State-of-the-art of sustainability assessment methodologies and methods and their fit for the evaluation of MOONSHOT initiatives

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BACKGROUND

We face a climate and energy challenge that cannot be solved with incremental innovations alone, but where radical innovations are also needed to make the transition to a low-carbon economy and society. The MOONSHOT innovation program provides funding to realize such technological breakthroughs by 2050 to contribute to the achievement of the Flemish climate objectives.[1] Given the objective and timeline of the innovation program, it is crucial to use the resources in a targeted and most efficient way. There is a need for a harmonized framework that allows projects proposed and implemented within the MOONSHOT innovation program to be evaluated for their sustainability impact. This framework should allow to estimate the environmental and economic impact at low Technology Readiness Level (TRL) and from the project application onwards, to adjust the projects and project proposals in time.

Despite the availability of environmental, economic and integrated assessment methodologies and methods, there is no harmonized framework that can be directly applied to the MOONSHOT innovation program. Clear agreements on system boundaries, methodological choices and default values are needed to evaluate projects in an independent, objective, transparent and overarching manner.

This report is one of the deliverables from a project commissioned by Vlaio and Catalisti to develop a methodological framework for sustainability assessment in the framework of the MOONSHOT innovation program. This report starts by describing the state-of-the-art concerning sustainability assessment methodologies and methods and identifying the stakeholder needs for the evaluation of the sustainability impact of MOONSHOT projects. Based on these, a dedicated methodological framework is being developed that can be used within the MOONSHOT innovation program. The methodological framework is also being translated into a template that is publicly available and that aims to support applicants and project partners of the MOONSHOT innovation program. The framework and template are being tested on running MOONSHOT projects to prove its applicability. Finally, an article will be published for a broad audience to explain the advantage of using the developed methodological framework.

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[1] The Flemish energy and climate plan 2021-2030 aims to reduce carbon emissions in our region by 40% (compared with 2005 level) by 2030 (Vlaamse Regering, 2019. Algemeen kader voor de geïntegreerde nationale energie- en klimaatplannen.). The 40% (instead of 35% as foreseen in the original Flemish energy and climate plan) is based on additional measures taken by the Flemish Government in 2021 (Vlaamse Regering, 2021. Visienota aan de Vlaamse Regering. Betreft: Bijkomende maatregelen Klimaat.).

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LIST OF ACRONYMS

(D)PBP	(Discounted) Payback Period
CAPEX	Capital Expenditures
CBA	Cost Benefit Analysis
eLCC	Environmental Life Cycle Costing
EF	Environmental Footprint
ERA	Environmental Risk Assessment
ETEA	Environmental Techno-Economic Assessment
feLCC	Full Environmental Life Cycle Costing
fLCC	Financial Life Cycle Costing
FU	Functional Unit
GSA	Global Sensitivity Analysis
IRR	Internal Rate of Return
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCOE	Levelized Cost Of Energy
LSA	Local Sensitivity analysis
MFA	Material Flow Analysis
MSP	Minimum Selling Price
NPV	Net Present Value
OAT	One-at-a-time
OEF	Organisational Environmental Footprint
OEFSR	Organisational Environmental Footprint Sector Rules

OPEX	Operational Expenditures
PDF	Probability Density Function
PEC	Predicted Environmental Concentration
PEF	Product Environmental Footprint
PEFCR	Product Environmental Footprint Category Rules
PNEC	Predicted no-Effect Concentration
ROI	Return On Investment
SA	Sensitivity analysis
SFA	Substance Flow Analysis
sLCA	Social Life Cycle Assessment
sLCC	Social Life Cycle Costing
TEA	Techno-Economic Assessment
TRL	Technology Readiness Level
TSA	Techno-Sustainability Assessment

CHAPTER 1 INTRODUCTION

To enable a successful development and commercialization of the new technologies, the assessment of their environmental and economic sustainability at an early stage is key. Note that for a full sustainability assessment, also the social impact should be included, however, this is out of the scope of our project and therefore not included in this report. The stages of technology development can be categorized by means of the Technology Readiness Levels (TRLs). 80% of all environmental effects that are associated with a product or process are determined at an early TRL, more specific, the design phase (Tischner et al., 2000). Furthermore, most freedom degrees exist at low TRL so critical process steps should be identified as early as possible (Moni et al., 2019; Thomassen et al., 2019a; Thonemann et al., 2020). Also Cooper (1990) indicates that the most pivotal activities, those in which the differences between successes and failures are the greatest, are the early activities in the new product process. He said 'the seeds of success or failure are sown in the first few steps of the process'.

For the assessment of the economic and environmental sustainability of new technologies and processes, a plethora of methodologies exists. In this report, the state-of-the-art of the most prominent economic and environmental sustainability assessment methodologies and methods are discussed. In literature, a lot of confusion exists regarding terms such as framework, methods, methodology, tool and indicators. In this report the definitions from Sala et al. (2012), as illustrated in Figure 1, will be used.

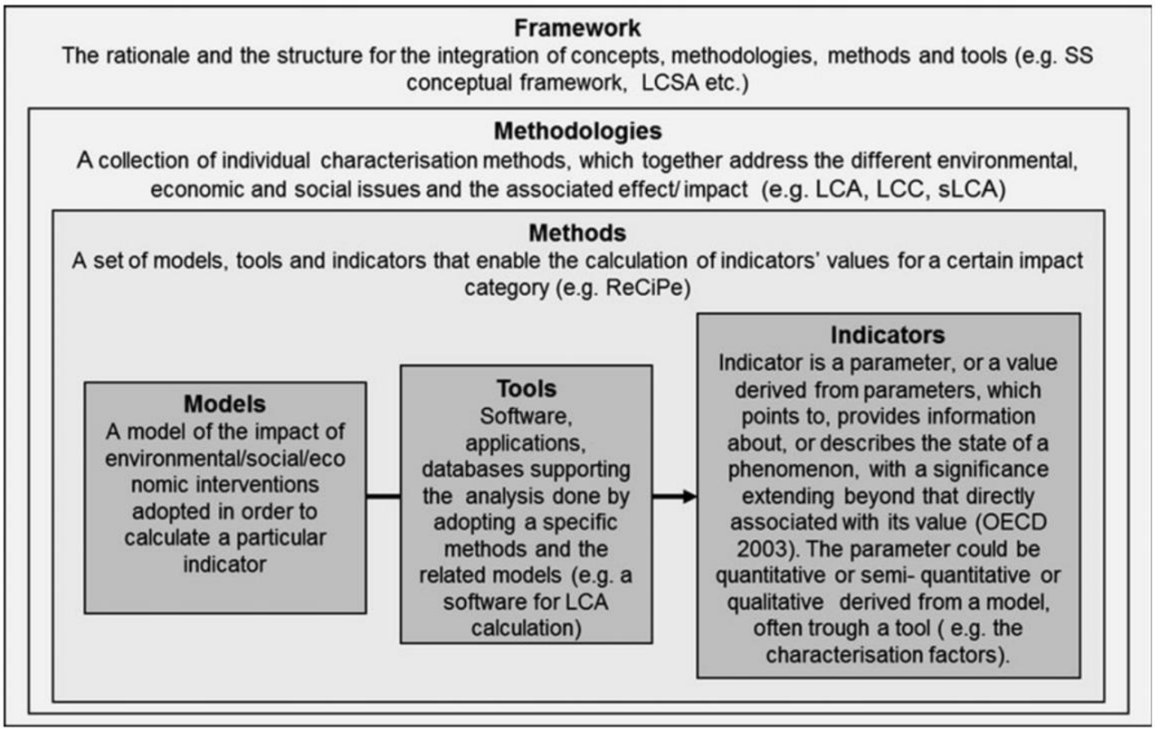


Figure 1. *Sustainability assessment framework as used in this report (Sala et al., 2012)*

In the next chapters, an overview of relevant methodologies is provided (Chapter 2-6). The goal of this overview is to determine the main methodologies and methods, their goal and scope, and define their differences. For the selection of state-of-the-art methodologies and methods described in this report, the main goal and scope of the MOONSHOT program is considered. For a more extended overview of assessment methodologies and methods, Annex A of this report can be consulted. The goal of this report is not to describe how the assessments need to be performed, but to describe what the assessment methodologies and methods entail. Based on this report and stakeholder consultations, a selection of methodological guidelines and indicators will be made. The details of the selected guidelines and indicators will be provided in the Deliverable 'Methodological framework for the sustainability assessment of MOONSHOT initiatives'.

The discussed methodologies and methods in this report are divided into five groups.

1. A first group of assessment methodologies are the **technical assessments**. In these methodologies, the physical flows are quantified but no further burdens or benefits are included. These technical assessments are often the backbone of economic and environmental sustainability assessment methods, however, they can also be used as such, for example for the calculation of indicators such as the recycling rate or the energy consumption (Chapter 2).
2. The second group of assessment methodologies focuses on the **economic feasibility** and economic sustainability of new technologies. In these assessments, the costs and revenues of new technologies and processes are quantified (Chapter 3).
3. The third group of assessment methodologies focuses on the **environmental impact assessment** of new technologies, processes and products. These methodologies go beyond the technical assessments as they quantify the burden on the environment of the physical flows. The economic and environmental assessment methodologies can start from a technical assessment, but they can also be limited to pure cost and environmental impact calculations (Chapter 4).
4. A fourth group of assessment methodologies **integrates both economic and environmental perspectives**. This way, trade-offs and mutual benefits can be identified (Chapter 5).
5. When assessing the technical characteristics, economic feasibility or environmental impact of a new process or product, 100% certainty on the results can never be achieved. This is because the assessments rely on models that, in turn, are approximations of reality, and therefore inevitably carry uncertainties due to mathematical relations, choices and assumptions, data, etc. Therefore, all these methodologies are often combined with uncertainty assessments. These **uncertainty assessments** will be discussed as a fifth group of assessment methods (Chapter 6).

In the next chapters, the selected state-of-the-art methodologies per group are described. A general description is provided, the indicators that are typically used are listed, as well as an overview of available methodological guidelines and tools. Finally, for each methodology, the main strengths and weaknesses (i.e. limitations) are described. Each chapter is closed with an overview of the available databases.

CHAPTER 2 STATE-OF-THE-ART TECHNICAL ASSESSMENTS

For the state-of-the-art of the technical assessments, material or substance flow analysis (MFA/SFA), circularity analysis, and (lifecycle) mass and energy balance based metrics are selected. Although the calculation of the mass and energy balance is often not considered to be a method in itself, it is the starting point for the calculation of a large number of metrics. For example, MFA is often used to calculate circularity metrics such as recycling rates. Therefore, it is a useful methodology to assess technologies aiming to contribute to a circular economy. Circularity analysis could therefore also be classified under the MFA/SFA section, however, we have included it separately to highlight its importance.

Besides mass, energy consumption is also an important parameter. In early-stage assessment, a low energy consumption is often targeted as a proxy for a low environmental impact (Huijbregts et al., 2010). If besides recycling rates, energy related metrics are required to be calculated, mass and energy balance metrics can be used as a second methodology. Depending on the scope of the assessment, a single process or whole life cycle perspective can be adopted.

2.1. MATERIAL OR SUBSTANCE FLOW ANALYSIS (MFA/SFA)

2.1.1. DESCRIPTION

A material or substance flow analysis tracks the materials (e.g. plastic) or substances (e.g. Cu) in a system. The methodology is based on physical flows and mass balances, where the sum of the total input mass should equal the sum of the total output mass. The system boundaries of a MFA/SFA in the value chain are illustrated in Figure 2 (although the system boundaries can also cover multiple processes in the value chain).

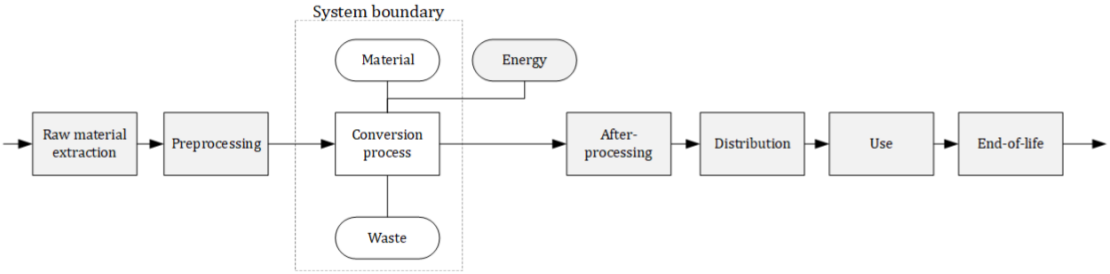
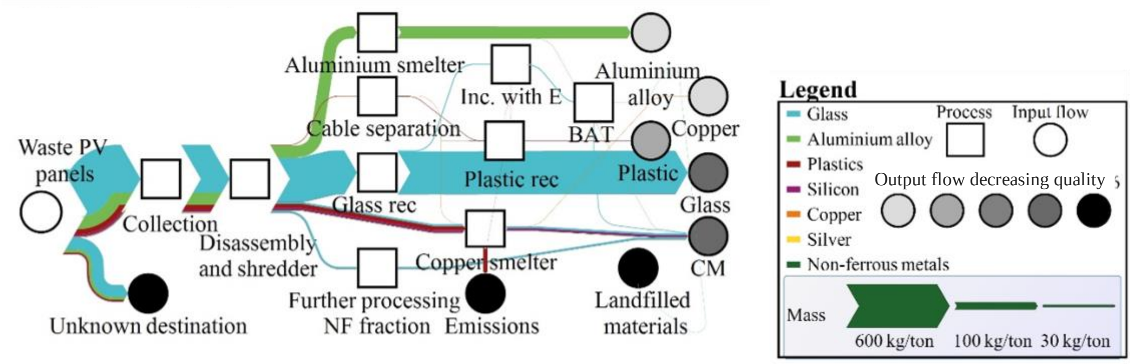


Figure 2. *System boundaries of a MFA/SFA*

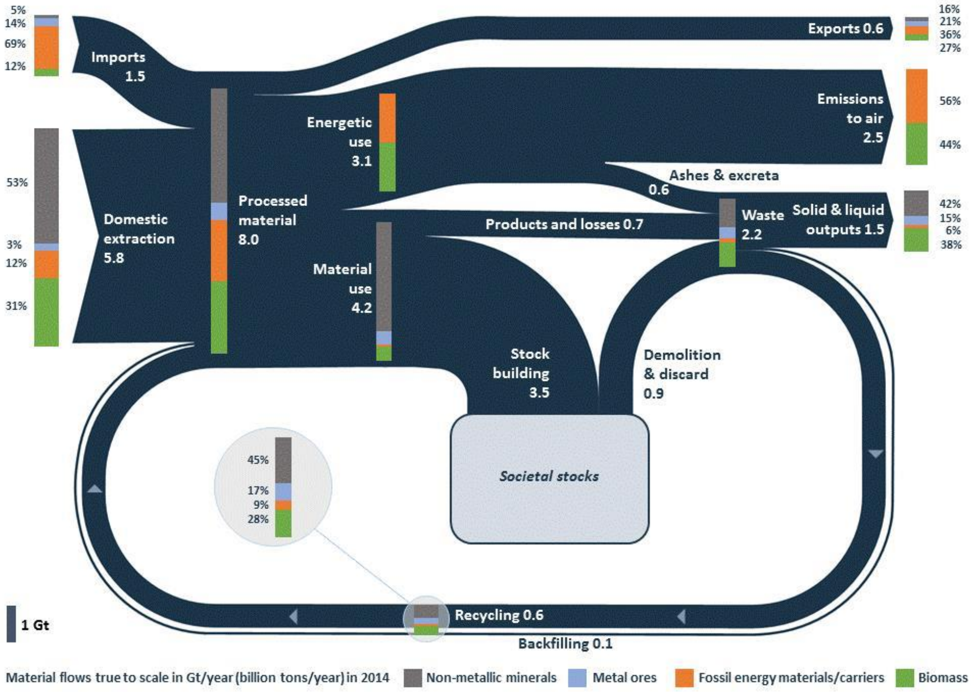
MFAs or SFAs can be executed on different levels. A SFA focuses on the flows of a substance, such as copper or lithium in a certain process, system or region. An MFA, on the other hand, focuses on materials composed of multiple substances, such as plastics or glass. An MFA/SFA can also include multiple substances and materials, for example by assessing the material flows in the waste management system of solar panels (Figure 3a). MFAs are also used on a macro level, for quantifying the material flows in an entire economy (Figure 3b). Static MFAs only cover a fixed point or period in time (for example, the total mass flows in 2022), while dynamic MFAs also take evolution over time into account. Static MFAs are often visualized by means of Sankey diagrams. In these Sankey diagrams, the width of the arrows illustrates the quantity of the flow.

a) MFA/SFA of PV waste management system in Belgium per ton waste PV panels (Thomassen et al., 2022)



(rec=recycling; NF=non-ferrous; Inc. with E=incineration with energy recovery; CM=construction materials)

b) MFA in the EU-28 from 2014 (Mayer et al., 2019)



Note: Numbers may not sum up to total due to rounding.

