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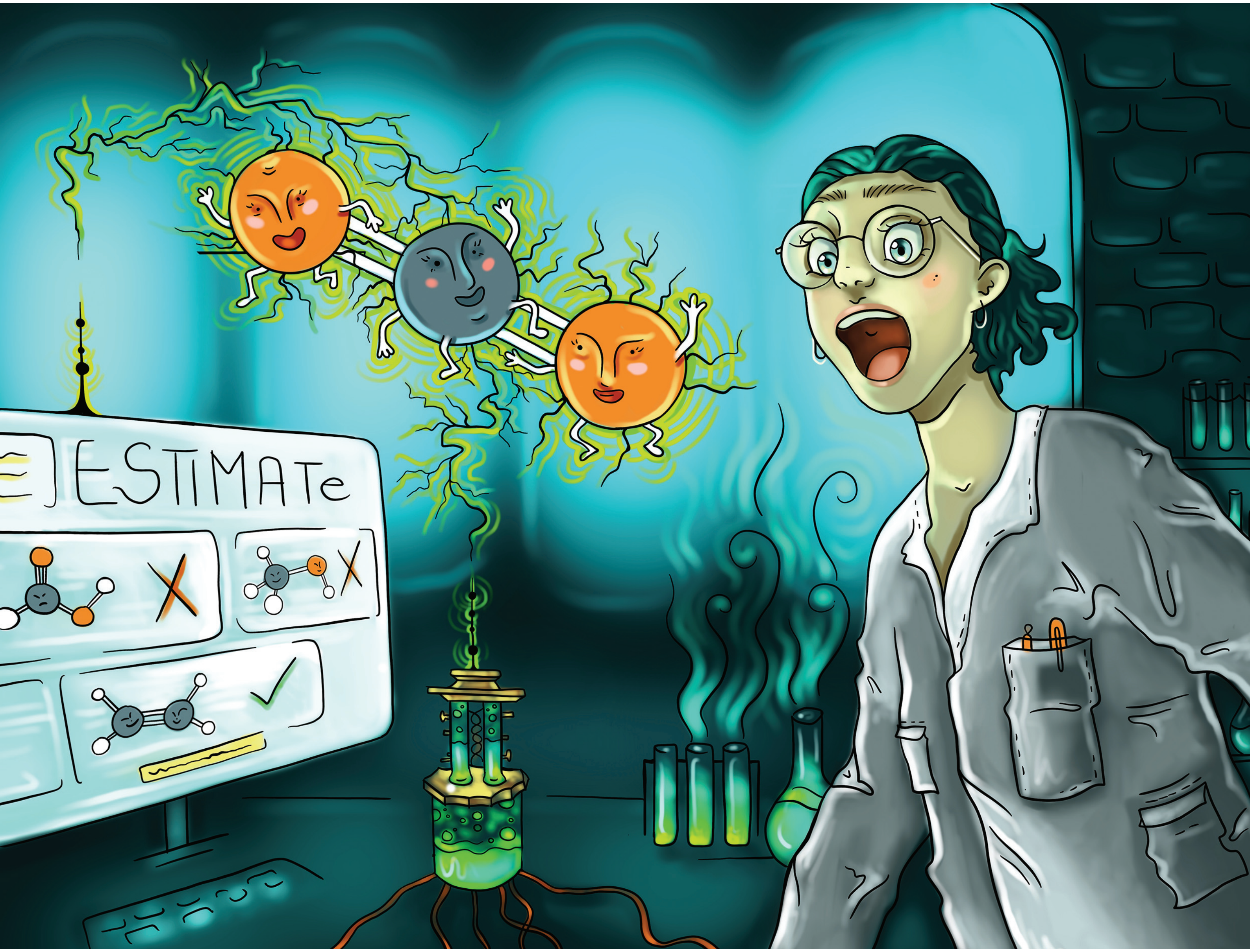

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Early-stage impact assessment tool (ESTIMATe) for the life cycle assessment of CO_2-based chemicals†

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In the pursuit of climate change mitigation, the chemical industry is developing carbon capture and utilization (CCU) processes to eliminate fossil carbon feedstock. Life Cycle Assessment (LCA) of CCU processes is crucial to verify climate change mitigation and identify potential burden shifting to other areas of environmental damage. Preferentially, this knowledge would be available already in early process development. However, LCA expertise is sparse and LCA studies are often data-intensive and complex, limiting the accessibility to non-LCA experts. To bridge this accessibility gap, we present ESTIMATe, an open-source Excel tool automating LCA assumptions and using estimation methods to streamline the LCA of CCU processes. ESTIMATe, designed for non-LCA experts, quickly provides simplified early-stage LCA results before a comprehensive LCA would usually be conducted. Our case studies demonstrate how ESTIMATe guides process development at different levels of process maturity by assessing climate change mitigation potentials, analyzing environmental impacts along the course of process development, and comparing the environmental performance of process alternatives. ESTIMATe is thus designed to complement rather than replace comprehensive LCA software, providing early access to LCA results and enabling process developers to incorporate environmental perspectives into their decision-making. The ESTIMATe tool is available for download at **https://doi.org/10.5281/zenodo.11060469**.

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1. Introduction

The chemical industry is responsible for 7% of CO_2 emissions and 10% of energy use globally.[1] To mitigate greenhouse gas emissions, novel processes are being developed that utilize low-carbon energy and eliminate fossil feedstock.[2] As an option to eliminate fossil feedstock, carbon capture and utilization (CCU) captures and converts CO_2 into value-added products.[3,4] Even if CO_2 from a fossil source is used, CCU products can potentially reduce greenhouse gas emissions compared to conventional fossil-based products.[5] However, climate benefits from CCU are not guaranteed, for instance when energy-intensive process steps are required.[4,6] Consequently, CCU process development requires a holistic environmental impact assessment.

The 12 principles of green chemistry,[7] introduced 25 years ago, have proven invaluable as qualitative guidelines for lowering the environmental impact of chemicals. These principles continue to shape environmentally conscious practices in a large community committed to sustainable chemical processes. Alongside these qualitative principles, the integration of quantitative approaches is essential for a more comprehensive evaluation of environmental impact.

One prominent quantitative method is Life Cycle Assessment (LCA),[8,9] highlighted as the gold standard for demonstrating a "green advance" in chemistry in a recent editorial.[10] LCA is a standardized method that quantitatively evaluates the environmental impacts of products and services over their entire life cycle and for a holistic set of environmental impact categories, *i.e.*, areas of environmental damage.[8,9] It is desirable to conduct LCA studies as early as possible in process development for several key reasons:[2,11–15] first, so-called early-stage LCA can evaluate the theoretical environmental potential of CCU process routes which allows to sort out unpromising options before investing time and money into subsequent development stages. Second, early-stage LCA informs process developers regarding possible burden shifting towards other areas of environmental damage.

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Third, investigating the sensitivity of the environmental performance towards process parameters and external variables provides valuable insights to improve process development.

However, early-stage LCA in general and the LCA of CCU technologies in particular present unique challenges that are not yet addressed in the LCA ISO standards. For LCA studies of CCU technologies, for instance, assumptions related to carbon accounting are especially crucial.[16–18] In early-stage LCA, methodological research is ongoing concerning a number of challenges related to comparability, scale-up issues, uncertainty and uncertainty communication, and data availability.[13,19] For instance, primary process data required for LCA are not available in the early stages of process development, causing data gaps.[11,19–23] Filling such data gaps leads to a trade-off between the early availability of LCA results and result accuracy. For a comprehensive discussion of the current challenges in early-stage LCA and approaches to overcome those challenges, readers are encouraged to refer to the recent review by Moni *et al.*[19]

To address the challenges in early-stage LCA of CCU technologies, the Global Carbon Initiative has published the CCU guidelines.[16] The CCU guidelines define typical methodological decisions, suggest methods to fill data gaps, and provide guidance to ensure a consistent assessment with meaningful results.

Still, despite the benefits of early-stage LCA, and efforts to simplify and standardize early-stage LCA for CCU technologies, LCA is not widely applied by chemists and process developers in green chemistry.[10] Expertise in the field of LCA is often scarce, and the practical application of LCA according to the standards and guidelines remains challenging for non-LCA experts. Instead, LCA experts are usually consulted only in later process development stages, *e.g.*, when a technology is introduced at large scale. To foster the application of early-stage LCA in the field of green chemistry, non-LCA experts should be able to conduct early-stage LCA studies with low effort.

In contrast to full LCA software such as SimaPro, GaBi, or Brightway, Excel-based LCA tools present a more accessible entry point for non-LCA practitioners.[24] In the landscape of Excel-based LCA tools, only a few options exist, the majority of which are tailored to the building sector.[25–27] However, three specific tools are relevant in the context of LCA for novel chemical products: first, the TECHTEST Excel Tool[28] allows techno-economic assessments, energy, and carbon balance calculations for novel technologies. The environmental assessment in TECHTEST comprises two categories: Climate Change Impact and energy use. The user is guided through the environmental assessment but must look up emission and energy use factors for material inputs manually in the NREL database. Most importantly, the user must make LCA methodological decisions. Furthermore, TECHTEST lacks data generation support and a focus on CCU technologies. Second, AssessCCUS[29] allows users to enter input data for Life-Cycle and Techno-Economic Assessments of CCUS technologies online and exports the assessment results as an Excel file. AssessCCUS calculates Manufacturing Costs, Climate Change Impact, and Water Use mainly from user-specified data, but provides emission factors for electricity, natural gas, and fuel oil. Impact categories other than Climate Change and Water Use are not supported, and data generation is outside of the scope of the tool. Third, the LCA Model for CCU[30] provides an interactive overview of the Climate Change Impact of CCU technologies from the literature. However, the model does not allow users to generate, enter, or assess their own process data. For conducting LCA studies, the model further lacks a holistic set of impact categories.

