours	€ ₂₀₁₈ (MWh) ⁻¹	30.04	43.08	20.70
Charges and levies				
min	€ ₂₀₁₈ (MWh) ⁻¹	11.25	0.60	0.41
max	€ ₂₀₁₈ (MWh) ⁻¹	42.80	33.90	22.90
Retail price—grid electricity				
Annual average min	€ ₂₀₁₈ (MWh) ⁻¹	55.72	66.13	40.51
Annual average max	€ ₂₀₁₈ (MWh) ⁻¹	89.60	99.43	63.00
4,000 h min	€ ₂₀₁₈ (MWh) ⁻¹	41.29	43.68	21.11
4,000 h max	€ ₂₀₁₈ (MWh) ⁻¹	72.84	76.98	43.60

Rounding to two decimals should not be understood as an indication of accuracy.

^aAdditional market mechanisms (e.g., supply and demand and regulations) have a high influence but are hard to predict.

^bCalculation results, see SI section 3.

^cThe values are taken from estimates for 2050. Due to the political requirement to achieve the 2050 targets as early as 2045 and the already considerable uncertainties, the 2050's values were used for the 2045's calculation.

TABLE 3 GHG emissions from electricity production (Fette et al., 2020; Wernet et al., 2016) and calculated results.

	Unit	2018	2030	2045
Power mix 8,000 h	kg CO _{2-eq} kWh ⁻¹	0.506	0.131	0.052
Power mix 4,000 h	kg CO _{2-eq} kWh ⁻¹	0.445	0.054	0.047
PV open space	kg CO _{2-eq} kWh ⁻¹	0.078	0.071	0.069
Wind onshore	kg CO _{2-eq} kWh ⁻¹	0.011	0.01	0.01
Wind offshore	kg CO _{2-eq} kWh ⁻¹	0.011	0.01	0.01

^aRounding to three decimals should not be understood as an indication of accuracy.

comparing different PtX processes concerning the use of “precious” electricity.

$$\eta_{PtF} = \frac{\sum \dot{m}_{Prod} \cdot LHV_{Prod}}{\sum P_{el}}. \quad (2)$$

Since there are various electrolysis systems with system-specific efficiencies, using η_{PtF} for comparison can be misleading if PtX processes use different electrolysis systems. By excluding the electrolysis from the efficiency, the remaining PtX process can be compared. In addition, if hydrogen were supplied from a source other than an electrolyzer, this balance limit could be used. In a minimal-example in Section 4, the corresponding balance limit is

depicted in Figure 4. In this case, the efficiency is called “hydrogen-to-fuel-efficiency” η_{HtF} , which is provided in Equation 3.

$$\eta_{HtF} = \frac{\sum \dot{m}_{Prod} \cdot LHV_{Prod}}{\dot{m}_{H_2} \cdot LHV_{H_2}}. \quad (3)$$

The carbon yield, Y_C , is obtained using Equation 4 as follows:

$$Y_C = \frac{\sum \dot{n}_{CP}}{\sum \dot{n}_{CE}}. \quad (4)$$

Here, $\dot{n}_{CP}$ is the carbon mole flow in the products, excluding waste, and $\dot{n}_{CE}$ is the carbon mole flow in the reactant. If there is a reaction with several products, e.g., Fischer–Tropsch pathway, the carbon efficiency to each

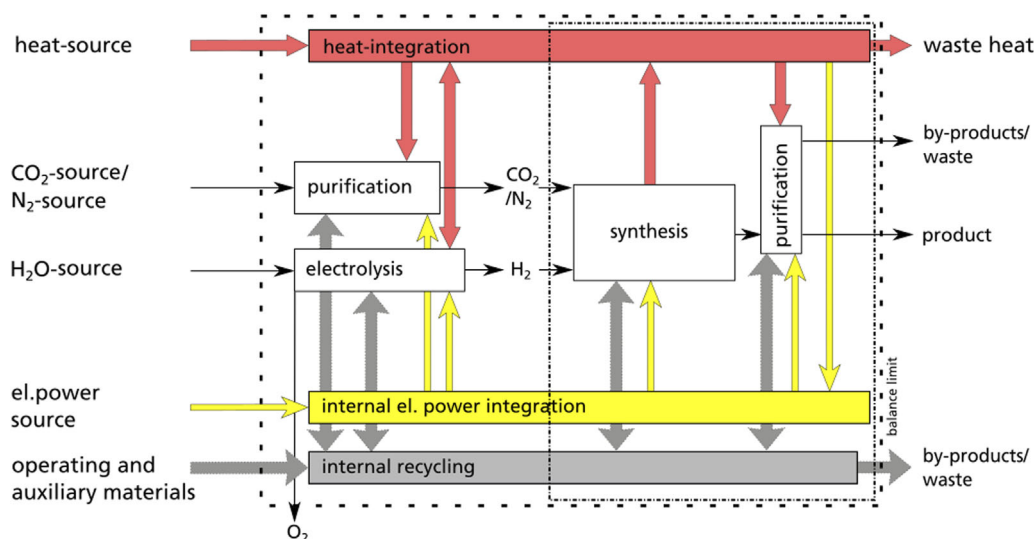


FIGURE 2
Schematic general PtX process with two possible balance limits (including and excluding electrolysis).

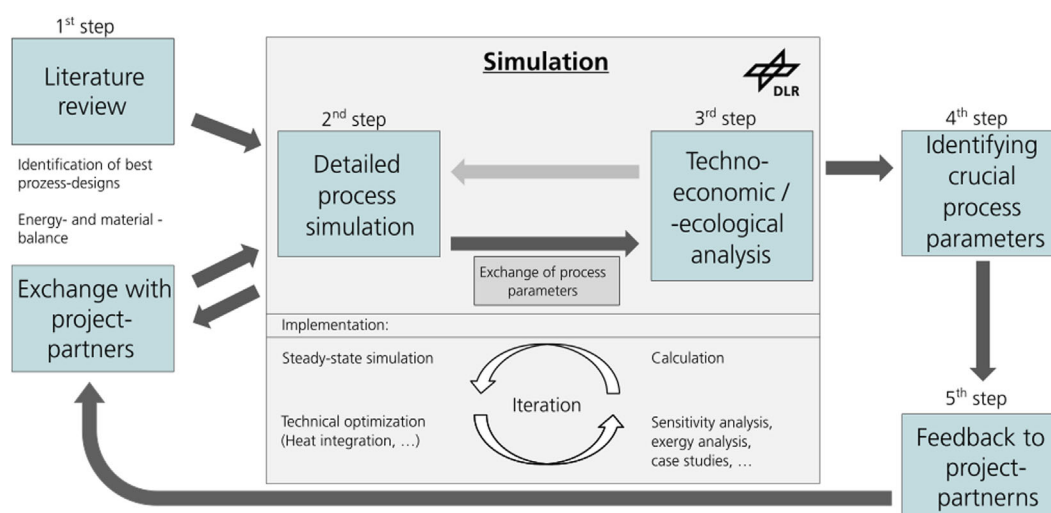


FIGURE 3
Schematic representation of a standardized TEA/LCA. (Albrecht et al., 2017).

product, Z_C , can be calculated using the following equation (Equation 5).

$$Z_C = \frac{\dot{n}_{TP}}{\sum \dot{n}_{CE}}. \quad (5)$$

Here, $\dot{n}_{TP}$ is the carbon mole flow of the target product.

