

# Apples and Apples: A Shortcut Assessment Framework for Early-Stage Carbon Capture and Utilization Technologies Based on Efficiency, Feasibility, and Risk

Arno W. Zimmermann,\* Georg A. Buchner, and Reinhard Schomäcker\*

Climate change is one of the largest current challenges to humankind, requiring a steep emissions reduction. One promising approach is using CO<sub>2</sub> as a resource. Research and development of carbon capture and utilization (CCU) technologies have increased in recent years, putting early-stage techno-economic assessment (TEA) in a key role to derive recommendations systematically, to allocate resources efficiently, and overall to push commercialization successfully. Shortcut TEA assessment approaches that reduce assessment detail and effort compared with conventional, full-scope studies have gained popularity in recent years but have been criticized as comparing apples with oranges. Several open methodological questions remain such as how to implement global assessment standards, how to reduce subjective judgments, and how to compare technologies at different maturities. Herein, a shortcut assessment framework for early-stage CCU technologies is proposed, based on the perspectives of efficiency, feasibility, and risk (Efferi). The Efferi framework implements the Global CO<sub>2</sub> Initiative's Guidelines, enables comparisons at different technology maturities, and systematically reduces subjective judgments. The Efferi framework provides a starting point for a more robust and easy assessment of early-stage CCU technologies, leading to clearer go/no-go recommendations at reduced assessment effort and enabling fairer, “apples to apples” comparisons.

limits to 2 °C or even 1.5 °C require net-zero emissions by 2100 and 2050, respectively,<sup>[2,3]</sup> making the removal of CO<sub>2</sub> from air necessary.<sup>[4]</sup> One technology concept addressing emission reduction and the removal of CO<sub>2</sub> from the atmosphere is carbon capture and utilization (CCU),<sup>[5–7]</sup> which means collecting carbon dioxide from flue gas or air and using it in products and services.<sup>[8]</sup> The potential of using CO<sub>2</sub> is estimated to be significant, but estimations vary—Hepburn et al. find 0.5 Gt<sub>CO<sub>2</sub></sub> a<sup>-1</sup>,<sup>[9]</sup> Chauvy et al. between 3.5 and 4.5 Gt a<sup>-1</sup>,<sup>[10]</sup> and the Global CO<sub>2</sub> Initiative between 1 and 7 Gt<sub>CO<sub>2</sub></sub> a<sup>-1</sup>.<sup>[11]</sup> Applications include chemicals, energy storage, fuels, and materials as well as processing solvents and recovery agents in resource extraction.

The first CO<sub>2</sub> utilization technology was described by Inoue et al. in 1969—a polymer synthesis from CO<sub>2</sub> and epoxides.<sup>[12]</sup> Since then research and development (R&D) of CCU technologies have strongly increased and many concepts are at an early maturity stage.<sup>[13]</sup> At early maturity, deci-

sions of researchers and developers typically have a large influence on process performance at a low cost of implementation, while with increasing maturity influence on process performance shrinks and implementation cost rises sharply (see **Figure 1**).<sup>[14]</sup> Assessment for decision-making at these early stages is therefore critical;<sup>[15]</sup> it enables the identification of promising next steps or helps to terminate projects and overall allows for the efficient use of R&D resources—“fail cheap and early.”

One common form of assessment is techno-economic assessment (TEA), which “includes studies on the economic impact of research, development, demonstration, and deployment of technologies”.<sup>[16]</sup> Together with a large number of practitioners, we developed a guideline for TEA, describing the three major practitioner groups: research, industry, and funding.<sup>[17–20]</sup> We further proposed a full-scope assessment framework for chemical technologies and a clarification of the technology readiness level (TRL) definitions for chemical technologies.<sup>[21,22]</sup> Further assessment guidance documents have been published by the US National Energy Technology Laboratory and the US National Renewable Energy Laboratory;<sup>[23,24]</sup> Sick et al. confirm a general agreement in the mentioned approaches but

## 1. Introduction

Global warming is one of the largest current challenges to humankind and the earth's biosphere.<sup>[1]</sup> To limit global warming, no additional, net-zero emissions need to be achieved—

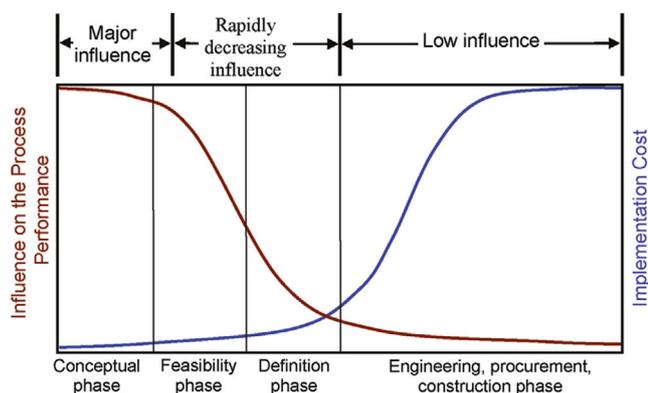
A. W. Zimmermann, Dr. G. A. Buchner, Prof. R. Schomäcker  
Institute of Chemistry  
Technische Universität Berlin (TU Berlin)  
Str. des 17 Juni 124, Berlin 10623, Germany  
E-mail: arno.zimmermann@tu-berlin.de; schomaecker@tu-berlin.de

Dr. G. A. Buchner  
Campus Straubing for Biotechnology and Sustainability  
Technical University of Munich (TUM)  
Am Essigberg 3, Straubing 94315, Germany

 The ORCID identification number(s) for the author(s) of this article can be found under <https://doi.org/10.1002/ente.202000691>.

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**Figure 1.** Influence on process performance and implementation cost in the chemical R&D process. Reproduced with permission.<sup>[14]</sup> Copyright 2012, American Chemical Society.

request further guidance in the stages of early-stage technologies.<sup>[25]</sup>

TEAs at early stages are challenging, as the substantial input data uncertainty of technical indicators is increased by the additional layer of economic parameters and calculations.<sup>[15]</sup> Assessments of CCU are especially challenging, as they do not only cover early-stage projects but also include a variety of disciplines reaching from fuels, polymers to civil engineering. The first TEA for CO<sub>2</sub> utilization technologies was conducted by Audus and Oonk in 1997 where the production of methanol and inorganic carbonates was analyzed based on three technical and three economic criteria.<sup>[26]</sup> In the 1990s and 2000s, CO<sub>2</sub> utilization concepts were discussed based on ideal or lab-validated reactions, using few criteria such as “market potential” or the “mass of CO<sub>2</sub> stored” for specific carbonate material applications or multiple applications.<sup>[27–29]</sup>

In the 2010s, shortcut TEA studies emerged in scientific CCU literature. Shortcut studies compare many alternatives on a low level of detail, in contrast to full-scope studies that compare a few technology alternatives on a high level of detail. Various indicators are used in scientific, industry, and governmental literature, such as energy efficiency,<sup>[30]</sup> energy consumption or demand,<sup>[31–33]</sup> relative added value,<sup>[10,33–35]</sup> production volume or market potential,<sup>[10,34–37]</sup> economic limitations or feasibility,<sup>[10,36,37]</sup> substitution of fossil fuels,<sup>[10,35]</sup> mass of carbon or CO<sub>2</sub> utilized as a rate or potential,<sup>[10,31,34,35]</sup> CO<sub>2</sub> emissions reduction as a rate or potential,<sup>[33–35,37,38]</sup> health and safety,<sup>[10,34]</sup> cost of CO<sub>2</sub> utilized,<sup>[34]</sup> cost of CO<sub>2</sub> avoidance<sup>[38]</sup> and technology maturity or availability.<sup>[10,35,36]</sup> Related methodological papers propose generic frameworks on how to merge environmental assessment with TEA<sup>[39,40]</sup> or propose a detailed list of 140 indicators including data needs.<sup>[14,41,42]</sup> Overall, a large variety of indicators are used in shortcut TEAs for CCU, which makes comparing these studies such as comparing apples and oranges.<sup>[8]</sup> However, current literature either leaves out one of the criteria domains, technical, environmental, or economic,<sup>[10,30–32]</sup> or does not specify equations for calculations of indicators or indicator weightings.<sup>[35–37,39,40]</sup> The remaining studies did not account for technology maturity.<sup>[14,34,38,41,42]</sup>

Recently, Bergerson et al. outlined evaluation techniques for different technology maturity stages; however, the work is limited to life cycle assessment and does not include specific

CCU guidance.<sup>[43]</sup> Also recently, Roh et al. present a TRL-based shortcut assessment framework for CCU, guiding the preparation of data and indicator calculation exemplified in four case studies. While the article provides a comprehensive overview of methods and data references, it does not yet include a coherent set of indicators specified by equations and reducing subjective judgments and comparisons of alternatives at different TRLs remain subject to future research.

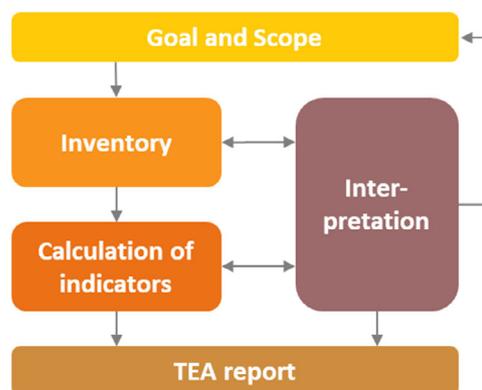
While recently including technology maturity, the existing literature on shortcut TEA does not yet provide a specific set of accepted indicators and equations allowing to reduce subjective judgments and to compare alternatives at different TRLs. Building on the recent methodological developments, we designed the here discussed shortcut assessment framework for CCU technologies, systematically based on the TEA guidelines and technology maturity, suggesting a coherent set of indicators and equations to reduce subjective judgments and uncertainty. We laid emphasis on an easy-to-apply assessment framework using the perspectives of researchers, industry managers, and funding agents allowing for an “apples to apples” comparison of early-stage CCU technologies at the same TRL or different TRLs.

## 2. Principles of the Framework Design

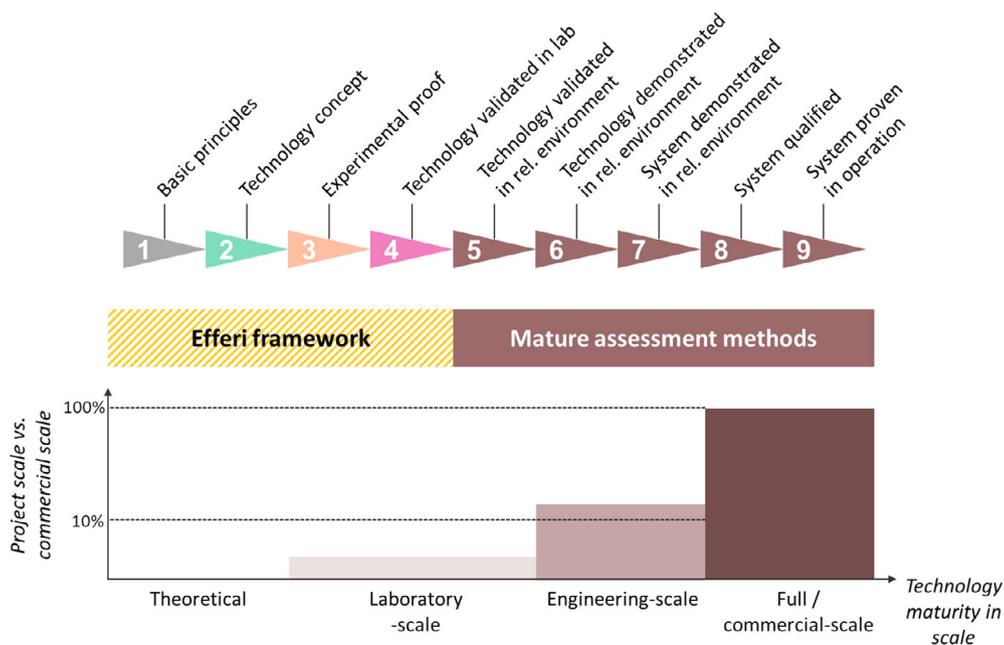
We considered the following principles for framework design: 1) compliance with the TEA guideline for CCU, 2) link of assessment to technology maturity, 3) use of maturity-as-a-scope, 4) use of shortcut indicators, 5) use of commonly accepted criteria and indicators, and 6) use of stakeholder perspectives.

We design the framework in *compliance with the TEA guideline for CCU*, especially following the “shall guidelines” and applying the assessment phases, which are discussed separately in each chapter (see **Figure 2**). Note that in contrast to the generally recommended functional-unit-based reporting, some indicators of the efficiency, feasibility, and risk (Efferi) framework remain free of units.

We *link the assessment to technology maturity*, in particular to the maturity concept of TRLs, as presented in Zimmermann and Schomäcker and similar to Roh et al.<sup>[15,44]</sup> TRLs categorize technology into nine levels of maturity and each level can be linked to a scale relative to a full-scale system.<sup>[45]</sup> While the first two stages



**Figure 2.** Phases of TEA and their dependencies. Reproduced under the terms of the CC BY 4.0 license.<sup>[17]</sup> Copyright 2018, The Authors, published by University of Michigan Library.