In this work, we present the ESTIMATe method and tool which enable non-LCA experts to conduct consistent early-stage LCA of CCU processes within minutes using Microsoft Excel.

Between other Excel-based LCA tools, ESTIMATe stands out as specifically tailored to assessing early-stage CCU processes yielding fuels and chemicals in a holistic set of impact categories. By automating LCA assumptions, supporting data generation, incorporating a background database, and applying scenario analyses, ESTIMATe minimizes required user input. In this way, non-LCA experts can obtain robust LCA results quickly.

ESTIMATe is based on the CCU guidelines[16] and specifically tailored to assess CCU processes for organic chemicals and their mixtures. The focus on chemicals allows the automatization of LCA assumptions and assessment steps, which reduces LCA knowledge required of the users. We implement our method in the open-access ESTIMATe Excel tool which:

(1) applies the LCA methodology consistently,

(2) employs estimation methods accepted in the LCA community to fill data gaps depending on data availability, and

(3) shows results for a holistic set of impact categories and provides concise explanations of assumptions and limitations to the user.

In section 2, we briefly introduce the ESTIMATe method and its underlying assumptions. Section 3 demonstrates the application of the ESTIMATe Excel tool with a focus on user inputs *vs.* tool outputs. For this purpose, we are assessing electrochemical CO_2 reduction to ethylene at different levels of data availability. In section 4, we discuss our results critically and conclude.

2. Method: calculation of environmental impacts *via* ESTIMATe

ESTIMATe calculates environmental impacts of CCU chemicals and their fossil benchmark technology. The tool is tailored for assessing organic chemicals and their mixtures, with a particular focus on high-volume basic organic chemicals, and has been specifically developed and tested for thermocatalytic conversion and electroreduction of CO_2. Since the environmental impacts of many CCU chemicals depend strongly on the energy input,[16] an automated scenario analysis is integrated to resolve the level of decarbonization in the background energy system. ESTIMATe provides both quantitative results and result figures, together with a summary of assumptions made during the LCA study.

To generate the LCA results, ESTIMATe consists of five steps (*cf.* Fig. 1): (1) goal definition, (2) LCA methodology, (3) data generation, (4) background system linkage, and (5) the calculation of LCA results. User input is required in the steps 1 (goal definition) and 3 (data generation), and optional in step 4 (background system linkage). Overall, the assessment in ESTIMATe requires the following minimum user input:

- a list of products and reactants,
- the specification whether the reaction is thermochemical or electrochemical, and
- the specification whether the product is used as an intermediate or a fuel.

With increasing technology maturity, further user input can be added to improve the estimation.

In the following subsections, we briefly introduce the methodology behind ESTIMATe by elaborating on the steps of the ESTIMATe method:

(1) Goal definition: Common goals accompanying process development (section 2.1)

(2) LCA methodology: Application of LCA standards in line with the goals (section 2.2)

(3) Data generation: Methods to close data gaps according to data availability and study goal (section 2.3)

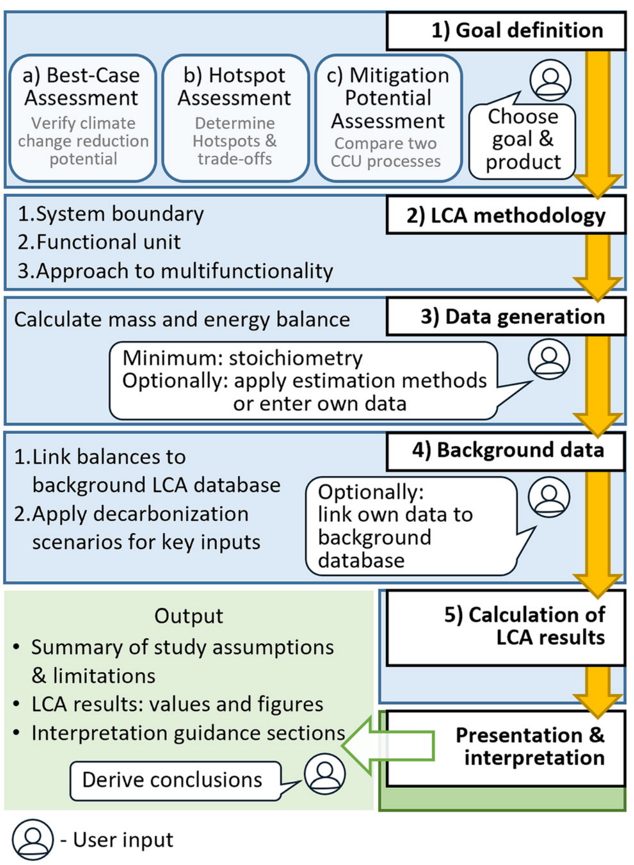

Fig. 1 Overview of the ESTIMATe method and user inputs in each step. CCU – carbon capture and utilization.

(4) Background system linkage: Scenario application for relevant utilities (section 2.4)

(5) Calculation of LCA results: multiple environmental impact categories (section 2.5)

Then, we summarize how ESTIMATe presents results and study assumptions (section 2.6). Finally, section 2.7 explains the data basis of ESTIMATe.

2.1. Goal definition

The first step of any LCA study is the definition of the study goal, *i.e.*, the central research question. In our discussions with process development specialists, three main questions emerged regarding the development of new processes:

Is the process (a) meeting minimum expectations, (b) competitive to the benchmark technology, and (c) the best choice compared to other novel processes?

Consequently, ESTIMATe offers three types of studies: Best-Case Assessment, Hotspot Assessment, and Mitigation Potential Assessment. All assessments in ESTIMATe are comparative LCA studies, *i.e.*, the environmental impacts of a new process are assessed in relation to a benchmark.

Best-case assessment. Best-Case Assessments verify the greenhouse gas reduction potential, support Go/No–Go decisions, and identify possible burden-shifting to other environmental impacts. For this purpose, a robust lower boundary of the Climate Change Impact is calculated from theoretical best-case assumptions for the new process. The best-case environmental impacts are then compared to the fossil-based benchmark process. Best-Case Assessments are in alignment with the LCA part of "Monitoring" studies according to the CCU guidelines,[16] tailored to the needs of decision-makers (*e.g.*, management).

Hotspot assessment. In Hotspot Assessments, the new process is investigated regarding its environmental hotspots and trade-offs. The new process is compared either to the current fossil-based benchmark or to a competing CCU route to the same product. Moreover, key contributors to the environmental impact are identified to support further process development. Hotspot Assessments correspond to the LCA part of "R&D support" studies as described in the CCU guidelines.[16]

Mitigation potential assessment. Finally, Mitigation Potential Assessments compare emission reductions and burden-shifting across two CCU processes. If the compared processes yield different products, the comparison takes place based on a shared resource under the assumption that each product replaces its fossil-based benchmark process. This study type supports decision-making under limited resource availability. If two processes producing the same product are compared, the comparison takes place on the basis of the same amount of product produced.

2.2. LCA methodological assumptions

LCA studies involve making several methodological choices in line with the LCA standards and the study goal to ensure valid results.

For instance, the *functional unit* quantifies the qualitative function of each system under study and must be identical for compared systems. The *system boundary* specifies which life-cycle stages are studied in the assessment, usually containing the complete life cycle ("cradle-to-grave"). In comparative LCA, identical life-cycle stages for compared systems may be neglected. Systems providing multiple functions (*e.g.*, co-production of two chemicals) require a *multi-functionality approach* to allocate environmental impacts to individual products.[8,9] Below, we describe the LCA-methodological assumptions in ESTIMATe.

Functional unit and system boundary. Functional unit and system boundaries for CCU products depend on whether the product is a chemical intermediate or a fuel, and on whether the product's chemical structure and composition are identical or different to the benchmark.[16] In early-stage assessments conducted *via* the ESTIMATe tool, the chemical structure is assumed identical to the benchmark for both chemical intermediates and fuels. This assumption limits ESTIMATe's current applicability to CCU chemicals and synthetic fuels identical to existing counterparts. A potential avenue for future research involves broadening ESTIMATe's applicability to assess differing synthetic fuels.

For Best-Case and Hotspot Assessments, chemical intermediates are evaluated using a mass-based functional unit, while fuels are evaluated with a functional unit based on energy.[16] Since identical products are assumed, the life cycle of the benchmark and the new process differs only up to the production process ("the gate"). All subsequent life-cycle stages are identical for both routes and may be neglected in the comparative assessment.[8,9,16] The system boundaries are thus "cradle-to-gate", including the whole supply chain up to the final product delivered at the factory gate.