Heat integration potentials are further determined in the technical analysis. This is crucial in order to achieve high efficiencies. A widely used method is the PINCH-analysis, as explained by Linnhoff and Lenz (1987).

The underlying heat transfer coefficients of the heat exchangers are listed in Section 2.2 of the supporting information (SI) and other technical parameters. Depending on the localization of a PtX plant, it could be possible to sell heat in the form of steam. For this case, assumed pressure levels for a German plant are listed in

the SI Section 1.4. Only if the balance limit and other technical assumptions are disclosed completely can technical results, such as energetic efficiencies and carbon yields, be compared.

2.2 Economic analysis

Chemical engineering cost estimation is a well-known procedure for standard large-scale chemical plants (Peters et al., 2004). In PtX-processes, it is often applied to small-scale decentralized plants because of high costs and low availability of renewable power and electrolyzers. This is only partially correct as the error bar of that estimation increases largely toward small-scale demo units, and the results are harder to compare. The main

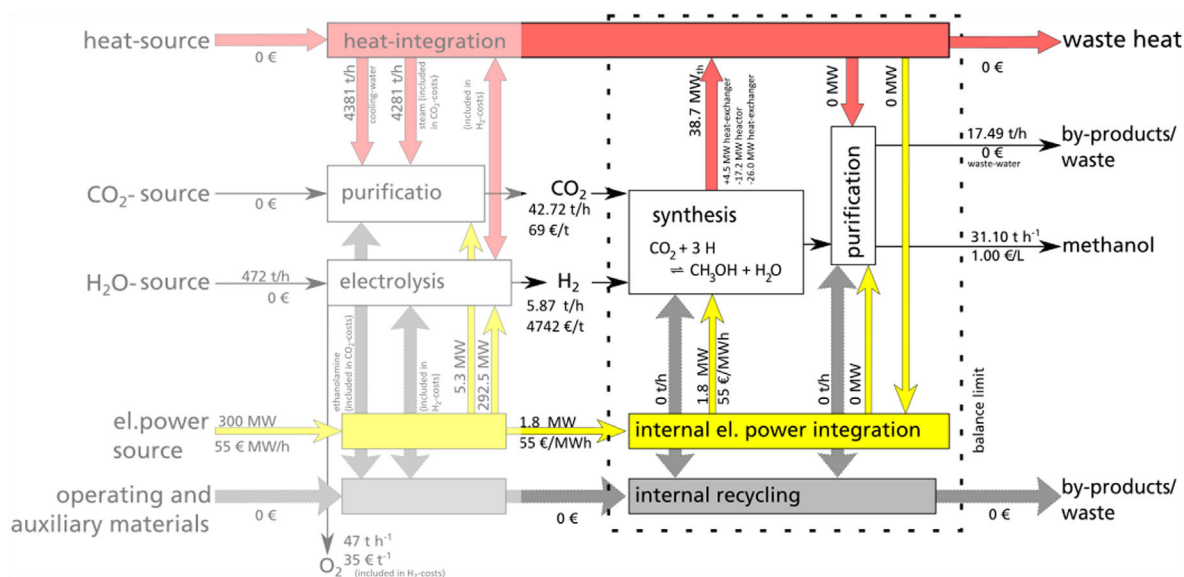


FIGURE 4
PtX example process flows and costs.

results of the economic analysis are capital expenditures (CAPEX), operating expenses (OPEX), and NPCs.

Depending on the available information, an economic analysis can be performed according to different levels of detail and, thus, estimation accuracy. Using the factor method and parameter models presented in this study, it is possible to achieve the estimation accuracy of a feasibility study (Christensen et al., 2005). For higher estimation classes, more extensive, cost-intensive, site-specific, non-generalizable, and significantly longer planning efforts would need to be carried out. However, since “semi-detailed costs” are used for major components, an estimation accuracy of CAPEX between 3 and 4 can be achieved, approximately $\pm 30\%$ (Christensen et al., 2005). For more detailed information on the accuracy of cost estimations, refer to Adelung (2022).

From the process parameters determined in the technical analysis, the CAPEX and OPEX are calculated. The CAPEX is reflected in the annual capital costs (ACCs). In order to calculate the ACC, individual equipment items (pumps, heat exchangers, etc.) need to be calculated using the equipment cost (EC_i) function (6) for the respective years with the given physical characteristics (Albrecht et al., 2017).

$$EC_i = f_i(S_{i,1}; S_{i,2}; \dots; S_{i,k}) \cdot \left(\frac{CEPCI}{CEPCI_{ref}} \right) \cdot F_{pre,i} \cdot F_{mat,i} \quad n, i, k \in \mathbb{N}. \quad (6)$$

Here, $f_i(S_{i,1}; S_{i,2}; \dots; S_{i,k})$ is the cost function of the individual pieces of equipment with defining properties. $S_{i,k}$ are the respective input variables, such as pressure, temperature, and throughput. The inflation adjustment can be determined using the chemical engineering plant cost index (CEPCI), where the current CEPCI is divided by the $CEPCI_{ref}$ of the reference year. Pressure and material factors $F_{pre,i}$ and $F_{mat,i}$ are used to adjust the previously calculated results to certain pressure levels or materials used. For further information, see SI chapter 1. Knowing the individual EC_i , fixed

capital investment (FCI) can be determined using Equation 7.

$$FCI = \sum_{i=1}^m EC_i \cdot \left(1 + \sum_{j=1}^{10} F_{ind,i,j} \right) \cdot \left(1 + \sum_{j=11}^{12} F_{ind,i,j} \right) \quad i, j \in \mathbb{N}. \quad (7)$$

A proposal for standard empirical factors $F_{ind,i,j}$ is provided in the SI in Supplementary Table S1. To calculate the total capital investment (TCI), Equation 8 is used.

$$TCI = FCI \cdot (1 - \text{working capital})^{-1}. \quad (8)$$

With the given values and the interest rate (IR), the annual capital cost (ACC) can be calculated according to Equation 9.

$$ACC \left[\frac{\text{€}}{\text{a}} \right] = FCI \cdot \left(\frac{IR \cdot (1 + IR)^y}{(1 + IR)^y - 1} + \frac{IR \cdot y}{9} \right). \quad (9)$$

Here, y is the plant operation time in years, and IR is the interest rate. For further information on production costs and cash flows during construction, see also Giglio et al. (2015). A subsequent sensitivity analysis allows the influence of different process parameters and input data on production costs to be investigated.

