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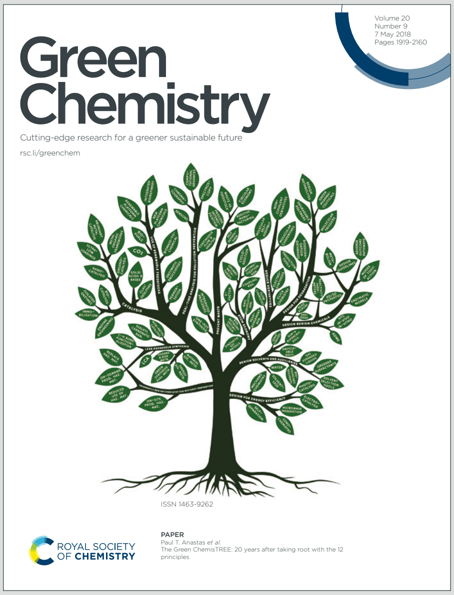

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How to assess the potential of emerging green technologies? Towards a prospective environmental and techno-economic assessment framework

Gwenny Thomassen,[a,b,c,d] Miet Van Dael[a,b], Steven Van Passel[a,c] and Fengqi You[*e]

For sustainable production and consumption, emerging green technologies need to be optimized towards a minimal environmental impact and a maximal economic impact. In an early stage of technology development, more flexibility is available to adapt the technology. Therefore, a prospective environmental and techno-economic assessment is required. The prospective assessment differs at the different stages of technology development, as also the data availability and accuracy evolves. This paper reviews the different prospective technological, economic and environmental assessment methods which have been used to assess the potential of new green chemical technologies. Based on the current best practices, an overarching framework is introduced to assess the technological, economic and environmental potential of an emerging green chemical technology at the different stages of technology development.

The need for a prospective green technology assessment

To reduce the environmental problems our society faces, the technologies used for our daily-life consumption pattern need to become more environmentally friendly. This need for environmentally sustainable production and consumption has also been stated as one of the Sustainable Development Goals.[1] To enable a more sustainable production, new green chemical technologies are being developed. For example, green chemicals from renewable feedstocks are under development that should contribute to a more sustainable chemical sector. However, these green chemical technologies can only contribute to a more sustainable society if their environmental impact is lower than the environmental impact of their conventional counterparts. Moreover, these emerging technologies will only be able to replace conventional technologies, if they can also economically compete with them. An assessment of the potential of these emerging green chemical technologies from life cycle environmental and techno-economic perspectives would therefore be important and necessary.

This assessment will differ in level of required accuracy and data availability, in accordance with the stage of maturity of the emerging technology. The stages of technology development can be defined by the Technology Readiness Levels (TRL), ranging from 1 to 9.[2] At a low TRL, the technology consist of a mere idea or general concept. The final specifications are still unclear and the technology is easily adaptable. As the technology proceeds alongside the TRLs, it becomes more mature until it is ready for market introduction. At this point, detailed data are available, but adaptations become more impractical and costly. The TRL scale is widely adopted for technology development management, and for example used by the European Union as a unified scale to better position project proposals.[3] A specific application of the TRL scale for the chemical industry has been formulated, which will be used throughout this study as well.[4] Most of the current technology assessments focus on mature technologies at a late TRL. However, 70%-80% of the production costs is determined at an early stage of technology development.[5, 6] In addition, the environmental impact will also be defined at this stage.[7] Yet, the mature stage is too late to optimize a new technology.[8] A prospective technology assessment, starting from an early stage of development, is required, including both a life cycle environmental impact assessment and a full techno-economic analysis.[9] A lot of methodological variations exist in economic and environmental prospective technology assessments over the different levels of technological maturity.[10] Consequently, there is an increasing demand for harmonized assessments, as formulated in numerous projects on emerging green technologies.[11-15] The harmonized assessment framework, as proposed in this study, could assist

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[a] *UHasselt, Centre for Environmental Sciences, Agoralaan, 3590 Diepenbeek, Belgium.*
[b] *VITO, Unit Separation and Conversion Technologies, Boeretang 200, 2400 Mol, Belgium.*
[c] *University of Antwerp, Department of Engineering Management, Prinsstraat 13, 2000 Antwerp, Belgium*
[d] *Ghent University, Research Group Sustainable Systems Engineering (STEN), Coupure Links 653, 9000 Ghent, Belgium.*
[e] *Robert Frederick Smith School of Chemical and Biomolecular Engineering, Cornell University, Ithaca, New York 14853, United States.*

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in providing an answer to this demand. As different sorts of data are available and different levels of accuracy are required at each TRL, the prospective technology assessment will also differ at each TRL. This difference will be translated in both the environmental and the economic assessment.

This review provides an overview of prospective technology assessment methods, covering both environmental sustainability and techno-economic aspects. After reviewing the different prospective technology assessment methods, a more in-depth review is performed of the different screening and streamlining methods, which can be adopted in these prospective technology assessment methods. Based on this review, best practices are gathered in an integrated prospective environmental techno-economic assessment (ETEA) framework. The prospective ETEA framework includes specific guidelines on how to perform a prospective green chemical technology assessment at each TRL, including both the economic assessment and an environmental assessment. Therefore, this framework can act as a guidance for the assessment of new green technologies along their development path.

Prospective technology assessment methods

Prospective environmental impact assessment

The most popular methodology to perform an environmental impact assessment of products or processes is the life cycle assessment (LCA).[16] In an LCA, the environmental impacts of a specific product or process are assessed, taking the entire product life cycle in account.

There are different types of LCA, depending on the goal of the assessment. An attributional LCA will assess which environmental impact can be attributed to a certain product or process, including the immediate physical flows. A consequential LCA, on the other hand, takes the broader consequences for the product system into account, including the effects of, for example, differences in demand.[17] Besides the two different types, there are also two different approaches to an LCA, being a process-based analysis and an input-output analysis. These two approaches can also be combined, resulting in a hybrid approach.[18] In a process-based LCA, the underlying technological process is modelled to quantify all resources and emissions. In an input-output analysis, economic input-output models are used which provide the monetary flows between different economic sectors. This economic input-output model can then be multiplied with the according resource use and emission data of the different sectors to obtain an estimate of the environmental impacts. In accordance with the specific goal and scope of the assessment, the appropriate type and approach towards an LCA can be selected.

The first LCAs have been performed in the 60s assessing the energy requirement of chemical products and the environmental impact of packaging. In this period, these studies where known as Resource and Environmental Profile Analyses (REPA) or Ecobalances and had a large methodological variation. To reduce this variation, different workshops were organized by the global Society of Environmental Toxicology and Chemistry (SETAC) in the 90s.[19] These workshops led to a harmonized assessment method, which was consolidated in ISO guidelines.[20] The term ‘life cycle assessment’ was also introduced in this period.[19] The ISO standards define for example the four steps of the LCA methodology.[21] The first step of an LCA is the definition of goal and scope. In this step, the type and approach of the LCA should be defined. An LCA is usually oriented towards a product, but can also be used to assess the environmental impacts of an organization, consumer or country.[16] The system boundaries, the functional unit and the allocation procedure of the LCA are also defined in the first step. The functional unit of the LCA defines for which function the environmental impact will be assessed. Allocation is required when a process has multiple output products and the environmental impact for each output product separately is required. In this case, the total environmental impact will have to be divided over the different end products. The second step of the LCA is the life cycle inventory. In this step, an inventory list is made including all elementary inputs and outputs. An elementary input is an input coming directly from the environment and not from another process. To list all elementary inputs and outputs, all upstream and downstream processes need to be assessed as well. As this can amount to a very large scope, the definition of the system boundaries is crucial.[22] The third step of the LCA is the impact assessment step. Different impact indicator sets exist, which can be used to characterize the environmental impact of the elementary flows of the life cycle inventory. After the calculation of different indicators, they can be normalized and weighted for comparison. However, as this encompasses the inclusion of subjective choices, the ISO does not allow this for comparative analyses intended to be disclosed to the public. For other analyses, the results prior to the weighting procedure should always be provided.[20] The fourth step is the interpretation step, where different analyses can be added to analyse the results, such as a contribution analysis, sensitivity analysis, or uncertainty analysis.[22] In the interpretation step, a data quality analysis can be added by means of a Pedigree matrix. The LCA method is still being developed further, for example towards a Product Environmental Footprint (PEF) by the European Commission.[23] On a global level, the Life Cycle Initiative has been launched in 2002 by the SETAC and UN Environment to facilitate the

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application of life cycle knowledge on a global agenda.[24] To perform and report a reliable LCA, responsible conducts have been formulated.[25] The LCA can adopt a relative approach, where the impact is compared to a benchmark or an absolute approach, where the total impact over the life cycle is calculated without comparison.

Due to the large data and time requirement, a full-scale LCA is considered not to be applicable during early TRLs.[26] To enable an early TRL LCA, streamlining methods are used to simplify the LCA methodology into a prospective LCA.[27] Different studies exist that discuss the necessity of prospective LCAs.[8, 26, 28, 29] In addition, multiple examples of prospective LCAs exist as well.[27, 30-33] As an extension from the prospective LCA concept, the anticipatory LCA approach was developed.[34] In the anticipatory LCA, stakeholders are also involved to underpin the methodological assumptions, such as system boundaries, when performing a prospective LCA. A case study on photovoltaics was used to illustrate this anticipatory LCA approach.[35] However, the term anticipatory LCA has also been used for prospective studies which do not exactly follow the suggested anticipatory approach.[36-38] To avoid discussion over terminology, the term prospective assessment is recommended for studies assessing a technology, which is not fully established in the market.