After assessing CCU chemicals separately, Mitigation Potential Assessments allow for the additional comparison of two CCU chemicals. The ISO standards specify that consistent comparisons in LCA require the compared processes to fulfill the same function, *i.e.*, supply the same functional unit. Consequently, if Mitigation Potential Assessments compare different chemicals that each provide a unique function, a mass-based functional unit is not applicable. Still, a comparison of the mitigation potential of two CCU products might be desirable, necessitating the definition of a suitable a basis of comparison for the products. To solve this issue, we adopt the approach proposed by Sternberg *et al.*[31] and analyse which product uses a scarce resource most efficiently. For this purpose, we quantitatively define the functional unit as the use of the scarce resource, for instance, 1 kg of captured CO_2 or 1 kWh of renewable electricity. This approach reflects that CCU technologies compete for a limited renewable feedstock or energy supply. Furthermore, we assume that each process's main product replaces its conventional counterpart (benchmark) and give a credit for avoiding the environmental impacts of the benchmark (as further discussed in the section "solving multi-functionality"). Consequently, a Mitigation Potential Assessment answers the question "Which process uses the scarce resource most efficiently?". Since Mitigation Potential Assessments examine the supply chain up to the desired products, "cradle-to-gate" system boundaries are again applied.

While suitable for assessments in ESTIMATe, "cradle-to-gate" system boundaries may lead to misinterpretation of results: the release of carbon captured within the product is not accounted for in the assessment scope, potentially giving the impression of "carbon-negative" chemicals. However, all captured carbon is most likely emitted at the end of the product's life. Only if carbon sourced from air is stored permanently (CCS), true carbon negativity may be achieved. To avoid misinterpretation, ESTIMATe calculates the amount of carbon present in the product and the corresponding stoichiometric CO_2 emissions in each assessment. The user is thus informed of probable end-of-life emissions. ESTIMATe prominently displays information on captured carbon and system boundaries wherever climate change impacts are presented, ensuring clarity for non-LCA experts.

Solving multi-functionality. Per default, ESTIMATe assumes all co-products to be combusted and emitted to the environment to overestimate rather than underestimate the environmental impact. At the user's discretion, individual co-products can be classified as by-products, for which a multi-functionality approach must then be applied. ESTIMATe employs two multi-functionality approaches outlined in the ISO standards: the avoided burden approach and, as a fallback, allocation.

The avoided burden approach assumes that the co-production of a given product replaces its benchmark production, thereby avoiding the environmental burden associated with the benchmark. Please refer to the ESI† for details on the avoided burden approach and an example of its application to CCU.

While the avoided burden approach is commonly used in LCA, results must be interpreted carefully to avoid misinterpretation. Specifically, the avoided environmental burdens depend on the assumption that by-products actually replace the benchmark process, and on the choice of benchmark process, which might improve or change in the future. Furthermore, assumed avoided emissions could be misinterpreted as true emission removal from the environment. ESTIMATe clearly distinguishes avoided burdens from other environmental impacts, *cf.* sections 3.3 and 3.4.

Only if no benchmark dataset is available for the avoided burden calculation, ESTIMATe employs allocation to solve multi-functionality. Allocation distributes the environmental impacts between two products based on flow properties such as mass, energy content, or economic value. In accordance with the literature,[18] ESTIMATe recommends the economic criterion because of its broad applicability. Users with experience in LCA can perform a sensitivity analysis on the multi-functionality approach in ESTIMATe.

2.3. Data generation

LCA studies generally require a "process inventory", *i.e.*, detailed mass and energy balances of the studied process.[8,9]

In the early stages of process development, however, comprehensive data on the industrial-scale process are not available yet. Consequently, suitable estimation methods are required to fill data gaps such as reactant masses and utility demands.

The minimum required user input for data generation in ESTIMATe is a list of products and reactants, from which ESTIMATe calculates a stoichiometric mass balance for the Life Cycle Assessment. Since the data availability increases with the process development, the CCU guidelines recommend more accurate methods to close data gaps depending on the Technology Readiness Level (TRL).[16] All estimation methods recommended in the CCU guidelines that are applicable to early-stage CO_2-based chemical production (up to TRL 4) are implemented in ESTIMATe. In this way, *e.g.*, energy demands for product separation and purification can be incorporated into ESTIMATe assessments. For an overview of all implemented methods, the reader is referred to the ESI.† When assessing technologies above TRL 4, results from process design software or measured data from real plants may be manually entered into the ESTIMATe tool.

Via a simple questionnaire, ESTIMATe supports the user in selecting the most accurate method for the current data availability. Each estimation method is explained, its source referenced, and a comment on data quality and limitations is provided. In particular, the tool supports the consistency of estimation methods with the study goal. For instance, Best-Case Assessments require optimistic/"best-case" estimation methods to provide a reliable lower boundary of environmental impacts.

At TRL 1 and 2, the CCU guidelines recommend mostly stoichiometry-based estimation methods and heuristics. In ESTIMATe, mass and energy balances resulting from these methods are automatically scaled to the study's functional unit.

At TRL 3 and 4, estimation methods are based on simple process design equations for individual equipment, such as distillation columns or dryers. Although ESTIMATe does not generate a flowsheet connecting individual units, ESTIMATe calculates utility demands per mass throughput of individual units. Users may copy and paste the resulting utility demands into their assessment.

Finally, the user may adapt the process inventory in Hotspot Assessments manually. In that way, the user can add *e.g.*, solvents, inerts, catalysts, or additional energy demands to the assessment as the process development progresses. When LCA experts assess a process at a later stage of development, transferring modeled processes from the ESTIMATe tool to established commercial LCA software is easy, since ESTIMATe lists reference products, amounts, and linked background processes from the LCA database ecoinvent (*cf.* section 2.7).

2.4. Background data linkage

Langhorst *et al.*[16] identify differing supply chain assumptions as the key cause for diverging results of LCA studies in the CCU context. Scenario analysis allows to evaluate the new process in multiple supply chain contexts, which in turn yields a more comprehensive understanding of the expected environmental impact.

For relevant reactants and utilities, ESTIMATe applies four scenarios representing different decarbonization levels. We use the scenarios provided in the CCU guidelines[16] for electricity, heat, hydrogen, carbon dioxide source, and natural gas supply. In all scenarios, the capture of feedstock carbon dioxide mitigates Climate Change Impact, either by avoiding emissions from a coal-fired power plant or by removal of CO_2 from the atmosphere *via* direct air capture. As a relevant utility to the chemical industry, we add steam production datasets that correspond to the scenarios for heat production with additional energy losses for water evaporation. Table 1 summarizes the four decarbonization scenarios. Experienced users have the flexibility to diverge from these predefined scenarios by opting for ecoinvent processes or self-modelled processes instead.

We use ecoinvent data for utilities. Processes not included in the ecoinvent database (*e.g.*, methanation) are modelled from literature sources specified in the CCU guidelines. Despite neglecting details such as leakages and emissions from the construction phase, for instance for constructing the CO_2 capture systems, the literature process inventories are considered satisfactory since they are modeled as recommended in the CCU guidelines. We model steam production based on our own assumptions. All modelled process inventories are included in the ESI.†

While decarbonization scenarios are applied to processes modelled within ESTIMATe, the scenario analysis is not extended to processes from the ecoinvent database. The assumption of constant ecoinvent environmental impacts presents a recognized limitation of ESTIMATe, particularly when using ecoinvent data as a benchmark or avoided burden. In such cases, where a new process with decarbonization scen-

Table 1 Overview of the four decarbonization scenarios in ESTIMATe, based on the scenarios from Langhorst *et al.*[16] Electricity scenario source: International Energy Agency[40]

	Status quo	Low-decarbonized	High-decarbonized	Full-decarbonized
Electricity	IEA ETP reference	IEA ETP 2 °C scenario, year 2030	IEA ETP 2 °C scenario, year 2050	Wind power
Hydrogen	Steam methane reforming	Alkaline electrolysis	Alkaline electrolysis	Alkaline electrolysis
Feedstock CO_2	Coal-fired power plant	Coal-fired power plant	Direct air capture	Direct air capture
Heat	Natural gas vessel	Electrode boiler	Electrode boiler	Electrode boiler
Steam	From heat	From heat	From heat	From heat
Natural gas	Natural gas grid mix	Natural gas grid mix	Methanation (CO_2-based)	Methanation (CO_2-based)

arios is compared to a fossil process under current boundary conditions, it is essential to exercise caution in result interpretation as detailed in section 3. Despite this limitation, the constant ecoinvent impact is a valuable initial data point enabling a swift preliminary assessment. Users may further enhance their assessment by modelling benchmark and avoided burden processes within ESTIMATe, presenting a practical solution to integrate decarbonization scenarios. Addressing the limitation of constant ecoinvent impacts is a potential future focus for ESTIMATe, for which the adoption of a dynamic LCA approach as discussed in the literature[32–34] seems promising.

2.5. Calculation of LCA results

LCA is not limited to climate change impact assessment but considers a holistic set of impact categories to avoid environmental burden shifting to other areas. Multiple Life Cycle Impact Assessment methods are available in the literature. For ESTIMATe, we select two methods: firstly, ReCiPe Midpoint V1.13[35,36] due to its widespread application in the literature and, secondly, Environmental Footprints 3.0 (EF 3.0), which is recommended by the European Commission's Joint Research Center.[37] In each assessment, results are calculated for all environmental impact categories of the ReCiPe and EF methods. The ESTIMATe manual in the ESI† offers instructions for users with LCA expertise to incorporate additional impact assessment methods if desired.

ESTIMATe calculates climate change impacts from by-product emissions under the assumption of complete combustion to CO_2 and H_2O.

2.6. Result presentation and interpretation guidance

Early-stage LCA with the ESTIMATe method examines environmental impact contributions of each entry in the process inventory, which allows the user to identify opportunities for improving processes and supply chains. Furthermore, the comparison to a benchmark process allows providing context, simplifying the evaluation of the new process.