Figure 3. *Examples of MFA/SFAs visualized in Sankey diagrams*

2.1.2. INDICATORS

By using a MFA/SFA, different sorts of mass-based indicators can be included. If the MFA/SFA is performed on a macro-level (economy-wide MFA), indicators such as direct material input and total material requirement can be calculated. For a discussion on the economy-wide MFA of Flanders, including these macro-indicators, the report of Christis and Vercalsteren (2020) can be consulted. For the assessment of new technologies, MFA/SFA on a smaller scale are of more interest. Indicators such as the recycling rate, collection rate, reuse rate, recovery rate or recycled content can be calculated to quantify the contribution to a circular economy of this new technology or process. These circularity indicators will be discussed in more detail in the next section.

Besides quantitative indicators, also more qualitative indicators can be discussed. For example, if a specification of materials is included in the MFA, it is possible to assess which of these materials belong to the list of critical raw materials, as defined by the European Commission. This list of materials which are important for our economy, but also have a high supply risk, was first constructed in 2011. In 2020, a fourth update was published, including 30 materials (European Commission, 2020a). Besides a qualitative description, there are also quantitative methods to define a criticality score (Tran et al., 2018).

Antimony
Baryte
Beryllium
Bismuth
Borate
Cobalt
Coking coal
Fluorspar
Gallium
Germanium
Hafnium
Heavy rare earth elements
Light rare earth elements
Indium
Magnesium
Natural graphite
Natural rubber
Niobium
Platinum group metals
Phosphate rock
Phosphorus
Scandium
Silicon metal
Tantalum
Tungsten
Vanadium
Bauxite

Figure 4. *2020 list of critical raw materials (European Commission, 2020a)*

2.1.3. METHODOLOGICAL GUIDELINES

A standard work for MFA and SFA is the book by Brunner and Rechberger (2004), covering methodological assistance, potential application possibilities and multiple examples of MFA and SFA studies. Another guideline is the manual written by the OECD (2008). This document aimed to provide guidance on methodological and measurement issues related to MFA, also covering related indicators and the development of material accounts.

2.1.4. TOOLS

Tools for MFA and SFA include STAN (freely available at https://www.stan2web.net/) and e!Sankey (iPoint, 2021). An example of an MFA made by means of the e!Sankey software was provided in Figure 3. Figure 5 provides an example of an MFA of the life cycle of PET, made using the STAN software. A more basic tool to make Sankey diagrams is the Sankeymatic website (SankeyMATIC: Build a Sankey Diagram).

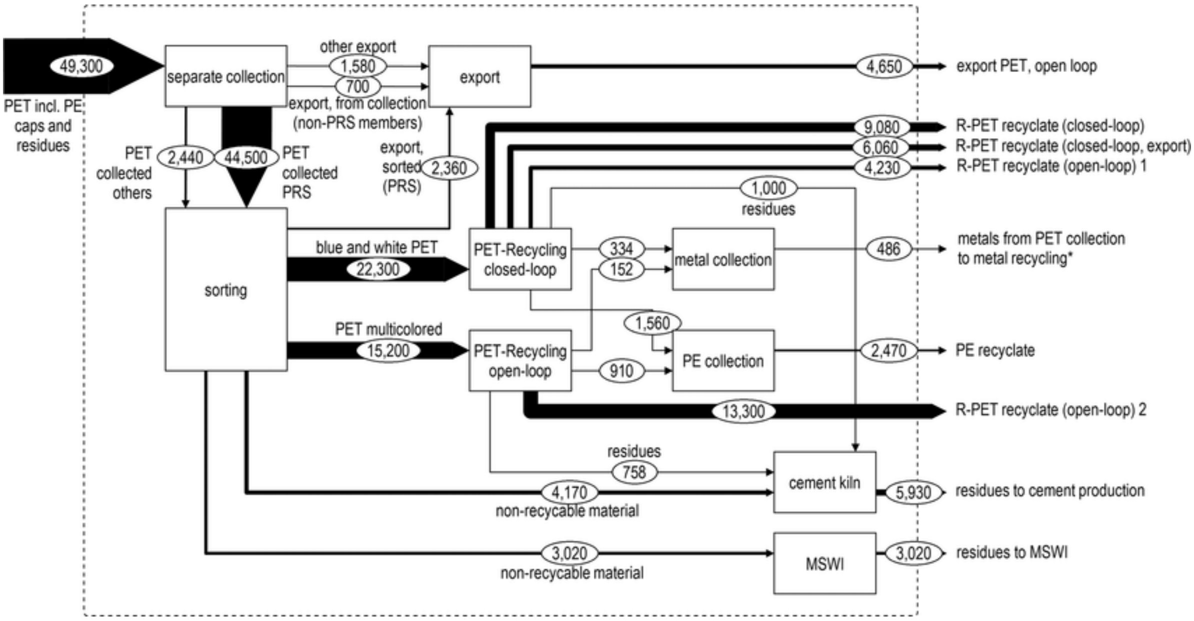


Figure 5. *MFA of the lifecycle of PET, made using the STAN software (Haupt et al., 2017)*

2.1.5. STRENGTHS AND LIMITATIONS

Strengths:

- Clear visualization, easily communicated to non-experts;
- Able to calculate how a system performs with regards to policy targets, as these are often based on recycling rates;
- Possibility of data reconciliation (using the mass balance to fill in missing data or further specify data points when uncertainty ranges are given);
- Potential stepping stone for more advanced assessments, as they often start with quantifying the mass flows (i.e. life cycle assessment (LCA) and techno-economic assessment (TEA)).

Limitations:

- Depending on the goal of the assessment, only a limited amount of input and output flows are included (for example, energy flows are usually excluded);
- No burden related indicators can be calculated;
- Only limited information on an individual process level.

2.2. CIRCULARITY ANALYSIS

2.2.1. DESCRIPTION

In the current context, where the transition to a clean and circular economy is a top priority on the European political agenda, the estimation of relevant indicators that can measure the circularity of a product or service are essential. Circular economic models aim to close material loops, maintaining the value of resources as long as possible, minimize waste and emissions, and decouple economic growth from resource consumption.

Circularity analysis aims to assess how a specific system, process or product contributes to the circular economy. The concept has gained an increasing amount of attention over the last decades.

Regarding circularity and circular economy, a wide range of different definitions has been provided by academics, organizations, and governments. Based on these definitions certain common characteristics are identified. The concept of ‘circularity’ describes the relation between the economy, natural resources, production and further components of the relevant value chain (Ellen MacArthur Foundation, 2013). In a business-as-usual approach, a linear value chain will strain the environment and its resources during the production and consumption of goods and end-of-life stage. In this system the components’ value depreciate during their use stage and are subsequently disposed. The linear economy is often described as a take-make-waste system. A circular economy will shift this paradigm towards a system where materials keep a high value, the end-of-life stage is postponed or eliminated and several aspects are taken into account such as materials, energy, health, biodiversity and well-being. The circular economy concept is illustrated in Figure 6.

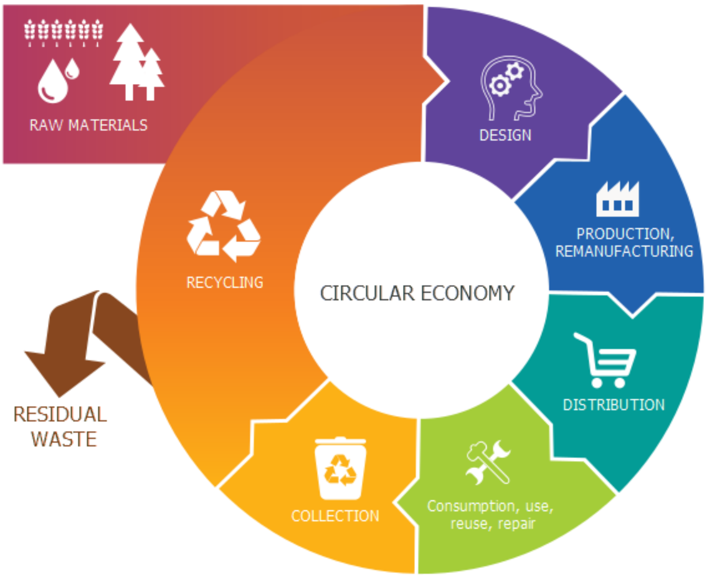


Figure 6. *The circular economy concept*

To transition towards a circular economy, different strategies can be followed: (1) narrowing the loops, (2) closing loops, and (3) slowing loops (Figure 7). The first strategy is to optimize the use of raw materials and energy, the second strategy is focusing more on reuse and recycling of materials and the third is mainly focused on life prolongation. Also, a fourth strategy, substituting fossil or environmentally polluting materials for more sustainable materials can be adopted (Hanemaaijer et al., 2021). Certain aspects of design for disassembly can be used to reduce and/or prevent waste and increase resource efficiency by encouraging alternative considerations at the project definition phase. The application of adaptability concepts and principles can minimize the need for unnecessary removal and new production, by repurposing or modifying assets to renew their service life, hence slowing the loops.

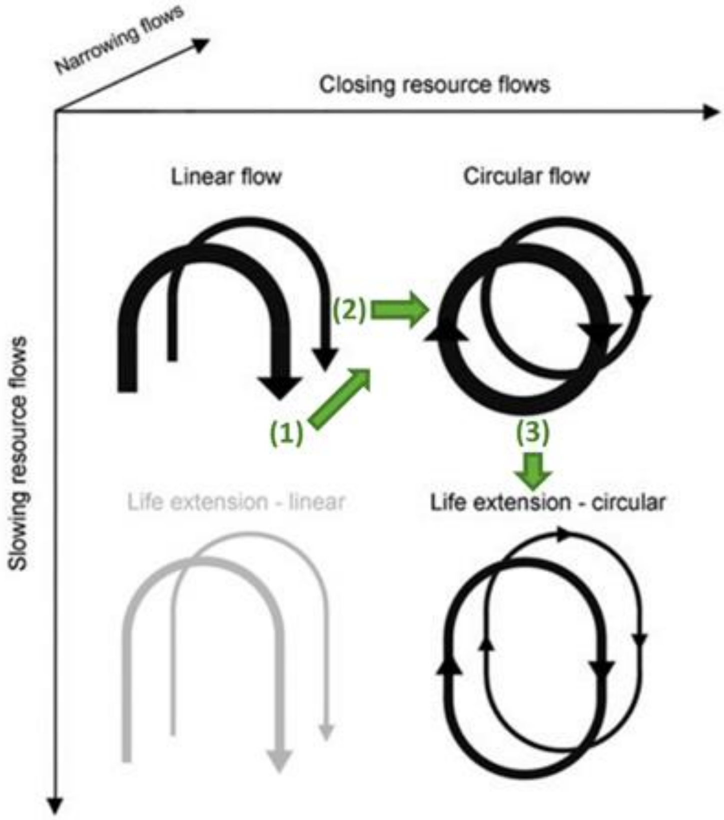


Figure 7. *The main approach applied to group the user requirements (adopted from (Bocken et al., 2016)).*

2.2.2. INDICATORS

A large amount of circularity indicators exists. A few examples are:

- % reuse or recycled content of inflow
- % recycling rate of waste
- % water circularity
- % renewable content

For a review of such indicators, the study by Moraga et al. (2019) can be consulted. They classified the indicators based on how they take into account technological cycles, if they follow a life cycle thinking approach and if they include effects on the environmental, social or economic dimension. Another example is the work of Saidani et al. (2019) that classified 55 circularity indicators based on criteria such as the implementation level (micro, meso, or macro), the type of loops (maintain, remanufacture/reuse, or recycle), and possible purposes (informative, action-oriented, communicative, or educational). The majority of the 55 identified circularity indicators are non-sector specific.

A widely known circularity indicator is the Material Circularity Indicator, introduced by the Ellen MacArthur Foundation. This indicator provides a circularity index based on the lifetime of the product, the intensity of use (amounts of uses), the primary resource consumption (virgin materials) and the amount of unrecoverable waste (not recovered, recycled or reused) (Ellen MacArthur Foundation and ANSYS Granta, 2019). The required information on material flows to calculate this indicator is illustrated in Figure 8.

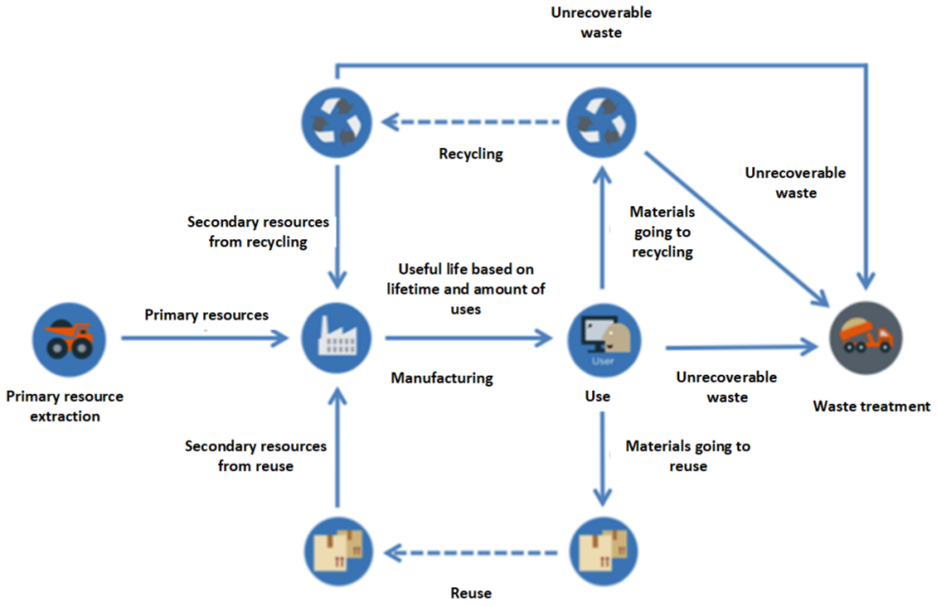


Figure 8. *Material flow information to calculate the Material Circularity Indicator (based on Ellen MacArthur Foundation and ANSYS Granta (2019))*

Recently the European Energy Agency published a report describing a monitoring framework to measure Europe's circular economy following The Bellagio Declaration (https://www.eea.europa.eu/themes/waste/measuring-europes-circular-economy/measuring-europes-circular-economy). To standardize CE principles and measurement and assessment methods and indicators, work is ongoing in the ISO/TC 323.

In Flanders, the Circular Economy Monitor was created by the Circular Economy Policy Research Center. This monitor gives an overview of more than 100 indicators, illustrating the transition to a circular economy in Flanders on a regional (macro), sectorial (meso), and product group (micro) level. Examples of such indicators are, the circular material use rate (CMUR) and the total amount of reuse in Flanders (macro), the material footprint of consumption goods and the valorisation rate of old tyres (meso). The Policy Research Center also introduced indicators on a product/material level, such as the in-use occupation of materials, quantifying the maintenance of materials in a useful state in products for as long as possible (Moraga et al., 2021). While research is still ongoing, the defined indicators and results for Flanders can be found at: https://cemonitor.be/.