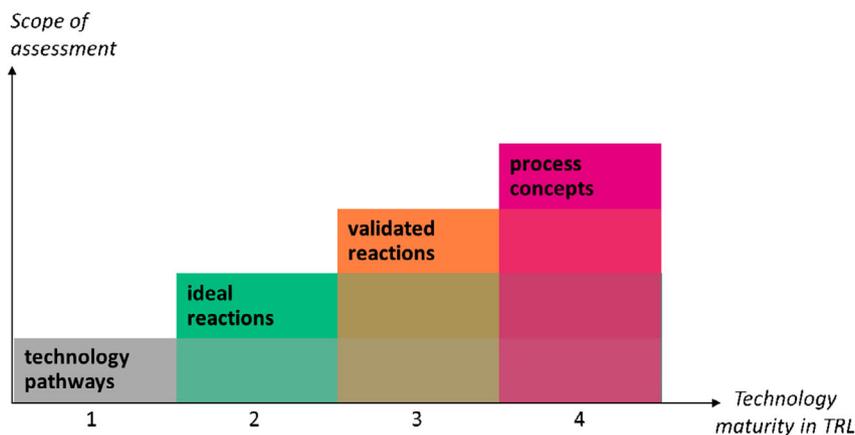
**Figure 3.** TRL levels, scales, and assessment methods, showing the nine levels of maturity and the increasing technology scale.

remain theoretical, levels 3–5 reach lab scale, levels 6 and 7 engineering scale, and levels 8 and 9 full scale (see **Figure 3**). We apply the TRL specifications for the chemical industry, which provide detailed evaluation criteria based on an expert survey and therefore allow for a more objective form of evaluation.<sup>[22]</sup> Data availability and technology maturity go hand in hand: the TRL evaluation can be partly based on the evaluation of what data are available, and in return, a TRL signifies what data are available for assessment. We focus this assessment framework on early-stage technologies from TRL 1 to TRL 4. For later TRL, mature “full-scope” assessment methods are available in the literature.

We use *maturity-as-a-scope*, meaning that we mainly include data points that are available at high certainty and exclude data points that require estimation and heuristics, as presented in Zimmermann and Schomäcker and similar to Roh et al.<sup>[15,44]</sup> Conventionally, novel and incumbent technologies are compared with heuristics<sup>[46]</sup> or in an in-operation scenario, meaning at the

highest possible maturity level, at TRL 9. However, as new technologies have not reached this maturity level, practitioners need to make many assumptions, leading to an increased input data uncertainty and high assessment effort when looking at too many scenarios or risking leaving out important solutions when looking at too few scenarios. In the proposed assessment framework, we reverse this approach and suggest to assess novel and benchmark technologies on the “common denominator maturity” level, based on the chemical R&D process and TRL scheme (see **Figure 4**).

First, this means that the assessment is conducted at the maturity level of the least mature technology element. Second, the assessment acts as if the benchmark technology would be on the same, early maturity level as the new technology. Third, results from prior TRLs are included in the subsequent TRL. Applying the maturity-as-a-scope-principle, we can make use of similar indicators and boundary conditions for all technologies, allowing for a comparison at the same TRL or different TRLs.



**Figure 4.** Scheme of the maturity-as-a-scope-principle, showing the enlarging scope of the assessment at an increasing level of technology maturity.

When the new technology completes a TRL and moves to the next one, the scope of assessment can simply be extended, and further aspects can be easily included in the prior assessment.

Using this maturity-as-a-scope-principle is expected to rule out fewer solutions than a conventional, full-scope approach, resulting in a larger set of recommended solutions. For example, a product system at early maturity with a challenging separation would be excluded using the conventional heuristics of a full-scope approach, while being included using this shortcut approach where separation is out of scope at early maturity.

The impact of a larger set of solutions is expected to be minor, as the amount of resources required for each solution remains low at early maturities. Furthermore, the size of the set will be reduced when the scope of the assessment is extended at later maturity. In addition, this larger set might include unconventional solutions that would be ruled out using conventional heuristics otherwise. Overall, applying the maturity-as-a-scope-principle provides the key advantage of reducing assessment effort and at the same time increasing input data certainty, which leads to cheaper assessments and reduced risk of decision-making.

In addition, we *apply shortcut indicators* to overcome knowledge gaps for technology assessment. Such shortcut indicators have been used for the assessment of chemical production from fossil resources<sup>[47]</sup> and CO<sub>2</sub>.<sup>[15,31,35]</sup> Shortcut indicators bypass conventional, “full-scope” indicators, as they decrease the level of detail. The advantage of using shortcut indicators is that recommendations can be made requiring fewer data and effort; the disadvantage is a less detailed and therefore less thorough assessment. We apply shortcut indicators in this assessment framework to provide recommendations for decisions with enough certainty in an environment with many unknowns, such as early-stage R&D projects. While shortcut indicators seem suitable in early-stage assessments or screening assessments, practitioners should avoid them for assessments of late-stage projects and when detailed data are available, for example, for decision-making at production scale or involving large budgets.

We *use commonly accepted criteria and indicators* to avoid “reinventing the wheel.” We derived this set from our recent literature study.<sup>[8]</sup> We first collected the indicators from literature and clustered them. Second, we created generalized indicators from each cluster. Implementing this set of commonly accepted criteria and indicators reduces the subjective judgment of practitioners, as all assessments following the Efferi framework apply the same criteria. The coherent set further ensures that the framework remains relevant for practitioners, while at the same time it includes as many aspects of assessment as possible.

The *use of stakeholder perspectives* recently became a popular approach in product design and business development, as in the frameworks of business model canvas or design-thinking; however, this thinking does not yet seem to be common in R&D. Currently, different taxonomies for chemical R&D indicators exist, such as the taxonomy of “four E”—efficiency, energy, economy, and environment<sup>[41]</sup>—or the three pillars of sustainability—economy, environment, and society.<sup>[48]</sup> While the former taxonomy is not mutually exclusive, the latter enforces “disciplines thinking,” requiring the involvement of a larger number of experts and leading to more communication efforts and errors. Instead of disciplines thinking, we take the perspectives from stakeholders: a small-scale/efficiency perspective

commonly found in research, a large-scale/feasibility perspective commonly found in industry, and a risk/return perspective commonly found in funding and investment.

### 3. Efferi Assessment Framework

#### 3.1. Overview and General Remarks

Following the identified assessment gap and pursuing the six principles mentioned earlier, we developed a framework incorporating an assessment of technology elements by readiness level and by shortcut indicators that takes on the three perspectives of efficiency, feasibility, and risk, further called Efferi assessment framework. The framework is developed for applied research covering TRL 1–TRL 4. A comprehensive set of ten indicators, based on a literature review, is proposed—mass, energy, value, global warming impact (GWI), and CO<sub>2</sub>—each for the efficiency and feasibility perspective as well as for each TRL.

The third perspective analyzes risk, defined generally in ISO 73:2009 as “the effect of uncertainty on objectives,”<sup>[49]</sup> and more specifically for TEA as “the possibility of one or more unwanted outcomes to occur and its potential economic loss.”<sup>[50]</sup> In contrast to the efficiency and feasibility perspectives, which use indicators, the risk perspective uses the established approach of the interpretation phase in TEA and life cycle assessment (LCA) described, for example, in the ILCD handbook—a four-step process of characterization of uncertainty, uncertainty analysis, sensitivity analysis, and improvement of data quality.<sup>[17,51–53]</sup> Suitable methods and further details for each of the four steps are described by TRL later. Furthermore, we recommend to improve data iteratively and to focus on improving key data, which are data with significant contribution and sensitivity on results and recommendations. This established four-step process covers general aspects of risk analysis and risk management defined in ISO 73:2009, such as analyzing the nature of risk, determining the level of risk, and identifying pathways to reduce risk.<sup>[49]</sup>

Practitioners need to adjust the system boundaries to the goal of the study; typically TEA studies include cradle-to-gate boundaries,<sup>[17,18]</sup> but Efferi can be used at any boundary and can cover product life cycles from cradle to grave, similar to LCA or life cycle costing (LCC). The Efferi framework suggests taking all conversion steps of the product system into account, including all reactants and products. Material flow inputs and outputs to the product system are described as reactants (r) and products (p), respectively. Products can be further specified to targeted products (p,t). The intention for performing the reaction or process is to obtain the targeted product and a process can have multiple targeted products. Other, nontargeted products can be by-products or side products and are typically of low or even negative value; waste products or emissions are also counted as other products. As it is good practice for any technology assessment, deriving recommendations need to be aligned to the goal and scope of the study also when using the Efferi framework; furthermore, the reporting of the results needs to be tailored to the stakeholders’ and the audience’s needs.

The Efferi assessment framework is further described and discussed later for each TRL, assessment phase, and assessment perspective. Summary tables of the indicator sets can be found in the Appendix. A summary of the assumptions is shown in **Table 1**.

**Table 1.** Efferi framework assumptions by TRL.

	TRL 1	TRL 2	TRL 3	TRL 4
Reaction/process	Ideal reactions, 100% yield, neglecting kinetic limitations		Nonideal reactions, measured selectivity, and yield	Preliminary process concept, simulated selectivity, and yield
Temperature and pressure		Standard ambient temperature and pressure (29 815 K and 100 kPa)		
Energy and work	Ideal conversion of energy to work without losses		Input energy: ideal conversion, output energy: exhaust heat not recovered, accounting for exergy losses	Input and output energy accounting for exergy losses
Entropy	Change in entropy is neglected			
Heat losses		Heat losses are neglected		
Product	Identical functionality of old and new products			
Supply and demand volume		Energy supply and demand is assumed as infinitely available in a region		
Prices	Complete market penetration by a new product, constant market sizes; all sales replace products at the end of their lifetime			
Cost	Constant prices, taking historic price data averages for current and future reference (past 10 years), neglecting change in prices and volumes during market entry			
Cost	Neglecting indirect operational expenditure (OpEx), assuming written-off plants—neglecting capital expenditure		Neglecting indirect OpEx, piping, and infrastructure cost	
	Neglecting overhead cost and general expenses (e.g., sales, administration, research, and so on) and interest			
GWl and CO <sub>2</sub> storage	GWl reduction and CO <sub>2</sub> storage are independent of scale			

### 3.2. TRL 1—Idea: Technology Pathways

#### 3.2.1. TRL 1: Scope and Activities

At TRL 1, basic research is translated to applications and general opportunities are identified.<sup>[22]</sup> For TRL 1, we suggest a macroscopic view, evaluating technology options in general with explorative concepts such as brainstorming or qualitative screening. For assessment at TRL 1, practitioners need to perform a literature study on existing observations of basic principles; including observations from own experiments is optional.

#### 3.2.2. TRL 1: Inputs and Assumptions

For an assessment at TRL 1 in the Efferi framework, the following inputs are necessary: 1) identification of suitable application for a technology, 2) definition of benchmark products/services for this application, and 3) data on inputs and outputs of mass and energy of benchmarks systems and the product system in focus (e.g., market prices, cumulative energy demand, GWl, notable environment, health, and safety features).

For assumptions, see Table 1.

#### 3.2.3. TRL 1: Efficiency Assessment

We suggest to keep efficiency assessment criteria and indicators at TRL 1 qualitative: practitioners should conduct a qualitative assessment of technical, economic, and environmental efficiencies, comparing the proposed technology option(s) to benchmark solution(s). As criteria, we recommend comparing the efficiency in mass and energy conversion, sales prices, GWIs, and CO<sub>2</sub> consumption—in analogy to the quantitative indicators in TRL 2–TRL 4.

#### 3.2.4. TRL 1: Feasibility Assessment

Similarly, we suggest keeping feasibility assessment criteria and indicators at TRL 1 qualitative as well, with a focus on technical, economic, and environmental feasibility. As for feasibility criteria, we recommend comparing the demand or supply of reactants, products, or energy as well as the overall generated value, greenhouse warming potential, and CO<sub>2</sub> consumption—in analogy to the quantitative indicators in TRL 2–TRL 4.

#### 3.2.5. TRL 1: Risk Assessment and Interpretation

To discuss risk at TRL 1, practitioners should qualitatively weigh potential benefits of technology option(s) with their qualitative uncertainty and sensitivity, for example, by using a rating system (e.g., traffic lights) and by discussing the alternatives in different scenario conditions. A typical goal is the rough identification of key factors of uncertainty and sensitivity, providing priorities for R&D.

#### 3.2.6. TRL 1: Recommendations

Practitioners should derive recommendations for technology pathways based on the assessment perspectives discussed earlier. We recommend using a variety of criteria and avoiding one endpoint criterion that is derived by normalization and weighting at this stage. A common conclusion at TRL 1 would be a go/no-go recommendation for R&D.

### 3.3. TRL 2—Concept: Ideal Reactions

#### 3.3.1. TRL 2: Scope and Activities

At TRL 2, the technology concept or application is drafted<sup>[22]</sup>—the assessment scope sharpens from the macroscopic view of

TRL 1 to a large set of chemical reactions ( $> 5$ ).<sup>[54]</sup> Limitations from kinetics such as side reactions are out of scope at this stage. We recommend defining the location for production as a region. Existing studies from the literature provide data for validation. Own laboratory experiments can be used to reproduce and validate literature data. Finally, a concept for an application is clearly defined.