When interpreting LCA results, it is crucial to consider the study assumptions to come to correct conclusions. For this purpose, all assumptions, including their influence on result interpretation, are summarized in the ESTIMATe tool using text boxes. These summaries contain the assumptions on data sources, functional unit, system boundary, and scenarios. For instance, it is important to recognize that negative impacts resulting from avoided burden assumptions (*cf.* section 2.2) are due to the methodology, and do not represent a net removal of carbon dioxide from the atmosphere. Another instance of potential misinterpretation arises with negative Climate Change Impacts which can occur due to the "cradle-to-gate" system boundaries of LCA studies in ESTIMATe. To avoid misinterpretation of negative total impacts as "negative emission technologies", ESTIMATe indicates to the user how much captured CO_2 is bound in the product at the end of the assessment scope. ESTIMATe further explains that all captured CO_2 will likely be emitted at the product's end-of-life and only technologies achieving permanent CO_2 storage may achieve net carbon negativity (*cf.* section 2.2).

2.7. Data basis of ESTIMATe

For environmental impact data, ESTIMATe relies on ecoinvent,[38] the largest environmental impact database. While users require a license for ecoinvent, the use of ecoinvent data in an Excel format allows the integration of the database directly into ESTIMATe, avoiding the need for users to search for background data themselves. Furthermore, automatic linkage of products to ecoinvent processes is possible, for instance for the benchmark processes of chemicals, or for common process inputs such as cooling water. While ESTIMATe has been developed using the attributional ecoinvent version 3.8 cut-off, it is in principle possible to include other database versions, including the consequential system model. However, please note that slight modifications to the import of ecoinvent into ESTIMATe might be necessary, which would require LCA expertise.

As mentioned in section 2.4, ESTIMATe further extends the ecoinvent database with literature data to include decarbonized background system processes. In a separate worksheet in ESTIMATe, the user can explore the environmental impacts of these literature data through the four decarbonization scenarios.

ESTIMATe contains a default list of 97 organic chemicals and their chemical properties[39] for generating data through stoichiometric calculations and ideal thermodynamics. However, users can supplement the list with additional organic chemicals. The same list contains the substance "characterization factors", sourced from the ecoinvent website.[38] Characterization factors quantify the environmental impact of a substance's emission in each of the impact methods mentioned in section 2.5.

Users may extend the chemical database with chemicals relevant to their assessment consisting of the elements carbon, hydrogen, oxygen, and nitrogen. Additionally, ESTIMATe provides the functionality to create pseudo-components for representing fuel mixtures, enabling assessments of synthetic fuels. The reader is referred to the manual provided in the ESI† for a synthetic fuel assessment example.

In summary, the environmental impact and chemical property data integrated in ESTIMATe reduce the user's effort for data research and thus facilitates environmental assessments.

3. Results

This section demonstrates the practical application of ESTIMATe with a focus on user input and the resulting tool output. For this purpose, we study the example of electrochemical CO_2 reduction to ethylene in four study setups. While ESTIMATe enables assessments for any organic chemicals and their mixtures, we select the ethylene case study due to the availability of literature data from different stages of process development. The four case studies allow us to illustrate how the ESTIMATe tool accompanies chemical process development, and each study highlights different features of ESTIMATe: first, a Best-Case Assessment establishes a Climate Change Impact reduction potential before starting process development (section 3.1). Second, a laboratory-scale Hotspot Assessment illustrates ESTIMATe's data generation process and the use of estimation methods (section 3.2). As an exemplary sensitivity study, we demonstrate the implementation of a CO_2 recycle and its impact on environmental impacts. Third, a hotspot assessment based on data from process design software shows how ESTIMATe supports data input and handles by-products (section 3.3). Finally, a Mitigation Potential Assessment compares the environmental impact of electrochemical CO_2 reduction to ethylene to another promising CCU technology at the process design scale, namely, CO_2 hydrogenation to methanol (section 3.4). Together, the four sections illustrate the process design guidance offered by ESTIMATe across multiple stages of process development. All figures in this section are sourced directly from ESTIMATe. Climate change impacts are determined using the EF3.0 impact assessment method (*cf.* section 2.5). While assessment-specific limitations are discussed in each results section, ESTIMATe's general limitations are summarized in the conclusion (section 4).

3.1. Best-case assessment

In the first case study, we assess the greenhouse gas reduction potential of electrochemical CO_2 reduction to ethylene by establishing a robust lower boundary of the Climate Change Impact. For this purpose, we conduct a Best-Case Assessment starting from only a list of products and reactants. We make ideal assumptions for the novel process and compare the assessment results to the fossil benchmark technology.

User input and required steps in ESTIMATe. We choose the Best-Case Assessment goal, specify the process name and designate ethylene as the main product to create a new assessment spreadsheet (goal definition, *cf.* section 2.1). At the top of the created sheet (Fig. 2), we review the LCA methodological assumption (*cf.* section 2.2) on intended product use to ensure that ethylene is assessed as a chemical intermediate on a mass-basis instead of as a fuel. ESTIMATe preselected the ecoinvent dataset "market for ethylene" as benchmark technology, representing a current technology mix for ethylene production, mainly composed of steam cracking.

In the data generation step (section 2.3), we enter the reactants (CO_2 and water) and products (ethylene and oxygen), and specify the reaction type as electrochemical. ESTIMATe then computes the gross reaction equation and process energy demand based on idealized assumptions, *i.e.*, 100% CO_2 conversion, perfect selectivity, and thermodynamic minimum energy demand. Based on the gross reaction equation, ESTIMATe calculates and displays the process energy and mass balance, giving the user the option to double-check the balances and the background system linkage (section 2.4).

For the final step (calculation, section 2.5), ESTIMATe generates results across four decarbonization scenarios. The results are presented both numerically and in figures which illustrate the contribution of individual process inputs and outputs to the overall environmental impact. Overall, conducting this Best-Case Assessment takes as little as one minute.

Results and conclusions for process development. Due to the idealized nature of Best-Case Assessments, a key limitation is that the real process can never achieve the performance reported in the results, as the results represent a theoretical lower boundary of environmental impacts. Consequently, the Climate Change Impact has only two main contributors: electricity generation and the CO_2 capture process. The CO_2 capture process has a negative Climate Change Impact due to avoiding CO_2 emission to the atmosphere. Consequently, the Climate Change Impact reaches negative values in low-, high-, and full-decarbonized background system scenarios (Fig. 3). The Climate Change Impact of the best-case electrochemical CO_2 reduction to ethylene decreases as the decarbonization level of the background system increases. Negative Climate Change Impact values are possible since ESTIMATe examines only the environmental impacts of production ("cradle-to-gate" study), and carbon emitted to the atmosphere at the end of the life cycle of ethylene is outside of the assessment scope. However, the storage of carbon in ethylene is not permanent, as it would be in a Carbon Capture and Storage (CCS) technology. Instead, carbon bound in ethylene will most likely be emitted to the atmosphere at the end-of-life of the product. A text box adjacent to Climate Change Impact graphs in ESTIMATe

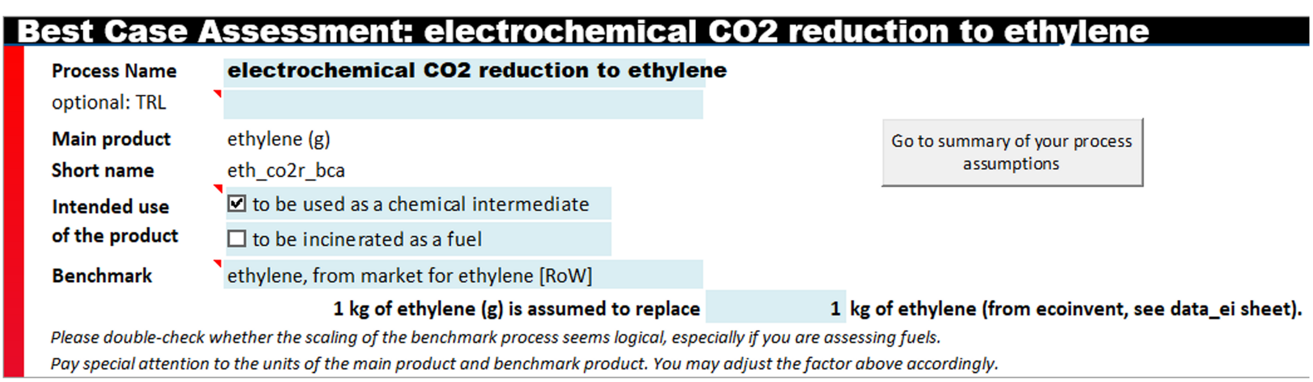

Fig. 2 The study setup section in ESTIMATe for the Best-Case Assessment of electrochemical CO_2 reduction to ethylene.