2.2.3. METHODOLOGICAL GUIDELINES

As circularity in general focusses on the mass flows in a system, the methodological guidelines in Chapter 2.3 can be used as basis for the calculation of different metrics. The wide range of indicators also induces a large range of indicator-specific guidelines. They will not be further discussed here as the specific calculation methods for indicators selected for the Moonshot initative is described in the deliverable ‘‘Methodological framework for the sustainability assessment of MOONSHOT initiatives” and falls therefore outside the scope of this deliverable.

2.2.4. TOOLS

Some tools are available and are almost all focused on a company-level assessment, e.g.:

- Circular Transition Indicators (CTI) tool from WBCSD developed by KPMG. The tool is developed for companies as a self-assessment to determine the circular performance of a company (open access after registration);
- Circle assessment tool for companies to measure circularity and identify opportunities for circular strategies based on 7 key areas of the circular economy by Circle economy. (licence required);
- Circularity check by Ecopreneur. This is an online self-assessment tool with ca. 60 questions that provide a circularity score for a specific product or service. https://ecopreneur.eu/circularity-check-landing-page/ (open access);
- Circulytics by the Ellen Macarthur Foundation can be used on a company-level to assess how circular it is across its operations (open access after registration);
- Circularity calculator by IDEAL & Co is developed for designers (license – required).

2.2.5. STRENGTHS AND LIMITATIONS

Circularity frameworks and tools mentioned above are not coordinated yet. Moreover, the multitude of definitions and indicators regarding circularity does not contribute to a coherent systematic approach, leading to divergent interpretation and results (Cottafava and Ritzen, 2021). To provide a more harmonized monitoring of circularity in Flanders, the Circular Economy Monitor was created by the Circular Economy Policy Research Center[2]. Another limitation of the circularity concept is that it is often used on a system scale and not on a product or process scale as the recycling of materials requires a multiproduct and multiprocess perspective. A strength of this type of metrics is that circulariy metrics, when process specific, are often easy to be calculated (for example, % renewable materials) and can be used as a base for more extended sustainability assessments in a later TRL.

Note that under ISO/TC 323 one is also working on standardization in the field of Circular Economy which can solve part of the limitations mentioned above. One of the documents under preparation, more specifically ISO/CD 59020 specifies a framework for organizations to measure and assess circularity. The framework is applicable at multiple levels (i.e. regional, inter-organizational, organizational and the product level).

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[2] https://cemonitor.be/

2.3. (LIFECYCLE) MASS AND ENERGY BALANCE BASED METRICS

2.3.1. DESCRIPTION

The mass and energy balance extends the MFA of a product by adding energy requirements as well. This way, a full overview of inputs and output flows in the defined system is provided. This concept is illustrated by Figure 9.

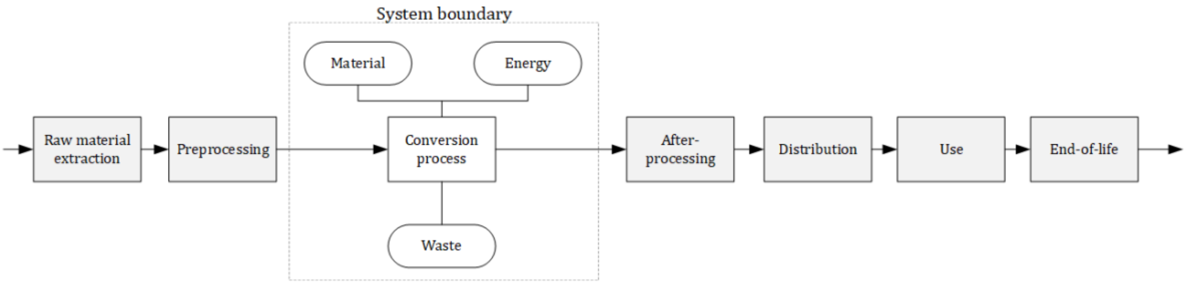


Figure 9. *System boundaries of mass and energy balance based metrics*

These metrics can both be defined on a process level, as well as on a product level. To define these metrics on a product level instead of on a process level, a lifecycle perspective is important. With this perspective, all life cycle stages of a product are taken into account. The different lifecycle stages of a product include in general raw material extraction, feedstock production, manufacturing, distribution, use and the end-of-life of the product (Figure 10). The inclusion of all life cycle stages following a lifecycle perspective avoids that by minimizing the costs or impacts of one process the costs or impacts in another process in the same value chain would be increased. This transfer of burden can lead to higher costs and environmental impact on a product level, while the individual process could claim to be cheap and environmentally friendly. If all lifecycle stages are included, the assessment is called a cradle-to-cradle assessment, or cradle to grave, depending on if recycling processes occur at the end-of-life stage. If the assessment starts at the raw material extraction and stops at the company gate, for example after the afterprocessing, the assessment is called cradle to gate. Lastly, if the assessment only covers one company, the assessment is indicated as a gate-to-gate assessment.

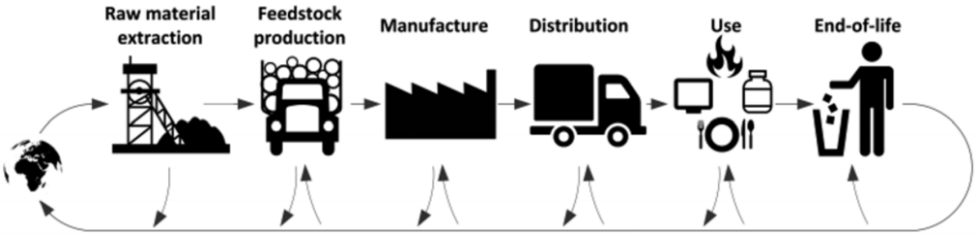


Figure 10. *The general life cycle phases of a product (Thomassen et al., 2019a)*

In case of a lifecycle mass and energy balance-based methodology, the mass and energy balances cover the entire lifecycle. This concept is illustrated in Figure 11. The indicators are therefore based on the life cycle inventory (LCI). In a LCI, not only all inputs and outputs of the upstream and downstream processes are quantified, but also the inputs and outputs in the up- and downstream processes of the in- and outputs themselves. In contrast to LCA, no life cycle impact assessment (LCIA) is done.

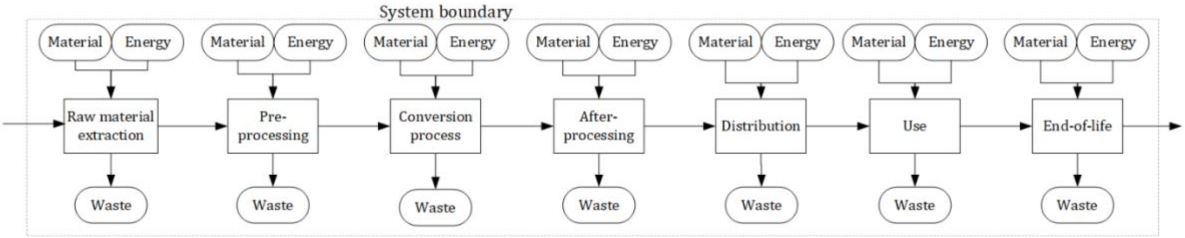
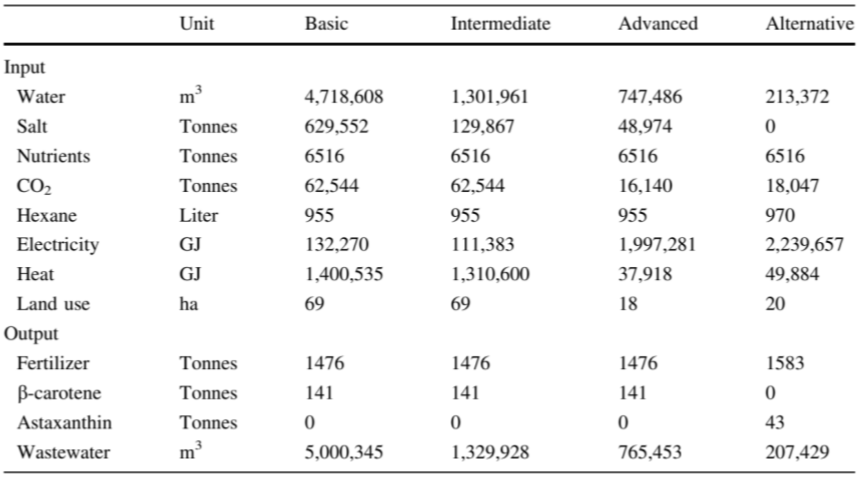


Figure 11. *System boundaries of lifecycle mass and energy balance based metrics*

Similar as for MFA, mass and energy balances are based on the law of conservation of matter (law of Lavoisier), stating that the mass in a closed system remains constant, no matter what kind of processes happen inside. Also the first law of thermodynamics (conservation of energy) is relevant here, stating that energy cannot disappear or appear out of thin air. The quantity of mass and energy flowing into a system should therefore always equal the mass and energy flowing out of a system (unless mass or energy is added to the stock). An example of a mass and energy balance is provided in Table 1.

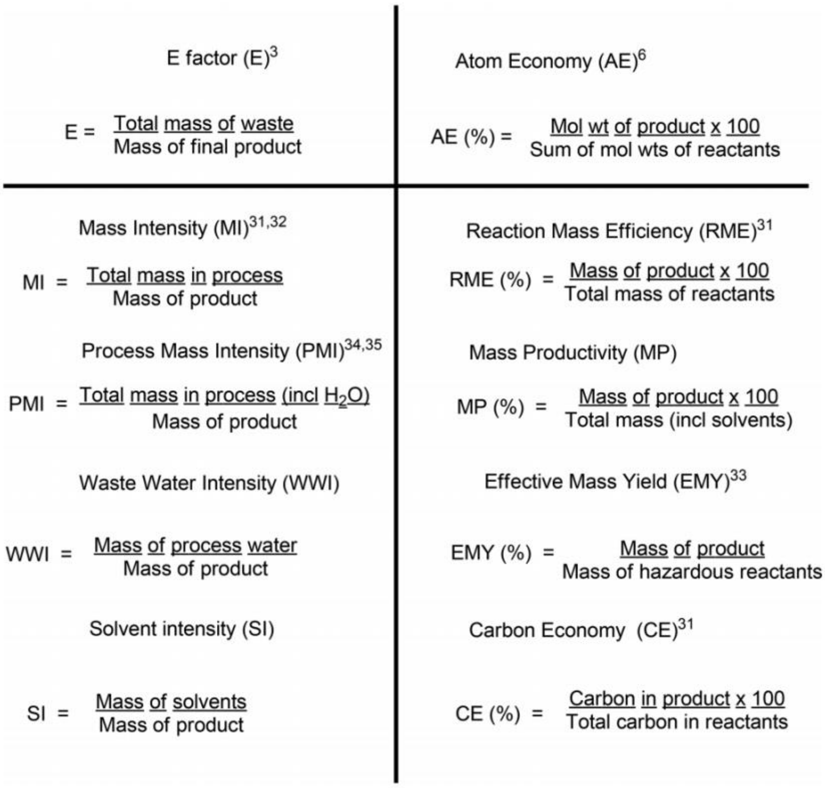
Table 1. *Mass and energy balance of an algae-based biorefinery (Thomassen et al., 2016) (note: as this figure provides only the summary of a mass and energy balance, not all inputs and outputs were included)*



	Unit	Basic	Intermediate	Advanced	Alternative
Input					
Water	m^3	4,718,608	1,301,961	747,486	213,372
Salt	Tonnes	629,552	129,867	48,974	0
Nutrients	Tonnes	6516	6516	6516	6516
CO_2	Tonnes	62,544	62,544	16,140	18,047
Hexane	Liter	955	955	955	970
Electricity	GJ	132,270	111,383	1,997,281	2,239,657
Heat	GJ	1,400,535	1,310,600	37,918	49,884
Land use	ha	69	69	18	20
Output					
Fertilizer	Tonnes	1476	1476	1476	1583
β-carotene	Tonnes	141	141	141	0
Astaxanthin	Tonnes	0	0	0	43
Wastewater	m^3	5,000,345	1,329,928	765,453	207,429

2.3.2. INDICATORS

Although the calculation of the mass and energy balance is often not considered to be a method on itself, it is the starting point for the calculation of a large amount of metrics, such as the green chemistry indicators or resource use indicators. Green chemistry is based on twelve principles, formulated by Anastas and Warner (1998): (1) Waste prevention before remediation, (2) atom efficiency (3) less hazardous/toxic materials, (4) safer products by design, (5) innocuous solvents and auxiliaries, (6) energy efficient by design, (7) renewable rather than depleting raw material, (8) shorter synthesis, (9) catalytic rather than stoichiometric reagents, (10) design products for degradation, (11) analytical methods for pollution prevention, (12) inherently safer processes. An overview of the main mass-based green chemistry metrics is provided in Figure 12. If only these mass-based green chemistry metrics are used, a process-based MFA could also be used as a methodology.

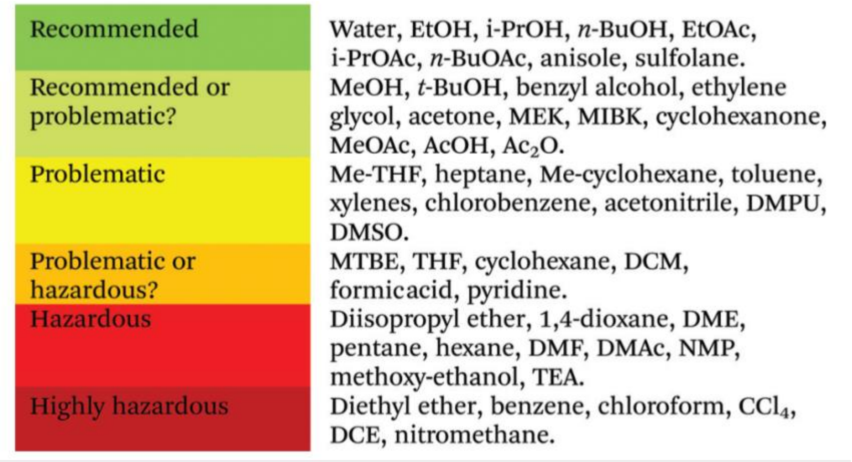


E factor (E)[3] $E = \frac{\text{Total mass of waste}}{\text{Mass of final product}}$	Atom Economy (AE)[6] $AE\ (\%) = \frac{\text{Mol wt of product} \times 100}{\text{Sum of mol wts of reactants}}$
Mass Intensity (MI)[31,32] $MI = \frac{\text{Total mass in process}}{\text{Mass of product}}$	Reaction Mass Efficiency (RME)[31] $RME\ (\%) = \frac{\text{Mass of product} \times 100}{\text{Total mass of reactants}}$
Process Mass Intensity (PMI)[34,35] $PMI = \frac{\text{Total mass in process (incl } H_2O\text{)}}{\text{Mass of product}}$	Mass Productivity (MP) $MP\ (\%) = \frac{\text{Mass of product} \times 100}{\text{Total mass (incl solvents)}}$
Waste Water Intensity (WWI) $WWI = \frac{\text{Mass of process water}}{\text{Mass of product}}$	Effective Mass Yield (EMY)[33] $EMY\ (\%) = \frac{\text{Mass of product}}{\text{Mass of hazardous reactants}}$
Solvent intensity (SI) $SI = \frac{\text{Mass of solvents}}{\text{Mass of product}}$	Carbon Economy (CE)[31] $CE\ (\%) = \frac{\text{Carbon in product} \times 100}{\text{Total carbon in reactants}}$

Figure 12. *Overview of the main mass-based green chemistry metrics (Sheldon, 2017)*

In essence, all indicators for which only information on direct inputs and outputs to the process is required can be calculated. In case of a lifecycle mass and energy balance, all indicators related to the LCI, including all inputs and outputs in the value chain, can be calculated with this methodology. Also energy related indicators are often calculated, for example (cumulative) energy demand and (cumulative) exergy demand. Also raw material consumption, water use, non-renewable energy use or emission-related metrics such as the carbon footprint are potential indicators that can be calculated based on the mass and energy balance.