Prospective LCAs use in general three different streamlining strategies.[39] In the first streamlining strategy, the system boundaries are limited by, for example, excluding the capital goods. However, capital goods can have a relatively large environmental impact.[40] Also other significant parameters, such as the enzymes in the lignocellulosic ethanol production process, were found to be excluded.[41] Cut-off criteria are typically subjective, as many excluded processes have never been assessed before. [18] Therefore, the statement that these excluded processes do not have a significant impact is more an assumption than a fact. A second strategy is the use of general indicators.[42] However, the most widely used environmental indicators, such as carbon footprint, are not necessarily the most important ones.[43] The streamlining of the indicator set can lead to replacement of environmental impacts to other indicators and does not give a general view on the environmental potential of a new technology.[44] A third strategy is the use of proxy data, by using average or general estimates when specific data are not available. Although a prospective LCA is performed during technology development, the technology itself is projected on a future industrial scale to enable comparisons with conventional established technologies.[28] Significant differences exist between lab-based LCAs and LCAs projected on an industrial scale.[45] Proxy data can serve as an approximation of this industrial scale data. The use of different streamlining methods, enables an LCA continuum, where the environmental impact is assessed alongside technology development.[39] A stepwise procedure for LCA during process development has been proposed.[46] However, guidelines on how to convert the lab-based data into industrial scale data are rare. For this conversion, an integration with the technological analysis is required, which has been advocated before.[47] This integration is also found in the parameterization approaches, where raw data and formulas are used instead of fixed numbers.[48]

Prospective techno-economic assessment

The economic profitability of a new green chemistry technology can be assessed by different methods. A method that gained recent popularity is the techno-economic assessment (TEA).[49] In this method a technological assessment is integrated with an economic assessment. In this way, an alteration in a technological parameter is directly translated into an altered economic indicator. According to Web of Science, the oldest publication including the term techno-economic assessment was published in 1983, assessing the recovery of chemical elements from seawater and brine. Although the amount of published techno-economic assessments has increased, methodological discussions are still rare.[49] In general, the methodology is based on cost engineering estimate practices and cost-benefit analyses. Recommended practices for these cost engineering estimates have for example been formulated by the American Association of Cost Engineers (AACE). However, in published TEA studies, a large variation still exists concerning for example indirect costs and scale-up measures, which can largely impact the results.[10] To harmonize these assessments, Van Dael et al.[49] provided a general methodology for the TEA, based on current best-practices. This TEA methodology consists of four steps. In the first step, a market study is performed so the prices and market volumes can be determined. In addition, the market potential for the new product or technology can be assessed here. In the second step, the process flow diagram (PFD) and mass and energy balances are calculated. The third step is the economic analysis, where investment criteria are used to assess the profitability of the system. These investment criteria can include the net present value (NPV), or the internal rate of return (IRR), which specifies the discount rate for which the NPV equals zero and the (discounted) payback period.[50] In the fourth step, a risk analysis is included to assess the influences of uncertainty on the indicators.

In contrast to prospective LCAs, not much literature is available on prospective TEAs. TEAs are in general used for technologies under development and therefore mostly prospective. Although a lot of TEAs have been performed, prescriptions on the methodology itself and how this methodology incorporates the TRLs are scarce.[49] As the technological

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process underlying the prospective economic and environmental assessments is equal, the same streamlining methods can be used. Similar to prospective LCAs, prospective TEAs assume a future industrial plant, i.e. the nth plant design. The nth plant indicates that the facility under development is the nth plant of its kind. Major technical challenges have been overcome, and required equipment are commercially available.[51] Other methods such as Life Cycle Costing (LCC) have been used as well to assess the economic potential.[52] However, in these methods important costs such as labor and equipment costs are often excluded, which makes conclusions on the crucial drivers of an economically profitable technology infeasible. Moreover, LCC focusses more on the total cost distribution of the product over its total life cycle, while TEA analyses the economic profitability from an investor's perspective.

Prospective integrated assessment

Currently, the environmental impact and the cost of a technology are usually assessed separately at different TRLs. As the system boundaries are different, the results can hardly be compared.[10] An integrated assessment takes multiple dimensions into account in one assessment. As a result, the decision maker has multiple criteria to consider. There are various ways to deal with this multi-criteria decision making. A first approach is by multi-criteria analysis (MCA), where different criteria are weighted and analysed. The aim of an MCA is to select the best scenario out of a set of known scenarios. MCA assigns weights to the different criteria or objectives to obtain one output value.[53] Both quantitative and qualitative criteria can be used.[54] Another approach is to perform first a multi-objective optimization (MOO).[55] The use of MOO can result in a set of Pareto-optimal scenarios, instead of one optimal scenario. A Pareto-optimal scenario is a scenario which cannot be improved in one dimension without deteriorating in another scenario.[55] After performing a MOO, an MCA can be added to weigh the Pareto-optimal scenarios and obtain one optimal scenario. However, in a prospective technology assessment, the main objective is to obtain a broad perspective on the economic and environmental impacts of the emerging green technology. A broad range of indicators is therefore more appropriate than a limited set of aggregated indicators at this point of technological maturity.

Besides economic and environmental perspectives, sustainability also has a social dimension. Sustainability also includes a social dimension. However, in contrast to the environmental and economic dimensions, only limited work has been done on social technology assessment.[56] Therefore, it has not been included in this framework, but is considered as an interesting path for further research.

The integration of environmental and economic perspectives alongside technology development is not a new concept.[57] Also, an integrated environmental, economic and social assessment for chemical process design has been proposed before.[58] In this study, the environmental assessment was streamlined by using a single simplified indicator, the waste reduction (WAR) algorithm. For the economic assessment, the NPV and the IRR were calculated. The social assessment was included in a qualitative way. An overall strategy for a design methodology integrating techno-economic assessment, LCA, pinch analysis, supply chain analysis and multi-criteria decision has also been proposed.[59] These existing studies focus mostly on providing an overarching methodological structure or on comparing technologies with a limited amount of indicators. The indicators have often been streamlined, but no information is given on how to handle scale-up of early TRL data. Scale-up procedures are also available. However, they have not been combined with an overarching framework to optimize new technologies towards economic and environmental objectives over the different TRLs, which is the main purpose of this paper.

An integrated environmental techno-economic assessment (ETEA) methodology can assist in harmonizing the economic and environmental dimensions of sustainability.[60] The framework will follow the strategy for an overarching method, as has previously been proposed and is based on the integration of the LCA and TEA methdology.[59] As data availability and accuracy are different at each stage of technology development, the ETEA methodology will differ at each TRL. Therefore, a framework that is applicable over different TRLs is required, so that a continuum is constructed between a screening ETEA at a low TRL, a streamlined ETEA at middle TRL and a full-scale ETEA at TRL 9. As the ETEA methodology is based on an integrated LCA and TEA, streamlining methods from these underlying methodologies are incorporated. These streamlining methods are based on the best-practices, which are currently available. Streamlining methods are required in the definition of the system boundaries, the gathering and processing of the technological, economic and environmental data and the handling of uncertainty. The different screening and streamlining methods that can be adopted in prospective technology assessment are reviewed in the next section. This way, an overview of different methods is provided that can be used to define the potential of an emerging green technology.

Screening and streamlining methods

Screening analysis

In the first TRLs (1-3), limited quantitative data is available. Therefore, screening tools can be applied. Screening methods

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provide a first glance on the potential of an emerging green technology. These methods are often qualitative or semi-quantitative and can be considered as a first rough prospective assessment.

The Sustainability SWOT (Strengths, Weaknesses, Opportunities, Threats) is a qualitative tool that can assist in the brainstorming process by providing first insights on the economic, environmental and social potential of the new technology.[61] For the environmental analysis, different matrix approaches exist.[62-65] In these methods the impact of the different life cycle phases on general indicators is scored in a qualitative way. An example of such a screening matrix is the MET matrix, which includes material, energy and toxicity considerations.[66] According to an industry review of sustainability assessments in early design stages, these qualitative screening tools should be simple and visual.[67] It can be translated through a color code or simple criteria to score the performance of the new technology. For these criteria, the twelve principles of green chemistry can be used.[68] These green chemistry principles have also been used by Cespi, et al. [69], together will other full LCA indicators, for their early-stage assessment of a process intensification technology. Also an extension with twelve principles of green engineering was elaborated, which can also be used in the matrix.[70] An interesting screening analysis has also been developed for the Lifecycle Screening of Emerging Technologies method (LiSET).[71] LiSET uses a traffic light color code to compare different technologies at the early TRLs. A decomposition analysis is used to decompose the technology into its different components, being the material, energy and service flows which are directly used for the technology or which are used to produce the input in upstream life cycle stages. These decomposition terms are then further translated in life cycle aspects, which present evaluable metrics. An example of such a metric could be the scarcity of a material that is used as an input. These metrics are then evaluated in relative terms for the different technology alternatives by means of a traffic light color code.[71] The main goal of the matrix approach is not to provide an accurate estimate of the potential of the emerging technology, but to provide insights on the sustainable hotspots, which are expected to have a large influence on this potential.