With the plant operating time and the annual production quantities, the NPCs can then be calculated according to Equation 10.

$$NPC \left[\frac{\text{€}}{\text{kg}} \right] = \frac{ACC + \sum OPEX_{ind} + \sum OPEX_{dir} + t_{labor} c_{labor}}{\dot{m}_{Prod}}. \quad (10)$$

Here, t_{labor} is the sum of man-hours, and c_{labor} is the mean hourly labor costs. The product $t_{labor} c_{labor}$ is referred to as operating labor (OL). In order to normalize the costs of the product, several bases can be used: volume, energy, or mass flow of the product, among others. The following reference quantities are proposed: $\text{€}_{\text{year}}/\text{L}$, $\text{€}_{\text{year}}/\text{MJ}_{\text{LHV}}$, or $\text{€}_{\text{year}}/\text{kg}$. To account for inflation, the year should always be specified. Furthermore, it is important to state the concentration of the target product within the presentation of the results or in the assumptions.

2.3 Ecological analysis

For sustainable PtX production, an economic analysis or LCA should be carried out to obtain information on the environmental impacts. It should be carried out according to standardized DIN ISO 14040 (DIN, 2020) and 14044 (DIN, 2018). The following scope of the calculations is proposed:

- **System boundary:** The LCA is performed for the most relevant input flows for the PtX process. For the supply of electricity, hydrogen, and CO₂, the environmental impacts from cradle-to-gate of the technologies and materials are considered. This means that the resource, energy supply, and emissions associated with the construction of the plants are included.
- **Functional unit:** Depending on the technology, the following functional units are proposed: 1 kWh of electricity, 1 kg of hydrogen, or 1 t of CO₂. For the PtX process, a functional unit can be defined by the LCA practitioner. In our exemplary calculation in Section 4, all emissions refer to the flow of the produced methanol in 1 hour.
- **Data:** The data used for the LCA is based on the results of the calculation of the electricity. Example data for a German production are based on the German electricity grid mix and the subsequent technological assessment of hydrogen and carbon dioxide supply. Data for the production of the plants can be derived from technical analysis, literature, or a given production plant. The sources are documented in the chapters of each technology, respectively. In addition to these foreground-data, some data are from secondary databases. The so-called background data includes the supply chain, e.g., material supply. In this work, this is carried out using the database ecoinvent[®] 3.6 (Wernet et al., 2016).
- **Allocation:** In the production of PtX, co-products can occur. The environmental impacts have to be allocated to all products. Therefore, an energetic allocation is proposed.
- **Impact category:** For the life cycle impact assessment, only one impact category, “climate change,” is chosen since the reduction of greenhouse gas emissions is the main motivation for the energy transition. To obtain the CO₂-equivalent of all greenhouse gases, the characterization factors from Intergovernmental Panel On Climate Change (2014) for global warming potential over an integration period of 100 years are used.

More detailed information on the methodology and data used in this study for LCAs of PtX products can be found in the methodology guide for LCAs of e-fuels (Pichlmaier et al., 2021).

3 Assumptions

For comparable results, balance limits and other assumptions must be identical. The assumptions in this study are partly standard approaches and partly assumptions that have been proven valuable in projects with several project partners (e.g., BEniVer). Set example values, like year, size, interest rate, and lifetime, are exchangeable. It is important for comparison that they are defined equally for all analyzed processes.

3.1 Comparability and completeness

For assessment of PtX processes, a list of necessary assumptions is presented in Table 1 in column one. If any of this information is missing from an assessment, the results are not comparable. The second column includes example values, which have been set within BEniVer. These could be used for comparison with the results of the BEniVer project. In the third column, explanations and further information (sources) are given. As an example of how to use the methodology and assumptions, a simplified case is included in Section 4. A comprehensive study using the methodology presented in this study, along with the example values and additional input values, was performed by Rahmat et al. (2023).

To account for changes due to technological progress, the following approach is proposed: The plant is designed for a total nominal capacity of 3 MW_{el} or 300 MW_{el} in 2018. In the following years, the plant is operated with the same material flows, but different efficiencies are assumed, resulting in decreased input power, while the product flow remains the same. This approach allows simulations to be easily adapted to other years.

3.2 Power supply

Electricity represents the most important energetic input to a PtX process. Depending on the electricity source, electricity costs, availability, and environmental impact have to be considered. Detailed explanation and presentation of the underlying data can be found in the SI in chapter 3.

Levelized cost of electricity (LCOE) is calculated according to Equation 11 (IRENA, 2020):

$$LCOE = \frac{\sum_{t=1}^n \frac{I_t + M_t + F_t}{(1+r)^t}}{\sum_{t=1}^n \frac{E_t}{(1+r)^t}} \quad (11)$$

Here, I_t represents the CAPEX of the power plant in year t , M_t represents the operating and maintenance costs in year t , F_t represents the fuel expenses in the year t , and E_t represents the full-load hours in year t . r represents the imputed interest rate, and n represents the depreciation period or the life of the system. Using the assumptions defined in Supplementary Table S11 and the minimum and maximum rates for taxes and levies, the following possible retail prices for grid electricity were calculated.

At present, the German grid mix is not 100% renewable; therefore, PtX products based on that are not “green” *per se*. For more in-depth information and data for 100% renewable sources, see SI section 3. GHG emissions from electricity production are determined using LCA, including the upstream chain of energy sources (e.g., coal) and plant construction (e.g., coal power plant and wind turbine) and disposal. Based on the composition of the respective electricity mix and year, the share of each technology is calculated using the appropriate emission factor from the LCA database ecoinvent[®] (Wernet et al., 2016). The exact allocation is explained in Section 3.5 of the SI. For renewable technologies, emission factors from ecoinvent[®] are also used.