Besides quantitative indicators, such as discussed above, also qualitative indicators can be assessed based on the mass and energy balance. For example, different solvents can be classified according to their hazard level. A summary of such a solvent classification guide is illustrated in Figure 13 (Prat et al., 2014). Also this metric, as no energy consumption information is required, could be used with MFA/SFA as well.



Recommended	Water, EtOH, i-PrOH, *n*-BuOH, EtOAc, i-PrOAc, *n*-BuOAc, anisole, sulfolane.
Recommended or problematic?	MeOH, *t*-BuOH, benzyl alcohol, ethylene glycol, acetone, MEK, MIBK, cyclohexanone, MeOAc, AcOH, Ac_2O.
Problematic	Me-THF, heptane, Me-cyclohexane, toluene, xylenes, chlorobenzene, acetonitrile, DMPU, DMSO.
Problematic or hazardous?	MTBE, THF, cyclohexane, DCM, formicacid, pyridine.
Hazardous	Diisopropyl ether, 1,4-dioxane, DME, pentane, hexane, DMF, DMAc, NMP, methoxy-ethanol, TEA.
Highly hazardous	Diethyl ether, benzene, chloroform, CCl_4, DCE, nitromethane.

Figure 13. *Summary of solvent selection guide (Prat et al., 2014)*

2.3.3. METHODOLOGICAL GUIDELINES

To calculate the mass and energy balance, process modelling is often required. Guidelines on process modelling can be found in chemical engineering handbooks or case-specific literature. As assessments at early TRL require some assumptions, specific guidelines for such early stage assessments have been published as well (Hassim et al., 2012; Roh et al., 2020; Thomassen et al., 2019a).

2.3.4. TOOLS

To facilitate process modelling, licence-based tools such as ASPEN(-Plus) and ChemCAD are available, but do not always include new innovative processes. Also the open access engineering toolbox is a popular tool (https://www.engineeringtoolbox.com/).

For lifecycle mass and energy balance, also LCI databases can be consulted. These databases contain quantitative information on the inputs and outputs of specific processes. Also input-output tables can be used, which provide the flows of specific product groups from one sector to another. An overview of these databases is provided in section 2.4.

2.3.5. STRENGTHS AND LIMITATIONS

Strengths:

- Easy to understand and communicate;
- No estimations required on the further burdens of the specific substances;
- Specifically for lifecycle mass and energy balance (or LCI): No trade-offs between different processes in the lifecycle can happen.

Limitations:

- Limited information on the impact;
- Limited ability to compare processes or products;

- Specifically for lifecycle mass and energy balance (or LCI): A large amount of data is required;
- Specifically for lifecycle mass and energy balance (or LCI): No information is given on the effect of the emissions or resource use (e.g. impact on global warming).

2.4. DATABASES OR OTHER DATA SOURCES

An overview of databases that can be used for the technical assessments is provided in Table 2.

Table 2. *Overview of databases and other sources for technical assessments*

Database	Description	Accesibility
Engineering toolbox	Overview of standard values for process modelling	Open access
Ecoinvent	License-based LCI data on energy supply, resource, extraction, material supply, chemicals, metals, agriculture, waste management services and transport services (Wernet et al., 2016)	Licence required
The Evah Pigments database	LCI data on pigments	Licence required
LCA Commons	LCI data representative for the USA	Licence required (USDA Commons version is open access)
IDEMAT	LCI data on product design	Academic licence Open access
Carbon Minds (cm.chemicals)	LCI data chemicals	Licence required
Environmental footprints	LCI data to perform PEF	Open access
Evah OzLCI2019	LCI data focused on Australia-Asia	Open access
IDEA	LCI (hybrid) focus on Japan	Licence required
Agri-footprint	LCI for agriculture and food	Licence required
Exiobase	Multi-regional environmentally extended supply and use/input output database	Open access
ARVI	LCI data on the value-chain of wood-polymer composite production	Open access

Agribalyse	LCI data for agriculture and food, focus on France	Open access
Needs	LCI data on future transport services, electricity and material supplye	Open access
ESU World food	LCI data related to agriculture, food processing and consumption activities	Licence required
ELCD	LCI of the JRC	Open access
ProBas	LCI data on energy, materials and products and transportation services and waste, focus on Germany	Academic licence Open access
Bioenergiedat	LCI for bioenergy supply chains, focus on Germany	Open access
Worldsteel	LCI on steel	Open access
Ökobaudat	LCI on construction materials, focus on Germany	Licence required
One Click LCA database	LCI and LCC on construction products	Licence required

CHAPTER 3 STATE-OF-THE-ART ECONOMIC ASSESSMENTS

In this chapter the following economic methodologies are described: Cost Benefit Analysis (CBA), Techno-Economic Assessments (TEA), and Life Cycle Costing (LCC). As these methodologies are closely related, a description of the differences and similarities is added as well.

3.1. COST BENEFIT ANALYSIS (CBA)

3.1.1. DESCRIPTION

Cost Benefit Analysis (CBA) is a policy assessment method that quantifies in monetary terms the value of all consequences of a policy to all members of society. Nevertheless, the methodology is also used by businesses. The European Commision defines cost benefit analysis as an analytical tool for judging the economic advantages and disadvantages of an investment decision by evaluating its costs and benefits/opportunities to assess the welfare change attributable to it. It is a micro-economic approach that assesses a project's impact on society as a whole. Note that this means that not only individual costs and benefits are included, but all social costs and benefits. Hence, CBA is sometimes referred to as social CBA. Typically, direct employment and external environmental effects are included in the calculated economic indicators. In case external environmental effects are included in the calculation, these are often translated into an actual currency, i.e. monetized.

Traditionally, CBA is mostly used ex-ante, however, it can also be used as an ex-post evaluation. The latter is less interesting in the framework of the Moonshot program as it is focused on low TRL technologies. The ex-ante approach is focused on making go/no-go decisions. It is clear that uncertainty is considerable at this stage.

In short, all costs of a project or decision are summed up and are extracted from the total estimated benefits the project or decision will generate. If the benefits outweigh the costs, it is a good decision to make.

The general steps that are followed are (Boardman et al., 2017):

1. Describe context and definition of goals and objectives;
2. Decide whose benefits and costs count;
3. Identify impact categories, catalogue them and select measurement indicators;
4. Predict impacts quantitatively over the life of the project;
5. Monetize all impacts;
6. Discount benefits and costs to obtain present values;
7. Compute the net present value (NPV) of each alternative;
8. Perform sensitivity analysis;
9. Make a recommendation.

Essential for a CBA is an uncertainty or sensitivity analysis to check the robustness of the CBA results. Often a what-if analysis is used. A more detailed description of uncertainty and sensitivity analysis is provided in Chapter 6.

3.1.2. INDICATORS

Calculated indicators are typically:

- Total costs;
- Total benefits;
- NPV, the indicators below are calculated as well, however, the NPV is the most appropriate criterion as it does always provide a correct answer (Boardman et al., 2017);
- Internal rate of return (IRR);
- Return on investment (ROI);
- Benefit-cost ratio.

3.1.3. METHODOLOGICAL GUIDELINES

- Guide to cost-benefit analysis of investment projects of the European Commission. These guidelines are specifically designed to support CBA for policy projects; https://ec.europa.eu/regional_policy/sources/docgener/studies/pdf/cba_guide.pdf
- Handbook 'Cost-Benefit Analysis: concepts and practice' by Boardman AE, Greenberg DH, Vining AR and Weimer DL.

3.1.4. TOOLS

No dedicated tools for CBA are available. The tools that are available are more focused on project management (e.g. smartsheet, miro cost benefit analysis template or FolgekostenSchätzer) instead of technology assessment.

3.1.5. STRENGTHS AND LIMITATIONS

Strengths:

- Data-driven decision methodology that can help make investment decisions and that helps to think about all costs and benefits related to the investment;
- Strong decision support methodology for governments where societal costs and benefits are key to make sound decisions.

Limitations:

- Difficult to quantify all costs and benefits which might make the decision less accurate, especially if the time horizon is long;
- No dedicated tools available;
- Other non-monetary reasons can play a role in the decision and these are not captured by the CBA methodology;

- The NPV results in the more efficient allocation of resources amongst the alternatives evaluated, it does not necessarily result in the most efficient allocation of resources;
- Distribution of the impacts across different stakeholders is not directly considered.

3.2. TECHNO-ECONOMIC ASSESSMENT (TEA)

3.2.1. DESCRIPTION

The use of TEAs is significantly increasing, however, no clear accepted definition exists of what constitutes a TEA, despite several efforts that have been made. We will base ourselves on the book chapter published by Van Dael et al. (2014b) as a reference. For a more detailed description we refer to this work.

In the book chapter the definition provided by Kuppens (2012b) is used in which a TEA is defined as '*The evaluation of the technical performance or potential and the economic feasibility of a new technology that aims to improve the social or environmental impact of a technology currently in practice, and which helps decision makers in directing research and development or investments*'.

Following the previous definition, a TEA is applied for a project that is still in its development stage (i.e. ex-ante). However, a TEA can also be used for a project that has already been implemented and that is either expanding or re-evaluating its conditions (i.e. ex-post). This is also confirmed in the methodological guidelines provided by the Global CO_2 Initiative (Zimmermann et al., 2018).

Performing a TEA at an early development phase provides an initial assessment on (1) the overall technical and operational barriers to overcome, (2) an optimal sizing for the project in terms of feedstock availability or plant capacity, (3) desirable product yields and waste management and (4) an indication of the (preliminary) economic feasibility or the main technical or financial factors that limit its feasibility.

A TEA is divided into four different phases and performed in an iterative way with a go/no-go decision after every iteration (see Figure 14). First, a market study is performed. Second, a preliminary process design is defined and translated into a simplified process flow diagram and mass and energy balance. Third, this information is directly integrated into a dynamic economic evaluation. From this analysis, the profitability is identified. Fourth, an uncertainty analysis is performed to identify the potential barriers. The inclusion of this fourth step is essential for a decision-driven TEA. Note that both technological, as well as economic barriers can be identified thanks to the direct integration. Based on the results of a cycle, risk reduction strategies and specific research targets can be formulated for follow-up research trajectories.

In most cases a TEA starts from a private-investors point of view and focuses on the manufacturing phase. Upstream processes are included via market prices that are taken into account for the different feedstocks and utilities used. The same reasoning applies for the downstream processes where for example a cost is included for certain waste treatment steps. Only if the goal of the TEA is to also optimize the upstream or downstream processes, a detailed mass and energy balance for these is included.

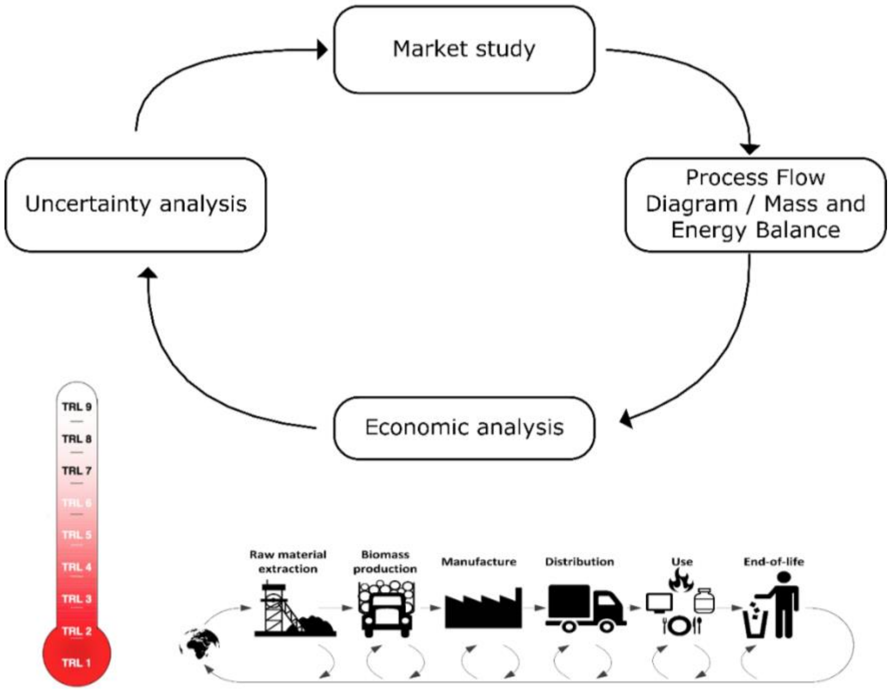


Figure 14. *TEA (based on Van Dael et al. (2014a) and Thomassen et al. (2019a))*

3.2.2. INDICATORS

Typical indicators calculated in a TEA are the following:

- Minimum Selling Price (MSP);
- Capital expenditures (CAPEX);
- Manufacturing (i.e. expenses necessary to make the product)/production cost (i.e. expenses associated with a company doing business) (OPEX);
- Levelized cost of energy (LCOE) or levelized cost of hydrogen (in case of energy technologies). See section 3.3.2 for a more detailed description;
- Revenues;
- NPV;
- IRR;
- (Discounted) Payback Period ((D)PBP).

3.2.3. METHODOLOGICAL GUIDELINES

For methodological guidelines we refer to the following documents:

- Book section with methodological guidelines on how to perform a TEA (Van Dael et al., 2014b);
- Guidelines Global CO_2 Initiative – dedicated to CCU related projects (https://assessccus.globalco2initiative.org/).

3.2.4. TOOLS

- Open access template to perform a TEA from the Global CO_2 Initiative: Excel template that follows their guidelines to perform a TEA specifically for CCU processes (https://assessccus.globalco2initiative.org/).

3.2.5. STRENGTHS AND LIMITATIONS

Strengths:

- Data-driven decision methodology that supports in making sound investment decisions.

Limitations:

- The private investors point of view of the methodology, ignores initially the inclusion of monetized external environmental benefits. Note that these can be included, e.g. via the CO_2 price;
- Difficult to quantify costs and benefits which might make the decision less accurate. This requires a more extended uncertainty and sensitivity analysis to provide sufficient insights for the decision maker;
- The NPV results in the more efficient allocation of resources amongst the alternatives evaluated, it does not necessarily result in the most efficient allocation of resources.

3.3. LIFE CYCLE COSTING (LCC)

3.3.1. DESCRIPTION

Life cycle costing (LCC) is a methodology used in Europe since the ‘70s to support decision and policy making (Hoogmartens et al., 2014). LCC can be described as a product related assessment, and may include the cost of externalities (such as greenhouse gas emissions). It allows assessing the economic performance (costs) of a product throughout its whole life cycle, identify hotspots or points of improvement, and compare the costs of products similar in function. The main cost categories included in an LCC analysis are related to the following five different life cycle stages: (1) research, development, and design, (2) primary production, (3) manufacturing, (4) use, and (5) disposal (Huppes et al., 2004).

Depending on the goal of the study (i.e., assessing financial, environmental or social concerns), four LCC types have been introduced: **fLCC, eLCC, feLCC, and sLCC** (Finkbeiner et al., 2010). Hoogmartens et al. (2014) explain these four types as follows:

1. Conventional LCC assessments that only focus on private investments from one actor (a firm or consumer) are categorized as **financial LCC (fLCC)**. Generally, only costs borne by the actor matter, and environmental costs or external end-of-life costs are omitted.
2. An **environmental LCC (eLCC)** builds upon data of fLCC and extends it to life cycle costs borne by other actors. The full life cycle of a product is considered, but focus remains on real cash flows that are internalized or expected to be internalized. There is no conversion from environmental emissions to monetary measures. Examples of costs included in an eLCC are

waste disposal costs, CO_2 taxes that are expected to be implemented and global warming adaptation costs. Discounting is not applied.