System boundaries

In TRL 4, the screening assessment evolves into a first quantitative streamlined assessment. A streamlined prospective assessment covers the same scope as a full-scale technology assessment, but uses different streamlining methods to cover for the lack of industrial data. The first aspect that needs to be streamlined is the system boundary. The system boundary defines which part of the life cycle will be used and which level of detail will be adopted. A technology does not stand on its own, but is part of a product lifecycle. This lifecycle starts from raw material extraction and ends with the end-of-life phase (Fig. 1). Multiple recycling loops are possible to enhance a circular life cycle instead of a linear concept.[72] The inclusion of all life cycle stages is important to avoid the replacement of costs and impacts to other life cycle phases.

Consequently, all inputs and outputs need to be modelled, until the final elementary inputs from the environment and elementary outputs into the environment are obtained. The elementary inputs from the environment are the resources that are extracted directly from the environment for the entire product life cycle. The elementary outputs into the environment are the emissions from all different life cycle phases that end up in the environment. The quantification of all elementary inputs and outputs encompasses a large system, which cannot be completely modelled due to time and budget constraints. Two main streamlining methods are used to solve this problem: excluding parts of the life cycle or simplifying the required data. In the first streamlining method, the system boundaries are limited and parts of the life cycle of the product or process are not incorporated in the assessment. As advocated by Graedel, this streamlining method has the risk of excluding important parts of the life cycle.[39] Different strategies exist to determine which products and processes can be included or excluded. For example, this can be based on the relative quantity, impact or cost. However, these strategies rely on information, which has not been gathered yet. As this information was available, these products and processes could be easily included. Therefore, related or similar technologies are often used to identify the product or process that can be excluded. Another method to deal with the low data availability at this TRL is the use of key elementary flows.[73] Key elementary flows are substances, which have a crucial impact on a specific environmental impact indicator. For example, CO_2 is a key elementary flow for the global warming potential indicator. Besides the known inputs and outputs, the occurrence and quantity of these key elementary flows can be included as well.

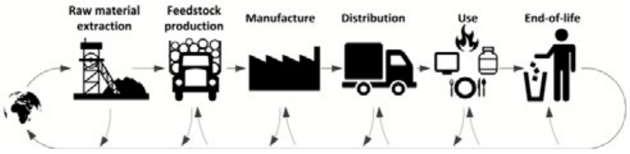

Fig. 1 General life cycle phases of a product or process including recycling streams

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A second streamlining method is to divide the system in foreground and background systems. The foreground system is specifically modelled, but for the background system, generic data from databases can be used (Fig. 2). The foreground system boundary is defined by the inputs and outputs to the foreground processes. Using this streamlining method, only foreground data needs to be obtained from the process or product under consideration. Background data can be obtained elsewhere, for example in databases such as ecoinvent or Gabi.[74, 75] Background processes can occur before (upstream) or after the specific product at the limit of the foreground system boundary (downstream). In the background processes, the level of detail will also be limited compared to the foreground process. This level of detail can vary from a black-box perspective, where only the main inputs and outputs are defined, to a full-scale technology characterization, including all underlying parameters.

In conclusion, the use of these two streamlining methods leads to the identification of the system boundaries and the classification of these system boundaries in a foreground and background system. Inside the overall system boundaries, a harmonized assessment is required. The cost and environmental impact of a specific technology can differ if it is used or produced at a different location or point in time. Consequently, the temporal and geographical scope of both the background and the foreground processes should be harmonized.[28]

Technological data

After the system boundary is determined, the required technological data needs to be gathered. Technological data includes process parameters, which can be used to model the required quantities of mass and energy flows.

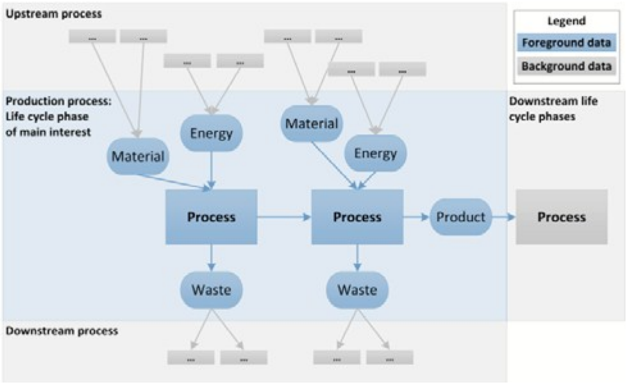

Fig. 2 Foreground and background data in the life cycle of a chemical product, focussing on a specific chemical process in the foreground

During the development of a new technology, the technological specifications of the n^{th} plant design have not been established yet. These technological specifications will be altered at the different TRLs. At the first TRL, the technology should be characterized based on a conceptual design. At TRL 4, laboratory data becomes available, which can be used in the prospective technology assessment. This data will increasingly resemble the n^{th} plant characteristics when the technology matures into the demo and pilot plant TRLs. However, when the laboratory, demo or pilot plant data are directly used in the prospective technology assessment, the results will differ and no estimate of the potential of the mature n^{th} plant design can be obtained. Therefore, scale-up procedures are required as streamline methods to upscale technological data from early TRL to an n^{th} plant design. [76] These scale-up procedures provides equations and rules-of-thumb to identify and quantify the industrial scale alternative of an early TRL parameter or process. As the industrial process flow diagram and mass and energy balance are not available yet, these streamline methods can assist in filling up the blanks to allow for an assessment of an n^{th} plant design. The required scale-up procedure is therefore identified by the required data. Piccinno *et al.* provided engineering-based scale-up procedures for certain batch reactions, purification and isolation processes.[76] This procedure also advocated the inclusion of fugitive emission estimates.[77, 78] Fugitive emission estimates were also provided by Smith *et al.*, who used computer-aided simulation and estimation models for emissions and land use in chemical manufacturing processes.[79] Another useful scale-up procedure was proposed by Simon *et al.*[80] Their scale-up framework included the scale-up of the PFD based on the laboratory procedures; a quantitative upscaling of the process characteristics; and an estimation of the working characteristics, such as yield and power requirements, based on similar industrial processes. Tecchio *et al.* used a combination of pilot and stoichiometric data and also formulated scale-up functions for the technological data.[7] Van der Spek *et al.* used preliminary rigorous modelling results and projected them on an industrial scale using simplified methods.[81] Wernet *et al.* proposed a tiered approach using molecular-structure-based models to determine the relevance of the parameters and applying process models to estimate the most relevant components.[82] A method to select appropriate proxy values through expert elicitation was proposed by Subramanian and Golden, including an estimate for the associated uncertainty of the proxy value.[83] Judl *et al.* proposed the use of general checklists to include frequently used unit processes in a standardized form.[84] Van Kalkeren *et al.* used general rules of thumb, partially based on the framework of Hischier *et al.*, which was also used in ecoinvent, to calculate the required process data.[33, 85] Solvent use can constitute a major part of the environmental impact of a chemical or pharmaceutical product.[86] Methods for optimal solvent selection were developed by Gani *et al.* and Henderson *et al.* [87-89] An environmental assessment of fifty organic

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solvents was performed by Capello *et al.*, who also developed the ecosolvent tool to assess the environmental impact of waste-solvents.[90] They formulated specific recommendations and rules of thumb for waste-solvent procedures.[91, 92] A review on different green solvent selection guides can be found in Byrne *et al.*[93]

As the background processes are not specifically modelled, general data needs to be obtained from databases or modelling. For the upstream background processes, the ecoinvent or GaBi database can be used to obtain the mass and energy balance for the products limiting the foreground system boundaries.[74, 75] Ecoinvent also includes the mass and energy balance for basic equipment like pump and tank. To model the downstream background processes, modules or general equations can be used, for example for end-of-life scenarios.[94, 95] For the transportation and disposal, average values can be included.[46] When no information is available over the mass and energy balances of an input or output, the foreground system boundary will need to be extended to include the proceeding upstream or subsequent downstream process as well.

To decrease uncertainty on the technological process, stakeholders need to be involved as well to underpin the assumptions, similar to the anticipatory LCA approach.[34] Integration tools from process system engineering, such as pinch analysis and water integration, can be included to reduce utility consumption.[96]

Economic data

If a TEA is performed, only foreground economic data is required, because a TEA follows an investor's perspective. However, when no price for the foreground product is available, background data can be used to estimate the price. In an LCC, the background economic data is also required.