TABLE 4 TEA and LCA values for generic hydrogen.

	Unit	2018	2030	2045
H ₂ costs—minimum for 8,000 FLH ^{a,b}	€ ₂₀₁₈ kg ⁻¹ H ₂	4.74	3.96	2.34
H ₂ costs—maximum for 8,000 FLH ^b	€ ₂₀₁₈ kg ⁻¹ H ₂	6.43	5.51	3.33
H ₂ costs—minimum for 4,000 FLH ^c	€ ₂₀₁₈ kg ⁻¹ H ₂	6.09	3.79	2.02
H ₂ costs—maximum for 4,000 FLH ^c	€ ₂₀₁₈ kg ⁻¹ H ₂	7.66	5.3	3.01
Electricity demand ^d	kWh kg ⁻¹ H ₂	49.84	46.77	43.98
GHG emissions ^{b,d}	kg _{CO₂-eq} kg ⁻¹ H ₂	24.8	6.1	2.3

^aRounding to two decimals should not be understood as an indication of accuracy.

^bFull-load hours.

^cFor 8,000 FLH electricity, German grid mix.

^dFor 8,000 FLH electricity, German grid mix.

^eAEL, PEM, and SOEC, each 1/3 carbon dioxide.

3.3 Hydrogen supply

In the case of electrolysis being outside the balance limit, example cost and environmental impact data for German production are presented below. Considered electrolysis technologies are alkaline electrolysis (AEL), proton exchange membrane electrolysis (PEM), and high-temperature solid oxide electrolyzer cell (SOEC). The AEL and PEM processes can produce pure oxygen, which can potentially be sold. In this work, it is proposed that this is feasible at a scale of approximately 300 MW_{el}, and thus, the revenue is deducted from the H₂ costs. Based on the technical and economic parameters of the electrolysis and the electricity costs from Section 3.2, an individual TEA has been calculated for each electrolyzer according to the methodology from Section 2.2. The economic values include capital expenditures for the entire system, the stack's share of capital expenditures, and specific maintenance costs. The individual results of the respective types of electrolysis are listed in the SI section 4. Individual LCA for each process has also been carried out using the methodology described in Section 2.3.

For the GHG emissions, energy and material flows from the technical analysis and the plant construction are considered. The material input of plant construction is based on the following studies: AEL (Liebich et al., 2020), PEM (Bareiß et al., 2019), and SOEC (Wulf and Kaltschmitt, 2018). Considering the stack and plant lifetime, the plant construction is normalized to kg of hydrogen produced. Furthermore, the purchased electrical energy, water consumption, and consumption of other operating materials, such as potassium hydroxide, are considered for the operating phase. The energy and material flows in the operating phase were linked to datasets from the ecoinvent® database and calculated using LCA software.

For generalized German hydrogen production, it is still unknown which technology will capture which market share as each technology has its advantages and disadvantages. Therefore, generic values have been defined and proposed, assuming that AEL, PEM and SOEC each take up one-third. Table 4 provides the costs for large-scale generic production of hydrogen at a specified transfer

TABLE 5 Composition of “generic CO₂” by year.

Source	2018	2030	2045
DAC	0%	5%	10%
MEA: cement	70%	60%	45%
MEA: GS ^a	15%	20%	25%
MEA: MVA	15%	15%	20%

^agas and steam power (GS) plant.

pressure of 50 bar and a temperature of 50 °C, along with the energetic and ecologic values.

Anion exchange membrane (AEM) electrolysis is not considered in this study since the technology was only available at the beginning of EiV in the “single-digit kW range” (Sunfire GmbH, 2023). Equivalent results can be calculated in the same manner as described for the other electrolysis technologies.

3.4 Carbon supply

Considered CO₂ sources are direct air capture (DAC) and extraction from point sources. The compositions of point sources are listed in Supplementary Table S24 in SI. Within BEiV, the following CO₂ sources were assumed to exist until 2045: cement plant, combined gas and steam (GS) plant, and waste-to-energy plant (MVA). Based on the technical and economic parameters of the DAC and the process simulations of an ethanolamine (MEA)-scrubber, an individual TEA is performed for each CO₂ supply option. The results are presented in the SI section 5. In order to make different approaches more comparable, “generic CO₂” is proposed in addition to data for specific CO₂ sources. Due to a lack of informed data, educated estimates of the contributions of CO₂ sources to the average German CO₂ mix are shown in Table 5.

TABLE 6 TEA and LCA of generic CO₂.

	Unit	2018	2030	2045
CO ₂ costs—minimum (8,000 h ^a)	€ ₂₀₁₈ t _{CO₂} ⁻¹	68.95	82.19	89.61
CO ₂ costs—maximum (8,000 h ^a)	€ ₂₀₁₈ t _{CO₂} ⁻¹	73.13	87.52	93.42
CO ₂ costs—minimum (4,000 h ^b)	€ ₂₀₁₈ t _{CO₂} ⁻¹	87.27	107.33	123.34
CO ₂ costs—maximum (4,000 h ^b)	€ ₂₀₁₈ t _{CO₂} ⁻¹	91.16	112.66	127.85
Steam 4 bar	t t _{CO₂} ⁻¹	1.77	1.80	1.83
El. power consumption	kWh t _{CO₂} ⁻¹	123.25	160.05	200.85
Cooling water	t t _{CO₂} ⁻¹	100.20	97.28	96.29
GHG emissions ^a	t _{CO₂-eq.} t _{CO₂} ⁻¹	0.07	0.03	0.02
GHG emissions (incl. CO ₂ capture) ^a	t _{CO₂-eq.} t _{CO₂} ⁻¹	-0.93	-0.97	-0.98

^aRounding to two decimals should not be understood as an indication of accuracy.

^aFor 8,000 FLH electricity, German grid mix.

^bFor 4,000 FLH electricity, German grid mix.

Table 6 provides the resulting costs for a large-scale generic supply of carbon dioxide at transfer conditions of 3 bar and 35 °C, along with the energy and environmental impacts.

The ecological impact considers the energy and material flows determined in the TEA, such as raw materials, auxiliaries, and plant construction. Material data from the following sources are used for the ecological balance of plant construction. For DAC, data from Lozanovski (2019) were applied. For the selection of background processes from ecoinvent[®], the process designations from the appendix of Liebich et al. (2020) were used. For flue gas scrubbing with MEA, the data from Liebich et al. (2020) were used. Considering the plant lifetime, the plant construction was related to one ton of CO₂. In the operation phase, the purchased electrical energy, water consumption, and consumption of other operating materials, such as cooling water and MEA, were considered.