### 3.3.2. TRL 2: Inputs and Assumptions

Practitioners applying the Efferi framework at TRL 2 require the following inputs: 1) update of inputs from TRL 1, 2) definition of the targeted product(s) of ideal reaction, 3) stoichiometric formulas for all reaction steps, summed up and in the form of 1 mol of targeted product, 4) higher heating value (HHV)/standard enthalpy of combustion for each substance and input/output energy, 5) market-average, secondary prices of reactants, products, and energy—a few, secondary sources are enough, 6) GWI of each substance—GWI estimation methods may be applied to bridge data gaps. If applied, practitioners shall report methods and assumptions, and 7) market size (mass) of each substance and application.

For assumptions, see Table 1. In the following all indicators are presented separately; a complete list can be found in Annex A, Table A1.

#### 3.3.3. TRL 2: Efficiency Assessment

**Mass Efficiency of an Ideal Reaction:** At TRL 2 the ideal reaction is defined. We can therefore extend the assessment scope to an ideal reaction and move from qualitative to quantitative efficiency assessment. The first efficiency indicator, mass efficiency, evaluates how much of the input mass is chemically bound in the targeted product. This indicator is also known as “atom economy”<sup>[55]</sup> and has been used for CCU assessments in a similar form.<sup>[31,56]</sup> In the calculation (Equation (1)), the stoichiometric mass of the targeted product ( $m_{p,t}$ ) is divided by the total stoichiometric mass of all reactants ( $m_r$ ), derived from the molar mass ( $M$ ) and the stoichiometric coefficient ( $\nu$ ). If the reaction contains several steps, net reactants from all steps must be included.

$$\eta_{\text{mass,TRL2}} = \frac{\sum_{p,t} m_{p,t,\text{react}}}{\sum_r m_{r,\text{react}}} = \frac{\sum_{p,m} (M_{p,t} * \nu_{p,t})}{\sum_r (M_r * |\nu_r|)} \quad (1)$$

Mass efficiency ranges between zero and one: a value of zero means that the ideal reaction produces no targeted products, and a value of one means that a reaction only produces targeted products.

**Energy Efficiency of the Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify efficiency assessment—in the following for energy. As a second efficiency indicator, we define energy efficiency, measuring how much of the input energy and energy from reactants is bound in the targeted product(s) or is released. The importance of using energy efficiency as an indicator was highlighted in the literature<sup>[30,32]</sup> and used in similar calculations in various studies.<sup>[26,31,57,58]</sup> In the calculation (Equation (2)), the sum of HHVs of the targeted product(s) ( $\text{HHV}_{p,t}$ ) and output energy ( $Q_{\text{out,react}}$ ) as an absolute value is

divided by the sum of HHVs of reactants ( $\text{HHV}_r$ ) and input energy ( $Q_{\text{in,react}}$ ). The HHV can also be expressed by the standard enthalpy of combustion ( $\Delta_c H^\circ$ ). We include released or output energy in the calculation as it could be used for other purposes.

$$\eta_{\text{energy,TRL2}} = \frac{\sum_{p,t} \text{HHV}_{p,t} + |Q_{\text{out,react}}|}{\sum_r \text{HHV}_r + Q_{\text{in,react}}} \quad (2)$$

$$= \frac{\sum_{p,t} (|\Delta_c H^\circ_{p,t}| * \nu_{p,t}) + |Q_{\text{out,react}}|}{\sum_r (|\Delta_c H^\circ_r| * \nu_r) + Q_{\text{in,react}}}$$

Energy efficiency ranges between zero and one: a value of zero means that none of the energy from reactants or input energy is contained in the target products or is released, and a value of one means that all input energy is contained in the target products or is released. Energy efficiency is reduced if by-products contain significant amounts of energy.

**Value Efficiency of an Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify efficiency assessment—in the following for value. As a third efficiency indicator, we define value efficiency, measuring how much monetary value is created or lost in the reaction. This indicator was used in a similar form, for example, as “relative added value” in the literature.<sup>[10,35,46]</sup> In the calculation (Equation (3)), the value created by all target products and output energy, each weighted by their corresponding prices ( $\pi$ ), is divided by the value of all required inputs and input energy, again weighted by their corresponding prices.

$$\eta_{\text{value,TRL2}} = \frac{\sum_p (m_{p,t,\text{react}} * \pi_{p,t}) + Q_{\text{out,react}} * \pi_Q}{\sum_r (m_{r,\text{react}} * \pi_r) + Q_{\text{in,react}} * \pi_Q} \quad (3)$$

Value efficiency can range between zero and any positive number with a threshold of one: a value lower than one means that target products and output energy are worth less than reactants and input energy—value is lost; in contrast, a result larger than one means that value is gained. Please note that for electrochemical reactions, practitioners should use the price of electricity, and for thermochemical reactions, practitioners should use the price of relevant heat sources (e.g., midpressure steam). Good references for price data of reactants, products, or energy are data from similar plants or market average price data.

**GWI Reduction Efficiency of an Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify efficiency assessment—in the following for GWI. As the fourth efficiency indicator, we define GWI reduction efficiency, measuring how to target products and output energy, each weighted by their respective GWIs, relate to the GWI of reactants and input energy (Equation (4)). As GWIs either values from benchmark processes or average GWI values (e.g., average mix of electricity of a country) may be used. The indicator is used in a similar form in various studies, for example, in Chauvy et al.<sup>[10]</sup>

$$\eta_{\text{GWI,TRL2}} = \frac{\sum_{p,t} (m_{p,t,\text{react}} * \text{GWI}_{p,t}) + Q_{\text{out,react}} * \text{GWI}_Q}{\sum_r (m_{r,\text{react}} * \text{GWI}_r) + Q_{\text{in,react}} * \text{GWI}_Q} \quad (4)$$

GWI reduction efficiency, in most cases, ranges between zero and any positive number with a threshold of one. A value lower than one means that the GWI of the target products and output energy achieved by standard processes is lower than the GWI of

reactants and input energy of the selected reaction, signaling an increase in GWI; a value larger than one means a decrease in GWI. When dealing with negative CO<sub>2</sub> emissions, the indicator can also result in a value below zero. “Negative emission” in this context means that CO<sub>2</sub> is not sent out, “emitted,” to the atmosphere, but instead brought back from the atmosphere. For negative carbon emissions to occur, the emissions of the product system have to be set in relation to the environment. Net negative emissions can only occur if three conditions are fulfilled: CO<sub>2</sub> needs to be captured from the atmosphere, CO<sub>2</sub> needs to be permanently stored at the end of life, and the amount of CO<sub>2</sub> emitted during the life cycle is lower than the amount of CO<sub>2</sub> captured and stored.<sup>[59]</sup>

**CO<sub>2</sub> Efficiency of an Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify efficiency assessment—in the following for CO<sub>2</sub>. The fifth efficiency indicator, CO<sub>2</sub> efficiency, measures how much CO<sub>2</sub> is chemically contained in products, similar to the description by ISO 27912 and CCU assessment literature.<sup>[10,31,35,60,61]</sup> For calculation we divide the mass of reactant CO<sub>2</sub> by the total mass of all reactants (CO<sub>2</sub> and coreactants), derived from molar mass and stoichiometric coefficients, similar to mass efficiency (Equation (5)).

$$\eta_{\text{CO}_2, \text{TRL2}} = \frac{m_{r, \text{CO}_2, \text{react}}}{\sum_r m_{r, \text{react}}} = \frac{M_{\text{CO}_2} * \nu_{\text{CO}_2}}{\sum_r (M_r * \nu_r)} \quad (5)$$

CO<sub>2</sub> efficiency describes to what extent the input CO<sub>2</sub> is consumed in the reaction or process and can range from zero to one; zero means no CO<sub>2</sub> is consumed in the reaction, and one means only CO<sub>2</sub> is consumed in the reaction.

### 3.3.4. TRL 2: Feasibility Assessment

**Maximum Mass and Energy Flow Potential of Ideal Reaction:** Similar to efficiency assessment, we extend the assessment scope of feasibility assessment to an ideal reaction and move from qualitative to quantitative efficiency assessment at TRL 2. The first two feasibility indicators, maximum mass flow potential ( $\dot{m}_{\text{max}}$ ) and maximum energy flow potential ( $\dot{Q}_{\text{max}}$ ), indicate the largest mass and energy turnover possible for the reaction if all production and consumption options are fully used. These indicators have been discussed in similar ways, for example, as “market potential,” “production volume,” or “demand availability” in CCU literature.<sup>[10,26,29,35–37,56]</sup>

In the Efferi framework we calculate them in three steps: first, the total mass flow of any reactant or product  $i$  ( $\dot{m}_{\text{total},i}$ ) is estimated by adding all mass flows of possible production or consumption options  $j$  (e.g., annual world market for each application or annual production capacity, see Equation (6)). Second, the limiting substance  $l$  and its maximum mole flow ( $\dot{n}_{\text{max},l}$ ) is determined by identifying the minimum among all total mass flows weighted by their molar mass and stoichiometric coefficient (Equation (7)). Third, the maximum mass flow potential of any reactant or product  $i$  ( $\dot{m}_{\text{max},i}$ ) can be derived from the maximum mole flow of the limiting substance (Equation (8)), which is especially relevant for the targeted product(s). As we assume that the limiting factor is mass and that energy is supplied or consumed without a limit in a region that is relevant for this assessment, the maximum energy flow potentials can be

simply derived from the maximum mole flow (Equation (9)). Assuming limited energy and including this restriction in the calculations of the maximum flows is also possible. Note that the calculations presented here are repeated at TRL 3 and TRL 4, which is why no subscript “<sub>react</sub>” was added.

For  $i, l \in p, r$ , and  $j \in$  all options of production or consumption:

$$\dot{m}_{\text{total},i} = \sum_j \dot{m}_i \quad (6)$$

$$\dot{n}_{\text{max},l} = \text{Min} \left( \frac{\dot{m}_{\text{total},i}}{|\nu_i| * M_i} \right) \quad (7)$$

$$\dot{m}_{\text{max},i} = \dot{n}_{\text{max},l} * |\nu_i| * M_i \quad (8)$$

$$\dot{Q}_{\text{max},\text{in}}, \dot{Q}_{\text{max},\text{out}} \sim \dot{n}_{\text{max},l} \quad (9)$$

In general, large maximum mass and energy flow potentials show that there is no shortage of input material supply, input energy supply, product demand, or output energy demand and that the scale of production can be increased tremendously. Small maximum mass and energy flow potentials indicate a shortage of one of the aforementioned factors and a small scale of production.

**Maximum Value Potential of Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify feasibility assessment—in the following for value. The third feasibility indicator, maximum value potential ( $\dot{\Pi}_{\text{Value,TRL2}}$ ), measures how much value could be generated if the ideal reaction is scaled to its maximum. The commonly known indicator “market potential” is similar but analyzes the product side only. We calculate maximum value potential as follows: we add the sum of the maximum reactant mass flows weighed by their respective prices to the maximum energy input weighted by its price and multiply this expression by the value efficiency (see Equation (10)); alternatively, maximum value potential can be calculated from maximum target product and output energy flows. Large values signal value gain, which may result from large mass or energy flows or high prices.

$$\dot{\Pi}_{\text{Value,TRL2}} = \left( \sum_r (\dot{m}_{\text{max},r,\text{react}} * \pi_r) + \dot{Q}_{\text{max},\text{in},\text{react}} * \pi_Q \right) * \eta_{\text{Value,TRL2}} \quad (10)$$

**Maximum GWI Reduction Potential of Ideal Reaction:** With the scope of an ideal reaction at TRL 2, we further quantify feasibility assessment—in the following for the GWI. The fourth feasibility indicator, maximum GWI reduction potential ( $\Delta \text{GWI}_{\text{max,TRL2}}$ ), measures by how much emissions can be reduced when the reaction is scaled to its maximum. This indicator has been applied in a similar form, for example, by Otto et al. and others.<sup>[10,35,37]</sup> For the calculation we add the maximum flow of reactant mass and input energy multiplied by their respective GWIs and weigh this expression by GWI efficiency (Equation (11)); alternatively, maximum GWI reduction potential can be calculated from maximum target product and output energy flows. Large values signal a large emissions reduction, which may result from large mass or energy flows or high GWIs.

$$\Delta G \dot{W}_{I_{\max, \text{TRL}2}} = \left( \sum_r (\dot{m}_{\max, r, \text{react}} * G \dot{W}_{I_r}) + \dot{Q}_{\max, \text{in, react}} * G \dot{W}_{I_Q} \right) * (\eta_{G \dot{W}_{I, \text{TRL}2}} - 1) \quad (11)$$

*Maximum CO<sub>2</sub> Storage Potential of Ideal Reaction:* With the scope of an ideal reaction at TRL 2, we further quantify feasibility assessment—in the following for CO<sub>2</sub> storage. The fifth feasibility indicator, maximum CO<sub>2</sub> storage potential, measures how much CO<sub>2</sub> can be stored when the reaction is scaled to its maximum. The indicator has been discussed and applied in CCU literature in similar forms.<sup>[28,35,62]</sup> We calculate this indicator by multiplying the sum of all maximum reactant mass flows with CO<sub>2</sub> efficiency (Equation (12)). Large values signal a large CO<sub>2</sub> storage potential, which may result from large mass flows or high consumption of CO<sub>2</sub>.

$$\dot{m}_{\text{CO}_2, \text{storage, TRL}2} = \sum_r \dot{m}_{\max, r, \text{react}} * \eta_{\text{CO}_2, \text{TRL}2} \quad (12)$$

### 3.3.5. TRL 2: Risk Assessment and Interpretation

To discuss risk at TRL 2, we recommend extending the scope of analysis from TRL 1. While uncertainty analysis can remain largely qualitative, its scope can be extended, for example, by increasing the detail of analysis from a simple ranking at TRL 1 to a ranking matrix at TRL 2 (e.g., a pedigree matrix used by Fernandez-Dacosta,<sup>[63]</sup> but in a simpler version). Nevertheless, practitioners should try to quantify uncertainty analysis where possible, for example, for input data or by deriving threshold values. Practitioners can also extend the scope of sensitivity analysis from TRL 1, for example, by including a one-at-a-time or local sensitivity analysis, for a small set of key variables. Based on the sensitivity analysis, practitioners should be able to derive first hotspots and priorities for R&D.