For a screening assessment in the first TRLs, expert estimates can be used. In a streamlined assessment, investment criteria can be calculated by adding the operational, equipment, indirect costs and revenues from the end-products. Cost engineering principles can be used to find the appropriate cost data.[97] The prices for operational costs can be found in databases like Eurostat or by contacting the specific supplier.[98] The price of the equipment can be found through price quotes. However, these prices need to be harmonized to the appropriate production capacity, location and year of production. If the price quotes for the equipment are not in accordance with the required production scale, the procedure, as illustrated in Fig. 3, can be used to incorporate the economies-of-scale.[99] If more than one price estimate is available, a regression function can be constructed. If the fit of this function is sufficient (e.g. $R^2>0.90$), and the required capacity falls within the range of the regression function, the regression function can be used to estimate the price quote at the required capacity. If only one price estimate is known, the six-tenth rule can be used. Specific exponents for typical equipment types such as pumps, reactors or separators are available.[97] If no price estimate is available, the equipment can be brought back to its individual components, for which a price needs be obtained. In this case, the production of the equipment needs to be included in the system boundaries. To harmonize the price quotes to the appropriate year, a price index, such as the Chemical Engineering Plant Cost CEPCI index (CEPCI) can be used.[100] Lastly, location factors and exchange rates can be used to adapt the price quote to the appropriate location.[101] Industrial investment costs decrease when the cumulative capacity increases due to learning effects.[102] This effect can be included by adopting learning rates for analogous technologies.[81] Additional direct and indirect costs such as buildings, electrical systems and installation costs need to be included as well. If they are not provided elsewhere, they can be included as fixed percentages of the delivered-equipment cost.[97] If a specific price cannot be found in databases or through price quotes, estimation techniques, as reviewed by Niazi *et al.*,[103] can be used. These techniques can also be used if downstream life cycle costs such as end-of-life costs are required to estimate the predicted product price. The NPV calculation includes a discount rate selection. This discount rate reflects the risk of the investment. Its typical values are 10% for the cost improvement of conventional technologies, 15% for conventional technology expansion, 20% for product development, and 30% for speculative venture, respectively.[49] This discount rate can be used directly to discount future positive cash flows or can be used to calculate the weighted average cost of capital (WACC). The WACC also takes into account that a certain part of the investment will be credited by the bank, which shares the risk. Therefore, it is a more

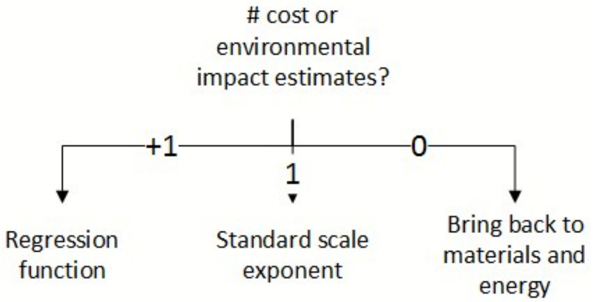

Fig. 3 Procedure for capacity harmonization dependent on the amount of cost or environmental impact estimates (based on Gerber *et al.*, 2011)[106]

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realistic measure than the direct use of the discount rate. Another important assumption is the project lifetime, typically 10-15 years.[49] Besides the project lifetime, the lifetime of the individual equipment also needs to be taken into account so reinvestments can occur when necessary. At the end of the project lifetime break-down costs for the project and residual estimates are available, although these values are often ignored at lower TRLs.

Environmental data

The mass and energy balance as provided by the technological analysis is also the basis for the quantitative environmental analysis. As the entire life cycle has been included in the background system, the mass and energy balance of the background system will entail the life cycle inventory. To calculate the environmental impact based on this inventory, characterization factors are required to provide the impact of each mass and energy component to the environmental indicators. A full range of environmental indicators, such as the ReCiPe set, is recommended to obtain a first complete perspective on all potential environmental impacts caused by the emerging green chemical technology.[104] The characterization factors can be found online or in databases such as ecoinvent. As ecoinvent also includes the background technological data, it can be used to calculate the foreground environmental data automatically. The use of databases such as ecoinvent to transform the quantity of an input per functional unit into the total environmental impact per functional unit is illustrated in Fig. 4. The database can be used to obtain the emission inventory data and resource use data, as well as the characterization factors. In the inventory, the manufactured product is translated into a list of elementary emissions and resources, which is then completed by providing the characterization factors for these elementary emissions and resources. Multiplying the elementary emissions and resources with their respective characterization factors and summing them all up leads to an estimate of the total environmental impact per functional unit.

Similar to the economic data, the environmental impact of the equipment may also need to be harmonized. Scaling the data to the appropriate scale can have crucial effects on the results.[44] A similar economies-of-scale relation as for the costs of the equipment was found.[105] If the power exponent of a certain equipment is not known, the same power exponent for the costs can be used as a proxy.[105] Guidelines on the specific exponents to use, based on the availability of databases, have been proposed in the literature.[106] Therefore, the procedure from Fig. 3 can also be used for the environmental impacts, which was also advocated by Gerber *et al.*[106] Harmonization to the production year is only required when the production process has changed in which case the updated inventory of the new production process needs to be used. However, in a prospective assessment, assumptions can be included about a future state. Care should be taken that the same temporal scale is used for the foreground and background processes.[28] Harmonization to the appropriate location can be done by selecting local production processes, for example for the electricity mix. Additional direct and indirect costs can be included by searching for specific inventories, such as chemical factories or labor.[107] However, no general estimates, as found for the economic analysis, are available.

Uncertainty

As the streamlining methods are used to approximate the future potential of the prospective technologies, uncertainty is inherent in the models. To enable a correct interpretation of the results of the prospective technology assessment, the impact of this uncertainty should always be assessed. There are three main types of uncertainty influencing the outcome: uncertainty in the input data, uncertainty due to choices, and uncertainty in the modelling.[108] Different methods exist to deal with these different types of uncertainty, which enable to put the resulting indicators of the prospective assessment in the right perspective.

To deal with uncertainty in the input data, uncertainty and sensitivity analyses can be included and a data quality analysis can be performed. The effect of choices can be assessed by including a what-if analysis or scenario analysis. The last type of uncertainty, modelling uncertainty, can be countered by a harmonized assessment strategy, as provided in this review.

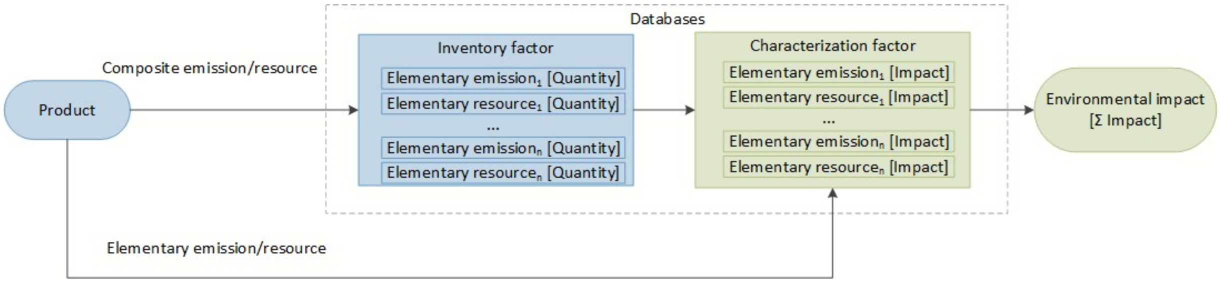

Fig. 4 Transformation from technological data to environmental impact data, incorporating the full life cycle inventory of the product, including all elementary emissions and resources and their corresponding characterization factors

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A sensitivity analysis identifies the most important parameters in the model and has been identified as the most successful streamlining method.[109] Different sorts of sensitivity analyses exist. The most basic form of a sensitivity analysis is a contribution analysis, where the contribution of the different processes or life cycle stages to the end indicators is assessed. The contribution analysis can also be used to assess the contribution of the midpoint indicators to the endpoint indicators to identify the most important midpoint indicators for each endpoint indicator. Similarly, the contribution analysis can also be used to assess the impact of the different cost components on the overall economic indicator.

A more advanced form of a sensitivity analysis assesses the impact of the underlying parameters in the model (Fig. 5). An identical distribution (for example -10% and +10%) is provided for all parameters. Subsequently, a large amount of iterations (e.g. 10,000) is performed to identify the parameter, which has the largest influence on the output indicators. In this sort of sensitivity analysis, the goal is not to obtain an uncertainty range of the indicators, but to identify the most crucial parameters. Therefore, this sensitivity analysis can be performed without knowing the uncertainty distribution of all the parameters and assuming a general distribution, such as a triangular distribution on all parameters. In a partial sensitivity analysis, only a part of the parameters are included. For a global sensitivity analysis, a real uncertainty distribution for the different parameters is obtained and included.[110] The inclusion of this uncertainty distribution enables an uncertainty analysis, where the ranges of possible outcomes for the indicators are defined. (Fig. 6). However, the identification of this uncertainty range is in general not possible at an early TRL, where even an accurate most-likely value of all parameters is hard to obtain. If also a worst and best-case value are known, a triangular distribution can be used instead.[111]

To classify the uncertainty in the data, a data quality analysis can be used. Here, different types of data are classified. As the data availability differs over the TRLs, different data quality types are used: (i) primary data, which is directly generated by the analysis; (ii) secondary data, which is based on experimental studies on an appropriate scale; (iii) average data, which takes multiple studies into account; (iv) calculations, which are based on theoretical principles or general rules of thumbs; and (v) assumptions, which are based on expert opinions.