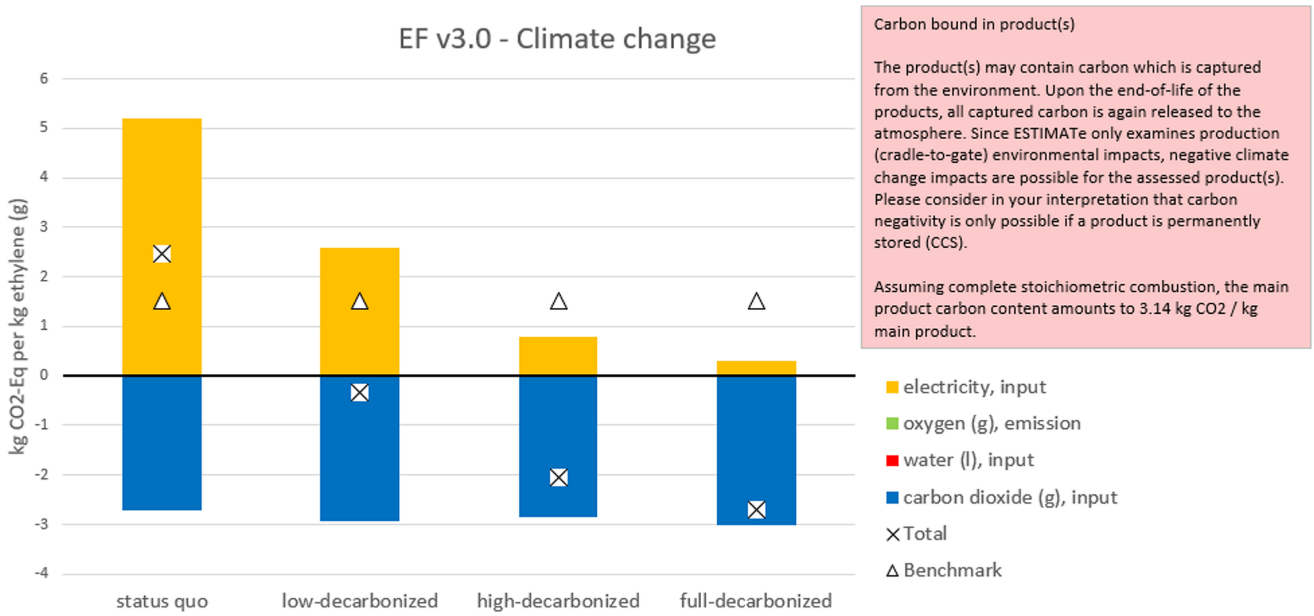

Fig. 3 Climate Change Impact of the Best-Case Assessment of electrochemical CO_2 reduction to ethylene in the ESTIMATe tool. The different bars correspond to the different background system scenarios defined in section 2.4.

emphasizes the temporary storage of CO_2 and specifies the amount of carbon dioxide released at the end-of-life of the product to avoid misinterpretation by the user. For instance, per kg of ethylene, 3.14 kg of CO_2 are emitted at the end-of-life assuming stoichiometric combustion. The "cradle-to-grave" Climate Change Impact of ethylene production is thus always positive if the product is incinerated at the end of life.

Compared to the benchmark, electrochemical CO_2 reduction achieves a lower Climate Change Impact in all scenarios except for the *status quo*, indicating that further development of the process is promising. However, the performance in the *status quo* scenario also shows that the potential for Climate Change Impact reduction depends on the background system – even for the technology's theoretical best case.

Furthermore, environmental burden is shifted to other impact categories (Fig. 4), which aligns with burden-shifting observed in renewable energy systems in general.[2,34] The main contributor to this burden-shifting is increased electricity use in combination with a shift towards renewable electricity sources. For instance, "Material resources: metals/minerals" impacts soar as more wind and solar power plants are needed (Fig. S2 in the ESI†). Since fossil-based technologies have been optimized over decades and modeled in detail in LCA databases, the benchmark often outperforms the new technology in categories other than the Climate Change Impact. ESTIMATe qualitatively displays all impact categories (*cf.* Fig. 4). For each impact category, the recommendation level from the Joint Research Center (JRC) of the European Commission is also reported as a measure for the underlying uncertainty within the impact category: the higher the recommendation level, the higher the uncertainty. A higher deviation in impact is then expected for more uncertain categories, as observable in Fig. 4, for instance in the "Material resources: metals/minerals" category. Users can examine the key contributors to the environmental impact in each impact category in ESTIMATe.

3.2. Hotspot assessment at laboratory scale

In a laboratory-stage assessment of electrochemical CO_2 reduction to ethylene, we examine the environmental impacts in comparison to the benchmark process and compare the results to those of the Best-Case Assessment (section 3.1). Further, we identify areas of improvement for the environmental performance of electrochemical CO_2 reduction to ethylene. Laboratory data for this case study section is taken from the literature, with an optimistic assumption of 25% single-pass conversion.[41,42]

User input and required steps in ESTIMATe. Similarly to the first assessment, we choose the study goal, select ethylene as the main product, and review the automated assumptions. The data generation step (*cf.* section 2.3), however, differs from the Best-Case Assessment since laboratory results instead of ideal stoichiometric values are used. ESTIMATe requires a list of all reactants and by-products according to the laboratory data, the single-pass CO_2 conversion, the energy efficiency, and selectivities towards each by-product (all case study data are provided in the ESI†). Based on this input, the process mass and energy balances are calculated, and the resulting process inventory is displayed.

In the process inventory generated by ESTIMATe, unreacted CO_2 is assumed to be emitted to the atmosphere as a worst-case assumption. For the present case study, this assumption leads to high carbon losses and thus also high amounts of CO_2 required as process input. Consequently, we observe large

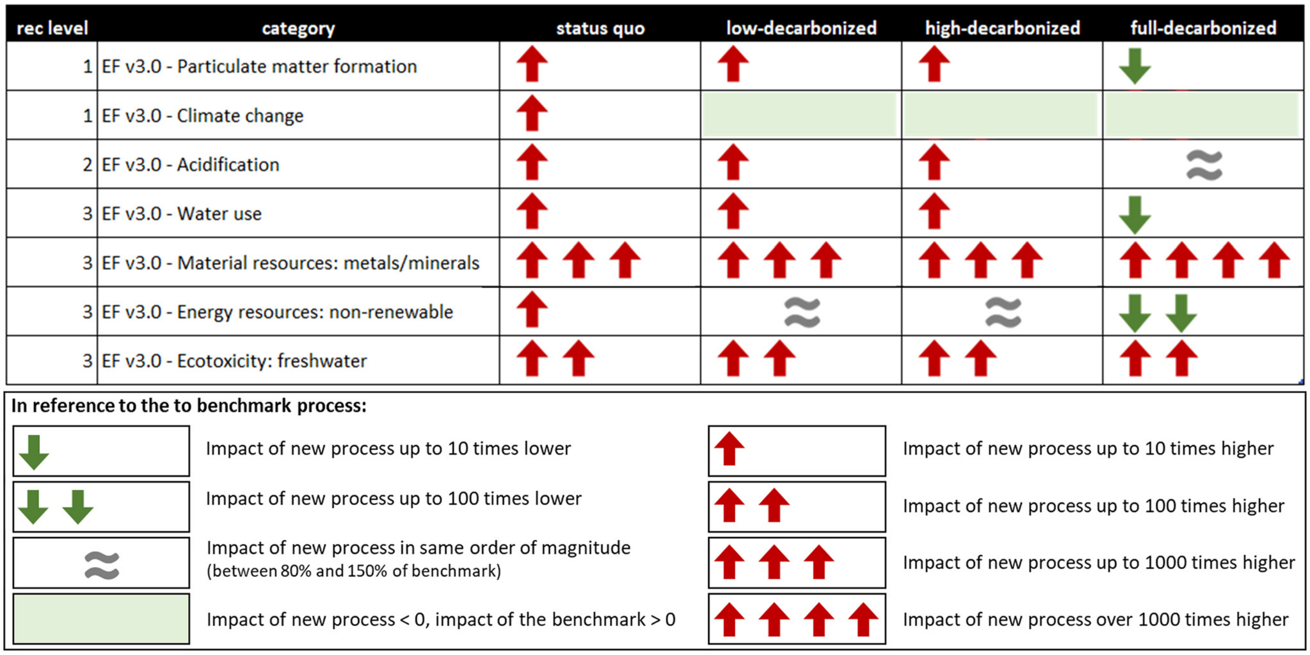

Fig. 4 Qualitative overview of impact trends in selected impact categories in the ESTIMATe tool. Symbols indicate the performance of best-case electrochemical CO_2 reduction to ethylene compared to benchmark technology. "rec level" refers to the recommendation level from the Joint Research Center (JRC) of the European Commission, a measure for inherent uncertainty in each impact category: the higher the recommendation level, the higher the uncertainty.

contributions of CO_2 capture and CO_2 emissions when calculating the Climate Change Impact of this process setup (Fig. 5A).

This worst-case scenario is used to derive a more realistic setup of the case study: as a reasonable assumption for the electrochemical CO_2 reduction to ethylene at larger scales, we implement a CO_2 recycle, considering a purge of 4% of the CO_2 at the reactor outlet. The addition of the recycle requires three steps in ESTIMATe: first, manual adaptation of CO_2 input and emission amounts in the process inventory according to the purge assumption. Second, approximation of the separation energy demand using an estimation method based on ideal thermodynamics within ESTIMATe.[23] Third, addition of the separation energy demand to the inventory and selection of electricity as background database process (background system linkage step, *cf.* section 2.4). For future reference, ESTIMATe stores all user assumptions in a central location.

Results and conclusions for process development. As expected for a non-ideal process, the Climate Change Impact results of laboratory-scale electrochemical CO_2 reduction to ethylene are substantially higher than in the Best-Case Assessment (Fig. 5B). Still, the Climate Change Impact of CO_2-based ethylene is lower than the benchmark environmental impact for high- and full-decarbonized background system scenarios, indicating a potential Climate Change Impact reduction for the process. Similar to the Best-Case Assessment, negative Climate Change Impacts are again achieved due to the "cradle-to-gate" assessment scope, which is explained in a text box next to the figure.