### 3.3.6. TRL 2: Recommendations

To derive recommendations at TRL 2, we recommend comparing multiple ideal reaction product systems with each other and with the ideal benchmark reaction(s) based on the three assessment perspectives discussed earlier. Normalization and weighting to use a single criterion is optional and requires the disclosure of schemes and metrics. Practitioners can derive go/no-go recommendations as well as qualitative and quantitative targets and priorities for R&D.

## 3.4. TRL 3—Proof of Concept: Validated Reactions

### 3.4.1. TRL 3: Scope and Activities

At TRL 3, applied laboratory research is started, to prove the functional principle or the reaction mechanism and predict the observed reaction.<sup>[22]</sup> At TRL 3, we refine the scope from a large set of reactions (>5) at TRL 2 to only a few alternatives of reactions (≤5). At TRL 3, the Efferi framework includes side reactions and by-products in the assessment. If a reaction has multiple steps, practitioners need to take the whole reaction network

into account, including all main and side reactions. Detailed laboratory experiments and analytics become necessary at TRL 3, showing a proof-of-concept for critical functions (catalyst, reaction, or similar) and providing data necessary for the assessment. In addition, practitioners should perform first market research and a client survey.

### 3.4.2. TRL 3: Inputs and Assumptions

Following the Efferi framework at TRL 3, practitioners need to update data inputs from TRL 2. Reaction formulas of main and side reactions (reaction networks) based on data from laboratory experiments need to be included. The following data become necessary at TRL 3: 1) measured mass and energy balances, selectivity and yield of each reaction step, 2) reaction conditions (pressure, temperature, energy input/outputs), 3) overall reaction rate (macrokinetics), 4) HHV of reactants and products, 5) price adjustment factors for functionality and sustainability, and 6) lifetime of product or application.

For assumptions, see Table 1. In the following all indicators are presented separately; a complete list can be found in Annex A, Table A2.

### 3.4.3. TRL 3: Efficiency Assessment

*Mass Efficiency of Validated Reactions:* At TRL 3, practitioners validated the reaction in focus and other related reactions in laboratory experiments and summarized them in a reaction network. We can therefore extend the scope of mass efficiency from ideal reactions to an overall reaction network (react net), including side reactions and by-products based on measured yield and selectivity (Equation (13)).

$$\eta_{\text{mass, TRL}3} = \frac{\sum_{p,t} m_{p,t, \text{react net}}}{\sum_r m_{r, \text{react net}}} \quad (13)$$

*Energy Efficiency of Validated Reactions:* Similar to mass efficiency, we extend the scope of energy efficiency to the overall reaction network at TRL 3. In addition, we make use of the stated reaction temperature to account only for the part of output energy that can be converted into work depending on the temperature level, output exergy ( $B_{\text{out, react net}}$ ) (Equation (14)).

$$\eta_{\text{energy, TRL}3} = \frac{\sum_{p,t} \text{HHV}_{p,t} * m_{p,t, \text{react net}} + B_{\text{out, react net}}}{\sum_r \text{HHV}_r * m_{r, \text{react net}} + Q_{\text{in, react net}}} \quad (14)$$

*Value Efficiency of Validated Reactions:* Similarly, we extend the scope of value efficiency to the overall reaction network and exergy ( $B_{\text{out, react net}}$ ) at TRL 3 (Equation (15)). The price of exergy ( $\pi_B$ ) can be approximated from the price of energy. Furthermore, value efficiency is extended to include adjustments of functionality and sustainability. The product's functionality and resulting performance might be improved or reduced compared with its competitors, changing the willingness to pay of customers. We include this by introducing a price adjustment for functionality ( $\pi_{p,f}$ ). Practitioners can derive this positive or negative adjustment, for example, from a price-functionality-ratio or price-performance-ratio for the identified application, mapping prices,

and functionalities to competitor products. Similarly, a product's sustainability indicators might be increased or decreased, for example, reduced toxicity or lower GWI, changing the willingness to pay. We include this by introducing a product price adjustment for sustainability ( $\pi_{p,s}$ ). Practitioners can derive this positive or negative adjustment, for example, from a general price of carbon or by deriving a "price-sustainability-ratio" for the application, mapping prices, and sustainability indicators of competitor products. If applied, functionality and sustainability price adjustments should be supported by literature and market data or in expert interviews.

$$\eta_{\text{value,TRL3}} = \frac{\sum_p (m_{p,t,\text{react net}} * (\pi_p + \pi_{p,f} + \pi_{p,s})) + B_{\text{out,react net}} * \pi_B}{\sum_r (m_{r,\text{react net}} * \pi_r) + Q_{\text{in,react net}} * \pi_Q} \quad (15)$$

*GWI Reduction Efficiency and CO<sub>2</sub> Efficiency of Validated Reactions:* Similarly, we extend the scope of GWI reduction efficiency and CO<sub>2</sub> efficiency to the overall reaction network (react net) and exergy ( $B_{\text{out,react net}}$ ) at TRL 3 (see Equation (16) and (17)).

$$\eta_{\text{GWI,TRL3}} = \frac{\sum_p (m_{p,t,\text{react net}} * \text{GWI}_{p,t}) + B_{\text{out,react net}} * \text{GWI}_B}{\sum_r (m_{r,\text{react net}} * \text{GWI}_r) + Q_{\text{in,react net}} * \text{GWI}_Q} \quad (16)$$

$$\eta_{\text{CO}_2, \text{TRL3}} = \frac{m_{p,\text{CO}_2, \text{react net}}}{\sum_r m_{r,\text{react net}}} \quad (17)$$

#### 3.4.4. TRL 3: Feasibility Assessment

*Maximum Mass and Energy Flow Potentials of Validated Reactions:* In parallel to efficiency assessment, we extend the scope of maximum mass and energy flow potentials to the overall reaction network and output exergy at TRL 3. We include yields and selectivity from laboratory data as well as for the overall reaction network with side reactions and by-products. Note that for mass flows, we consider the mass of products sold for replacement and potential market growth only and that the stoichiometric coefficients need to be recalculated according to the net overall reaction. The calculation at TRL 3 is the same as at TRL 2.

*Maximum Value Potential, GWI Reduction, and CO<sub>2</sub> Storage Potential of Validated Reactions:* Similarly, we extend the scope of maximum value, GWI reduction, and CO<sub>2</sub> storage potentials to the overall reaction network and output exergy at TRL 3 to include yields, selectivity, side reactions, and by-products (see Equation (18)–(20)). The latter two indicators are extended to also account for the lifetime ( $t_{p,t}$ ) of the targeted product or application at TRL 3.

$$\dot{\Pi}_{\text{Value,TRL3}} = \left( \sum_r (\dot{m}_{\text{max},r,\text{react net}} * \pi_r) + \dot{Q}_{\text{max,in,react net}} * \pi_Q \right) * \eta_{\text{Value,TRL3}} \quad (18)$$

$$\Delta \text{GWI}_{\text{max,TRL3}} = \left( \sum_r (\dot{m}_{\text{max},r,\text{react}} * \text{GWI}_r) + \dot{Q}_{\text{max,in,react net}} * \text{GWI}_Q \right) * (\eta_{\text{GWI,TRL3}} - 1) * t_{p,t} \quad (19)$$

$$\dot{m}_{\text{CO}_2, \text{storage,TRL3}} = \sum_r \dot{m}_{\text{max},r,\text{react net}} * \eta_{\text{CO}_2, \text{TRL3}} * t_{p,t} \quad (20)$$

#### 3.4.5. TRL 3: Risk Assessment and Interpretation

To discuss risk at TRL 3, practitioners need to extend uncertainty analysis from TRL 2 and focus on including further quantitative information. For example, the uncertainty of input data and its propagation to results can be specified in intervals or box plots depending on data availability. However, the sole multiplication of intervals typically leads to large ranges of uncertainty and inconclusive results. Where no data are available, an expert opinion on uncertainty, or alternatively an overall uncertainty of the assessment could be used, which Association for the Advancement of Cost Engineering (AACE) lists as  $-50\%$  to  $+100\%$  for TRL 3.<sup>[21,64]</sup> Based on the uncertainty analysis, practitioners should be able to derive threshold values.

At TRL 3, practitioners can optionally extend the sensitivity analysis by including scenarios with more details and by optionally accounting for further factors in the local sensitivity analysis, which can be well presented in linear coefficient graphs or tornado diagrams. As at TRL 2, the analysis at TRL 3 should enable practitioners to confirm existing or identify further hotspots and key priorities for R&D.

#### 3.4.6. TRL 3: Recommendation

To derive recommendations at TRL 3, practitioners need to compare the validated reactions with each other and with validated benchmark reaction(s) based on the three assessment perspectives discussed earlier. As for prior TRLs, practitioners can focus on go/no-go recommendations as well as quantitative targets and priorities for R&D. Normalization and weighting are optional.

### 3.5. TRL 4—Preliminary Process Development: Process Concepts

#### 3.5.1. TRL 4: Scope and Activities

At TRL 4, the reaction concept is validated in a laboratory environment and the preparations for a scale-up are started.<sup>[22]</sup> At TRL 4, we refine the scope from a few alternatives of reactions to a few alternatives of process concepts, including system elements before and after the reaction such as reactant treatment or product separation. The assessment scope should include the overall process, ranging from reactants to the targeted products. Capacity, operating time, location, and time scenario (current or future) of the process concept should be specified. However, the design of individual system elements may remain preliminary, supporting, or interacting processes that do not need to be included at this stage. At TRL 4, we suggest showing at least a draft of a process flow diagram including specifications for main equipment, as well as proof of reproducible and predictable experimental results and further research on applications and users.

### 3.5.2. TRL 4: Inputs and Assumptions

At TRL 4, practitioners need to update data inputs from TRL 3. In addition, the Efferi framework requires a process concept including different system elements. The following additional data become necessary at TRL 4: 1) lower heating value (LHV) for reactants and products; 2) input and output energy in the form of work; 3) time and location-specific, market-average, secondary prices of reactants, products, energy, and price adjustment factors—a few, secondary sources are enough; and 4) prices of main equipment and equipment operation time.

For assumptions, see Table 1. In the following, all indicators are presented separately; a complete list can be found in Annex A, Table A3.

### 3.5.3. TRL 4: Efficiency Assessment

*Mass Efficiency of Process Concepts:* At TRL 4, practitioners specified the process concept. We, therefore, extend the scope of mass efficiency from the validated reaction network to process concepts, including mass flows of targeted products ( $\dot{m}_{p,t,process}$ ) and reactants ( $\dot{m}_{r,process}$ ) (Equation (21)). Mass flow data can be retrieved from the results of process simulation.

$$\eta_{mass,TRL4} = \frac{\sum_{p,t} \dot{m}_{p,t,process}}{\sum_r \dot{m}_{r,process}} \quad (21)$$

$$\eta_{value,TRL4} = \frac{\sum_p (\dot{m}_{p,t,process} * (\pi_p + \pi_{p,f} + \pi_{p,s})) + \sum_i (W_{i,out,process} * \pi_{W_{i,out,process}})}{\sum_r (\dot{m}_{r,process} * \pi_r) + \sum_i (W_{i,in,process} * \pi_{W_{i,in,process}}) + \sum_j \frac{\Pi_{equipment,j}}{t_{operation,j}}} \quad (23)$$

*GWI Reduction Efficiency and CO<sub>2</sub> Efficiency of Process Concepts:* Similarly, we extend the scope of GWI reduction efficiency and CO<sub>2</sub> efficiency to process concepts at TRL 4 (Equation (24) and (25)). For GWI efficiency, we recommend weighing individual workstreams with their respective GWIs and including the mass

$$\eta_{GWI,TRL4} = \frac{\sum_p (\dot{m}_{p,t,process} * GWI_{p,t}) + \sum_i (W_{i,out,process} * GWI_{W_{i,out,process}})}{\sum_r (\dot{m}_{r,process} * GWI_r) + \sum_i (W_{i,in,process} * GWI_{W_{i,in,process}}) + \sum_j \frac{m_{equipment,j}}{t_{operation,j}} * GWI_j} \quad (24)$$

$$\eta_{CO_2,TRL4} = \frac{\dot{m}_{r,CO_2,process}}{\sum_r \dot{m}_{r,process}} = \frac{\sum_{in} \dot{m}_{r,CO_2,process} - \sum_{out} \dot{m}_{r,CO_2,process}}{\sum_r \dot{m}_{r,process}} \quad (25)$$

### 3.5.4. TRL 4: Feasibility Assessment

*Maximum Mass and Energy Flows of Process Concepts:* At TRL 4, and similar to efficiency assessment, we extend the scope of maximum mass and energy flows to process concepts at TRL 4; we include mass flows based on data from process simulation. Note that the stoichiometric coefficients need to be recalculated according to the mass flows in the process. The calculation at TRL 4 is the same as at TRL 2.