3. The **full environmental LCC (feLCC)** FeLCC extends eLCC with monetized, non-internalized environmental costs that can be identified by an environmental assessment method such as environmental LCA.
4. In a **societal LCC (sLCC)** all costs borne by anyone in society, whether today or in the future, and associated with the life cycle of a product are taken into account. Impacts such as public health and human wellbeing have to be quantified and translated into monetized measures. sLCC uses discounting, and given the social perspective, low discount rates are mostly preferred.

The LCC methodology follows the LCA framework, which will be described in detail below. The framework outlines the steps that allow to define the goal and scope of the study, including the definition of the functional unit (FU), which is the unit reference of the assessment, and system boundaries. The latter represent the life cycle stages and processes included in the assessment. More information on the steps to be followed and the definition of the FU and system boundaries can be found in Section 4.1. An LCC should include an uncertainty/sensitivity analysis.

Compared to an LCA, where flows are expressed in physical quantities and translated into environmental impacts, an LCC expresses all units in monetary terms. Moreover, in an LCC, the price of a process input is representative of the upstream costs, which are therefore aggregated in the unit price. A detailed knowledge of upstream processes is then not required.

Altough the term LCC is focused solely on costs, LCCs can include benefits as well (revenues/negative costs), for example when co-products are produced during the life cycle of the product under study or when a recycling process enables the valorization of the recycled products of materials (Maienza et al., 2020; Miah et al., 2017; Sharma and Chandel, 2021).

3.3.2. INDICATORS

In general, an LCC leads to the calculation of **the life cycle costs** to study the economic feasibility. In some cases the scope of the assessment is limited, leading to a calculation of indicators such as manufacturing costs and total costs of ownership. These can also be included as additional indicators, to obtain more information on the importance of the different life cycle stages.

For energy technologies, it is advisable to utilize a levelized cost (a similar reference for value of money) to increase the significance of the LCC analysis concerning concept comparison. LCC results can be levelled by expected energy production. This allows a better analysis and evaluation of risk and total cost during the life span. The LCOE, also referred to as the levelized cost of electricity or the levelized energy cost (LEC), is a measurement used to assess and compare alternative methods of energy production.

In literature examples can be found where the scope is more wide, including indicators such as NPV, Present Value (PV), PBP, IRR, etc. Depending on the exact scope and goal, the TEA, LCC, CBA methodologies can overlap and so can the indicators.

3.3.3. METHODOLOGICAL GUIDELINES

- The Society of Environmental Toxicology and Chemistry (SETAC) published a code of practice for eLCC, which builds further on the SETAC-Europe Working Group on LCC in 2008 (Hunkeler et al., 2008). The code of practice can be bought for $12 online on www.setac.net (Swarr et al., 2011);
- ISO 15686-5:2017. Buildings and Constructed Assets – Service-life Planning – Part 5: Life-cycle Costing;
- The ORIENTING project also includes an in-depth analysis of the LCC methodology (Bianchi et al., 2021).

3.3.4. TOOLS

- One click LCA (construction sector);
- Life cycle vision (construction sector);
- D-LCC;
- BridgeLCC (construction sector);
- Open LCA, i.e. open source LCA software (open source);
- GaBi LCA software, including LCC;
- The European Commission has developed a series of sector specific LCC calculation tools which aim to facilitate the use of LCC amongst public procurers. More information can be found here: https://ec.europa.eu/environment/gpp/lcc.htm.

3.3.5. STRENGTHS AND LIMITATIONS

Strengths:

- LCC provides vital economic information to help decision makers understand full costs (and benefits) involved (Miah et al., 2017);
- Looks at the entire life cycle of a product.

Limitations:

- LCC focuses on the economic costs over the entire life cycle, not on the economic feasibility of a specific process in this life cycle;
- Sensitivity towards discounting. *"Although discounting is a generally accepted practice, the applied discount rate is often controversial. In business circles high discount rates are applied such that current financial flows have a higher weight. In contrast, from a societal or environmental point of view, low discount rates are preferred to avoid the fact that current activities impose large costs on future generations."* (Hoogmartens et al., 2014).

3.4. DIFFERENCE BETWEEN CBA, TEA, AND LCC

Within the economic dimension, three popular methods can be distinguished: the CBA, the TEA and the LCC. In the previous sections we described each of these methodologies, however, in literature these are often used interchangeably, therefore, we summarize the main differences here.

- A **CBA** was initially a policy instrument that focuses on the quantification in monetary terms of the value of all consequences of a policy to all members of society. This implies that all costs and benefits of a project over its lifetime, also indirect effects, are included in the assessment. A CBA is originally developed as an ex-ante evaluation approach.
- A **TEA** focuses on a project and takes the perspective of the technology developer and aims to assess the economic feasibility and identifies technological and non-technological barriers by a risk analysis to define clear technological development targets (Kuppens et al., 2015). The most efficient pathways for technology development are mapped by directly linking (i.e. integrating) technological and economic parameters. For the economic feasibility, both costs and benefits are included. As a TEA aims to provide valuable information to a process developer, it follows by nature an ex-ante approach. TEA is more focused on one actor, i.e. often the investor, that can produce multiple products.
- **LCC** is focused on the cost distributions of a product, considering all phases of its life cycle. It focuses on one product, but multiple actors. It does not focus on the economic feasibility of a specific process in contrast to TEA or CBA. Similar to LCA it was initially constructed for ex-post analysis, however, is more and more often used for ex-ante analysis as well.

Despite the different inherent perspectives of the assessments, the underlying methodology for the economic calculations, e.g. defining the costs and/or benefits and sensitivity analysis, is the same for all methodologies. The main differences are in the choice of the goal and scope and the level of detail in the technical calculations as described above. In case the goal and scope are defined the same, the methodologies are also the same. One additional difference that is not yet stressed, is that LCC can be seen as a comparative assessment tool that compares products, while TEA and CBA are typically used for autonomous project evaluation. Indeed, for CBA and TEA the calculation of the NPV has a meaning without comparison to other projects (Hoogmartens et al., 2014). The differences between the system boundaries and in- or exclusion of externalities in CBA, LCC and TEA are displayed in Figure 15. The background boundaries are included but in an indirect way, by means of the costs of the inputs that provide a proxy for the costs in their upstream lifecycle phases. Note that we took the inherent perspective of the different methodologies to make this figure and that in practice the boundaries can be put differently because of the defined goal and scope.

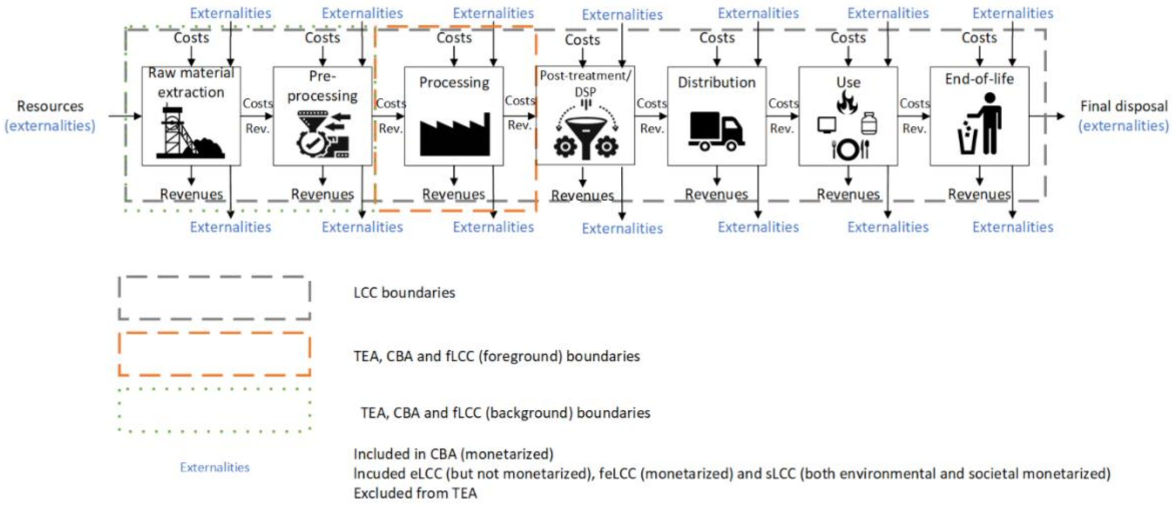


Figure 15. *Differences in system boundaries and in- or exclusion of externalities in CBA, LCC and TEA (based on Rebitzer and Hunkeler (2003), Wunderlich et al. (2021) and Thomassen et al. (2019a))*

3.5. DATABASES OR OTHER DATA SOURCES

An overview of databases and other sources that can be used for economic assessments is provided in the table below.

Table 3. *Overview of databases and other sources for economic assessments*

Database	Description	Accessibility
ICIS	Industrial price data, market reports	License required
Alibaba	Industrial price data (China)	Open access
S&P global	Industrial price data, market reports (former IHS Markit ENR and Platts)	License required
Argus	Industrial price data, market reports	License required
Eurostat	Statistical data EU	Open access

CHAPTER 4 STATE-OF-THE-ART ENVIRONMENTAL ASSESSMENTS

This section discusses environmental impact assessment methodologies. As discussed in the literature, LCA and environmental risk assessment (ERA) are the two main methodologies used for the characterization of environmental and toxicological impacts of products/processes and their chemical releases (Linkov et al., 2017). To this end, the discussion will be limited to these two.

4.1. LIFE CYCLE ASSESSMENT (LCA)

4.1.1. DESCRIPTION

LCA is an internationally standardized and commonly used methodology to assess the environmental impacts of a product, a process, a service or a system throughout its whole life cycle. It allows quantifying all emissions and waste, resources and energy used, and related environmental impacts along the life cycle of the system under study.

A general (conceptual) methodological framework for LCA has been defined by ISO in its 14040 (ISO, 2020a) and 14044 standards (ISO, 2020b). The LCA framework as described by ISO includes four main steps, as presented in the figure below: (i) goal and scope definition, (ii) LCI, (iii) life cycle impact assessment (LCIA), and (iv) interpretation. The figure shows that the 4 phases are not independent of each other.

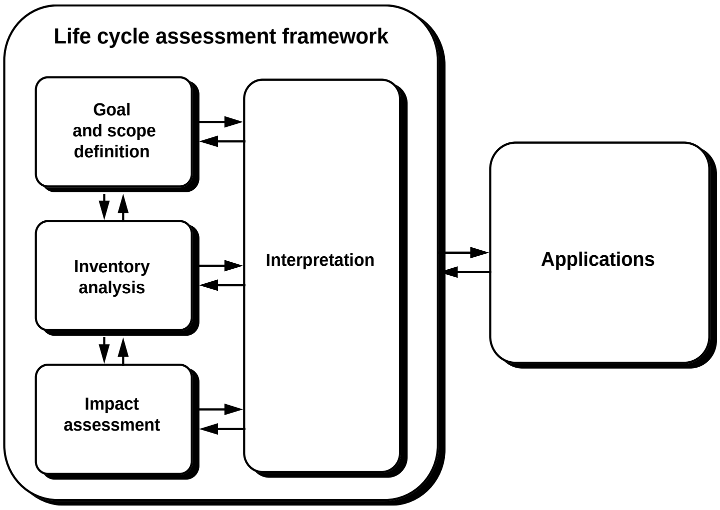


Figure 16. *LCA methodological framework (ISO, 2020a, b)*

In the first phase of an LCA (i), the **intended use of the LCA (the goal) and the breadth and depth of the study (the scope)** have to be clearly defined. The scope definition has to be consistent with the goal of the study. The **LCI step** (ii) involves **data collection and calculation procedures** to quantify the inputs and outputs that are associated with the product system(s) under study. This includes use of resources, energy and water as inputs, and releases to air, water and soil, waste and (by)products as outputs. Procedures of data collection and calculation should be consistent with the goal and the scope of the study. For each of the life cycle phases as described in the system boundaries, input and output data are to be collected. The LCI step of the LCA is the most challenging and time consuming, due to the often lack of data. Data can be collected based on specific data, estimations, experiments, as well as reports or literature studies. (Commercial) databases are also available, such as the Ecoinvent database, to support the modeling of the processes. The LCI data is then used to model all processes within the scope of the assessment (FU and system boundaries).

Based on the LCA model, environmental impacts are calculated in step (iii) of the LCA framework, the LCIA. In the LCIA, the results of the LCI are linked to specific environmental damage categories (e.g. CO_2 emissions are related to damages to human health caused by climate change, SO_2 emissions are related to damages to the ecosystem caused by acidification, etc.). It is important to note that the inventory results generally do not include spatial, temporal, dose-response or threshold information. Therefore, the LCIA can not and is not intended to identify or predict actual environmental impacts. Instead, the impact assessment predicts potential environmental damages (impacts) related to the system under study. Several LCIA methods have been developed, and are under development, such as CML 2001, EDIP 2003, Impact 2002+, ReCiPe, Eco-Indicator 99, USEtox, TRACI 2.1, Carbon footprint, Water footprint. Almost all methods operate on the assumption that a product's entire life cycle should be analysed. Differences among the methods lie in the models used to estimate the characterization factors (CFs), which can translate in differences in magnitude and unit of the impacts. As a result, this can lead to ‘confusion and mistrust in environmental performance information’ (European Commission, 2013). To obtain more harmonized LCA results, the European Commission launched the so-called Environmental Footprint (EF) method to measure the environmental performance of a product (good or service) or an organization throughout their whole life cycle using one common method (European Commission, 2021; Manfredi et al., 2012).

The EF method is developed by the Institute for Environment and Sustainability (IES) of the Joint Research Centre (JRC). It is a supporting method to the EC’s objective to “establish a common methodological approach to enable Member States and the private sector to assess, display and benchmark the environmental performance of products, services and companies based on a comprehensive assessment of environmental impacts over the life-cycle ('environmental footprint')”. The EF method was adopted by the Commission on 9 April 2013 and has been evaluated since 2014 in several PEF (Product Environmental Footprint) and OEF (Organisation Environmental Footprint) pilot projects. The PEF/OEF initiative has also delivered LCI data that fulfill strict quality requirements and are meant to support the implementation of the method through the Product Environmental Footprint Category Rules (PEFCRs) or Organisational Environmental Footprint Sector Rules (OEFSRs). PEFCRs and OEFSRs include a very rigorous definition of the data quality requirements and the required documentation and transparency of the data. It includes specific rules and default values for specific product categories, namely product category rules or organization sector rules (European Commission, 2017). Such rules outline the guidelines to calculate the EF of the product/organization in scope, including specific EF_compliant datasets. In addition, a set of 19 environmental impact categories, including climate change and other impacts to air, water and soil was selected.

The **interpretation** step (iv) is conducted throughout the whole LCA, as the analysis is considered an iterative approach and depends on the available data, assumptions and simplifications made. This interpretation step includes a check if the obtained results answer to the goal and scope, an analysis of data quality and additional potential analyses on the contribution of different life cycle stages, sensitivity of the included parameters and the uncertainty on the results.

Existing LCA guidelines, ISO 14040 and 14044 are well suited for established technologies, however, there are several methodological challenges to perform LCA of emerging technologies (Moni et al., 2019). Recently, an increasing number of papers have been published, proposing new methodologies to assess the sustainability of emerging technologies (Hung et al., 2018; Moni et al., 2019; Thomassen et al., 2019a; Thonemann et al., 2020; Zimmermann et al., 2018). These are often referred to as prospective LCA or ex-ante LCA. Such approaches focus on the assessment of technologies that are under development or which have been tested at lab and/or pilot scale, but which need to be modelled at a future phase or commercial scale (Arvidsson et al., 2017; Cucurachi et al., 2018). They allow estimating, often via multi scenario analysis, alternative future performance. They do not, however, aim to predict the future, but rather to estimate possible ranges of performances. These assessments at an earlier stage of technological development are of great importance to identify, during the R&D phase, the parameters and processes that could be changed to improve the technology's environmental performance. These approaches can support technology developers towards improved and more sustainable designs (Kazemi et al., 2018; Villares et al., 2016). Nevertheless, several challenges arise in the assessment of emerging technologies. Challenges include data quality and availability, scaling and comparability issues with mature technologies, rapid technology change and fast assessment during the design stage, and isolation of environmental from technical research inhibit application of LCA to developing technologies (Arvidsson et al., 2017; Hetherington et al., 2013; Wender et al., 2014). While some of these challenges (see data availability) can be related to retrospective LCA, they become more relevant and critical when assessing novel technologies, and lead to different types of uncertainties that need to be addressed. It is then crucial to describe the market and technological characteristics as they influence the outcome of a prospective LCA of emerging technologies (Buyle et al., 2019). The spatial and temporal variability of background systems is also important to consider when addressing emerging technologies, not to underestimate their applicability in different conditions. Research is being conducted to consider such challenges and uncertainties, and support technological development towards more sustainable solutions.