With the CO_2 recycle, the main Climate Change Impact driver in the laboratory-scale process is the electricity demand (Fig. 5B). Consequently, process development should prioritize decreasing the specific energy demand for ethylene production. Possible approaches could be improving the overall energy efficiency or increasing the selectivity towards ethylene. Other than electricity, direct emissions from the process contribute to the Climate Change Impact, and their relative contribution increases with background system decarbonization. The default assumption of emitting by-products to the environment is intended to provide worst-case impacts but is not a realistic option in practice. Process developers should thus try to avoid co-product emissions, either by prioritizing increased selectivity towards ethylene or by considering purifying co-products instead of emitting them, to thereby replace their benchmark production. Another option to explore for the large-scale process is to incinerate co-products and recycle obtained CO_2, while potentially recovering heat. The user can try out the effect any of these process adaptations on the environmental impact by adapting the process inventory accordingly and repeating the assessment, as we have done for the CO_2 recycle.

Based on the assumed minimum separation energy demand, the recycling of CO_2 is reasonable from an environmental perspective in all decarbonization scenarios and all impact categories. While the additional use of electricity increases the environmental impact, the increase is outweighed by avoided emissions related to CO_2 capture. Implementing the recycle reduces GHG emissions between

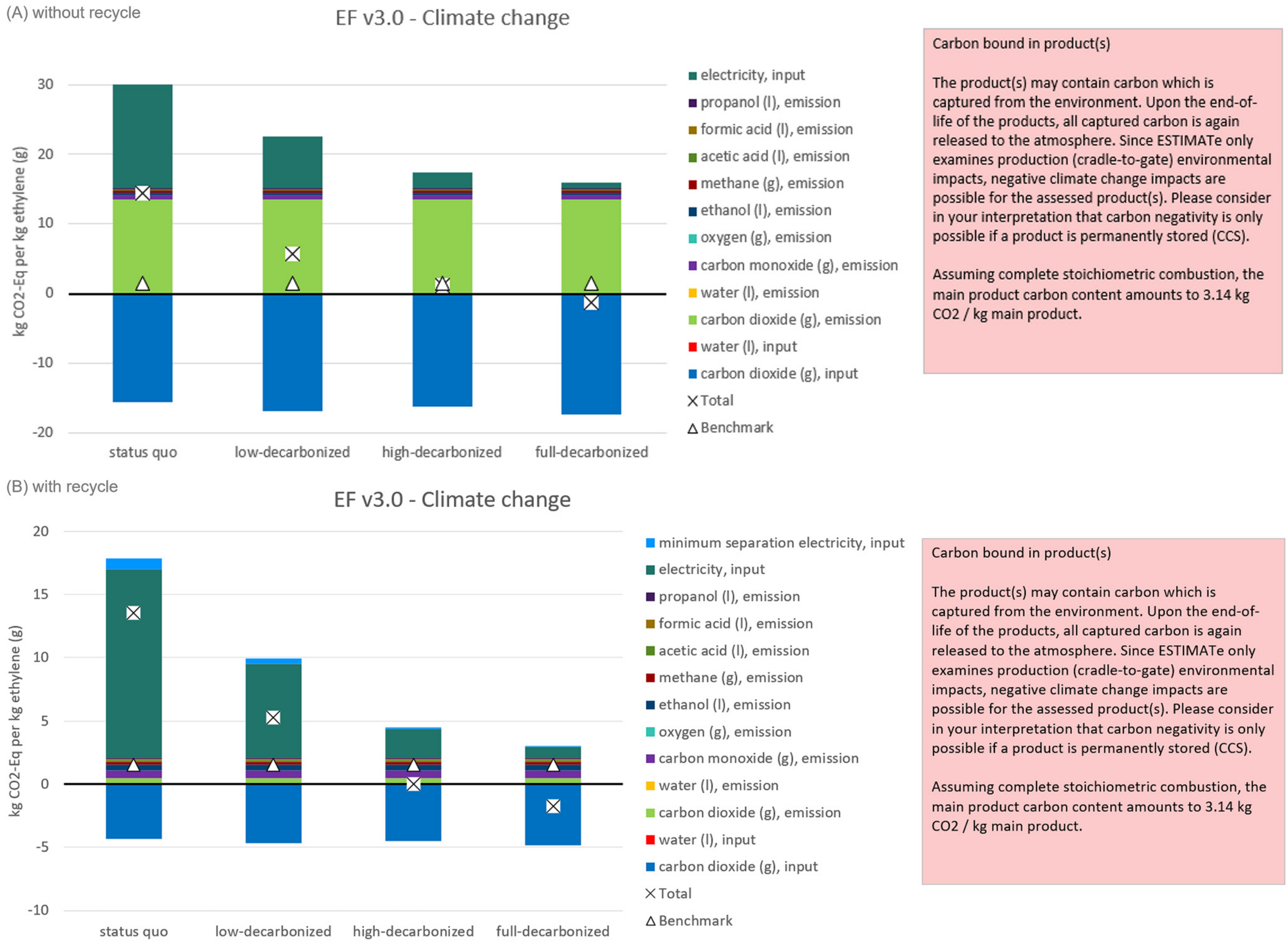

Fig. 5 Climate Change Impact of laboratory-scale electrochemical CO_2 reduction to ethylene in the ESTIMATe tool. (A) Without recycle of unreacted CO_2, (B) including a recycle of unreacted CO_2. Note the different scales of the *y*-axes. The different bars correspond to the different background system scenarios defined in section 2.4.

0.45 and 1.15 kg CO_2-eq per kg of ethylene, depending on the decarbonization level. Since the estimation of the separation energy demand has been optimistic and electricity still contributes substantially to the process's environmental impact, the determination of a more accurate separation energy demand should be prioritized. A quick adjustment in the process inventory in ESTIMATe reveals that doubling the assumed separation energy demand still leads to a Climate Change Impact reduction in three out of four scenarios, while the break-even point of zero Climate Change Impact reduction is reached in the low-decarbonized scenario. Such sensitivity analyses allow process engineers to define target values for parameters such as energy demand. The evaluation of the added CO_2 recycle illustrates how ESTIMATe allows users to explore trade-offs in process design. In similar studies, users may investigate further scenarios such as, for example, increased selectivity at the cost of lower CO_2 conversion.

As discussed above, some environmental impact categories display much higher values for electrochemical CO_2 reduction than for the optimized benchmark process. The contribution analysis in ESTIMATe allows to identify the source of these trends. *E.g.*, the ecotoxicity category suggests prioritizing efficient wastewater management and focusing on eliminating acetic acid emissions. In terms of human toxicity impact, carbon monoxide is the main contributor which could easily be avoided by flaring, potentially with heat recovery.

In summary, the Hotspot Assessment of lab-scale electrochemical CO_2 reduction to ethylene identifies both challenges and advantages. Notably, the process exhibits a significantly lower Climate Change Impact than the benchmark process. However, a limitation of our assessment lies in assuming the validity of lab data for comparison with the industrial-scale benchmark process.[43] In reality, scale-up may necessitate process adaptations affecting the process performance positively or negatively. ESTIMATe enables the exploration of trade-offs and consequences on environmental impact related to such process design decisions. The identified pathways for improving environmental performance provide valuable guidance for further process development.

3.3. Hotspot assessment at process design scale

At later stages of process development, data from process design software may be entered into the ESTIMATe tool. During this process, ESTIMATe's autofill and input check features support the user in data entry. We use this hotspot assessment as an example of by-product handling in ESTIMATe.

Again focusing on electrochemical CO_2 reduction to ethylene, we explore the environmental impacts of the technology at process-design scale in comparison to the fossil benchmark and the laboratory-scale process. Process-design scale data for this section is obtained from Ioannou *et al.*[44] The goal of the analysis is to identify areas of improvement for the process.

User input and required steps in ESTIMATe. In the data generation step (*cf.* section 2.3), we skip the stoichiometric calculations and directly enter the process inventory according to the process design software results. Specifically, all inputs and outputs of the process with corresponding amount and unit are listed and categorized as input, emission, by-product, or waste. For this study, we assume that pure hydrogen and oxygen are by-products that replace their production benchmark instead of being emitted. In the background system linkage step (*cf.* section 2.4), each flow is linked to a process from the background LCA database to quantify the environmental impacts associated with the flow. ESTIMATe suggests linked processes where possible, for instance for key inputs such as electricity, heat, and steam, and for database chemicals if naming conventions are followed.

Upon starting the LCA calculation, the user is alerted of unit inconsistencies between the process inventory and the background database. Furthermore, a simple check of the process mass balance is performed. The user may then double-check and adapt the inventory accordingly, or proceed.

Results and conclusions for process development. Process-design-scale electrochemical CO_2 reduction to ethylene shows the potential of Climate Change Impact reduction compared to the fossil benchmark in the high- and full-decarbonized scenarios (Fig. 6). Compared to the laboratory process, a slightly lower Climate Change Impact is achieved due to improved process integration. Again, the largest contributor to the Climate Change Impact is the electrolyser electricity demand, underlining once more the importance of improving energy efficiency as top priority in process development. Consequently, the technology should only be employed where low-carbon electricity is available. Beyond the climate change impact, electricity production is also the main contributor to all other impact categories. The production of potassium hydroxide used as a utility in the electrochemical CO_2 reduction process contributes to increased freshwater ecotoxicity values (Fig. S4, ESI†), which suggests investigating the recovery of potassium hydroxide.