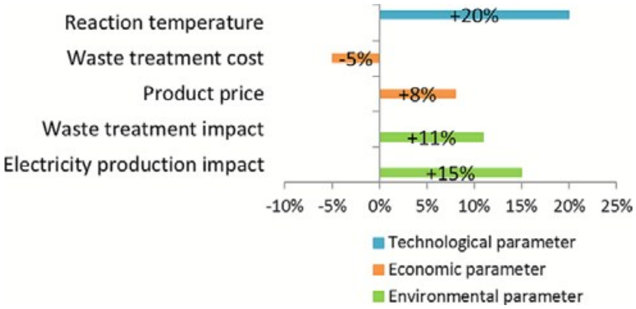

Fig. 5 Example of a sensitivity analysis, illustrating the impact of the process parameters on the output indicator

A data quality analysis, for example by means of a Pedigree matrix can be used to assess the reliability of the parameters.[22] A cost extension of the Pedigree matrix is available as well.[112] The sensitivity analysis can be linked with the Pedigree matrix by classifying the parameters in multiple quality classes according to their sensitivity.[113] Uncertainty factors for the parameters, based on the Pedigree matrix, have been obtained and can be used for an uncertainty analysis on the output indicators.[114] A protocol to handle uncertainty on primary and secondary data is also available.[115] To conclude, multiple methods to deal with uncertainty in input data exist.[116]

A second type of uncertainty is the uncertainty due to choices. One of the choices, which induces uncertainty, is the selection of the scenario. This can be countered with a what-if analysis. In a what-if analysis, the impact of a change in one parameter on the outcome is assessed. The calculation of such an additional what-if analysis only requires a small effort, but the added value is large.[117] To assess the implications of varying multiple parameters at the same time, a scenario analysis can be performed. Multiple scenarios, e.g. a best-case and a worst-case scenario, can be assessed to identify the optimal process conditions. A what-if analysis and scenario analysis assess the impact of a variation of one or multiple parameters on the indicators. An optimization analysis on the other hand, assesses a continuous range of one or multiple parameters. The goal of an optimization analysis is not to assess the effect of an alternative value of one or more parameters, but to find

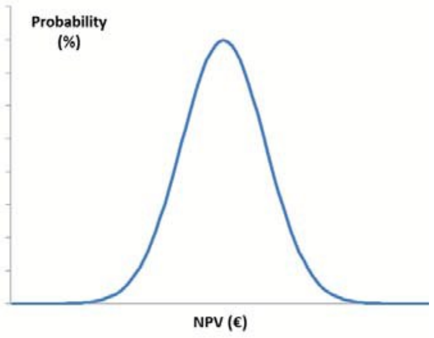

Fig. 6 Example of an uncertainty analysis, illustrating the uncertainty distribution on the NPV

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the optimal value for one or more parameters. Accordingly, this optimal value corresponds to the minimum or maximum value of the output indicator.

Besides optimizing the defined scenarios, the process design itself can also be optimized, selecting the optimal process design according to the stated objective. For this analysis, a superstructure can be included, consisting of various technology alternatives. When multiple output indicators exist, a MOO can be used to identify the optimal scenario according to multiple indicators. In this analysis, the optimal scenarios, giving technological, economic and environmental objectives, are defined.[118, 119] In addition, the optimal process design can also be identified in a MOO, using a superstructure of technology alternatives In a MOO, the Pareto frontier, consisting of all scenarios and process designs, which cannot improve for one indicator without deteriorating for another indicator, is identified (Fig. 7). This Pareto frontier contains all optimal scenarios and process designs and can be used by the decision-maker to make a final decision. In the selection of the appropriate method, care must be taken that the global optimum can be found. The ETEA framework uses modules, where each module specifies a technical process. This enables the construction of a superstructure, where the different modules are interchangeable, for optimization purposes. Instead of calculating all potential process designs, only the modules need to be calculated.[95]

Another choice, which induces uncertainty, is the scope of the assessment. Prospective LCAs will follow in general an attributional approach, focussing on the physical flows of the specific product system. However, external factors to the specific product system can have an influence on the potential of an emerging technology as well. The introduction of a new technology to the market will alter the market conditions and have an influence on other sectors. This might induce a response, which will consequentially influence the product system. This consequential LCA can be obtained by including economic models such as partial or general equilibrium models. A review on the use of consequential LCA was provided by Earles and Halog.[17]

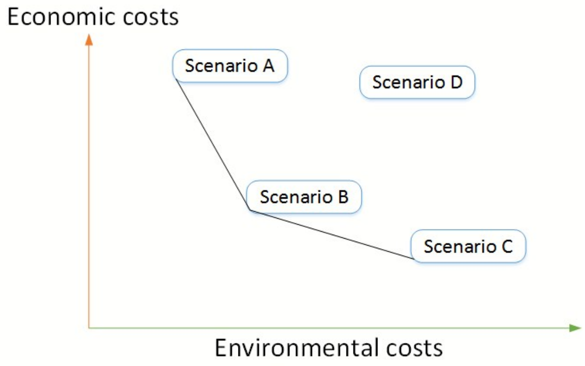

Fig. 7 Example of a Pareto-frontier, consisting of three Pareto-optimal scenarios

To combine the different assessments, a tiered-approach has been proposed for LCAs.[120] The different tiers of this approach are: 1) contribution analysis; 2) sensitivity analysis; 3) uncertainty analysis; 4) uncertainty propagation analysis, which is similar to the global sensitivity analysis; 5) combined sensitivity analysis, where different scenarios are included for multiple parameters. Therefore, this can be considered as an optimization analysis.

The Environmental Techno-Economic Assessment framework

Based on the reviewed methods, the best practices can be gathered in an overarching ETEA framework, which acts as a guideline for prospective technology assessment. Such a harmonized guideline can be used to ensure that emerging green technologies are assessed in a comparable way. The framework is directed both at technology developers as to policy makers. For technology developers, the ETEA framework can assist in highlighting the hotspots that need to be optimized in further technology development. As the framework can be used alongside the different stages of technological maturity, the assessment can follow the same rationale from an early stage on. When the technology matures, the ETEA model becomes more elaborated and more accurate. The ETEA framework is in particular useful for research projects and R&D trajectories within companies to illustrate the potential of the emerging technology to attract the required funding. From the opposite perspective, policy makers can use the ETEA framework to assess emerging green technologies to allocate subsidies and research funds. A harmonized, integrated framework is crucial to ensure a fair comparison of the potential of emerging green technologies. The need for such an integrated harmonized assessment framework over the different stages of technological maturity has also been highlighted by multiple European research projects, such as the MEASURE, STYLE and SAMT projects.[11-13] Also the formulation of specific methodological guidelines for a TEA and LCA of CCU technologies alongside technological maturity levels illustrates the importance of the proposed framework.[121]

The TRL scale will be used to classify the different streamlining methods considered in the review alongside the appropriate stages of technological maturity. At each TRL, the specific goal of the assessment should be defined and different methods for the technological, economic and environmental assessment are reviewed. Finally, the inclusion of additional analyses, such

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as sensitivity or uncertainty analyses, needs to be discussed for each TRL. This way, the framework makes a division between the 'must haves' for a reliable prospective assessment of emerging green technologies at each TRL and the 'nice to haves'.

The ETEA methodology for green chemistry technologies and chemical processes consists of five different steps. The first step is the market study, where the market potential of the new technology is assessed. The main objective and the scope of the assessment are also determined in this step. In the second step, the process flowsheet is constructed and the mass and energy balance are calculated. Here, the industrial process of the nth plant is modelled. In the third step, the economic analysis, the costs and the profits of the new technology are assessed, based on the technological analysis in the previous step. The fourth step includes the environmental analysis, including a broad range of environmental indicators, also based on the technological analysis. The last step of the ETEA is the interpretation step. Here, different additional analyses are added to deal with the uncertainty of the analysis, including a contribution analysis of the different life cycle or production phases, a sensitivity analysis of the underlying parameters, an uncertainty analysis of the results, and the data quality analysis.

The five steps of the ETEA methodology are used alongside the framework, but will differ due to differences in data availability, uncertainty of the results, the main objective of the assessment, flexibility, and costs of technological changes at the different TRLs. The ETEA methodology follows a stage-gate approach as illustrated in Fig. 8.[122] After each stage, the ETEA methodology provides information for a go/no-go decision. In case of a 'go', the technology can pass the gate to the next stage, while in case of a 'no-go', the technology needs to be adapted or abandoned.

Table 1 provides an overview of the ETEA framework over the different TRLs. At each TRL, a different goal is set and a different main question needs to be answered. In the first stage of technology development, the goal of the prospective ETEA is a first check of the potential of the concept. Can the revenues be higher than the costs? What are the environmental hotspots in the process? It is a rough assessment and the results could be relatively inaccurate. At TRLs 3-4, the main result is still the identification of the most crucial drivers. In addition, there should be potential for a realistic case to be feasible. For this realistic case, assumptions about further improvements can still be made. At TRLs 5-6, the focus remains on the identification of the main drivers, but at this level, the defined case should also be feasible. At the next TRLs 7-8, not only the defined case should be feasible, but also a realistic uncertainty range on the different parameters need to be provided, indicating a good probability of a positive outcome. At TRL 9, the technology is mature, so the true economic and environmental potential can be assessed.