Captured CO₂ enters the life cycle assessment as negative emissions. Captured CO₂ can be attributed either to the supply side, if it is captured from air, to process-related emissions, or to the fuel itself (Ausfelder and Dura, 2018). Since this has not yet been decided in regulations, the results are shown in Supplementary Table S29 in SI. The resulting values are depicted in Table 6 in case it is allocated to energy and material flows.

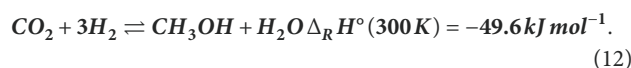
4 Result

To illustrate the application of the methodology and proposed assumptions, a simplified and idealized example of methanol synthesis is presented. In this section, the application of the presented methodology can be observed. Furthermore, the presented cost data (H₂, CO₂, and electricity) for German

production are integrated to facilitate understanding of their use. In contrast to realistic plants, no recycle streams are included, no catalyst is considered, and reaction kinetics are omitted. All these effects are neglected, resulting in an idealized outcome. However, for a basic understanding of the methodology, this example is sufficient. For deeper insights into the methanol synthesis, see, for example, Rahmat et al. (2023).

4.1 Assumption example process

For the stoichiometric direct conversion of CO₂ and H₂ to methanol, the chemical sum equation is defined as shown in Equation 12:



For simplicity, the chemical equilibrium is not considered, but a theoretical 100% yield in an artificial super reactor is assumed. CO₂ and H₂ with min costs for 8,000 FLH (see Tables 4,6) are mixed stoichiometrically and compressed to 40 bar using a compressor. Then, the reaction with an assumed 100% conversion rate takes place with no by-products but water. In the next step, a 100% separation of water and methanol is assumed. It is known to the authors that the separation of the product in reality would take place in a two- to three-stage rectification, where product losses occur. In this study, for simplification, no energy or material losses are assumed, nor are costs and revenues for heat, water, by-products, and waste. In order to present the methodology for calculating equipment cost, the cost calculation of one compressor is shown in Table 8. All other equipment costs for synthesis or purification are calculated similarly for a valid process model but are not necessary for the presentation of the methodology here and are therefore assumed to be 0.

Furthermore, the following values were assumed.

If one of these values is missing or if the main input values are defined differently, a comparable analysis cannot be achieved. For instance, if the hydrogen source is defined differently, it will have an influence on the technology (depending on the quality of H₂), costs, and GWP. Different target purities of methanol have a significant influence on the technology and energy demand. In this study, an oversimplified example has been selected. In reality, several distillation columns would be needed.

4.2 Technical analysis

Using Equation 13, the values given in Table 7, and the simulation, the energy efficiency η_{PIF} is 57%.

$$\eta_{PIF} = \frac{31,101\text{kg h}^{-1} \cdot 5.5\text{kWh kg}^{-1}}{292,561\text{kW}_{(\text{electrolysis})} + 5,265\text{kW}_{(\text{CO}_2\text{purification})} + 1,813\text{kW}_{(\text{compression})}} = 57\%. \quad (13)$$

In the literature, η_{PIF} efficiencies range from 40% (Adnan and Kibria, 2020) to 56% (Andersson et al., 2014). With a generic hydrogen source for 2018, 66.8% of the electrical energy is converted into the LHV of hydrogen. Other losses occur in CO₂ purification due to compression and the exothermic reaction, as also indicated

TABLE 7 Assumption of the oversimplified example process (values not mentioned: set as in Table 1).

Assumption	Value	Remark
General		
Country	Germany	
Year	2018	
Balance limit	Electrolyzer and CO ₂ extraction excluded	
Size	300 MW	
Technical		
Compressor	Compressor single stage	Aspen Plus® ; SI Supplementary Table S7
Recycle	No	Simplification
Reactor pressure	40 bar	
Conversion	100%	Simplification
Target purity	100% methanol at 30 °C and 1 bar	Simplification
Equation of state	Peng Robinson	
Catalyst	Not present	Simplification
Distillation columns	No	Simplification
Heat integration	No	Simplification
Economic		
Electricity cost	55.72 € ₂₀₁₈ (MWh) ⁻¹	Retail price grid electricity. Annual average minimum 2018; Table 2
H ₂ cost	4.74 € ₂₀₁₈ kg ⁻¹ H ₂	H ₂ costs minimum for 8,000 FLH; Table 4
CO ₂ cost	68.95 € ₂₀₁₈ t _{CO2} ⁻¹	CO ₂ costs minimum for 8,000 FLH; Table 6
O ₂ -sale	Already considered in generic H ₂	Chapter 3.3
Cost heat, water, auxiliary materials, reactor, columns, etc.	0 €	Simplification
<i>t</i> _{labor}	1,200 h a ⁻¹	1.5 persons assumed
<i>m</i> _{methanol}	31.1 t h ⁻¹	Simulation result
Equipment used	Compressor, centrifugal, stainless steel	Peters et al. (2004) See also SI Supplementary Table S7
Ecological		
Heat source	Waste heat	Enters system without the emission factor
Oxygen for synthesis	Emission factor: market for oxygen, liquid	ecoinvent®
Simulation result		
H ₂ mass flow	5.87 t h ⁻¹	Resulting from overall power demand
CO ₂ mass flow	42.72 t h ⁻¹	Stoichiometry

TABLE 8 Example process compressor EC_i (Peters et al., 2004).