The use of by-products to replace benchmark production can render the studied process more promising from the environmental point of view, and even competitive to the benchmark process in the low-decarbonized scenario (Fig. 6). Most environmental by-product credits are related to oxygen production in CO_2 reduction, which is assumed to replace benchmark oxygen production, *i.e.*, air separation. While these impact reductions might be achieved by the novel process, caution must be used in interpreting the results: Climate Change Impact reductions can occur only if the by-product oxygen in fact replaces an air separation process. Furthermore, the amount of avoided GHG emissions depends on the replaced oxygen production technology, which might change or improve in the future. Given that ecoinvent processes do not incorporate decarbonization scenarios (*cf.* section 2.4), the impact credits for oxygen production remain constant throughout the scenarios. However, in reality, the environmental impacts of air separation are expected to improve as the share in renewable electricity increases. Oxygen might even be available in such abundance in the future that it would no longer

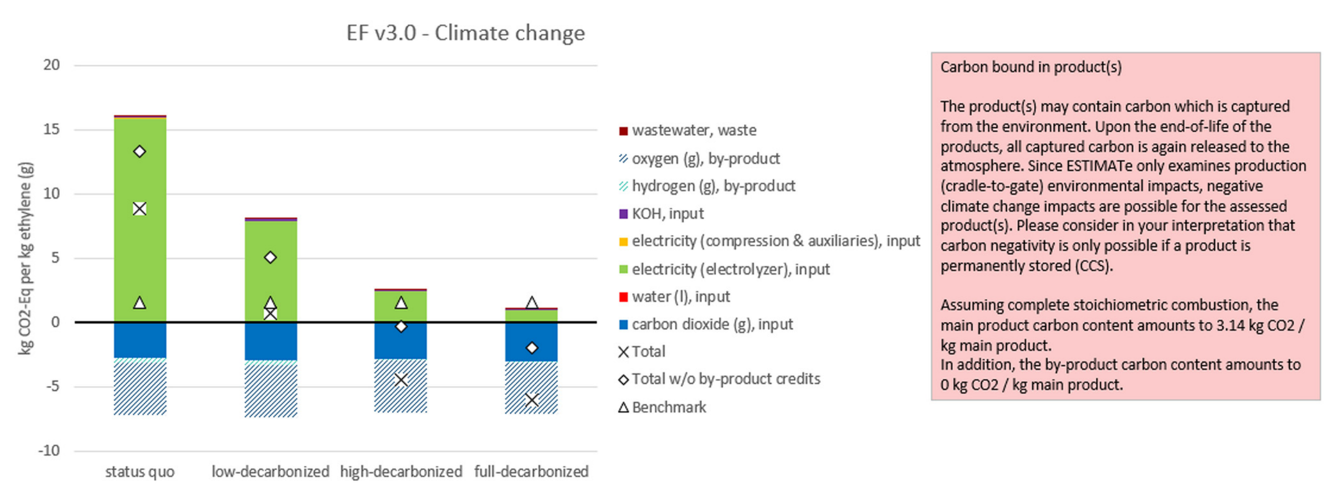

Fig. 6 Climate Change Impact of process-design-scale electrochemical CO_2 reduction to ethylene calculated by the ESTIMATe tool. The different bars correspond to the different background system scenarios defined in section 2.4.

be considered a valuable by-product. The unpredictable future context for by-product credits represents a main limitation of our process design-scale Hotspot Assessment, which is inherent in any analysis of an uncertain future. Since by-product credits always depend on such variables beyond the scope of the developed credits in addition to the result including by-product credits. Still, trends on by-product use can be valuable in process design, encouraging process integration and raising site-specific questions: can oxygen be supplied to another process? Would a change in oxygen source achieve emission mitigation? Could another by-product with higher mitigation potential be produced with low effort?

Beyond the scope of our ethylene case study, the future environmental impact of oxygen production generally requires research. Oxygen is a by-product in many electrochemical processes, prominently including water electrolysis. Today, oxygen produced *via* water electrolysis is typically vented to the atmosphere. However, water electrolysis can meet current oxygen purity standards, which are required for instance for medical applications,[45] and thus theoretically replace conventional production and improve the economics of water electrolysis.[46] Moreover, increased oxygen availability may in turn unlock new applications. Future oxygen production and applications remain a blind spot in the current LCA of electrochemical processes, warranting future research.

3.4. Mitigation Potential Assessment

Mitigation Potential Assessments within ESTIMATe allow direct comparisons of Hotspot Assessments. When assessing processes with the same main product, Mitigation Potential Assessments determine which process achieves higher environmental impact mitigation per unit of the main product. Furthermore, Mitigation Potential Assessments allow for the comparison of processes with different main products but a shared limited resource, addressing which process exhibits a higher mitigation potential using one unit of that resource. In the mitigation calculation, ESTIMATe assumes that the main product replaces its benchmark production.

As a starting point for a Mitigation Potential Assessment, both processes to be compared must be modelled in ESTIMATe as Hotspot Assessments. In this section, we compare the assessment of process design-scale electrochemical CO_2 reduction to ethylene[44] (section 4.3) to a Hotspot Assessment of CO_2 hydrogenation to methanol,[47] also at the process design scale. We aim to answer the question: "Given 1 kg of captured CO_2, which process mitigates more Climate Change Impact?"

User input and required steps in ESTIMATe. We select the two Hotspot Assessments for comparison. The Hotspot Assessment data, including assumptions, process inventory, and results, are automatically copied to the Mitigation Potential Assessment, allowing an overview of both processes. If comparing processes with different main products, ESTIMATe generates a list of shared resources as possible bases of comparison (here: feedstock CO_2 and electricity). For our assessment, we select feedstock CO_2 as the shared resource.

ESTIMATe then calculates the amount of main product produced from one unit of shared resource and scales the process inventory and all results accordingly. For our assessment, 1 kg of captured CO_2 can yield either 0.32 kg of ethylene or 0.69 kg of methanol (*cf.* Fig. 7). ESTIMATe calculates the environmental impacts of each process, as well as the impact of an equivalent amount produced *via* the corresponding benchmark process, a current market mix mainly composed of natural gas reforming. The results are displayed in a contribution analysis, as shown in Fig. 8.

Results and conclusions for process development. In Fig. 8, the totals refer to the impact change through implementing the new process instead of the benchmark process. Consequently, negative totals indicate impact mitigation, while positive totals indicate superior performance of the benchmark process. For both compared processes, Climate Change Impact is mitigated at high and full levels of background system decarbonization. In the *status quo* scenario, employing either process would increase Climate Change Impact compared to the benchmark. In the low-decarbonized scenario, the methanol process has a slightly higher Climate Change Impact than the benchmark process. In contrast, the ethylene process may reduce Climate Change Impact if the benchmark production of oxygen can be replaced, indicated by the difference between the totals with and without by-product credits (*cf.* discussion of by-products in section 4.3).

The main contributors to the Climate Change Impact of ethylene and methanol production are electricity and hydrogen production, respectively. Since hydrogen is supplied from water electrolysis in all but the *status quo* scenarios, the importance of electricity for the production of CO_2-based chemicals is again emphasized. Steam supply to the methanol production contributes 7 to 10% to the positive Climate Change

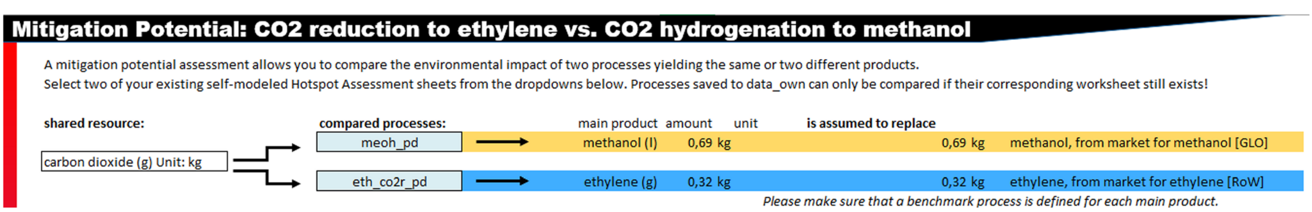

Fig. 7 Header of the Mitigation Potential Assessment sheet comparing electrochemical CO_2 reduction to ethylene and CO_2 hydrogenation to methanol in the ESTIMATe tool.