4.1.2. INDICATORS

Based on different life cycle impact assessment methods summarized above, different impact categories can be used to assess the environmental impact of a product, a process or a service. These impact assessment methods are often classified in two different groups, i.e. midpoint and endpoint categories. Midpoint and endpoint categories differ based on the level of aggregation of the results, as they look at different stages in the cause-effect chain. The endpoint categories represent areas of protection (such as human health, ecosystem quality or natural resources). Midpoint impacts are further classified according to the area of protection they affect. Although they might be more difficult to interpret because of the large number of impacts, midpoint results offer a higher level of detail. This enables to identify trade-offs between products/scenarios.

The table below summarizes the environmental impact categories of the EF method. For all indicators, the characterisation factors from the JRC of the European Commission needs to be applied[3].

Table 4. *Environmental impact indicators, units and models according to the EF method*

Impact category	Unit
Climate change – total (= fossil + biogenic + luluc)	kg CO_2 eq.
Climate change - fossil	kg CO_2 eq.
Climate change - biogenic	kg CO_2 eq.
Climate change - land use and land use change	kg CO_2 eq.
Ozone Depletion	kg CFC 11 eq.
Acidification	mol H+ eq.
Eutrophication aquatic freshwater	kg PO_4 eq.
Eutrophication aquatic marine	kg N eq.
Eutrophication terrestrial	mol N eq.
Photochemical ozone formation	kg NMVOC eq.
Depletion of abiotic resources – minerals and metals	kg Sb eq.
Depletion of abiotic resources - fossil fuels	MJ, net calorific value
Water use	m^3 world eq. deprived
Particulate matter emissions	Disease incidence
Ionising radiation, human health	kBq U235 eq.
Ecotoxicity (freshwater)	CTUe
Human toxicity, cancer effects	CTUh
Human toxicity, non- cancer effects	CTUh
Land use related impacts / soil quality	dimensionless

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[3] http://eplca.jrc.ec.europa.eu/LCDN/developerEF.xhtml

4.1.3. METHODOLOGICAL GUIDELINES

The LCA framework is defined under the ISO 14040/14044 norms (ISO, 2020a, b).

Other relevant references for LCA are:

- Commission Recommendation of 16.12.2021 on the use of the Environmental Footprint methods to measure and communicate the life cycle environmental performance of products and organisations. Can be downloaded here: https://ec.europa.eu/environment/system/files/2021-12/Commission%20Recommendation%20on%20the%20use%20of%20the%20Environmental%20Footprint%20methods_0.pdf
- Tools, documents and packages related to the EF scheme: https://eplca.jrc.ec.europa.eu/LCDN/developerEF.xhtml
- European Commission - JRC. (2011). ILCD Handbook: Recommendations for Life Cycle Impact Assessment in the European context. Vasa. https://doi.org/10.278/33030
- JRC. (2010). *International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance* (First edit). Luxembourg. Publications Office of the European Union. https://doi.org/10.2788/38479
- Rebitzer, G., Ekvall, T., Frischknecht, R., Hunkeler, D., Norris, G., Rydberg, T., … Pennington, D. W. (2004). Life cycle assessment Part 1: Framework, goal and scope definition, inventory analysis, and applications. *Environment International*, *30*(5), 701–720. https://doi.org/10.1016/j.envint.2003.11.005
- Pennington, D. W., Potting, J., Finnveden, G., & Lindeijer, E. (2004). Life cycle assessment Part 2: Current impact assessment practice, *30*, 721–739. https://doi.org/10.1016/j.envint.2003.12.009

4.1.4. TOOLS

- Global CO_2 Initiative tool provides an Excel template to perform an LCA specifically for CCU related processes (Open access);
- SimaPro LCA software;
- GaBi LCA software;
- Umberto LCA software;
- Brightway LCA software (Open access);
- One Click LCA software;
- Open LCA software (Open access);
- EASETCH LCA software (Open access, however payed training required).

4.1.5. STRENGTHS AND LIMITATIONS

Strengths:

- Commonly used to support policy and decision-making;
- Allows a broader and value chain perspective;
- It allows assessing the impacts throughout the whole life cycle of the product or service under study;

- Addresses multi-media emissions (soil, water, air);
- Addresses a large range of impacts at both global, regional and local scale.

Limitations (Laurent et al., 2014a; Laurent et al., 2014b; Obersteiner et al., 2007):

- Results are relative to the scope of the analysis (FU and system boundaries);
- The broad scope of the LCA often requires generalized models that do not reflect local conditions;
- Methodological choices influence the definitions of system boundaries, time frame of the assessment, LCIA method, etc.;
- Impacts are calculated based on standard environments;
- LCA emissions are aggregated over time and space, and are considered as pulse emissions with single effects. This could lead to the under or overestimation of the impacts;
- Data quality and availability is a limiting factor for many assessment methods, leading to assumptions and simplifications;
- Not all environmental impacts have generally accepted and scientifically sound characterization methods (e.g. noise, marine litter, biodiversity);
- LCIA and data gathering and structuring are under development. There is a need to take into account the related uncertainties, as well as to keep updated on the evolutions and state of the art.

4.2. ENVIRONMENTAL RISK ASSESSMENT (ERA)

4.2.1. DESCRIPTION

In general, risk assessment is a management tool used in decision making in, for example, regulation, business, as well as finance. Risk management allows understanding the nature and magnitude of the risk and the potential way to manage it. Risk assessment is a term that refers to different types of assessments that cover, for example, a different scope. ERA aims at assessing the likelihood and magnitude of the effects on the environment of the occurrence of a hazard, such as a chemical leakage, a disease, or the occurrence of an event. A common distinction is made between ERA of accidents and ERA of substances, the latter being the focus of this section (Finnveden & Moberg et al., 2005).

In the ERA of accidents, the probability, or frequency, of occurrence of unplanned events, and their consequences for the environment are assessed. Such assessment is often conducted ex-ante for projects (broader scope). ERA of substances aims, instead, at characterizing the nature and magnitude of the risks to human health and the environment from potential hazards, such as emissions, and considering specific exposure scenarios. The analysis of specific exposure scenarios makes the assessment site-specific and conducted at local level, although impacts could also be estimated at a broader level (for example for air emissions). ERA assesses the effects of substance releases at local level.

The ERA of substances, which is here defined as addressing risks to human health and the environment, is conducted following three main steps: (i) hazard assessment, (ii) exposure assessment, (iii) risk characterization (Flemström et al., 2004).

- The hazard assessment includes the identification of the hazard sources and its potential effects (hazard identification). A dose (concentration)-response (effect) analysis allows estimating the severity of the effect based on the dose and level of exposure to a substance.
- The exposure assessment allows instead to determine the concentrations to which the targets (humans or environmental compartments) may actually be exposed. This is conducted via a fate and transport modeling of the emission to the target via potential exposure pathways.
- The risk characterization is conducted to estimate the magnitude of the potential effects to the target(s). To do so, the results of the previous steps are compared to ensure that the predicted environmental concentration (PEC) of the released substance is lower than the predicted no-effect concentration (PNEC). The results represent the severity of the risk.

A further step could be integrated by quantifying the actual probability of occurrence of the hazard/adverse event.

ERA can be conducted either by only assessing the characteristics of the exposure pathways and potential effects of a hazard, or by determining the magnitude and severity of the risk based on normative or ecotoxicological limits.

Compared to the LCA described previously, the ERA has a more local focus, and aims at quantifying the potential effect and exposure of a hazard to a target and considering a site-specific release pathway.

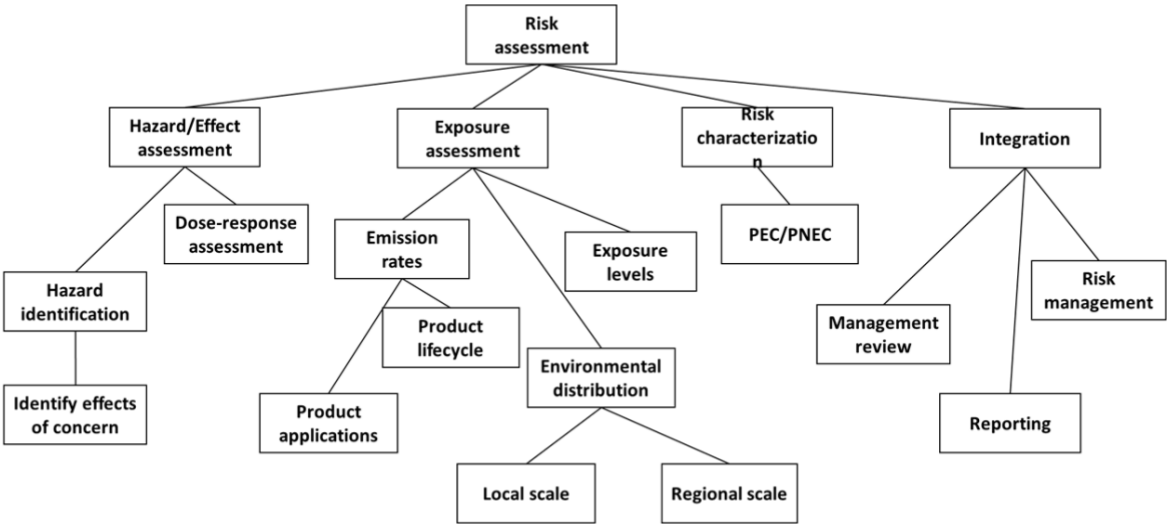

Figure 17. *Logic structure of the ERA (Flemström et al., 2004)*

4.2.2. INDICATORS

- Risk quotient (PEC/PNEC): the risk quotient determines if the risk is acceptable (<1) or not (>=1);
- Risk = probability*magnitude;

4.2.3. METHODOLOGICAL GUIDELINES

Literature studies that address ERA:

- Flemstrom, K., Carlson, R., & Erixon, M. (2004). *Relationships between Life Cycle Assessment and Risk Assessment*.
- Kaplan, S., & Garrick, B. (1981). On the quantitative definition of risk. *Journal of Risk Analysis*, *1*, 11–27. https://doi.org/https://doi.org/10.1111/j.1539-6924.1981.tb01350.x
- Aven, T., & Renn, O. (2009). On risk defined as an event where the outcome is uncertain. *Journal of Risk Research*, *12*(1), 1–11. https://doi.org/10.1080/13669870802488883

4.2.4. TOOLS

The tools for RA depend on the type and focus of the analysis. Examples of tools include:

- Risk matrix;
- Failure mode and effects analysis;
- Event tree analysis;
- Bowtie model.

Tools/software for risk assessment can be developed by companies and organizations:

- OECD Environmental Risk Assessment Toolkit;
- Lakes software;
- U.S. EPA. (2001). Indoor Air Quality Building Education and Assessment Model (I-BEAM), [CD-ROM];
- U.S. EPA. Multimedia, Multipathway, and Multireceptor Exposure and Risk Assessment (3MRA);
- U.S. EPA. Exposure Analysis Modeling System;
- For more tools developed by the U.S. EPA check https://www.epa.gov/risk/human-health-risk-models-and-tools.

4.2.5. STRENGTHS AND LIMITATIONS

Strengths:

- Realistic models of the process and emissions;
- The results can be compared directly with benchmarks, such as policy-based thresholds and background concentrations.

Limitations:

- Data quality and availability;
- As the methodology focusses on local impacts, the assessment of global impacts is limited (De Luca Pena et al., 2022);
- Assessing cumulative impacts from multiple stressors is challenging (De Luca Pena et al., 2022).

4.3. DIFFERENCES BETWEEN LCA AND ERA

Olsen et al. (2001) indicate in their study that the recommendations of LCA and ERA are different since they answer different questions, however, they are used in the same problem area.

LCA is a holist and multi-criteria assessment method. It aims to assess environmental impacts over the whole life cycle of the product/service on both a global, regional and local scale. It then allows assessing the impact of the total amount of emissions on different environmental targets (soil, water, and air) and on human health. LCA has therefore a broad focus, covering a broad range of impacts and allowing a multi-criteria assessment.

ERA has a more local focus and limited scope, aiming at quantifying the potential effect and exposure of a hazard to a target and considering a site-specific release pathway. ERA focuses on specific processes and chemical emissions. Impacts are determined based on the maximum concentrations at given points based on emission, fate and exposure models. Such emissions are then compared to threshold values to estimate the risk. Only local impacts can therefore be evaluated.

In LCA, the substances inventoried in LCA refer to a declared unit (DU) or a functional unit (FU), and are based on simplified relations and standard conditions. Moreover, the LCA is often dependent on the available database. Moreover impacts are calculated on a generalised level and standardised environment. ERA considers, instead, realistic models, with data accounted for specific local conditions at a given time interval. It is highly detailed as it assesses impacts at a local scale in time and space based on experiments and on-site measurements.

The table summarizes the differences between the two methodologies under the different perspectives mentioned above.

Table 5. *Differences between LCA and ERA*

LCA	**ERA**
Impact assessment: broader range of impacts compared to RA	Risk characterization (of chemicals): Hazards assessment (identification of hazards sources and effects), exposure assessment (emission rates, exposure levels), risk characterization (PEC/PNEC)
Global and average perspective: standardized environment, for a given period and global scale	Evaluation of effects on *local* scale in *space and time*
Impacts aggregated over time and space	Frequency and duration: long-term perspective + Site-related: exposure routes of contaminants, exposure pathways
Impacts associated to the chosen DU or FU	Benchmark with policy-based thresholds and background concentrations

Generalized modelling tool and databases: relative character of results	Results are supposed to describe reality in a more faithful way.

Although being methodologically very different also in terms of data quality and type of assessment, LCA and ERA can be integrated for a more comprehensive environmental assessment of scenarios (Olsen et al. 2001). A more detailed and local risk assessment combined with a more relative and global perspective of the impacts of waste management solutions could lead to a better identification of critical parameters for the environmental and health impacts. Nevertheless, the integration is not straightforward. Several efforts have been made in the literature at different levels and to address different challenges/uncertainties.

4.4. DATABASES OR OTHER DATA SOURCES

The table below provides an overvies of databases and other data sources for environmental assessments. The databases are mostly used for LCA. Multiple databases for the LCI have already been listed as well in section 2.4 with the technical assessments, as they can also be used for life cycle mass and energy balance based metrics.