Property	Value	Remark/source
Nominal power P	1,813 kW	
Material	Stainless steel	
$f_i(S_{i,1}; S_{i,2}; \dots S_{i,k}) = f_i(P) =$	$3034.997 \cdot P^{0.678}$	
$F_{mat,i}$	2.5	Stainless steel
Cost	\$ 1,230,135	
Reference year	2002	
Exchange rate 2018	0.8475 €/ \$	ExchangeRates.org.uk (2023)
CEPCI _{ref}	€ 395.6	Chemical Engineering (2025)
CEPCI	€ 603.1	
EC _i	€ ₂₀₁₈ 1,589,372	Equation 6

in Figure 4. Excluding the electrolysis process, the calculated hydrogen-to-fuel efficiency as shown in Equation 14 is 88%, which is in the range of literature data, which is between 82% (Rahmat et al., 2023) and 88% (Schemme et al., 2020).

$$\eta_{HtF} = \frac{31,101 \text{ kg h}^{-1} \cdot 5.5 \text{ kWh kg}^{-1}}{5,870 \text{ kg}_{H_2} \text{ h}^{-1} \cdot 33.3 \text{ kWh kg}^{-1}} = 88 \%. \quad (14)$$

Since no heat and no electricity are included in the equation, mostly the product losses are indicated in this efficiency. For full conversion, the carbon yields, as described in Equations 15,16, are equal to 100% since no purge is included. Thus, no carbon loss occurs.

$$Y_C = \frac{0.97 \text{ Mmol}_{methanol} \text{ h}^{-1}}{0.97 \text{ Mmol}_{CO_2} \text{ h}^{-1}} = 100 \% \quad (15)$$

In a real process, by-products would form. Unreacted educts would also have to be recycled. To prevent inert gases from accumulating in a recycle, a purge stream had to be included. Both effects result in a lower carbon efficiency as 73% in Schemme et al. (2020) and up to 96% in Rahmat et al. (2023).

4.3 Economic analysis

For Equation 6, the following information is needed, as listed in Table 8.

With the resulting EC_i and the factors provided in the SI in Supplementary Table S1, the FCI can be calculated as shown in Table 9.

With the given values, the TCI (Equation 16) can be calculated as follows:

$$TCI = \frac{M\text{€}_{2018} 8.005}{1 - 0.15} = M\text{€}_{2018} 9.41. \quad (16)$$

With an assumed interest rate of 5% (see Table 1) and using Equation 9, the ACC equals 1.53 M€₂₀₁₈ a⁻¹. Given the values

TABLE 9 Example process FCI based on Peters et al. (2004).

Source	j	Base	Factor ^a	Value in € ₂₀₁₈
			1	1,589,372
Equipment installation	1	EC	0.47	746,005
Instrumentation and control	2	EC	0.36	572,174
Piping (installed)	3	EC	0.68	1,080,773
Electrical (installed)	4	EC	0.11	174,831
Buildings including services	5	EC	0.18	286,087
Yard improvements	6	EC	0.10	158,937
Service facilities (installed)	7	EC	0.70	1,112,560
Total direct plant costs (D)			Total (D)	5,721,739
Engineering and supervision	8	EC	0.33	524,493
Construction expenses	9	EC	0.41	651,642
Legal expenses	10	EC	0.04	63,575
Total direct and indirect plant costs (D + I)			Total (D + I)	6,961,449
Contractor's fee	11	D + I	0.05	348,072
Contingency	12	D + I	0.10	696,145
			FCI	€ ₂₀₁₈ 8,005,666

^aIn this case, it is assumed that the compressor is not viewed as the “main compressor” as in Supplementary Table S1 of the SI.

in Table 7, the operational labor (OL) results in 0.49 M€₂₀₁₈ a⁻¹. In Table 10, the intermediate and the main results of the OPEX_{ind} calculation are shown.

Given the flows over the balance limit (Table 7) and the exemplary cost data for German production in 2018, the OPEX_{dir} results are shown in Table 11.

Using Equation 9 and the intermediate results, the NPC can be calculated as shown in Equation 17:

$$NPC \left[\frac{\text{€}}{\text{kg}} \right] = \frac{(1.53 + 0.92 + 247.1 + 0.5) \frac{M\text{€}_{2018}}{a}}{248,807.8 \frac{t}{a}} = 1 \frac{\text{€}_{2018}}{\text{kg}}. \quad (17)$$

The calculated NPC could be compared to other production processes that use the same input parameters and methodology.

Additionally, calculations of net present values could be carried out. These, however, have the disadvantage of adding

TABLE 10 Calculation of the OPEX_{ind} example process.

	j	Base	Factor	Intermediate results in € ₂₀₁₈	Value example process in € ₂₀₁₈
Operational labor (OL)				492,000	
Operation Supervision (OS)	1	OL	0.15		73,800
Maintenance: labor costs	2	FCI	0.01 ^a		79,951
Maintenance: cost of materials	3	FCI	0.01 ^a		79,951
Total maintenance (M)				159,902	
Operating supplies (OS)	4	M	0.15		23,985
Laboratory charges	5	OL	0.2		98,400
Insurances and taxes	6	FCI	0.02		159,902
Total labor costs (TLC)				645,751	
Plant overhead (PO)	7	TLC	0.5 ^a		322,876
Administrative costs	8	PO	0.25		80,719
Distribution and selling expenses	9	NPC	-		0
R&D Costs	10	NPC	-		0
			OPEX _{ind}		€ ₂₀₁₈ 919,584

^a(Peters et al., 2004).

TABLE 11 Example process energy and material flows OPEX_{dir}.

Power	$\dot{m}_{R\&B_i}$	Unit	$c_{R\&B_i}$	Unit	Value	Annual costs ^a in € ₂₀₁₈ a ⁻¹
Generic CO ₂ 2018 min	42.72	t h ⁻¹	68.95	€ ₂₀₁₈ t ⁻¹	2,945	23,562,74
Generic H ₂ 2018 min	5.87	t h ⁻¹	4,742	€ ₂₀₁₈ t ⁻¹	27,836	222,684,320
Electricity 2018 min ^b	1.81	MW	55.72	€ ₂₀₁₈ MWh ⁻¹	101	808,006
					OPEX _{dir}	247,055,067 € ₂₀₁₈ a ⁻¹

^a8,000 h a⁻¹.

^bElectricity is only considered a direct input to the methanol synthesis process since electricity costs have already been considered within the CO₂ and H₂ costs.

high uncertainties since future market prices of the products are not known.

An overview of the flows and resulting costs is depicted in Figure 4.

These results are only for illustrative purposes. What can be observed is that each of the costs for the input flows have to be set uniformly, as well as the calculation methodology, in order to make different process analyses comparable. A TEA of power-to-methanol based on rigorous process simulation and two reaction kinetic approaches carried out with BENiVer assumptions by Rahmat et al. (2023) resulted in a slightly higher NPC between 1.13 € kg⁻¹ and 1.48 € kg⁻¹.

The TEA is independent of the target audience and the intended application (see comments on Langhorst et al. (2022) in the introduction).