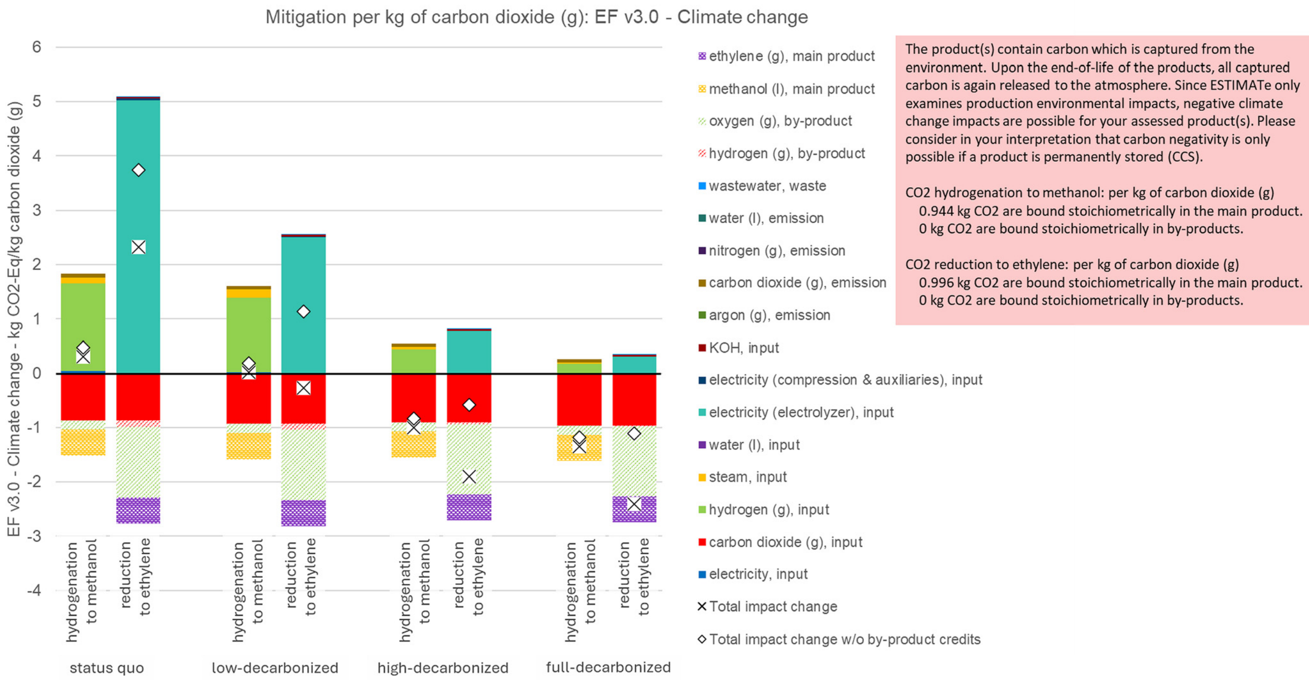

Fig. 8 Climate Change Impact results of the Mitigation Potential Assessment comparing electrochemical CO_2 reduction to ethylene (left bars) and CO_2 hydrogenation to methanol (right bars) in the ESTIMATe tool. The different bar clusters correspond to the different background system scenarios defined in section 2.4.

Impact in all scenarios. In contrast, direct emissions, wastewater treatment, and caustic soda production gain in relative importance with increasing levels of decarbonization: for ethylene production from 1 to 10%, and for methanol production from 4 to 26% from the *status quo* to the full-decarbonized scenario.

In terms of negative Climate Change Impact contributors, the impact of CO_2 capture is similar in both processes for each decarbonization scenario since both processes consume 1 kg of CO_2. However, the impact of the capture of 1 kg of CO_2 changes between the scenarios, due to changes in capture technology and electricity mix used for the capture. The avoided impact based on benchmark production amounts to 0.48 kg CO_2-eq both for 0.69 kg of methanol and for 0.32 kg of ethylene. Since no data is available on the future production methods of the products, a constant benchmark impact is assumed through all decarbonization scenarios (*cf.* section 2.4) which represents a limitation similar to the oxygen by-product credits in section 3.3. In our Mitigation Potential Assessment, by-product credits for oxygen are very high for ethylene production, as discussed in section 3.3. Since oxygen is produced in lower amounts, the credit is much smaller for methanol production.

Despite the limitations, important insights can be derived from this three-click preliminary Mitigation Potential Assessment: both processes exhibit Climate Change Impact mitigation potential at high levels of decarbonization. Neither process emerges as the obvious choice in Climate Change Impact mitigation. The order of prioritization between the processes hinges on the assumptions on by-product usage: if oxygen from ethylene production is considered emitted, the methanol production process shows higher Climate Change Impact mitigation. However, this changes when oxygen is considered a usable by-product, due to the avoided environmental burden of air separation. Since it is uncertain whether the avoided environmental burden of air separation is realized in practice, the Mitigation Potential Assessment results emphasize the importance of considering both processes in a future implementation context. At this point in process development, a full-scale LCA study becomes indispensable to address the limitations inherent in the simplified LCA scope in ESTIMATe. For LCA experts, the process inventories and results from ESTIMATe can form a starting point for further, more in-depth LCA studies.

4. Conclusion

While Life-Cycle Assessment (LCA) studies are desirable as early as possible in the development of Carbon Capture and Utilization (CCU) processes, the threshold to conduct LCA remains high for chemists and process engineers. The open-source ESTIMATe Excel tool offers an easy point of entry for non-LCA practitioners to perform early-stage LCA of CCU chemicals. The method behind the ESTIMATe tool is based on the LCA ISO standards[8,9] and conforms with the guidelines on LCA for early-stage CCU technologies.[16] By focusing the tool scope on CCU chemicals, methodological decisions and calculation steps could be automated and, thus, the user input is minimized.

While the minimum data input into ESTIMATe is a stoichiometric equation, the data quality can grow with process maturity. Specifically, ESTIMATe includes estimation methods and supports the user in selecting the most accurate LCA data depending on the data available from process development. To relieve data collection efforts, users must have access to the commercial ecoinvent database. Calculation of LCA results and application of decarbonization scenarios for key utilities is automated in ESTIMATe. Results are summarized in graphs, for which ESTIMATe provides short explanatory texts to facilitate interpretation.

As a simplified LCA tool, ESTIMATe must compromise between accessibility and functionality. The tool prioritizes features necessary to answer typical questions in early-stage CCU process development and standardizes assumptions to reduce user input. Thus, ESTIMATe has inherent limitations when compared to a standard full-scale LCA:

First, ESTIMATe's scope is limited to CCU products offering services of an existing counterpart. This limitation allows to simplify the assessment process and ensures comparisons are made between products with the same function. Hence, CCU products cannot be assessed that provide new services that are not offered by any chemical today.

Secondly, the tool is limited to three predefined study goals. These study goals have been identified to be particularly relevant for early-stage CCU process development. Still, the tool may not address all the questions that arise in a comprehensive LCA.

Thirdly, ESTIMATe applies predefined decarbonization scenarios to the modelled CCU processes only, neglecting potential decarbonization-related improvements in the environmental impact of fossil technologies. However, we consider this assumption to be reasonable, since the decarbonization of energy systems affects fossil technologies to a lesser degree than CCU technologies. Additionally, common environmental impact categories (*cf.* section 2) are preselected to reduce calculation time. Adding further categories is possible but requires some LCA expertise.

Lastly, while ESTIMATe addresses background system uncertainty through the application of four decarbonization scenarios in each assessment, it does not encompass other forms of uncertainty assessment. In contrast, a comprehensive LCA can consider additional types of uncertainty, such as input parameter uncertainty, to provide a more thorough analysis of environmental impacts.

These limitations underline that ESTIMATe's purpose is not to replace comprehensive full-scale LCA but to serve as a complementary tool, empowering non-LCA experts to carry out LCA studies before detailed results would usually be available. If ESTIMATe results indicate a promising process, LCA experts can leverage the data generated in ESTIMATe as a valuable starting point for a later full-scale LCA since both the process inventory and the assumptions made during data generation are easily accessible.

Our case studies show how non-LCA experts can perform assessments and derive environmental guidance across three study goals:

(1) Best-Case Assessments serve as a sanity check before starting process development, supporting go/no-go decisions.

(2) Hotspot Assessments allow users to generate or enter their own data and explore the environmental impact of their process. With Hotspot Assessments, users can identify the main contributors to the environmental impact, and thus determine levers for improved environmental performance both within the process (*e.g.*, a particularly damaging direct emission) and outside of the process scope (*e.g.*, the electricity mix). Furthermore, ESTIMATe offers users the flexibility to experiment with the tool, enabling them to gain an understanding of the environmental aspects associated with process design decisions.

(3) Mitigation Potential Assessments compare previously modelled processes. The user may thus check whether one process has environmental advantages over the other and identify variables for decision-making between the processes.

In conclusion, ESTIMATe provides a valuable preliminary understanding of environmental impacts and trade-offs in CCU process development. While ESTIMATe is intentionally designed for early-stage insights and may not encompass the detailed scope of full-scale LCA studies, the results can support decision-making about subsequent steps in process development. For example, ESTIMATe can be used to evaluate whether a basic engineering study, a front-end engineering design study, or full-scale LCA is warranted for a particular process. In this way, ESTIMATe contributes to informed decision-making in CCU process development.

The ESTIMATe tool, a user manual, and an Excel sheet to import ecoinvent data into ESTIMATe are available for download under the terms of the GNU General Public License version 3: **https://doi.org/10.5281/zenodo.11060469**

Author contributions

H. M.: Conceptualization, data curation, investigation, methodology, software, validation, visualization, writing – original draft, writing – review & editing. B. V.: Conceptualization, methodology, supervision, writing – review & editing. B. J.: Conceptualization, methodology, supervision, writing – review & editing. R. M.: Conceptualization, funding acquisition, methodology, supervision, writing – review & editing. C. R.: Supervision, writing – review & editing. A. B.: Conceptualization, funding acquisition, supervision, writing – review & editing.

Conflicts of interest

A. B. has served on review committees for research and development at ExxonMobil and TotalEnergies, oil and gas companies that are also active in polymer production. R. M. serves as

Managing Director of Carbon Minds GmbH, a company that is offering life cycle assessment databases, training and consulting to clients in the chemical industry. B. V. and B. J. are part of the R&D entity of TotalEnergies OneTech branch, particularly focusing on the development of innovative and sustainable technologies. The remaining authors have no conflicts of interest to disclose.

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