*Energy Efficiency of Process Concepts:* Similar to mass efficiency, we extend the scope of energy efficiency to process concepts at TRL 4. We now include LHV for both targeted products (LHV<sub>p,t</sub>) and reactants (LHV<sub>r</sub>) (Equation (22)). Using LHV makes use of the assumption that exhaust heat is not recovered. As process capacity is specified at TRL 4, we can use energy flows in the assessment. Practitioners can express input and output energy flows as work ( $W_{in,process}/W_{out,process}$ ); data can be retrieved from process simulation. If data for work are not available, data for exergy can be used as a proxy.

$$\eta_{energy,TRL4} = \frac{\sum_{p,t} LHV_{p,t} * \dot{m}_{p,t,process} + \sum_i (W_{i,out,process})}{\sum_r LHV_r * \dot{m}_{r,process} + \sum_j (W_{j,in,process})} \quad (22)$$

*Value Efficiency of Process Concepts:* Similarly, we extend the scope of value efficiency to process concepts at TRL 4 (see Equation (23)). The price of work ( $\pi_w$ ) can largely vary depending on the state of work, which is why we recommend pricing each workflow with a separate price (e.g.,  $\pi_{W_{i,out,process}}$ ). Furthermore, we recommend including the cost of equipment ( $\Pi_{equipment,j}$ ) of all system elements  $j$  (or process steps) weighted by their time of operation ( $t_{operation,j}$ ). Equipment cost is usually included in the results of process simulation.

of equipment ( $m_{equipment,j}$ ) weighted by time of operation and respective GWI, otherwise a justification for excluding equipment impacts needs to be provided. For CO<sub>2</sub> efficiency, we recommend accounting only for the net CO<sub>2</sub> consumed; any output flows of unreacted CO<sub>2</sub> need to be subtracted from the input flows.

*Maximum Value Potential, GWI Reduction, and CO<sub>2</sub> Storage Potential of Process Concepts:* Similarly, we extend the scope of maximum value, GWI reduction, and CO<sub>2</sub> storage potential to process concepts at TRL 4 to include mass and energy flows in the form of work, and equipment based on data from process simulation (see Equation (26)–(28)).

$$\dot{\Pi}_{Value,TRL4} = \left( \sum_r (\dot{m}_{max,r,process} * \pi_r) + \sum_i (W_{max,i,in,process} * \pi_{W_{i,in,process}}) + \sum_j \frac{\Pi_{equipment,j}}{t_{operation,j}} \right) * \eta_{Value,TRL4} \quad (26)$$

$$\begin{aligned} \Delta G \dot{W}I_{\max, \text{TRL}4} = & \left( \sum_r (\dot{m}_{\max, r, \text{process}} * GWI_r) \right. \\ & + \sum_i (W_{\max, i, \text{in, process}} * GWI_{W_i, \text{in, process}}) \\ & + \sum_j \left. \frac{m_{\text{equipment}, j}}{t_{\text{operation}, j}} * GWI_j \right) \\ & * (\eta_{GWI, \text{TRL}4} - 1) * t_{p, t} \end{aligned} \quad (27)$$

$$\dot{m}_{\text{CO}_2, \text{storage}, \text{TRL}4} = \sum_r \dot{m}_{\max, r} * \eta_{\text{CO}_2, \text{TRL}4} * t_{p, t} \quad (28)$$

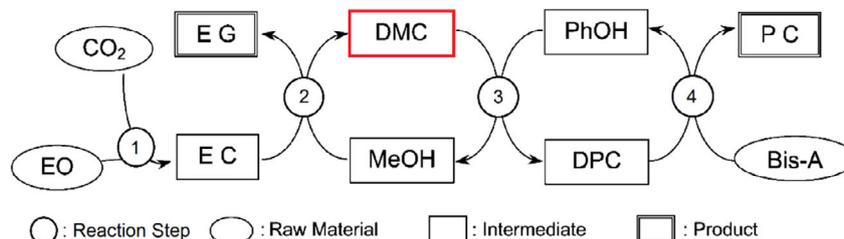
### 3.5.5. TRL 4: Risk Assessment and Interpretation

To discuss risk at TRL 4, practitioners need to extend the scope of analysis to the overall process concept. Characterization of uncertainty can remain qualitative; for input data uncertainty analysis, the degree of confidence approach's level of detail from prior TRLs, such as pedigree matrixes<sup>[63]</sup> and intervals, needs to be extended. If available, the distribution of input data and its propagation on results may be calculated, for example, in a Monte-Carlo analysis; however, such distributions should not simply be assumed, but supported by literature, market studies, or expert opinions. Context uncertainty can be analyzed qualitatively as for prior TRLs with the extension of scenario analysis at TRL 4. As for TRL 3, if data availability on overall uncertainty is limited, expert opinions or an overall uncertainty can be assumed, which AACE lists as -30% to +50% for TRL 4.<sup>[21,64]</sup> As for prior TRLs, threshold values can be derived.

We recommend extending sensitivity analysis from TRL 3 to include all major assumptions taken in the assessment. Furthermore, the analysis can be extended to a one-way or also n-way series.<sup>[65]</sup> As for prior TRLs, qualitative descriptions of key input variables and identified R&D hotspots should be discussed. Furthermore, we recommend extending threshold analysis from TRL 3 and increasing the level of detail of the local sensitivity analysis from prior TRLs.

### 3.5.6. Recommendations

To derive a recommendation at TRL 4, practitioners compare the proposed process concept(s) with the benchmark process concept(s) based on the three assessment perspectives discussed earlier. As for prior TRLs, practitioners can focus on go/no-go recommendations as well as quantitative targets and priorities for R&D. Normalization and weighting are optional.



**Figure 5.** Asahi reaction scheme, where CO<sub>2</sub> and EO are used to make PC and DMC forms an intermediate product. Reproduced with permission.<sup>[67]</sup> Copyright 1999, Royal Society of Chemistry.

## 4. Worked Example Dimethyl Carbonate

In this worked example, the Efferi framework is applied for TRL 2 and TRL 4 to two production processes for dimethyl carbonate (DMC). This worked example is based on process development data as provided in Kongpanna et al.<sup>[66]</sup> and extends prior work where just three indicators were analyzed.<sup>[44]</sup>

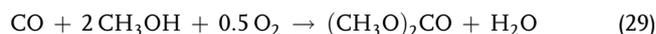
### 4.1. Goal and Scope

The goal of this worked example is the illustration of the Efferi framework, especially the comparison of a product system with a benchmark and a comparison at different development stages or TRLs. As both processes make DMC with an identical chemical structure, we chose the production of DMC as the function and the activities of a DMC producing company as system boundaries, starting with base chemicals and CO<sub>2</sub>, including reaction and separation. We apply all indicators presented in the Efferi framework which use unitless efficiencies and maximum annual flows as functional units.

We analyze two production routes: the rather novel Asahi process and the conventional Eni process as the benchmark. The Asahi process, introduced in the 2000s, is a production process for polycarbonate (PC), but also produces DMC as an intermediate. First, the Asahi process converts ethylene oxide (EO) and CO<sub>2</sub> to ethylene carbonate (EC). Second, EC is converted together with methanol (MeOH) to DMC, producing the by-product ethylene glycol (EG) (see **Figure 5**). EG and at TRL 4 also the remaining reactant of EC is also considered marketable, target products. The Asahi process is operated at 100–180 °C and 40–60 bar.<sup>[67,68]</sup>

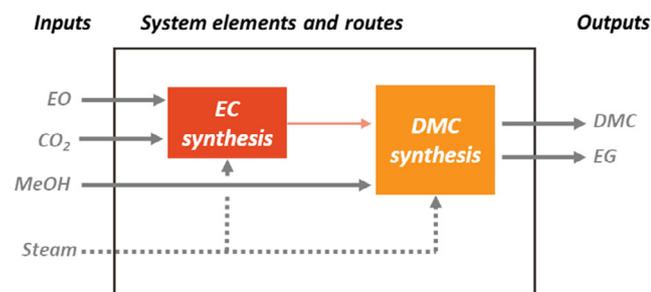
For TRL 2, we include synthesis steps for EC and DMC only (see **Figure 6**). At TRL 4, we include EC synthesis, EC separation, DMC synthesis as well as the separation of MeOH, DMC, and EG (see **Figure 7**).

The Eni process, introduced in the 1980s, converts oxygen, carbon monoxide (CO), and methanol to DMC. The reaction, a partial carbonylation, is operated at 120–140 °C and 20–40 bar, using a copper chloride (I) catalyst (see Equation (29)).<sup>[69]</sup>



At TRL 2, we consider only one system element—the DMC synthesis (see **Figure 8**). The product separation step (purification) remains challenging as DMC, methanol, and water form two binary azeotropes.<sup>[70]</sup> At TRL 4, CO<sub>2</sub> is added to the educts and three separation steps are added as system elements, where

**Asahi product system (TRL 2)**



**Figure 6.** Product system, Asahi process, TRL 2, where two system elements EC synthesis and DMC synthesis are included.

formaldehyde (FA), DMC, and water are separated in individual process steps (see **Figure 9**). For both TRLs, only DMC is considered as a marketable, target product.

**4.2. Inventory**

The inventory consists of process development and thermodynamic data, economic and GWI data as well as assumptions. Process development data are used as provided by Kongpanna et al.<sup>[66]</sup> and additional information provided by that author. For thermodynamic data, enthalpies of reaction were calculated based on the enthalpies of formation from the NIST Webbook and checked for plausibility with the Joback group contribution method.<sup>[71,72]</sup> LHV and HHV were calculated either based on the NIST Webbook, taken from literature values, or the Aspen Plus V10 software.

Economic data consist of production cost, sales prices, production capacities, and consumption demand as well as the chemical engineering plant cost index (CEPCI). Cost and prices were taken from the ICIS dashboard database, government websites, an average of online price quotes, and literature values. Where available, we used a 10-year price average and data for Germany or Europe or converted the price from USD or CNY to EUR based on the average annual exchange rate from the European Central Bank for the reported year. Capacities were taken as worldwide annual values for the latest years available from reports and databases of IHS Markit and Markets and Markets. The CEPCI values for 2013 (567.3) and 2019 (607.5)

were used to adapt the reported equipment cost by Kongpanna et al. to the most current price level. As GWI (100a) data were not available from just one database, it was taken from the databases UVEK LCI, PEF, soca v.1, and EuGeos. Where multiple values were reported, the higher one was chosen as a conservative approach.

All major values are provided in Annex B (see Table B1 and B2). The remaining assumptions are the operating time, which was defined as 7200 h a<sup>-1</sup> in Kongpanna et al., an operating period of 15 years of operation, and the neglect of GWI for equipment.

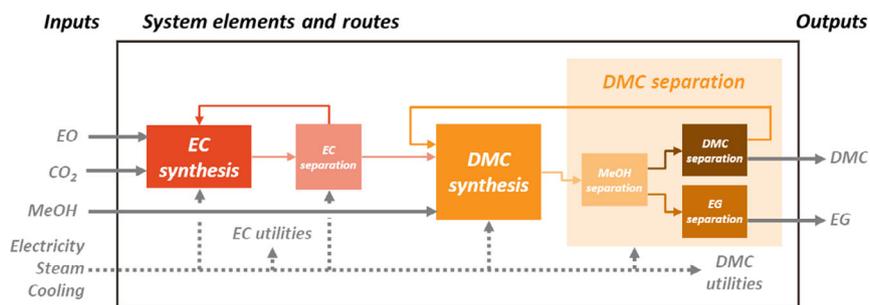
**4.3. Calculation**

The Efferi indicators of efficiency and feasibility are calculated as introduced in the prior chapters. The results are shown in **Table 2** and **3**.

In terms of mass, the Asahi process achieves higher efficiency than its benchmark, as not only DMC but also EG and at TRL 4 also EC are considered marketable target products whereas the Eni process has nonmarketable by-products only. In terms of energy, the Asahi process reaches a higher efficiency in the conversion at TRL 2 but ranges similar to the Eni process at TRL 4 due to a relatively energy-consuming process, indicating a potential for optimization. In terms of mass, the Asahi process achieves higher efficiency (1.00) than its benchmark (0.83), as not only DMC but also EG and at TRL 4 also EC are considered marketable target products whereas the Eni process has nonmarketable byproducts only. In terms of GWI, both processes reach a similar efficiency at TRL 2 and a value above 1, which indicates a potential GWI reduction. At TRL 4, the GWI efficiency of the Asahi process is lower than of the Eni process, which is related to the higher energy consumption. Note that we account for flue gas captured CO<sub>2</sub> here; when accounting for air captured CO<sub>2</sub>, for which no reliable GWI data seem to be published at the time of the study, the GWI efficiency of the Asahi process is expected to increase. In terms of CO<sub>2</sub> efficiency, the Eni process at TRL 2 does not consume CO<sub>2</sub>, resulting in an efficiency of zero. At both TRLs the Asahi process consumes larger amounts of CO<sub>2</sub> and therefore reaches a higher CO<sub>2</sub> efficiency.