4.4 Ecological analysis

For a comprehensive LCA, each material used for construction or within the process has to be assessed. Since a lifetime of 20 years, no by-products, no catalyst, and only one compressor are assumed, its influence on the environmental impact of the production is negligible for this minimal example. Therefore, a simplified LCA is

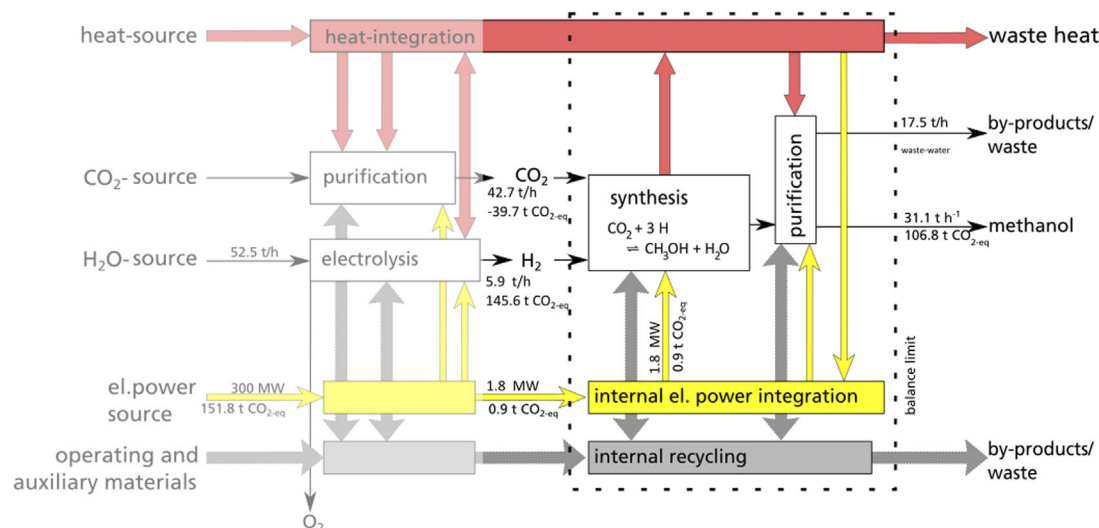


FIGURE 5
PtX example process results LCA.

conducted. Since a separate LCA for H₂, CO₂, and electricity has already been performed for German production, mass and energy flows from the technical analysis of the example process are used and connected with their CO₂-eq. footprint as shown in Figure 5. The underlying relative CO₂-eq. footprints for the streams are already presented in Table 3,4,6 and SI in Supplementary Table S23,S29. The resulting total GHG emissions are calculated to deliver the functional unit, which in this case, is a mass flow of 31.1 t h⁻¹.

The main influence on the overall GHG emissions is to be observed in the H₂ production. Since German grid electricity in 2018 is selected, it has a high share of non-renewable energy, which is reflected in the high CO₂-eq. allocated to H₂. The share of renewable energy is expected to increase in the future (see Supplementary Table S13 of SI). 100% renewable electricity for a German production facility currently comes with the drawback of reduced full-load hours, which would have to be assessed in more detail, including storage. For more information, see Raab et al. (2022), Ibáñez-Rioja et al. (2023). The assumed negative CO₂-eq. of the 2018 generic German CO₂ source can be achieved if it is allocated to the fuel. Currently, the regulations do not define where CO₂ has to be allocated to. The exemplary results presented in this study excluded materials such as steel, catalysts, and concrete in the LCA. These would increase the environmental impacts. Unless all material and energy streams are produced carbon-neutral, the product will always have a GWP greater than 0, but it might still be lower than that of fossil products. Additionally, transportation of the final product would also have to be assessed. A comparison of how close the simplified example is to more realistic processes is difficult since the main assumptions (CO₂ and H₂ source) are selected differently. Further impact categories might even be higher. For further information on LCA of PtX production and other impact categories, see Pichlmaier et al. (2021) and Weyand et al. (2023).

The LCA is independent of the target audience and the intended application (see comments on Langhorst et al. (2022) in

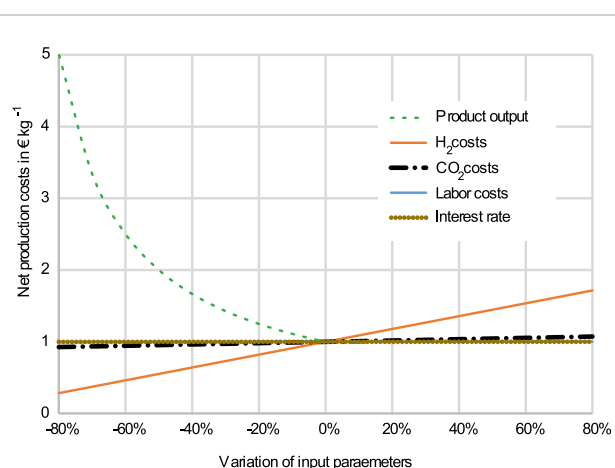


FIGURE 6
Sensitivity study NPC for the example process.

the introduction) but highly dependent on the setting of input parameters and the calculation methodology.

4.5 Adaption to other conditions

The analysis can be adapted to other conditions, such as country and prices, by changing the input parameters required in Table 1. For the first analysis, a sensitivity study can be carried out as shown in Figure 6 for the example process for ±80% of variance.

It can be observed that the product output has the highest influence on the NPC. So, if the plant runs with less FLH, the cost of the product would increase. However, this still might be necessary if fluctuating renewable energy has to be used. However, the electricity price for renewable energy and, therefore, the H₂ price could be lower. For other countries, the H₂ or CO₂ sources could vary, as

well as labor costs and interest rates. For a thorough analysis, all these parameters would be changed and an analysis carried out, but the sensitivity study provides first insights into the magnitude of influence on the result. An equal analysis could be carried out for the LCA.

For comparing other products or production processes, another synthesis would have to be defined, which is state of the art. All economic and ecological input values, such as year and H₂-source lifetime, would have to be set equally. The subsequent analysis would follow the same steps as defined in this work.

If “greenfield” is selected instead of “brownfield,” additional information would be needed. These include preparation of the land, foundations, roads, sewage treatment, electricity connection, steam generation, safety equipment, car parks, ecological compensation areas, additional storage, fees, and taxes. For all of these data, costs had to be defined and included into CAPEX- and OPEX-calculations (see also Peters et al. (2004)).