Table 6. *Overview of databases and other sources for environmental assessments (Life Cycle Initiative, 2022; OpenLCA Nexus, 2022)*

Database	Description	Accessibility
Ecoinvent	LCI database of products and processes worldwide	Licence required
Sphera (former Thinkstep) – Professional	Internal LCA database of GaBi software	Licence required
EN15804 add-on	LCI database for Environmental Product Declarations (EPDs) in the construction sector according to the EN15804 norm. Add-on for ecoinvent database	Licence required
UVEK LCI Data	LCI database for key areas (oil and gas, nuclear fuel and electricity, tansport and siposal services, forestry and timber industries) developed by the Swiss federal offices.	Licence required
The Evah Pigments Database	LCI database for pigments	Licence required
LCA Commons	LCI database providing US representative data	Licence required, but

		the USDA Commons version of the dataset is open access.
IDEMAT	LCI database developed by Delft University of Technology	Academic licence open access
Carbon Minds	Life cycle data of chemicals and plastics	Licence required
Environmental Footprint (EF)	Secondary LCI datasets intended to be compliant with the EF method, and a related EF impact assessment method.	Open access[4]
OzLCI2019	LCI database on Australian regional supply	Open access
Idea (v.2)	Hybrid inventory dataset for nearly all economic activities in Japan	Licence required
Exiobase	Detailed multi-regional environmentally extended supply and use input/output database[5]	Open access
Agri-footprint	LCI database for agricultural and food sectors	Licence required
ARVI	LCI for wood-polymer composite production	Open access
Agribalyse	French LCI database for the agriculture and food sector	Open access
EuGeos' 15804-IA		Licence required
Needs	LCI database on future transport, electricity and material supply	Open access

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[4] Only free of charge if you are conducting PEF or OEF studies exclusively under the approved product groups and sectors, which have been approved during the EF pilot phase and as defined in the PEFCRs and OEFSRs listed, and in accordance with the terms and conditions of the EULAs of all data providers exclusively until 31st December 2021 (permitted use)

[5] Input/output databases provide information about transactions between different sectors within an economy and can also be used to gather information on the value chain of a product

ESU World Food	LCI database for food	Licence required
LC-Inventories.ch		Licence required
bioenergythat	LCI database for bioenergy supply chains developed within the German BioEnergieDat research project	Open access
worldsteel	LCI on steelmaking processes	Open access
Ökobaudat	LCI database on construction materials	Licence required
EPA 2007 USEEIO model	Database with input/output data	Licence required
ELCD	Life cycle database of the JRC	Open access
Eurostat	Statistical data EU	Open access

CHAPTER 5 STATE-OF-THE-ART INTEGRATED ASSESSMENTS

To assess the environmental impact of new processes or products, a combination of the previously discussed assessment methods can be used. However, as these methodologies have often different scopes and system boundaries, it is not that straightforward to identify synergies and trade-offs between the economic feasibility and environmental impact. The integration of economic and environmental methodologies can provide a solution here, providing one integrated assessment methodology. For the integration of different methodologies, multiple strategies were identified by the study of De Luca Pena et al. (2022). Based on their review, two main integration strategies can be identified, focussing on the methodology itself (complementation of the driving method) or on the indicators (combination of results).

The **first strategy** focuses on providing one methodology, leading to multiple indicators. In this strategy, the system boundaries and assumptions are harmonized, and one common tool can be constructed. The environmental techno-economic assessment, as explained below, is an example of such an integrated methodology.

A **second strategy** focuses on the indicators, integrating both the economic as well as the environmental indicator results. For this integration, an aggregation into one single indicator is often performed. Alternatively, the results can also be combined without further aggregation. To aggregate multiple indicators into one single score, multi-criteria decision analysis can be used. An example of a methodology providing an integrated (combined, not aggregated) indicator is the eco-efficiency methodology and is explained below as well. Both strategies can also be combined, using an integrated methodology to calculate an integrated indicator.

5.1. ENVIRONMENTAL TECHNO-ECONOMIC ASSESSMENT (ETEA)

5.1.1. DESCRIPTION

According to Kuppens (2012a), there are three important questions a TEA should answer: 1) how does the technology work?; 2) is the technology profitable?; 3) is the technology desirable?. The TEA, as discussed in section 3.2 answers these two first questions. To answer the third question, an extended TEA is required (Van Dael et al., 2014a). Such an extended TEA, called ETEA, was proposed by Thomassen et al. (2018) and defined as '*The integrated evaluation of the technological performance, economic feasibility and potential environmental impact of a (new) technology and the identification of the most important underlying parameters that aims to help the decision makers in directing research and development or investments*'. The ETEA methodology integrates the TEA and LCA assessment, taking the investor's or technology developer's perspective. However, the entire lifecycle of the product should still be considered for the environmental impact assessment to avoid burden shifting from one lifecycle stage to another. The upstream life cycle is taken into account in an indirect way by means of prices and waste treatment is also included. However downstream costs of the targeted product itself, for example the cost of the use phase (for example, quantified in the total cost of ownership) or the end-of-life cost are not included. Still, it could be argued that the product price, which consumers are willing to pay would be lower if the downstream costs would be high.

The ETEA methodology consists of five steps, should cover the whole value chain in a direct or indirect way and can be performed at each TRL. This is illustrated in Figure 18. Although the ETEA can be performed at each TRL, the process under study is always projected on an industrial scale as this is the scale where the process will be commercial. Guidelines on how to perform an ETEA at the different TRLs are provided in Thomassen et al. (2019a).

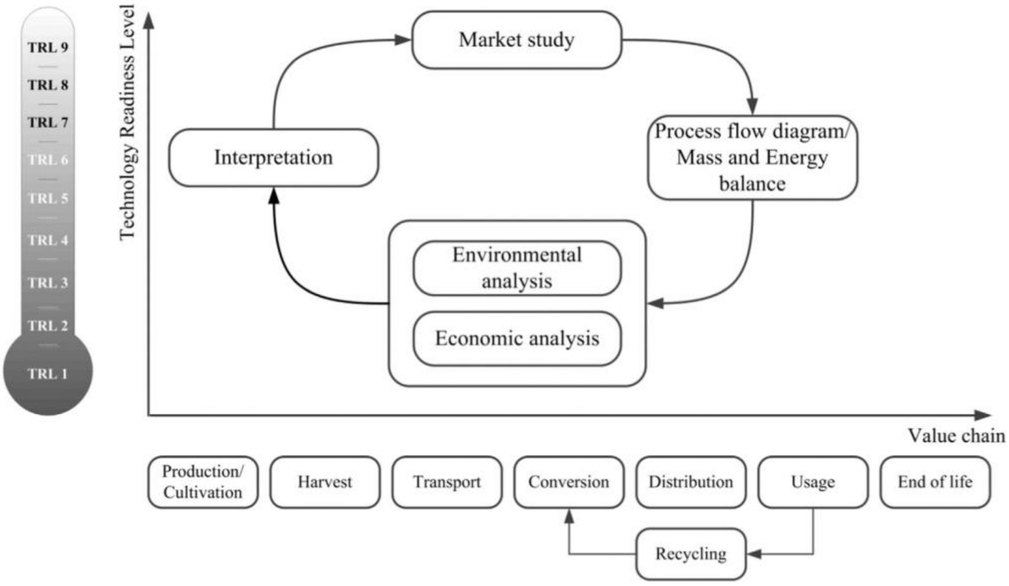
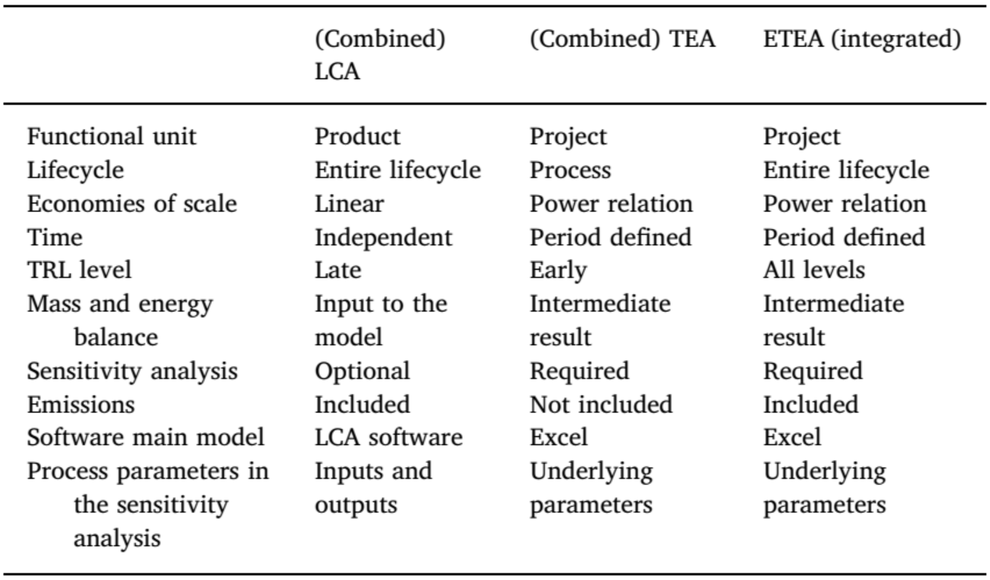


Figure 18. *Concept of the ETEA methodology (Thomassen et al., 2017)*

Integration of TEA and LCA is important as engineers and designers should simultaneously address economic benefits and environmental risks along with technical and other aspects while designing any process, product or service. This can better be done with an integrated assessment, than with a combined assessment. In addition, the integrated assessment allows for a multi-objective optimization, where the optimal scenario and parameters for both dimensions are calculated (Thomassen et al., 2019b). The differences between a combined LCA and TEA and an ETEA are provided in Figure 19. The ETEA has also been extended with a social impact assessment and a multi-criteria analysis towards a techno-sustainability assessment (TSA) by Van Schoubroeck et al. (2021). Guidelines for this TSA methodology can be found in Van Schoubroeck et al. (2022).



	(Combined) LCA	(Combined) TEA	ETEA (integrated)
Functional unit	Product	Project	Project
Lifecycle	Entire lifecycle	Process	Entire lifecycle
Economies of scale	Linear	Power relation	Power relation
Time	Independent	Period defined	Period defined
TRL level	Late	Early	All levels
Mass and energy balance	Input to the model	Intermediate result	Intermediate result
Sensitivity analysis	Optional	Required	Required
Emissions	Included	Not included	Included
Software main model	LCA software	Excel	Excel
Process parameters in the sensitivity analysis	Inputs and outputs	Underlying parameters	Underlying parameters

Figure 19. *Differences in approach between a combined LCA and TEA and an ETEA (Thomassen et al., 2018)*

5.1.2. INDICATORS

The ETEA methodology combines the indicators from a TEA (section 3.2.2) and from an LCA (section 4.1.2). It is therefore also possible to calculate combined indicators such as the NPV per CO_2-equivalent emitted.

5.1.3. METHODOLOGICAL GUIDELINES

Methodological guidelines for the ETEA methodology are provided in the tutorial review of Thomassen et al. (2019a).

5.1.4. TOOLS

No tool for ETEA is publicly available.

5.1.5. STRENGTHS AND LIMITATIONS

Strengths:

- Integrates technical, economic and environmental impacts, enabling the calculation of a large amount of indicators;
- The ETEA methodology can easily be used for a multi-objective optimization or a multi-criteria analysis;
- The ETEA methodology gives a lot of detailed insights on which parameters drive both technical, economic and environmental indicators.

Limitations:

- An ETEA can be time and data consuming;
- Expert knowledge is required for a reliable upscaling;
- ETEA is not used widely, as most studies focus either on LCA or on TEA;
- Knowledge on both economic feasibility assessments, environmental impact assessments and process engineering is required.

5.2. ECO-EFFICIENCY ASSESSMENT

5.2.1. DESCRIPTION

From the definition of the World Business Council of Sustainable Development (WBCSD), eco-efficiency is the ratio between the product or service value and the environmental impacts. The goal behind the use of eco-efficiency is to decouple economic growth from environmental impacts.

An eco-efficiency assessment is a quantitative methodology that takes into account the life cycle environmental impacts of a product system alongside its product system value to a stakeholder. It was originally developed by BASF and has its own ISO standards (Saling, 2016). The eco-efficiency assessment combines the LCA methodology (therefore also following the ISO 14040 standards) and a product system value assessment. For more information on the LCA part of this methodology, section 4.1 can be consulted. The product system value is the worth of a product system and is often expressed in monetary terms. This value should be a tangible and measurable benefit to the user and other stakeholders. For the quantification of this product system value, the FU should be used as a reference. The different steps of the eco-efficiency assessment are illustrated in Figure 20 (Saling, 2016).

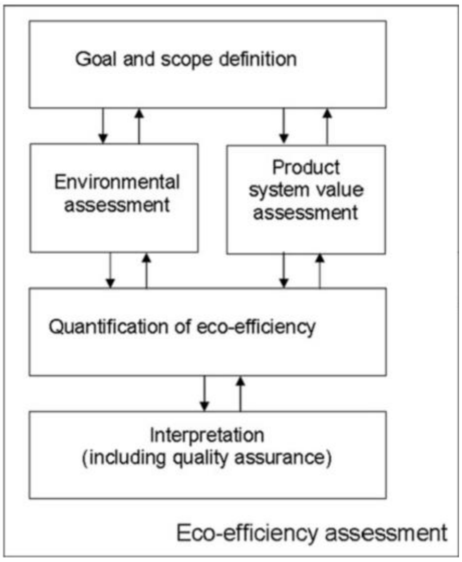


Figure 20. *Steps of an eco-efficiency assessment (Saling, 2016)*

The last step of an eco-efficiency assessment is the interpretation phase. In this step, visualizations are often used to illustrate both the environmental impact and the product system value. This visualization avoids the need for weighting both environmental and product value indicators, which is not allowed for comparative assessments disclosed to the public according to the ISO standards as it is subjective. In the case of such a comparative assessment disclosed to the public, also the environmental impact score should not be reported as a single overall score. An example of such a visualization is provided in Figure 21 (Saling, 2016).

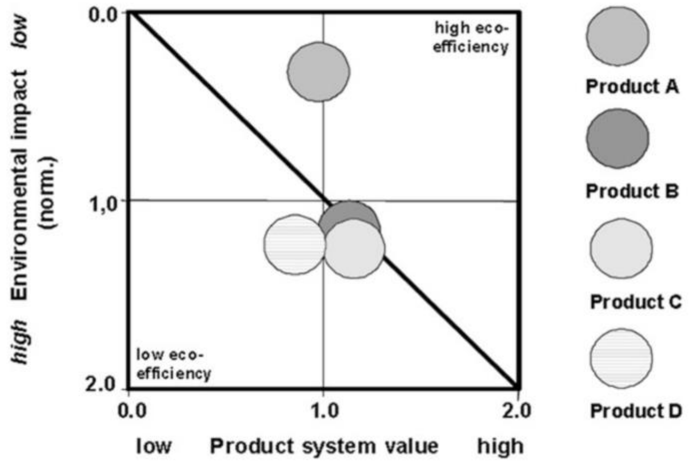
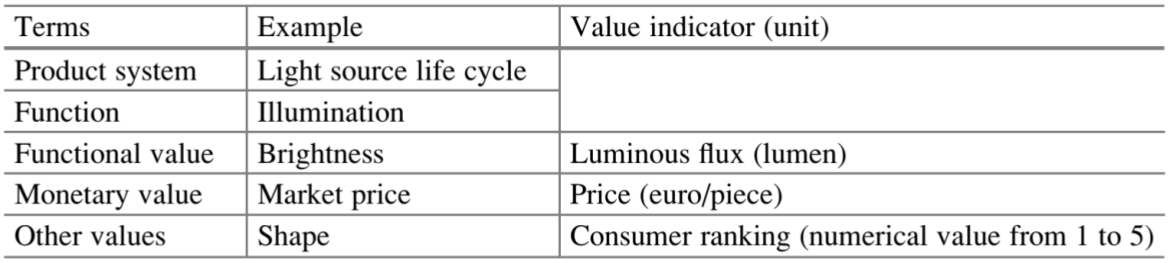


Figure 21. *Illustration of the results of an eco-efficiency assessment (Saling, 2016)*

5.2.2. INDICATORS

An eco-efficiency assessment uses the same indicators as an LCA for the environmental assessment. These can be consulted in Section 4.1.2. Potential indicators for this product system value are the costs, price, willingness to pay, profit, added value, but the indicators can also refer to aesthetics, brand and cultural and historical values. An example of product value indicators for a light source example is provided in Figure 22 (Saling, 2016).