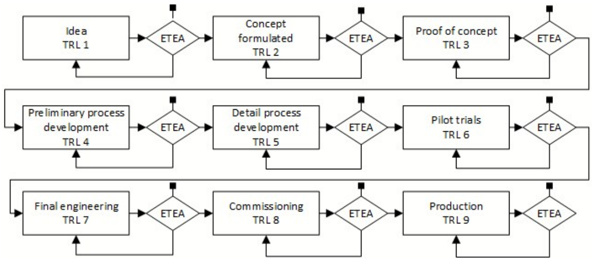

Fig. 8 Stage-gate approach for the ETEA framework, inlcluding go/no-go decisions at each gate

For the first step, the market study, it will increase in size and time requirement, starting from a simple online search to a full-scale market study at TRL 9. From TRLs 7-8, the market analysis can include the development of a business model canvas, which can also cover environmental and social perspectives.[123, 124] The PFD in the second step of the ETEA, will start from a blackbox perspective and gain more detail when the technology matures. At TRL 3-4, scale-up procedures, such as suggested by Piccinno *et al.*[1] and Simon *et al.*,[8] will be used. To include unknown emissions and resources, key elementary flows can be elaborated, including the main emissions and resources contributing to a specific impact category or entailing a specific cost. In addition, the fugitive emission method of Hassim *et al.*[77, 78] can be used. Fig. 9 illustrates how these methods contribute to defining the foreground system boundaries at TRLs 3-4.

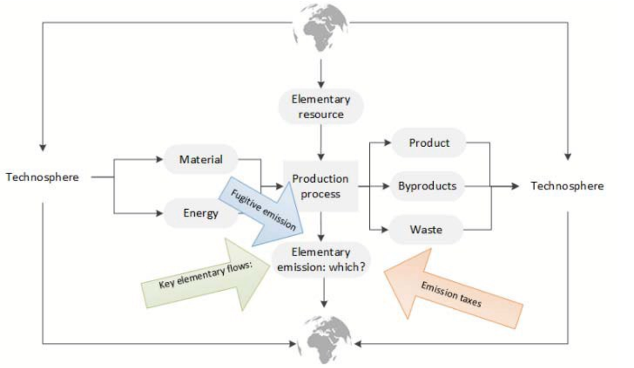

Fig. 9 Foreground system boundaries for TRLs 3-4, including the direct emissions to the environment that are included in the fugitive emission estimates, key elementary flows or emission taxes

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Table 1 Overview of the ETEA framework for the different TRLs, classifying which streamline measure and analysis can be used at each TRL

	TRL 1-2	TRL 3-4	TRL 5-6	TRL 7-8	TRL 9
Goal	Does it make sense? What are the main drivers?	What are the main drivers? Is a realistic case feasible?	What are the main drivers? Is the defined case feasible?	How big is the chance that the defined case will not be feasible?	Accurate value for the environmental and economic indicators
Market study	Online search	Patent analysis, market reports, environmental reports	Patent analysis, market reports, environmental reports	Business Model Canvas	Own market information
PFD and M&E balance	Blackbox perspective; stoichiometry, basic engineering equations	Scale-up procedures; Key elementary flows	MOO, Scale-up procedures; key elementary flows; calculations and assumptions not in sensitive foreground data	Scale-up procedures; piping and instrumentation diagram; calculations and assumptions only in background data	Real measured data, learning effects
Economic analysis	Screening economic analysis	Harmonization ; indirect costs	MOO, equipment cost dependent on regression function	No harmonization required in data	Real market data for all values
Environmental analysis	Matrix approach	Cradle-to-grave; Harmonization	MOO, Cradle-to-grave; Harmonization	No harmonization required in data, consequential LCA	Cradle to grave in foreground data
Interpretation	Sustainability SWOT, contribution analysis, what-if analysis, one-factor optimization	contribution analysis, sensitivity analysis, what-if analysis, one-factor optimization	Data quality analysis, contribution analysis, sensitivity analysis, what-if analysis, one-factor optimization	Uncertainty analysis, data quality analysis, contribution analysis, sensitivity analysis, what-if analysis, optimization	Uncertainty analysis, data quality analysis, contribution analysis, sensitivity analysis, what-if analysis, optimization

To include downstream processes of the life cycle, such as the distribution, use and end-of-life phase, standard models can be used. As the technology proceeds alongside the TRLs, the PFD and mass and energy balance will gain more detail. At TRLs 5-6 the most important parameters, as identified in the sensitivity analysis, should be based on foreground data and not on standard calculations. This is also the TRL where a first MOO becomes feasible. At TRL 7-8, the standard calculations should be limited to the background data only. At these TRLs, a detailed piping and instrumentation diagram should be added to the PFD. The PFD and mass and energy balances at TRL 9 should contain the final plant design, including primary data for the entire process. The third step, the economic analysis, is based on the mass and energy balances, and will therefore have the same system boundaries at each TRL. The economic data at TRLs 1-2 will be based on basic prices, found in standard databases, price quotes from suppliers or in e.g. reports and scientific articles. At TRL 3-4, price data should become more accurate. In addition, harmonization becomes important to ensure the price data is from the right period and scale. Indirect costs need to be added as well. At TRLs 5-6, this scale harmonization should be based on regression functions including multiple price estimates for multiple scales. Harmonization should not be necessary at TRLs 7-8, as price information on the specific scale should be available. However, for the MOO, harmonization remains required. At TRL 9, the real market costs are available and no estimates are required anymore. The environmental analysis, i.e. the fourth step, will start with a hotspot matrix, based on previous matrix LCA approaches, which were adapted to include the major technological processes of the life cycle steps.[62, 64, 125, 126]. At TRLs 3-4, a first quantitative environmental impact assessment is included, which follows the LCA prescriptions, including streamline measures. For the choice of the functional unit and the allocation methods, the ISO guidelines are followed. Harmonization is also needed for the appropriate timing, scale and location of the database estimates. Indirect impacts such as heating of the building and general utilities may also play a role. However, no estimates were found to quantify these indirect impacts. Similar to the economic analysis, the accuracy of the environmental impact data will increase at TRL 7-8. At these TRLs, it can also be interesting to expand the attributional LCA to include a consequential perspective. At TRL 9, the streamlined LCA will be transformed into a full-scale LCA. The fifth and final step, the interpretation, will add additional analyses over the TRLs. At TRLs 1-2 this will be limited to a sustainability SWOT and a small contribution analysis. Based on this contribution analysis, the main parameters can be varied in a what-if analysis and a one-factor optimization. At TRLs 3-4, a sensitivity analysis will be added to include all parameters in the model. A data quality analysis will be added at TRLs 5-6 to evaluate the accuracy of all the parameters. At TRLs 7-8, an uncertainty analysis and a global

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sensitivity analysis can be added as well. The ETEA framework follows the tier-based approach to deal with uncertainty as proposed by Clavreul *et al.*[120]

The environmental and economic indicators remain separate in the ETEA framework. Many studies have proposed the use of an aggregated indicator, which can also be done with the indicators from the ETEA framework by assigning weights to each indicator. However, weighting is in general subjective and can induce the loss of important information. Therefore, we advocate to leave the weighting decision to the final decision maker when taking the investment decision and not to the person performing the calculations. This way, all indicators can be taken into account by the final decision maker, according to his/her own perspective.

The use of a general software package as Excel enables a broad application of the framework, which is not restricted to people with specialized background. Currently, the three dimensions as assessed by the ETEA framework, being technology, economy and environment, are often tackled by different methods and tools. Some studies have proposed to combine them.[10] However, by combining the models, this division in expertise remains. Excel is an ideal software to build the ETEA model from an early stage on and to adapt and extend it in each iteration by people from all different backgrounds.

The use of LCA for the environmental impact assessment induces an allocation assumption if multiple output products are produced. The ISO guidelines state a hierarchical order for allocation measures.[20] The first choice is to avoid allocation by dividing the process in multiple subprocesses, which have one end product each. However, this is not always feasible. The second choice also avoids allocation by expanding the system to include all the end products in the functional unit. However, this does not lead to an environmental impact estimate per end product. Therefore, the next choice is substitution, where the environmental impact of a reference product for the by-products is subtracted from the total environmental impact of the end products. However, allocation based on substitution can lead to negative environmental impacts, when the reference products contain a large environmental impact. If substitution is not feasible, the ISO guidelines suggest allocation. Following this allocation strategy, the total environmental impact is divided over the different end products. Preferably, this allocation is based on a relevant characteristic. Alternatively, mass-based, energy-based or price-based allocation can be applied. For the economic analysis, the same hierarchy can be followed. When calculating specific investment criteria such as the NPV or the IRR, the functional unit includes the entire project, which is equal to the system expansion strategy. If the cost of a specific end product is the required indicator, substitution or allocation may be adopted. Therefore, depending on the selected indicator, a different allocation procedure can be followed for the environmental and economic analysis. However, it is important to communicate the adopted allocation procedure and to provide enough information to enable the calculation of the indicators using other allocation procedures. Moreover, if the least preferred option is selected for both the economic and environmental analysis, namely dividing the impact over the different end products, the relevant criteria which is used for this partitioning will be the same for both the economic and environmental analysis.