5 Summary and outlook

This publication addresses the problem of non-comparable analysis results of the PtX production pathway in the current literature by sharing a compact list of minimal required data, which are needed for a TEA and LCA (see Table 1). Its completeness and consistency provide the basis for standardized assessment. This represents a significant improvement in the current status of assessment comparability, as stressed in the introduction. For instance, in contrast to Langhorst et al. (2022), this study includes a definition of how the product is specified and a definition of the calculation methodology, and additional uncertainties are reduced by calculating the NPC instead of the net present value. A methodology for TEA and basic information for an LCA concerning the GWP were presented, based on DIN ISO 14040 (DIN, 2020) and 14044 (DIN, 2018). Furthermore, an easy-to-handle set of data and assumptions, used in the EiV-project (BMWK, 2017), was shared. It represents a defined set-point from which all processes can be compared, if intended. If an analysis is carried out at another set-point, the values for this new set-point would have to be presented completely. Table 1 helps ensure that no value is overlooked. Using the new set-point, a new comparable analysis could be carried out.

Within the presented dataset, estimated forecasts are presented. These have been calculated carefully, but technology and cost estimations for 2030 and 2045 are subject to great uncertainty. Current crises highlight the volatility of energy prices and commodity markets. Nevertheless, processes can be compared based on identical assumption, and their potential contribution to the climate change mitigation efforts in the transport sector, locally or worldwide, can be quantified.

Finally, a minimized example has been presented for explanatory purposes, knowing that the result is an oversimplification.

As an impact category example of the LCA, the GWP was selected since this is the main target parameter for decarbonizing the transport sector. A standardized assumption of the GWP for electricity, H₂ and CO₂ also enables better comparability. The analysis of further impact categories is necessary for real pathway assessment. Unfortunately, not all underlying data of the LCA could be shared due to the terms of use of the ecoinvent® database.

Adjustments, such as plant dimensions, synergies through suitable site selection, influences of individual process stages on the overall result, and other basic assumptions, can be addressed via sensitivity studies using the methodology presented (see chapter 4.5). This work presents a step toward a comprehensive comparison of all options for de-fossilization of the transport sector in Germany. However, this still requires an evaluation of the use and other aspects such as logistics, further environmental impact categories, infrastructure, taxation or subsidies, the application in the means of transport, and regulatory framework conditions.

In order to achieve climate goals, multi-megawatt scale plants are required to produce alternative fuels if current demand remains. However, neither renewable electricity volumes nor electrolyzer capacities are currently available at a refinery scale, so plants were considered at the scale of available demonstration plants and initial commercial scale.

The authors hope that this publication contributes to a more transparent comparison of PtX processes and thus facilitates the search for the best-suited solutions for the transition to greener alternatives.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material; further inquiries can be directed to the corresponding author.

Author contributions

NH: Visualization, Writing – original draft. MR: Conceptualization, Data curation, Writing – review and editing. NW: Data curation, Investigation, Methodology, Writing – review and editing. SH: Data curation, Methodology, Writing – review and editing. SP: Methodology, Writing – review and editing. R-UD: Data curation, Supervision, Writing – review and editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fenrg.2025.1297299/full#supplementary-material>

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Glossary

AEL	Alkaline electrolysis
AEM	Anion exchange membrane
BEniVer	Accompanying Research on the energy transition in transport (Ger. Begleitforschung Energiewende im Verkehr)
BMWK	German Federal Ministry for Economic Affairs and Climate Action (Ger. Bundesministerium für Wirtschaft und Klimaschutz)
CAPEX	Capital expenditures
CO₂-eq. km⁻¹	CO ₂ -equivalent per kilometer driven
DAC	Direct air capture
E-fuels	Electricity-based fuels
EiV	Energy transition in the transport sector (Ger. Energiewende im Verkehr)
FLH	Full-load hours
GHG	Greenhouse gas
GS	Gas and steam power plant
LCA	Life cycle assessment
LHV	Lower heating value
MEA	Ethanolamine
MVA	Waste-to-energy plant
NPC	Net production costs
OL	Operating labor
OPEX	Operating expenses
PEM	Proton exchange membrane
PFD	Process flow diagram
PtX	Power-to-X
PV	Photovoltaic
SI	Supporting Information
SOEC	Solid oxide electrolyzer cell
TEA	Techno-economic analysis
TKPI	Technical key performance indicator

Symbols

$\dot{m}_{\text{Educt}}$	[t h ⁻¹] Mass-flow educt
$\dot{m}_{\text{Prod}}$	[kg h ⁻¹] Mass-flow product
$\dot{n}_{\text{CE}}$	[kg _C h ⁻¹] Molar flow carbon in the educt
$\dot{n}_{\text{CP}}$	[mol _C h ⁻¹] Molar flow carbon in the product

$\dot{n}_{\text{TP}}$	[mol _C h ⁻¹] Molar flow carbon-targeted product
ACC	[€ a ⁻¹] Annual capital cost
ACC	[€ L ⁻¹] Annual capital cost
CEPCI	[€] Chemical engineering plant cost index
CEPCI_{ref}	[€] Chemical engineering plant cost index reference
c_{labor}	[€ h ⁻¹] Mean hourly labor costs
EC	[€] Equipment cost
EC_i	[€, \$, ...] Equipment cost
E_t	[€ ₂₀₁₈ (kW a) ⁻¹] Full-load hours in year t
FCI	[€] Fixed capital investment
F_{ind,i,j}	[-] Indirect cost factors
F_{mat,i}	[-] Material factor of component i
F_{pre,i}	[-] Pressure factor of equipment i
F_t	[€ ₂₀₁₈] Fuel expenses in the year t
IR	[%] Interest rate
LCOE	[€ ₂₀₁₈ (MWh) ⁻¹] Levelized cost of electricity
LHV_{Educt} [kJ kg⁻¹]	Lower heating value of the educt
LHV_{Prod} [kJ kg⁻¹]	lower heating value of the product
I_t	[€ ₂₀₁₈ kW ⁻¹] Specific investments in year t
M_t	[€ ₂₀₁₈ (kW a) ⁻¹] Operating and maintenance costs in year t
n	[a] Amortization period
NPC	[€ L ⁻¹] Net production cost
P	[kW] Sum of electrical input-power
r	[-] Interest rate
S_{i,k}	[p, T, kg h ⁻¹ , etc.] Input variable s(e.g., pressure, temperature, and throughput)
TCI	[€] Total capital investment
t_{labor}	[h] Man-hours
t_{labor}c_{labor} [€ a⁻¹]	Operating labor
y	[a] Plant lifetime
Y_c	[-] Carbon efficiency
Z_C	[-] Carbon efficiency-targeted product

Greek letters

η_e	[-] Energetic efficiency
η_{H2tF}	[-] Energetic efficiency: power to fuel
η_{PtF}	[-] Energetic efficiency: power to fuel