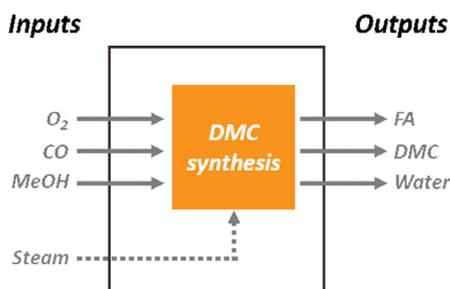
In addition, when looking at GWI and CO<sub>2</sub> efficiency together, this also shows that a process that consumes more CO<sub>2</sub> does not automatically have stronger emissions reductions.

**Asahi product system (TRL 4)**



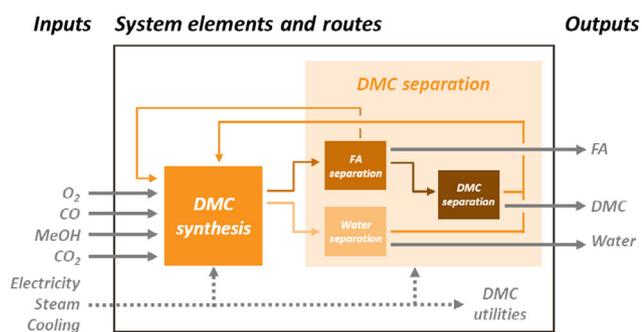
**Figure 7.** Product system, Asahi process, TRL 4, where the six system elements EC synthesis, EC separation, DMC synthesis, methanol (MeOH) separation, DMC separation, and EG separation are included.

**Eni product system (TRL 2)**



**Figure 8.** Product system, Eni process, TRL 2, where the system element DMC synthesis is included.

**Eni product system (TRL 4)**



**Figure 9.** Product system, Eni process, TRL 4, where the four system elements DMC synthesis, FA synthesis, DMC separation, and water separation are included.

**Table 2.** Efficiency indicators.

Indicator	TRL 2		TRL 4	
	Eni	Asahi	Eni	Asahi
Mass efficiency	0.83	1.00	0.72	0.97
Energy efficiency	0.60	0.72	0.53	0.51
Value efficiency	2.39	1.56	2.08	1.32
GWI efficiency	1.70	1.60	1.45	1.19
CO <sub>2</sub> efficiency	0	0.29	0.09	0.33

**Table 3.** Feasibility indicators.

Indicator	TRL 2		TRL 4	
	Eni	Asahi	Eni	Asahi
Maximum mass flow potential [kt a <sup>-1</sup> ]	1000	1000	1000	1000
Maximum energy flow potential [P] a <sup>-1</sup>	8.38	8.23	10.35	27.64
Maximum value flow potential [M€ a <sup>-1</sup> ]	1002	1570	1002	2091
Maximum GWI reduction potential [kt CO <sub>2</sub> -eq a <sup>-1</sup> ]	954	1266	754	691
Maximum CO <sub>2</sub> storage potential [kt a <sup>-1</sup> ]	0	489	118	679

In terms of feasibility, the maximum mass flow potential is the same for all processes as it is limited by the annual, global consumption of DMC, representing a small market for a bulk chemical. In terms of maximum energy flow potential, the Asahi process shows a strong increase between TRL 2 and TRL 4, indicating a high energy consumption of the suggested process design and again a potential for optimization. In terms of maximum value potential, the Asahi process reaches higher sales due to its marketable byproducts, which means that a company using the Asahi process could potentially realize a sales volume twofold of the Eni process sales volume based on the results at TRL 4. In terms of maximum GWI reduction potential, the Asahi process reaches a higher level than the Eni process at TRL 2 due to its multiple target products but a slightly lower level at TRL 4 due to its high energy consumption. In terms of maximum CO<sub>2</sub> storage potential, using the Asahi process shows a larger potential to temporarily store CO<sub>2</sub> in the economic cycle than the Eni process; however, the amount of 680 kt a<sup>-1</sup> is too low to be considered a large-scale emissions storage technology.

As expected, most efficiency results decrease from TRL 2 to TRL 4, as the scope of analysis becomes more exhaustive, and additional byproducts or energy burdens are included. The exception in this worked example is an increase in CO<sub>2</sub> efficiency in both cases as CO<sub>2</sub> is used as an additional input for the Eni process at TRL 4 and as CO<sub>2</sub> is also converted to the marketable product of EC for the Asahi process at TRL 4.

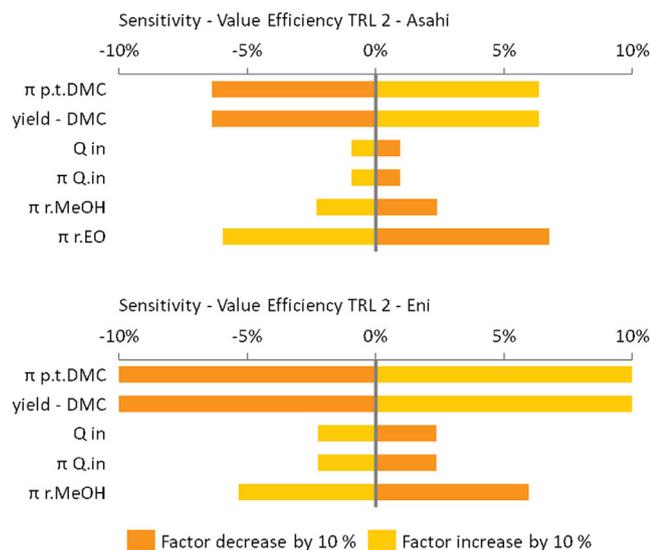
**4.4. Risk assessment and Interpretation**

**4.4.1. Sensitivity Analysis**

For TRL 2 we conduct a local sensitivity analysis focusing on six factors, the price of the target product DMC ( $\pi_{p,DMC}$ ), input energy ( $\pi_{Q,in}$ ), reactant methanol ( $\pi_{r,MeOH}$ ), and reactant EO ( $\pi_{r,EO}$ ) as well as DMC yield and amount of input energy ( $Q_{in}$ ). We vary these factors by 10% and observe the change in value efficiency. For both processes, the largest influencing factors on value efficiency are the price of DMC, DMC yield, and the price of methanol (see **Figure 10**).

For TRL 4, we extend the local sensitivity analysis by further factors, namely, the prices of the products EG ( $\pi_{p,EG}$ ) and EC ( $\pi_{r,EC}$ ), the price of reactant CO<sub>2</sub> ( $\pi_{r,CO2}$ ), the EUR-USD exchange rate, CEPCI, operating hours, years of operation, and the amount of work in the system elements DMC reaction, DMC separation, and DMC utilities for the Eni process and in addition also EC reaction, EC separation, and EC utilities for the Asahi process. As before we vary each factor by 10% and observe the outcome on value efficiency, but only report factors with a change larger than 0.1% (see **Figure 11**). The largest influencing factors on value efficiency are DMC yield, DMC price (for both processes), as well as the EO price for the Asahi process and the methanol price, and the EUR-USD exchange rate for the Eni process.

In addition, we analyze the thresholds where the processes break even, which means reaching a value efficiency of 1; we take into account the two most important factors identified by sensitivity analysis—DMC yield and price. As both factors have the same effect on value efficiency, only one threshold is reported.

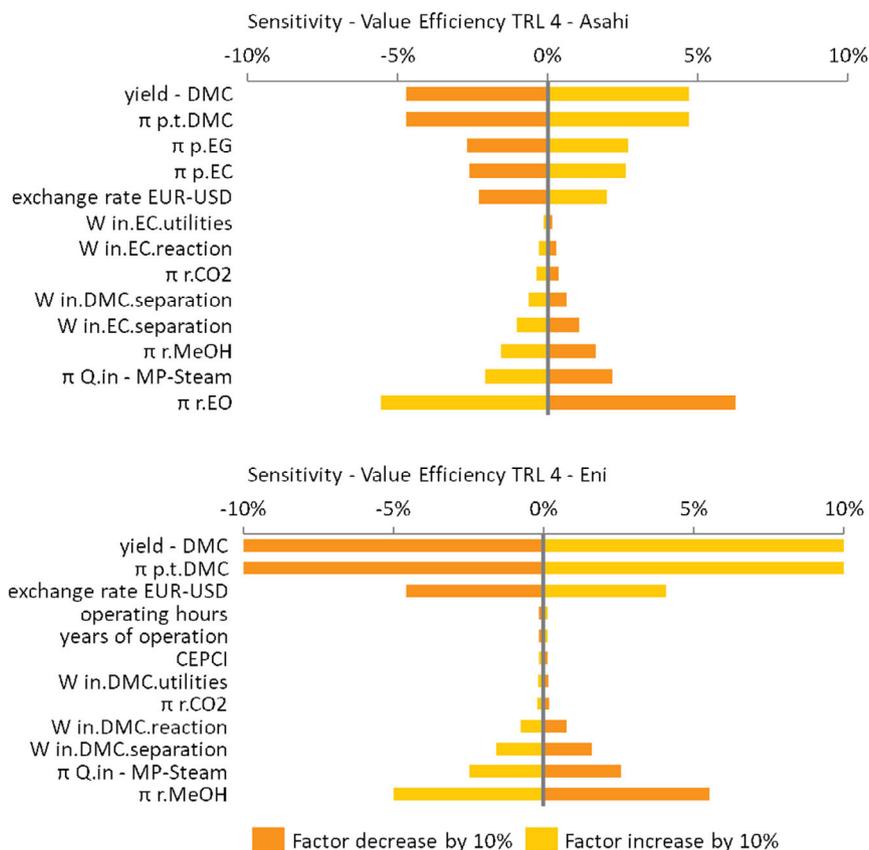


**Figure 10.** Sensitivity analysis at TRL 2 varying six factors by  $\pm 10\%$  and observing the change in value efficiency; for example, a decrease in the DMC price ( $\pi_{p.t.DMC}$ ) by 10% results in a reduction of value efficiency by 6.4% for the Asahi process and by 10% for the Eni process.

At TRL 2, the Asahi process breaks even at a DMC yield or price that is 56% lower than the base case; the Eni process breaks even at a DMC yield or price 58% lower than the base case. At TRL 4, both processes break even at a DMC yield or price 48% lower than the base case. All break-even thresholds are substantially lower than the base case, which means that there is a large buffer for variation of the most important parameters DMC yield and price.

#### 4.4.2. Uncertainty Analysis

For uncertainty analysis, we discuss input data, model, and context uncertainty. We chose to qualify input data uncertainty in a pedigree matrix. For both processes and TRLs, we rank and color-code input data quality from 0, red (no data), to 4, green (validated data). From TRL 2 to TRL 4 we increase the level of detail in the analysis (see Table 4, 5, and 6). At TRL 2, we use stoichiometric data, reaction enthalpies, and HHVs among others for our energy and mass balances, which also include CO<sub>2</sub> flows. We believe these data to be of a preliminary level of detail, which seems sufficient at TRL 2. At TRL 4, we replace the stoichiometric data with process development data, reaching the rigorous level. The remaining data stay at the detailed level which we



**Figure 11.** Sensitivity analysis at TRL 4 varying nineteen factors by  $\pm 10\%$  and observing the change in value efficiency—only changes larger than 0.1% are reported; for example, a decrease in the DMC yield by 10% results in a reduction of the value efficiency by 4.7% for the Asahi process and by 10% for the Eni process.

**Table 4.** Pedigree color code.

Pedigree rank	
4	Validated data
3	Rigorous data
2	Detailed data
1	Preliminary data
0	No data

**Table 5.** Pedigree matrix TRL 2.

	Eni	Asahi
Technical input data		
Mass flows and energy flows	1	1
Physical properties	2	2
Economic input data		
Sales price/production cost	2	2
Market size/production capacity	2	2
Environmental input data		
CO <sub>2</sub>	1	1
GWI	2	2

**Table 6.** Pedigree matrix TRL 4.

	Eni	Asahi
Technical input data		
Mass flows and energy flows	2	2
Design parameters	3	3
Boundary conditions	3	3
Physical properties	3	3
Economic input data		
Sales price/production cost	2	2
Market size/production capacity	2	2
Economic assumptions	2	2
Environmental input data		
CO <sub>2</sub>	2	2
GWI	2	2

consider sufficient at TRL 4; however, quantification of input data uncertainty was not possible as input data distributions were not accessible.