The streamlined ETEA includes subjective choices. Assumptions can be made in such a way that the technology is as cheap and environmentally friendly as possible. Therefore, the streamlined ETEA is mainly used to benchmark or identify optimization possibilities for the new technology. The ETEA framework can only be used to provide labels or to make final comparisons, when clear agreements have been formulated on adopted assumptions and full transparency on the data and assumptions is ensured in such a way that the analysis can be reproduced. To be able to use the absolute results of the full ETEA performed at TRL 9 for comparisons or labels, a certain modelling quality should be obtained restricting the type of data that can be used. To cope with the uncertainty that is introduced by the different assumptions, a full transparency is advocated on all used data. This would also allow for the ETEA to be reproduced. The results of the ETEA can only be interpreted with the used assumptions in mind. The result of using alternative assumptions regarding for example the choice of functional unit or allocation criteria should always be included to put the obtained results in the right perspective. In the next section, two examples of the ETEA framework will be elaborated further to illustrate different parts of the framework. A full ETEA is not provided as it can be found elsewhere. [60] In the first example, an example is provided of an environmental hotspot matrix as adopted at TRL 1-2. In the second example, scale-up procedures for an ETEA at TRL 5 are illustrated, based on an existing ETEA, which has been published before.[60]

Environmental hotspot matrix: example of an algal-based biorefinery

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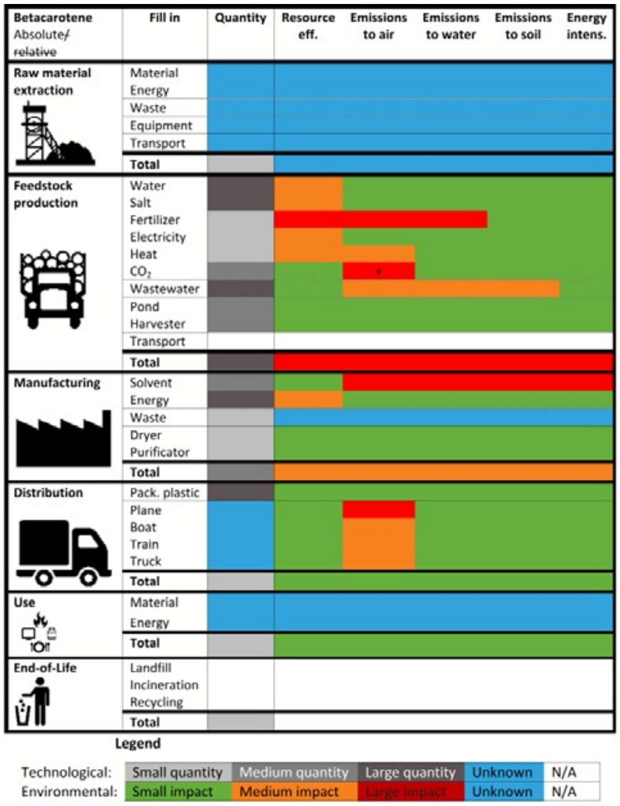

Betacarotene Absolute/ ~~relative~~	Fill in	Quantity	Resource eff.	Emissions to air	Emissions to water	Emissions to soil	Energy intens.
Raw material extraction	Material	🟦	🟦	🟦	🟦	🟦	🟦
	Energy	🟦	🟦	🟦	🟦	🟦	🟦
	Waste	🟦	🟦	🟦	🟦	🟦	🟦
	Equipment	🟦	🟦	🟦	🟦	🟦	🟦
	Transport	🟦	🟦	🟦	🟦	🟦	🟦
	Total	░	🟦	🟦	🟦	🟦	🟦
Feedstock production	Water	▓	🟧	🟩	🟩	🟩	🟩
	Salt	▓	🟧	🟩	🟩	🟩	🟩
	Fertilizer	░	🟥	🟥	🟥	🟩	🟩
	Electricity	░	🟧	🟩	🟩	🟩	🟩
	Heat	░	🟧	🟧	🟩	🟩	🟩
	CO_2	▒	🟩	🟥 +	🟩	🟩	🟩
	Wastewater	▓	🟩	🟧	🟧	🟧	🟩
	Pond	▒	🟩	🟩	🟩	🟩	🟩
	Harvester	▒	🟩	🟩	🟩	🟩	🟩
	Transport	⬜	⬜	⬜	⬜	⬜	⬜
	Total	▓	🟥	🟥	🟥	🟥	🟥
Manufacturing	Solvent	▒	🟩	🟥	🟥	🟥	🟥
	Energy	▓	🟧	🟩	🟩	🟩	🟩
	Waste	░	🟦	🟦	🟦	🟦	🟦
	Dryer	░	🟩	🟩	🟩	🟩	🟩
	Purificator	░	🟩	🟩	🟩	🟩	🟩
	Total	▒	🟧	🟧	🟧	🟧	🟧
Distribution	Pack. plastic	▓	🟩	🟩	🟩	🟩	🟩
	Plane	🟦	🟩	🟥	🟩	🟩	🟩
	Boat	🟦	🟩	🟧	🟩	🟩	🟩
	Train	🟦	🟩	🟧	🟩	🟩	🟩
	Truck	🟦	🟩	🟧	🟩	🟩	🟩
	Total	░	🟩	🟩	🟩	🟩	🟩
Use	Material	🟦	🟦	🟦	🟦	🟦	🟦
	Energy	🟦	🟦	🟦	🟦	🟦	🟦
	Total	░	🟩	🟩	🟩	🟩	🟩
End-of-Life	Landfill	⬜	⬜	⬜	⬜	⬜	⬜
	Incineration	⬜	⬜	⬜	⬜	⬜	⬜
	Recycling	⬜	⬜	⬜	⬜	⬜	⬜
	Total	░	⬜	⬜	⬜	⬜	⬜

Legend

Technological:	Small quantity	Medium quantity	Large quantity	Unknown	N/A
Environmental:	Small impact	Medium impact	Large impact	Unknown	N/A

Fig. 10 Example of the environmental analysis at TRLs 1-2 of the ETEA framework

The matrix approach as proposed for the environmental analysis at TRLs 1-2 is illustrated in Fig. 10. To illustrate the approach, a case study of microalgal-based biorefineries is presented. A microalgal-based biorefinery produces multiple products out of a microalgae feedstock. For this example, β-carotene and fertilizer are produced out of a feedstock of *Dunaliella salina*. A full-scale ETEA of this case study at TRL 5 has been published before.[60] The specific elaboration of this example can be found in the supplementary information.

As one-dimensional metrics fail to include the multidimensional nature of environmental impacts, the proposed matrix consists of multiple simple indicators.[26] The environmental assessment is a qualitative hotspot matrix, filled based on expert opinions or question lists. It is therefore based on the LiSET method.[71] However, in contrast to the LiSET method, it is not meant to compare multiple technology alternatives and for each decomposition term, the same simple indicators are used. This way, the hotspots within the different decomposition terms of the technology can be evaluated as well. For the comparison of different technology alternatives, different matrices can be constructed. The rows of the hotspot matrix provide the different composition terms, which follow the different stages of the life cycle and the inputs and outputs of these stages. In the columns of the hotspot matrix, the quantities of the input and output flows are displayed. Besides the quantities, five proxy environmental indicators are also included. For each indicator the severity of impact of the input or output to the indicator is defined. The first four proxy indicators are related to the uptake of resources out of the environment and the emissions to the air, water and soil. These four categories were selected as they indicate the direct flows between the environment and the production process. Energy intensity is added as a last category as this is a relatively easy indicator to estimate, and it can act as a good proxy indicator.[127] The amount of these categories is indicated with a qualitative color code, ranging from green to red. Blue signifies that there is not enough information to estimate the resulting color. The quantities are filled in with a grey scale, to elucidate the difference between the quantity and the impact of an input or output.

The environmental hotspots are indicated by inputs or outputs, which have a large quantity and/or a large impact on the environment. An input with a large quantity and a large potential environmental impact might not be so significant if the life cycle phase is less significant. This is for example the case for the solvent in the manufacturing stage. In the manufacturing phase, the quantity of solvent use is relatively high and the potential environmental impact is relatively high as well. However, compared to the feedstock production stage, the manufacturing stage is much less important. According to Fig. 10, the environmental hotspots for the algal-based biorefinery case are the salt, fertilizer and wastewater in the feedstock production stage. The screening ETEA from an early TRL can provide recommendations for later technology development and important measures, which can lower the cost and environmental impacts of the emerging technology.