We qualify model uncertainty, meaning how well the model reflects the analyzed system. Even though the assessment scope is significantly reduced, we use similar indicators and scopes for both processes, which is why we argue that this analysis remains a systematic comparison. We qualify context uncertainty as low to medium, as we keep the context for the analysis generic and do not follow a specific scenario, except for the base year 2019 and

the location of Europe/Germany. For the reason of brevity, the analysis of further scenarios is omitted in this worked example but has been described elsewhere before, for example, for oxy-methylene ethers.<sup>[73,74]</sup> As a heuristic, we follow the overall error ranges reported by AACE, originally reported at TRL 3 but used here also at TRL 2, of  $-50\%$  to  $+100\%$  and at TRL 4 of  $-30\%$  to  $+50\%$ .<sup>[21,64]</sup> The indicator results and their heuristic error ranges are shown in **Figure 12**.

We suspect that the AACE ranges overestimate the error and that a substantial difference in the results of Efferi indicators, a deviation exceeding  $\pm 33\%$ , allows us to derive significant conclusions. We observe significant differences at TRL 2 for value and CO<sub>2</sub> efficiency and the maximum potentials of value, GWI reduction, and CO<sub>2</sub> storage. At TRL 4 we observe significant differences for mass, value, and CO<sub>2</sub> efficiency and maximum potentials of energy, value, and CO<sub>2</sub> storage.

#### 4.5. Recommendations for Decision-Making

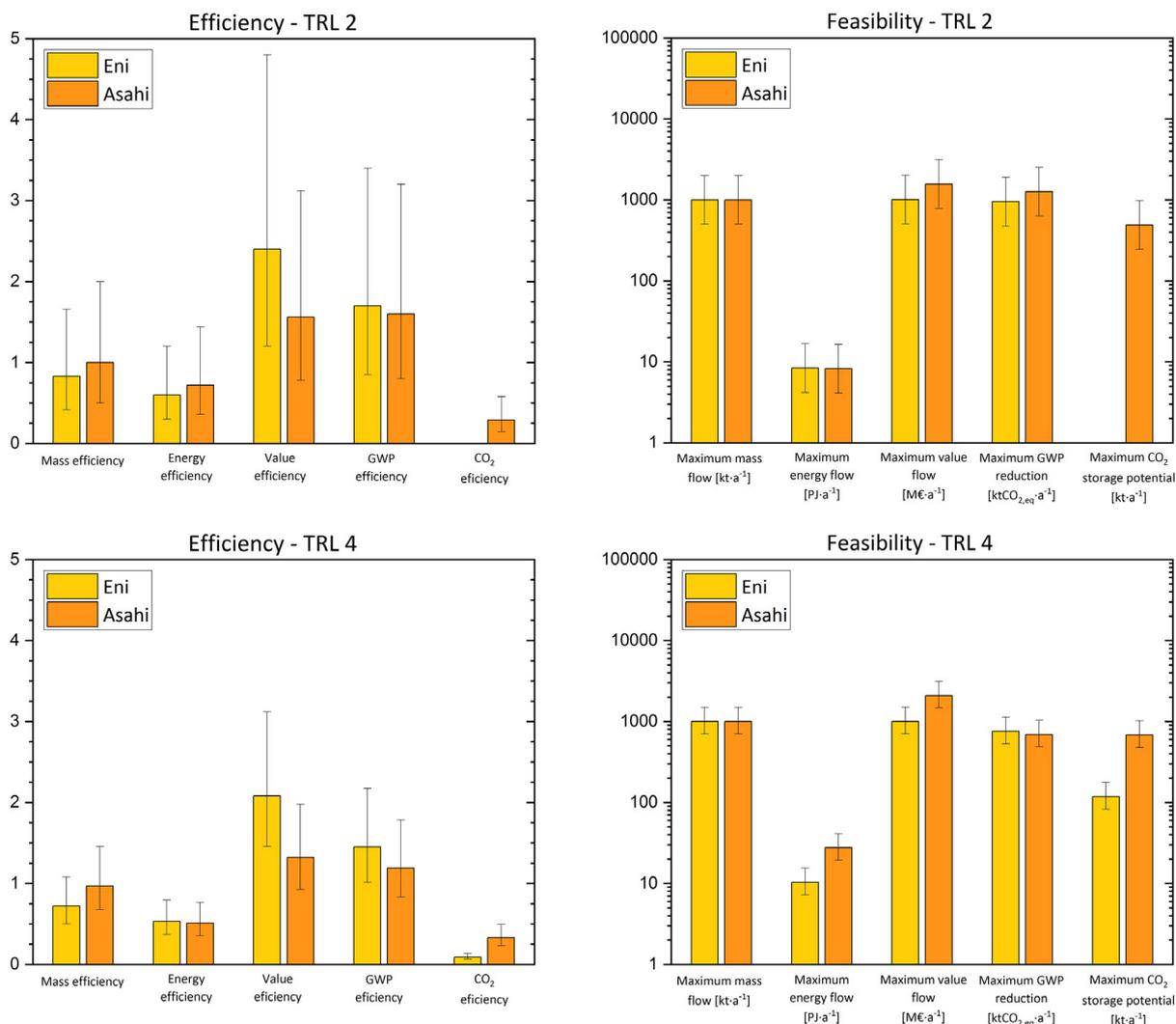
At TRL 2, the Asahi process performs significantly better at CO<sub>2</sub> efficiency, maximum value flow, maximum GWI reduction, and maximum CO<sub>2</sub> storage potential, while the Eni process performs significantly better at value efficiency. While value efficiency remains of concern, the required resources for development at TRL 3 and TRL 4 remain low and the continuation of the development of the Asahi process can be recommended. As focus points for the development, we suggest the improvement of DMC yield and energy efficiency in the process.

At TRL 4, the Asahi process performs significantly better at mass and CO<sub>2</sub> efficiency, maximum potential energy, and value flow as well as maximum CO<sub>2</sub> storage potential, whereas the Eni process again performs significantly better at value efficiency. In general, a continuation of the development of the Asahi process is recommended, mainly because of its most likely outperforming maximum value potential and additional CO<sub>2</sub> and GWI characteristics. If the only goal is to increase value efficiency, the continuation is, however, not recommended. The suggested development focus points from TRL 2 remain.

## 5. Discussion

In this article, we presented the Efferi framework, a method for assessing early-stage carbon capture and utilization technologies, implementing global standards for early-stage assessment, reducing subjective judgments, allowing for comparisons of alternatives at the same TRL or different TRLs, and taking the perspective of stakeholders. We presented a general overview as well as the framework in detail for each level from TRL 1 to TRL 4; we further presented an example application for the case of DMC at TRL 2 and TRL 4.

The Efferi framework follows all requirements (shall guideline rules) and some additional suggestions for more comprehensive assessment (should guideline rules) of the TEA guidelines for CCU.<sup>[17]</sup> The framework systematically combines commonly used indicators and their equations to a coherent set and provides specific guidance on goal, scope, inventory, calculation, and interpretation for each maturity level, forming a robust



**Figure 12.** Indicator values and heuristic error ranges, showing the results of the described efficiency and feasibility indicators at TRL 2 and TRL 4 for the Asahi and Eni processes including heuristic error bars.

and easy-to-use assessment method for practitioners that reduces subjective judgments. Results indicating a low performance of a product system are not likely to change considerably at a later TRL, which shows the reliability of the framework. Furthermore, a strong decrease from one TRL to the next shows that there remains, in theory, a large potential for improvement.

The selected shortcut assessment approach reduces input data uncertainty and assessment effort compared with conventional, “full-scope” assessments as the shortcut approach refrains from the use of estimation, or heuristics. For example, the Efferi framework leaves out heuristics which are, even though uncertain, conventionally judged by experience, such as separation processes at early development stages. Model uncertainty is expected to increase as the limited scope of assessment reduces the model’s complexity and thereby also how well it reflects the observed system. However, the influence on decision-making is

expected to be limited, as the assessments are repeated at increased scope with increasing maturity. Overall, the reduced input data uncertainty and an acceptable increase in model uncertainty can lead to clearer recommendations and lower risk in decision-making compared with conventional assessments—especially for go/no-go decisions. Furthermore, using the shortcut approach leads to a higher number of possible solutions, also including unconventional solutions that would have been ruled out using incremental factors and conventional logic.

While the Efferi framework provides a comprehensive set of criteria and indicators, practitioners might need to extend these criteria and indicators according to their goal. Further qualitative indicators, such as geographical constraints, or health and safety,<sup>[10]</sup> or quantitative indicators, such as other environmental impact categories, could be used to extend the scope of assessment. Enviro-economic indicators such as the cost of CO<sub>2</sub>

avoided and social criteria and indicators were so far excluded from the Efferi framework; the former has an additional layer of uncertainty,<sup>[15]</sup> which needs to be resolved first and the latter is currently not common in the assessment of early-stage CCU technologies<sup>[33]</sup> and its application is limited for the assessment in companies.<sup>[75]</sup> As the Efferi framework takes a cradle-to-gate assessment scope and analyzes one impact category, GWI, it only represents a preliminary environmental impact assessment; results have limited validity and shall be interpreted with caution.

To address the challenges of early-stage assessments,<sup>[25]</sup> the proposed Efferi framework links its assessment to technology maturity, applies maturity-as-a-scope, and uses shortcut indicators, similar to the recently published assessment framework of Roh et al.<sup>[15]</sup> Building on recent developments in the literature, the proposed Efferi framework is the first assessment method to systematically integrate the TEA Guidelines for CCU. In the case study, we have shown its applicability to a thermochemical process for the production of the chemical DMC. In addition to that we have applied the Efferi framework (in earlier versions) to thermochemical processes for the production of fuels,<sup>[73,74]</sup> minerals,<sup>[76]</sup> polymers<sup>[77]</sup> and an electrochemical process for the production of ethylene<sup>[78]</sup>—proving its applicability for all major technology fields of CCU.

To address the challenges of subjective judgments and comparisons between TRLs,<sup>[15]</sup> the here presented Efferi framework provides a standardized set of commonly accepted criteria and indicators that allows, in combination with the other principles of framework design, to not only reduce subjective judgments but also allow for comparisons at the same TRL or different TRLs. We further extend current literature by introducing a new stakeholder-perspective approach, using the perspectives of researchers, industry managers, and funding agents. Overall, the Efferi framework should

serve practitioners as an easy-to-use tool to systematically and reliably assess early-stage technologies in carbon capture and utilization.

Future research could include extending the Efferi framework to higher TRL, extending and specifying the Efferi framework to adjacent technology areas such as energy engineering and bioengineering, quantifying risk assessment, or specifying environmental and social criteria for early-stage technology assessment.

## 6. Conclusion

The here proposed Efferi framework offers a specific set of accepted indicators and equations allowing practitioners to reduce subjective judgments and to compare alternatives at the same and different TRLs, addressing current gaps in the literature. Furthermore, it is the first assessment framework for CCU to implement the TEA guidelines and incorporate stakeholder perspectives of researchers, industry managers, and funding agents. The Efferi framework provides specific guidance at each maturity level, forming a robust and easy-to-use assessment method for early-stage CCU technologies, allowing clearer go/no-go recommendations at reduced assessment effort and facilitating apples to apples comparisons. Future research could extend the Efferi framework to higher TRL or adjacent technology areas, quantify risk assessment, or specify environmental and social criteria for early-stage technology assessment.

## Appendix

### Annex A

**Table A1.** Efferi indicators of TRL 2—ideal reactions.

Perspective	Indicator	Equation	Eq.
Efficiency	Mass efficiency	$\eta_{\text{mass,TRL2}} = \frac{\sum_{p,t} \dot{m}_{p,t,\text{react}}}{\sum_r \dot{m}_{r,\text{react}}} = \frac{\sum_{p,t} (M_{p,t} * \nu_{p,t})}{\sum_r (M_r *  \nu_r )}$	(1)
	Energy efficiency	$\eta_{\text{energy,TRL2}} = \frac{\sum_{p,t} \text{HHV}_{p,t} +  Q_{\text{out,react}} }{\sum_r \text{HHV}_r + Q_{\text{in,react}}} = \frac{\sum_{p,t} ((\Delta_c H_{p,t}^0 * \nu_{p,t}) +  Q_{\text{out,react}} )}{\sum_r ((\Delta_c H_r^0 * \nu_r) + Q_{\text{in,react}})}$	(2)
	Value efficiency	$\eta_{\text{value,TRL2}} = \frac{\sum_{p,t} (\dot{m}_{p,t,\text{react}} * \pi_{p,t}) + Q_{\text{out,react}} * \pi_Q}{\sum_r (\dot{m}_{r,\text{react}} * \pi_r) + Q_{\text{in,react}} * \pi_Q}$	(3)
	GWl efficiency	$\eta_{\text{GWl,TRL2}} = \frac{\sum_{p,t} (\dot{m}_{p,t,\text{react}} * \text{GWl}_{p,t}) + Q_{\text{out,react}} * \text{GWl}_Q}{\sum_r (\dot{m}_{r,\text{react}} * \text{GWl}_r) + Q_{\text{in,react}} * \text{GWl}_Q}$	(4)
	CO <sub>2</sub> efficiency	$\eta_{\text{CO}_2, \text{TRL2}} = \frac{\dot{m}_{r,\text{CO}_2,\text{react}}}{\sum_r \dot{m}_{r,\text{react}}} = \frac{M_{\text{CO}_2} * \nu_{\text{CO}_2}}{\sum_r (M_r * \nu_r)}$	(5)
Large-scale feasibility	Maximum mass and energy flow potential	For $i, l \in p, r$ and $j \in$ all options of production or consumption	–
		$\dot{m}_{\text{total},i} = \sum_j \dot{m}_j$	(6)
		$\dot{n}_{\text{max},i} = \text{Min} \left( \frac{\dot{m}_{\text{total},i}}{ \nu_i  * M_i} \right)$	(7)
		$\dot{m}_{\text{max},i} = \dot{n}_{\text{max},i} *  \nu_i  * M_i$	(8)
		$Q_{\text{max},\text{in}}, Q_{\text{max},\text{out}} \sim \dot{n}_{\text{max},i}$	(9)
	Maximum value potential	$\dot{\Pi}_{\text{value,TRL2}} = (\sum_r (\dot{m}_{\text{max},r,\text{react}} * \pi_r) + Q_{\text{max},\text{in,react}} * \pi_Q) * \eta_{\text{value,TRL2}}$	(10)
Maximum GWl reduction potential	$\Delta \text{GWl}_{\text{max,TRL2}} = \left( \sum_r (\dot{m}_{\text{max},r,\text{react}} * \text{GWl}_r) + Q_{\text{max},\text{in,react}} * \text{GWl}_Q \right) * (\eta_{\text{GWl,TRL2}} - 1)$	(11)	
Maximum CO <sub>2</sub> storage potential	$\dot{m}_{\text{CO}_2, \text{storage,TRL2}} = \sum_r \dot{m}_{\text{max},r,\text{react}} * \eta_{\text{CO}_2, \text{TRL2}}$	(12)	

**Table A2.** Efferi indicators of TRL 3—validated reactions.

Perspective	Indicator	Equation	Eq.
Efficiency	Mass efficiency	$\eta_{\text{mass,TRL3}} = \frac{\sum_{p,t} \dot{m}_{p,t,\text{react net}}}{\sum_r \dot{m}_{r,\text{react net}}} \quad (13)$	(13)
	Energy efficiency	$\eta_{\text{energy,TRL3}} = \frac{\sum_{p,t} \text{HHV}_{p,t} * \dot{m}_{p,t,\text{react net}} + B_{\text{out,react net}}}{\sum_r \text{HHV}_r * \dot{m}_{r,\text{react net}} + Q_{\text{in,react net}}} \quad (14)$	(14)
	Value efficiency	$\eta_{\text{value,TRL3}} = \frac{\sum_p (\dot{m}_{p,t,\text{react net}} * (\pi_p + \pi_{p,f} + \pi_{p,s})) + B_{\text{out,react net}} * \pi_B}{\sum_r (\dot{m}_{r,\text{react net}} * \pi_r) + Q_{\text{in,react net}} * \pi_Q} \quad (15)$	(15)
	GWI reduction efficiency	$\eta_{\text{GWI,TRL3}} = \frac{\sum_p (\dot{m}_{p,t,\text{react net}} * \text{GWI}_{p,t}) + B_{\text{out,react net}} * \text{GWI}_B}{\sum_r (\dot{m}_{r,\text{react net}} * \text{GWI}_r) + Q_{\text{in,react net}} * \text{GWI}_Q} \quad (16)$	(16)
	CO <sub>2</sub> efficiency	$\eta_{\text{CO}_2, \text{TRL3}} = \frac{\dot{m}_{\text{CO}_2, \text{react net}}}{\sum_r \dot{m}_{r,\text{react net}}} \quad (17)$	(17)
Large-scale feasibility	Maximum mass and energy flow potential	Same as at TRL 2	–
	Maximum value potential	$\dot{\Pi}_{\text{value,TRL3}} = (\sum_r (\dot{m}_{\text{max},r,\text{react net}} * \pi_r) + \dot{Q}_{\text{max,in,react net}} * \pi_Q) * \eta_{\text{value,TRL3}} \quad (18)$	(18)
	Maximum GWI reduction potential	$\Delta \text{GWI}_{\text{max,TRL3}} = (\sum_r (\dot{m}_{\text{max},r,\text{react}} * \text{GWI}_r) + \dot{Q}_{\text{max,in,react net}} * \text{GWI}_Q) * (\eta_{\text{GWI,TRL3}} - 1) * t_{p,t} \quad (19)$	(19)
	Maximum CO <sub>2</sub> storage potential	$\dot{m}_{\text{CO}_2, \text{storage,TRL3}} = \sum_r \dot{m}_{\text{max},r,\text{react net}} * \eta_{\text{CO}_2, \text{TRL3}} * t_{p,t} \quad (20)$	(20)

**Table A3.** Efferi indicators of TRL 4—process concepts.

Perspective	Indicator	Equation	Eq.
Efficiency	Mass efficiency	$\eta_{\text{mass,TRL4}} = \frac{\sum_{p,t} \dot{m}_{p,t,\text{process}}}{\sum_r \dot{m}_{r,\text{process}}} \quad (21)$	(21)
	Energy efficiency	$\eta_{\text{energy,TRL4}} = \frac{\sum_{p,t} \text{LHV}_{p,t} * \dot{m}_{p,t,\text{process}} + \sum_j (W_{j,\text{out,process}})}{\sum_r \text{LHV}_r * \dot{m}_{r,\text{process}} + \sum_j (W_{j,\text{in,process}})} \quad (22)$	(22)
	Value efficiency	$\eta_{\text{value,TRL4}} = \frac{\sum_p (\dot{m}_{p,t,\text{process}} * (\pi_p + \pi_{p,f} + \pi_{p,s})) + \sum_j (W_{j,\text{out,process}} * \pi_{Wj,\text{out,process}})}{\sum_r (\dot{m}_{r,\text{process}} * \pi_r) + \sum_j (W_{j,\text{in,process}} * \pi_{Wj,\text{in,process}}) + \sum_j \frac{\dot{m}_{\text{equipment},j}}{t_{\text{operation},j}}} \quad (23)$	(23)
	GWI reduction efficiency	$\eta_{\text{GWI,TRL4}} = \frac{\sum_p (\dot{m}_{p,t,\text{process}} * \text{GWI}_{p,t}) + \sum_j (W_{j,\text{out,process}} * \text{GWI}_{Wj,\text{out,process}})}{\sum_r (\dot{m}_{r,\text{process}} * \text{GWI}_r) + \sum_j (W_{j,\text{in,process}} * \text{GWI}_{Wj,\text{in,process}}) + \sum_j \frac{\dot{m}_{\text{equipment},j}}{t_{\text{operation},j}} * \text{GWI}_j} \quad (24)$	(24)
	CO <sub>2</sub> efficiency	$\eta_{\text{CO}_2, \text{TRL4}} = \frac{\dot{m}_{\text{CO}_2, \text{process}}}{\sum_r \dot{m}_{r,\text{process}}} = \frac{\sum_{in} \dot{m}_{r,\text{CO}_2, \text{process}} - \sum_{out} \dot{m}_{r,\text{CO}_2, \text{process}}}{\sum_r \dot{m}_{r,\text{process}}} \quad (25)$	(25)
Large-scale feasibility	Maximum mass and energy flow potential	Same as at TRL 2	–
	Maximum value potential	$\dot{\Pi}_{\text{value,TRL4}} = (\sum_r (\dot{m}_{\text{max},r,\text{process}} * \pi_r) + \sum_i (W_{\text{max},i,\text{in,process}} * \pi_{W_{i,\text{in,process}}}) + \sum_j \frac{\dot{m}_{\text{equipment},j}}{t_{\text{operation},j}}) * \eta_{\text{value,TRL4}} \quad (26)$	(26)
	Maximum GWI reduction potential	$\Delta \text{GWI}_{\text{max,TRL4}} = (\sum_r (\dot{m}_{\text{max},r,\text{process}} * \text{GWI}_r) + \sum_i (W_{\text{max},i,\text{in,process}} * \text{GWI}_{W_{i,\text{in,process}}}) + \sum_j \frac{\dot{m}_{\text{equipment},j}}{t_{\text{operation},j}} * \text{GWI}_j) * (\eta_{\text{GWI,TRL4}} - 1) * t_{p,t} \quad (27)$	(27)
	Maximum CO <sub>2</sub> storage potential	$\dot{m}_{\text{CO}_2, \text{storage,TRL4}} = \sum_r \dot{m}_{\text{max},r} * \eta_{\text{CO}_2, \text{TRL4}} * t_{p,t} \quad (28)$	(28)

**Annex B**

**Table B1.** HHV and LHV.

Chemical	HHV [MJ kg <sup>-1</sup> ]	LHV [MJ kg <sup>-1</sup> ]	Reference
Oxygen	–	–	Per definition
Carbon monoxide	10.10	10.10	Aspen Plus V.10
Carbon dioxide	–	–	Per definition
Water	2.26	–	Calculated from NIST Webbook data
Methanol	23.88	21.10	Aspen Plus V.10
Ethylene oxide	29.50	27.65	Calculated from NIST Webbook data
Dimethyl carbonate	17.13	15.78	Calculated from NIST Webbook data
Ethylene glycol	16.81	14.85	Calculated from NIST Webbook data
Ethylene carbonate	20.02	18.71	Calculated from NIST Webbook data
Formaldehyde	18.65	17.30	Calculated from NIST Webbook data

**Table B2.** Production cost and sales prices of materials.

Chemical	Type	Value [EUR kg <sup>-1</sup> ]	Reference
Oxygen	Production cost	0.026	Rao, Muller (2007)
Carbon monoxide	Production cost	0.264	Natural gas based SMR und rWGS, expert guess
Carbon dioxide	Sales price	0.800	Expert guess
Water	Sales price	0.031	Boulamanti, Moya (2017)
Methanol	Sales price	0.332	ICIS database (10-year average 2010–2019)
Ethylene oxide	Sales price	1.306	ICIS database (10-year average 2010–2019)
Dimethyl carbonate	Sales price	1.002	Price quotes (17 quotes, Alibaba.com)
Ethylene glycol	Sales price	0.825	ICIS database (10-year average 2010–2019)
Ethylene carbonate	Sales price	1.369	Price quotes (7 quotes, Alibaba.com)
Formaldehyde	Sales price	0.654	Otto et al. (2015)

**Table B3.** Production cost of energy.

Energy	Type	Value [EUR G <sup>-1</sup> ]	Reference
Energy	Production cost (midpressure steam, 11 bar)	11.54	Turton (2012)

**Table B4.** Worldwide annual production capacities and consumption.

Chemical	Type	Value [kt a <sup>-1</sup> ]	Reference
Oxygen	Consumption	*	*Assumed to significantly larger than other capacities
Carbon monoxide	Consumption	320 042	Derived from SMR, IHS Markit (2019)
Carbon dioxide	Consumption	206 000	IHS Markit (2017)
Water	*	*	*Assumed to significantly larger than other capacities
Methanol	Production capacity	127 000	IHS Markit (2019)
Ethylene oxide	Production capacity	33 900	IHS Markit (2019)
Dimethyl carbonate	Production capacity	1000	Markets and Markets (2019)
Ethylene glycol	Production capacity	34 644	IHS Markit (2019)
Ethylene carbonate	Production capacity	1000	Markets and Markets (2019)
Formaldehyde	Production capacity	75 614	IHS Markit (2019)

**Table B5.** GWI 100a of materials.

Chemical	Type	Value [kgCO <sub>2</sub> -eq kg <sup>-1</sup> ]	Reference
Oxygen	Oxygen, liquid, at plant, Europe	0.3777	UVEK LCI Data (DQRv2:2018)
Carbon monoxide	Carbon monoxide, CO, at plant, Europe	1.5213	UVEK LCI Data (DQRv2:2018)
Carbon dioxide	Carbon dioxide liquid, at plant, Europe	0.8479	UVEK LCI Data (DQRv2:2018)
Water	Tap water production, conventional treatment (Europe without Switzerland)	0.0003	soca v.1
Methanol	Methanol, at plant, global	0.8090	UVEK LCI Data (DQRv2:2018)
Ethylene oxide	Ethylene oxide, at plant (Europe)	1.8204	UVEK LCI Data (DQRv2:2018)
Dimethyl carbonate	Dimethyl carbonate production, production mix, at plant, technology mix, 100% active substance	2.3158	PEF database
Ethylene glycol	Ethylene glycol, at plant, Europe	1.5561	UVEK LCI Data (DQRv2:2018)
Ethylene carbonate	Ethylene carbonate production, production mix, at plant, technology mix, 100% active substance (Europe)	1.6312	PEF database
Formaldehyde	Formaldehyde, production mix, at plant, Europe	1.1611	UVEK LCI Data (DQRv2:2018)

**Table B6.** GWI 100a of energy.

Energy	Type	Value [kgCO <sub>2</sub> -eq MJ <sup>-1</sup> ]	Reference
Energy	Heat and power cogeneration, natural gas, conventional power plant, 100 MW electrical   heat, district or industrial, natural gas	0.029	EuGeos' 15804_A2-IA System Processes

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## Conflict of Interest

The authors declare no conflict of interest.

## Author Contributions

A.W.Z. designed the framework, calculated the case study, and wrote the article. G.A.B. and R.S. contributed by discussing the framework and the case study and reviewing the article.

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