Scale-up measures: example of an algal-based biorefinery

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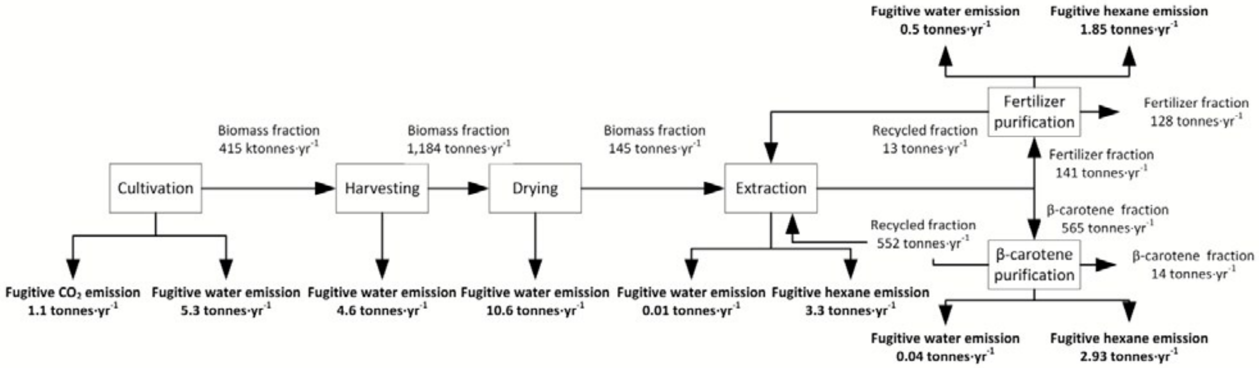

Fig. 11 Inclusion of fugitive emissions in the ETEA of an algal-based biorefinery[60]

The algal-based biorefinery has also been assessed in a more detailed ETEA at TRL 5. The results of this case study can be found in a previous paper and indicated that salt is a crucial driver for the environmental impact.[60] Therefore, a medium recycling step was introduced in the biorefinery process design to lower the overall wastewater production and salt and water consumption. A few scale-up measures as discussed in the framework have been used in this ETEA and will therefore be used as an example. Fugitive emission were included based on the framework of Hassim *et al.*[77, 78] For this purpose the total amount of equipment units in the PFD had to be calculated based on the production scale. The production scale of the assessment was based on the market volume of β-carotene, leading to a production scale of 11 ton of β-carotene per year. For this production scale, 30 tons of fugitive emissions per year were calculated based on the framework of Hassim *et al.*[77, 78] Fig. 11 illustrates the fugitive emissions at each stage of the process.

Another scale-up measure which was implemented was the harmonization of the price quote for a centrifuge to the appropriate capacity. After adding the direct and indirect costs that were not included in the price quotes, a regression function was calculated. Based on multiple price quotes a scale exponent of 0.56 was found for a range in capacities between 750 and 250,000 $l \cdot h^{-1}$. This regression function is illustrated in Fig. 12.

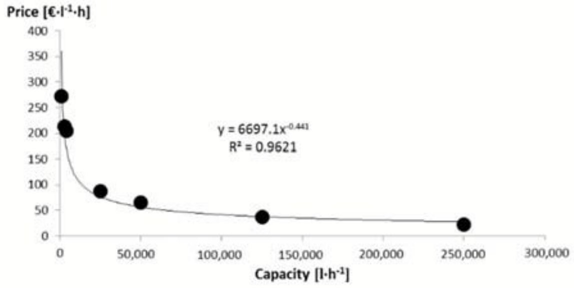

Fig. 12 Regression function of the investment costs of a centrifuge: example of a scale-up function[60]

Further perspectives

The provided framework entails guidelines on how to perform an integrated prospective technology assessment. Although a lot of streamlining methods are available, there are still important methods lacking. For example, the indirect cost of a production plant has been estimated, however, no similar estimates are available for the indirect environmental impact. In the input-output-based LCA, these indirect environmental impacts are included.[128] Therefore, they may be used to define rules-of-thumb or general estimates for the indirect impacts. For the key environmental impact, no hands-on list has been provided to check the important key elementary flows and emissions for each environmental indicator. In addition, only a few prospective technology assessment have been found, which adopted one of the proposed scale-up frameworks. This can be explained by the fact that most prospective technology assessments have been performed by technology developers, which are often no experts on the systematic assessment methods. Although a vast literature on the LCA methodology exist in comparison to the few studies discussing the TEA methodology and technological scale-up frameworks, the focus of the LCA methodological discussions still remains to a

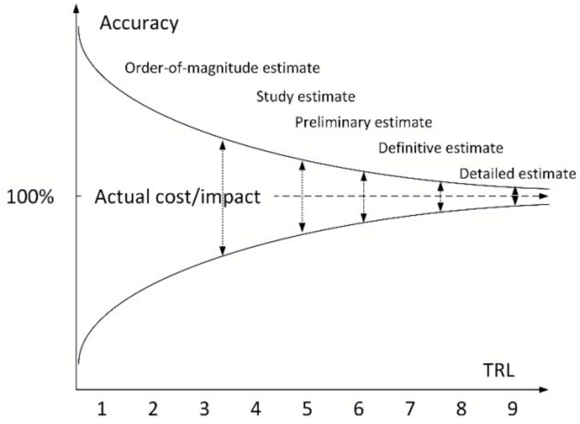

Fig. 13 Estimating accuracy trumpet, designating the increasing accuracy of the ETEA results at increasing TRLs[49]

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large extent on mature technologies. Moreover, as the LCA only includes the inventory and not the technological analysis, prospective LCAs often simply exclude unknown inputs or outputs. In contrast to the environmental input-output analysis, the process-based approach therefore currently leads to an underestimation of the environmental impact.[129] If the results from the environmental impact will only increase when the technology matures and the assessment becomes more accurate, the incentive to assess iteratively the environmental impact is scrutinized. Therefore, the streamlined methods in the provided ETEA framework are included to obtain an estimate for most inputs and outputs from an early TRL. Although this estimate may be inaccurate, the relevance of this parameter can at least be checked in the sensitivity analysis and the estimate can be further refined when the technology matures. The results from TRL 9 can then be used to improve the methods applied at lower TRLs. Therefore, further research is required on the uncertainty related to the provided streamline methods and scale-up frameworks.

The accuracy of the ETEA results differ at each TRL stage as illustrated in the estimating accuracy trumpet in Fig. 13. An interesting addition to the framework would be an estimation of this uncertainty range. Different classes exist for TEA cost estimates, ranging from an order-of-magnitude estimate with an uncertainty range of -50%/+100% to a detailed estimate with an uncertainty range of -10%/+15%.[49] However, as these classes did not incorporate the proposed scale-up measures and the environmental assessment has not been included, these error ranges will be different for the proposed ETEA framework.

This review discussed the opportunities for a more sustainable production by introducing a generic assessment method. However, the sustainable development goals not only cover sustainable production, but include both production and consumption. The linkage between production and consumption is therefore crucial. Sustainable production can lead to sustainable consumption only if this is communicated in an effective way. A major role is dedicated here to education. Innovative sustainable technologies can be developed, but if the consumer does not want them, they will unlikely be adopted. The ETEA methodology can assist in developing more environmentally sustainable technologies. However, it needs to be followed by a clear, transparent and universal way to communicate the results to a broader public and to policy makers to proceed towards a more sustainable consumption as well.

The economic and environmental potential of an emerging green technology can differ based on spatial variabilities. For the economic potential, prices can vary widely over different countries, leading to different results. For the environmental potential, upstream production processes can vary as well. For example the electricity production mix varies by countries and can have a large impact on the environmental impact results.[60] Spatial variabilities can also occur if different impact assessment methods are preferred in different regions. Different impact assessment methods have different characterization factors for the same elementary resources and emissions. Therefore, the environmental impacts of two technologies can only be compared if the same impact assessment method is used. The ETEA framework recommends the use of a general set of indicators such as the ReCiPe set. Currently, this is the major set of indicators covering a broad range of environmental impacts. However, methodological research on these impact methods can lead to improved methods which could then be incorporated further. To enable comparison of technologies with different impact methods, the provision of the full list of inputs and outputs to the technology is required. Temporal differences can also occur. Technologies evolve, prices change and also impact assessment methods improve over time. Therefore, it is important to identify and harmonize both the spatial and temporal scale of the assessment.

Conclusions

Green chemical technologies need to be developed with an optimal economic and environmental performance in mind. The current study provides a framework for this goal throughout all stages of technology development. The main application for this framework is therefore to act as a guidance during the development of green technologies. A second application of this framework is directed towards policy makers. A general framework to assess the economic and environmental potential of new technologies provides policy makers with a method to compare the potential of different technologies and to direct subsidies/taxes toward desired or undesired technology developments. Moreover, by identifying environmental and economic hotspots from an early stage of technology development, research can be supported and incentivized to lower these crucial impacts and costs. A third application of this framework is directed towards consumers and the communication of sustainable production practices. A generalized and harmonized assessment framework could provide a basis for ecolabels or other communication tools from producers to consumers. A harmonized approach towards environmental and economic sustainability facilitates sustainable decision making. For example, consumers may be willing to pay a green premium price for a product if they know that the higher production cost of this product is due to an improved environmental performance. Although this application as a communication tool between producers and

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consumers is specific for mature technologies at TRL 9, the ETEA framework at lower TRLs can assist in keeping the technology development on track to obtain the desired ecolabel.

The assessment of the economic and environmental potential is of major importance for the development of a new technology, and this importance will only be enlarged if we transition to a more sustainable way of production and consumption. For this transition, information on the drivers of environmentally sustainable technologies is indispensable. The ETEA framework aims to stimulate this transition by providing this crucial information for technologies in all stages of technology development. The application of this framework can be used for a large range of green chemical technologies. The use of a harmonized assessment method enables the comparison of different studies and encourages a more objective way of prospective technology assessment. By guiding technologies alongside their development, a more sustainable way of green chemical production can be accomplished.

Conflicts of interest

There are no conflicts to declare.

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