Terms	Example	Value indicator (unit)
Product system	Light source life cycle	
Function	Illumination	
Functional value	Brightness	Luminous flux (lumen)
Monetary value	Market price	Price (euro/piece)
Other values	Shape	Consumer ranking (numerical value from 1 to 5)

Figure 22. *Light source example of the selection of value indicators (Saling, 2016)*

5.2.3. METHODOLOGICAL GUIDELINES

The following methodological guidelines can be consulted:

- ISO 14045:2012. Environmental management – Eco-efficiency assessment of product systems – Principles, requirements and guidelines
- Saling et al. (2002). Eco-efficiency Analysis by BASF: The Method. *Int J LCA*.

- Saling, 2016. Eco-efficiency assessment. In: Special Types of LCA. Editor: Finkbeiner, M. Springer.

5.2.4. TOOLS

For the environmental impact assessment, the tools as used in the LCA (section 4.1.4) can be used. For the product value quantification, no specific tools are available.

5.2.5. STRENGTHS AND LIMITATIONS

Strengths:

- The methodology provides information on both environmental impact aspects and value aspects;
- The methodology includes clear visualizations (although this use is restricted when using in comparative assessments disclosed to the public);
- The methodology can include value indicators beyond the cost perspective (also non-monetary indicators) and has therefore a wider scope than the ETEA methodology;
- The methodology is currently applied by industry.

Limitations:

- The methodology is more a combination of an LCA and indicators on product value than a stand-alone methodology. This way, the guidelines are more conceptual than practical and not really hands-on. For more hands-on guidelines, the methodology refers to LCA guidelines. For the calculation of the product value, such hands-on guidelines, facilitating harmonized assessments, are not available. This way, the results from different eco-efficiency assessments may be challenging to be compared amongst each other;
- A large data and time effort, similar to an ETEA assessment, is required;
- Expert knowledge for the LCA is required.

5.3. DATABASES OR OTHER DATA SOURCES

For the environmental impact assessment, the databases from the LCA methodology can be used (see section 4.4).

CHAPTER 6 STATE-OF-THE-ART UNCERTAINTY ANALYSIS

Uncertainty analysis allows identifying limitations in scientific knowledge and analysing their implications for scientific results and conclusions. It is therefore necessary to strengthen the results and make conclusions more relevant for decision-making (Committee et al., 2018). Before describing the approaches to deal with uncertainty, it is best to introduce the concept and the different sources and types of uncertainty related to the discussed assessments. There is no clear definition of uncertainty in the literature in terms of concept and terminology.

A distinction is made, for example, between uncertainty and variability, with the former referring to the uncertainty that derives from the lack of knowledge, erroneous measurements, or unavailability of data, and the latter to the inherent spatial and temporal variability of the system under study (Björklund, 2002; Clavreul et al., 2012; Heijungs and Huijbregts, 2004; Huijbregts, 1998). In the literature, these two types of uncertainty are nonetheless both referred to as uncertainty, with the first type addressed as epistemic uncertainty, and the second as stochastic uncertainty. As assessments rely on models of the system under study, uncertainties (of both kind) are inevitable and inherent to the modelling and to all presented assessments.

The uncertainties can then be classified into three main categories (i) parameter, (ii) scenario, (iii) and model uncertainties. (i) Parameter uncertainties, or uncertainties in the input data, are due to the inherent variability of the parameter values, the potential lack of data, or errors in measurements (Björklund, 2002; Clavreul et al., 2012). (ii) Scenario uncertainties, also termed uncertainties due to choices, are related to the inevitable choices required in the different steps of the assessment. These include the choice of system boundaries, FU, allocation, choice of temporal or geographical scope, etc. (Clavreul et al., 2012). (iii) Model uncertainties, or uncertainties due to modelling, are instead related to the mathematical models used to represent the system under study (Clavreul et al., 2012; Heijungs and Huijbregts, 2004).

Uncertainty and sensitivity analyses are both approaches used to estimate the influence of these uncertainties on the model results. The differences between the approaches lie in their goal, the uncertainties they address, and the methods adopted in the analyses. It is, however, suggested to perform both an uncertainty analysis and a sensitivity analysis. The uncertainty analysis would first allow determining the uncertainty propagation of the parameter values on the results, improving the validity of the results. The sensitivity analysis would then allow identifying those parameters whose variation has a higher influence on the results, and that are responsible for the uncertainty of the results. Vice versa, performing first a sensitivity analysis would allow to apportion the variation of the output to specific factors/choices. However, the relative importance of the factor on the model results is dependent on its variance. An uncertainty analysis can be then performed to estimate the effect on the model results of the factor's variance (Saltelli et al., 2019). The following paragraphs provide more information on the two approaches.

6.1. UNCERTAINTY ANALYSIS

6.1.1. DESCRIPTION

Uncertainty analysis is used to determine the uncertainty in the model results due to the uncertainties in the input parameter values and data variability. It therefore aims at quantifying the uncertainty propagation from the input values to the results. Uncertainties in input values can be associated with different reasons, such as the lack of data, lack of representativeness of the data, measurement errors, incomplete or unclear data, statistical random sampling error, to name a few (Frey et al., 2006). Uncertainty analysis aims to support the LCI results by estimating the uncertainty of each parameter and propagating such uncertainty to the results (Björklund, 2002). To do so, statistical functions, such as probability density functions (PDF) for the parameter values, are required. Such probability distributions describe the uncertainty in the data by expressing the probability for a variable to take a value within a specific range. PDFs can be estimated, depending on the available data, by statistical analysis of measurements or expert judgment. A commonly adopted method for uncertainty propagation is Monte Carlo simulation, a probabilistic simulation technique that uses the PDFs for input variables to generate a probability distribution of the results. Model results are calculated N times, each time randomly sampling a parameter value from the PDF. The higher the number of iterations, the more accurate is the probability distribution of the results. Other approaches for uncertainty analysis include Latin hypercube sampling, analytical uncertainty propagation, and fuzzy interval arithmetic (Björklund, 2002; Groen et al., 2014). It must, however, be considered that a high uncertainty in the input parameter does not necessarily mean that the parameter contributes significantly to total uncertainty. For this reason, it is advised to couple uncertainty analysis with sensitivity analysis.

6.1.2. INDICATORS

The indicators correspond with the evaluation criteria (indicators used in LCA, TEA, etc.).

6.1.3. METHODOLOGICAL GUIDELINES

- 2006 IPCC Guidelines for National Greenhouse Gas Inventories, Chapter 3

6.1.4. TOOLS

- GaBi Analyst;
- EASETECH;
- OpenLCA;
- Excel;
- Matlab;
- Python;
- R.

6.1.5. STRENGTHS AND LIMITATIONS

Strengths:

- More robust results as it allows defining the probability distribution of results based on the probability distribution of input parameter values;
- Better supports decision-making.

Limitations:

- Long computation time depending on number of iterations and complexity of model;
- Often relies on assumptions on the mean, standard deviations and probability distribution function.

6.2. SENSITIVITY ANALYSIS

6.2.1. DESCRIPTION

Sensitivity analysis is a common risk analysis approach adopted to understand the effects on the results of variations in data, assumptions, and models. Saltelli et al. (2004) define sensitivity analysis as “the study of how uncertainty in the input of a model (numerical or otherwise), can be allocated to different sources of uncertainty in the model input”. Different sensitivity analysis approaches exist (Clavreul et al., 2012; Saltelli et al., 2019; Saltelli et al., 2007):

- **Local sensitivity analysis (LSA)**, or one-at-a-time (OAT) sensitivity analysis, allows defining the influence of the variation of parameter values on the model’s result. The analysis is conducted by varying the value of one parameter at a time (from which the name) of a certain %, commonly +/-10%. Results can be calculated in terms of sensitivity coefficients, partial derivatives used to describe how the output y varies with changes in the values of the input parameters x_1, x_2, …, x_n.
- **Global sensitivity analysis (GSA)** explores the input parameters space across its range of variation and then quantifies the input parameter importance based on a characterization of the resulting output response surface. GSA can be performed based on three different well-known methods: the Morris method (i.e., based on repetition of a set of randomized OAT design experiments), the Sobol method (i.e, a variance-based sensitivity analysis), and linear relationships measures (using correlation coefficients).
  While the Morris method provides a qualitative assessment, the Sobol method performs a quantitative analysis of the sensitivity, calculating a first-order and total-effect index. The first-order sensitivity index can estimate the contribution of the variation of one factor to the total results. In particular, it defines the expected reduction in the variance of the output model that would be achieved if one of the factors is kept constant. The total order sensitivity index estimates instead the contribution of the variation of one factor on the results of the model due to its variation with the other varying factors. This index provides information on which factors can be fixed without affecting the model results. It determines which factors are or area not influential.
  The Monte Carlo analysis is a common GSA approach, traditionally used to estimate Sobol indices. Monte Carlo analysis is based on performing multiple evaluations with randomly selected values of model inputs, and then using the results of these simulations to (1)

determine both uncertainty in the prediction of model outputs and (2) assign to each model input its contribution to the variance in model outputs.

- **Contribution, or hotspot, analysis** provides information on the main contributing processes/parameters, and the extent of their contribution (often reported in %), to the overall model results.

6.2.2. INDICATORS

- Sensitivity index is the separation between the means of two distributions in units of the standard deviation;
- Sensitivity coefficient shows how the input parameters are related to the calculated output;
- First order sensitivity index is the main or direct effect index of an input parameter;
- Higher order sensitivity index is the sensitivity of the output due to interactions between an input parameter and other input parameters;
- Total order sensitivity index measures the contribution to the output variance of an input parameter, including all its interactions with any other input parameter;
- % contribution.

6.2.3. METHODOLOGICAL GUIDELINES

Information on sensitivity and uncertainty analysis in the framework of TEA and LCA can be found in the paper of Faber et al. (2021) from the Global CO_2 Initiative. General method descriptions and applications from several practitioners can be found in Saltelli et al. (2000), a multi-author book (i.e., Handbook of Sensitivity Analysis).

6.2.4. TOOLS

- Oracle Crystal ball;
- “Sensitivity Analysis Knoll"/ “SensIt”/ “Sensitivity Analyzer” Add-In for Microsoft Excel;
- GaBi Analyst;
- STEM;
- Global CO_2 Initiative tool (open access);
- @risk.

6.2.5. STRENGTHS AND LIMITATIONS

Each type of sensitivity analysis will have its own strengths and limitations. The LSA has the strength to focus on the sensitivity in vicinity of a set of input values, but provides only a limited view of model sensitivity because the results can be influenced by other inputs and their interactions. GSA does vary all input parameters simultaneously and therefore the sensitivity is evaluated over the entire range of input factors. A global analysis requires higher computational power as compared to the local analysis. The choice of the type of sensitivity analysis will vary based on the research question of the decision-maker.

The general strengths and weaknesses of sensitivity analysis are the following:

Strengths:

- Defines the association between variables and facilitates more accurate forecasting;
- Defines the likelihood of success or failure of a project e.g., “what is the likelihood the NPV falls below zero?”.
- Provides more useful and robust/valid results by addressing uncertainties.

Limitations:

- Relies on assumptions: the assessor needs to be aware to have a credible selection of assumptions;
- Risk for a high computational cost. The computational cost is defined as the cost of carrying out a sensitivity analysis and varies significantly for different methods. The computational cost is commonly assessed in terms of the number of samples (model simulation runs) required for the method to generate statistically robust and stable results. For high-dimensional problems and intensive models, this cost can be large (Razavi and Gupta, 2015).

6.3. SCENARIO ANALYSIS

6.3.1. DESCRIPTION

Scenario analysis, also a risk analysis approach, is used to test different choices (scenario uncertainties), or modelling options, individually and assess their effects on the model results. Scenario analysis is sometimes considered a part of sensitivity analysis, as it has been introduced as an approach to perform sensitivity analysis on specific parameters. Scenario analysis, also referred to as ‘what-if’ analysis, involves analyzing the movement of a specific valuation or metric under different scenarios. With scenario analysis, you can predict the future value of an indicator, based on changes that may occur to your existing variables. For example:

- What happens if the price of the feedstock goes up?
- What if we use a higher discount rate?
- What if a technology under development would require less energy?

Typically, you might define a base-case scenario, a worst-case scenario and a best-case scenario. The base-case scenario is a baseline scenario based on your current and commonly accepted assumptions. Your worst-case scenario is all of the most negative assumptions. Your best-case scenario is your ideal projected scenario.

It is worth highlighting the dominant role of scenario analysis in prospective assessments. Scenario analysis has gained increasing interest as approach to define future potential scenarios of emerging technologies or, more generally systems. It allows addressing different uncertainties, such as the spatial and temporal variability of background and foreground processes.

6.3.2. INDICATORS

The indicators correspond with the evaluation criteria (indicators used in LCA, TEA, etc.).

6.3.3. METHODOLOGICAL GUIDELINES

Information on scenario analysis in the framework of TEA and LCA can be found in the work of Faber et al. (2021) from the Global CO_2 Initiative.

6.3.4. STRENGTHS AND LIMITATIONS

Strengths:

- Proactive risk management is possible because the impact of potential situations is assessed;
- Better decision-making as a result of investigating the benefits and risks of various options;
- Scenario analysis analyzes ‘the future’, which can help decision-makers to find opportunities or risks they may have otherwise overlooked.

Limitations:

- Knowledge of the field is required during the scenario-building process;
- Difficult not to focus on black and white scenarios or the most likely scenario (wishful thinking) during the scenario-building process (Mietzner and Reger, 2005).

6.3.5. TOOLS

- Oracle Crystal Ball;
- "What-If" functions in Excel;
- GaBi Analyst;
- Visyond;
- Synario;
- Global CO_2 Initiative tool.

CHAPTER 7 CONCLUSION AND RECOMMENDATIONS FOR MOONSHOT

In this report, we have discussed the state-of-the-art of technical, economic, and environmental assessment methodologies, integrated methodologies, and additional uncertainty analyses. For each of the methodologies, an overview of advantages and disadvantages was provided. For the economic, environmental and integrated assessment methodologies, common disadvantages were related to large data and time requirements. For technologies at an early TRL, these can pose an important obstacle. The problem of executing sustainability assessments at an early TRL has been widely discussed amongst others in the LCA community. For example, Thonemann et al. (2020) found three main challenges:

- Comparability: issues in defining the aim, functionality, and system boundaries, as well as specifying LCIA methodologies
- Data: data availability, quality, and scaling
- Uncertainty: uncertainty exists as an overarching challenge

The same challenges were identified by Hetherington et al. (2014) and Moni et al (2019). These challenges have an important effect on the accuracy of the results, which can be detrimental when these results are used to compare different technologies and make decisions without having good insights on the accuracy and impact. Therefore, early-TRL economic and environmental assessments are not fit to make such comparisons and this should not be its primary goal. Instead, the main objective for performing early TRL economic and environmental assessments is to identify important contributors and crucial parameters to further optimize the technology. This way, these assessments are used to guide technological development towards the most sustainable endpoint, although the exact value of this endpoint remains uncertain.

More simple metrics are usually based on technical assessment methodologies, requiring only data gathering on specific flows instead of the entire life cycle. The green chemistry metrics and the Metrics toolkit are examples of such indicators. Although these indicators do not give a full overview of the economic feasibility and environmental sustainability of a new technology, they can provide a first guidance at a (low) TRL where not much data is available yet, and when the time for executing the assessment is limited. Companies often follow several iterations where more detail is added when moving across the TRLs.

Based on the above and combined with the feedback that was received from the stakeholder assessment (i.e. separate task within this project), we recommend that a dedicated selection of indicators is made considering the goal and scope of MOONSHOT. Furthermore, we recommend that the level of detail increases with the TRL, but also with the stage of the project, i.e. idea generation, proposal phase, or project execution phase. Assessing the sustainability requires the availability of both time and data and therefore the requested level of detail should be in line with what can reasonably be expected at the different project stages and TRL. Finally, we recommend to use the sustainability assessment to define clear roadmaps to further guide technological developments and to set research goals, rather than to make statements on the exact sustainability impact as this is not possible at low TRL with the limited availability of data. The next step of our work is to further detail this recommended approach in concrete methodological guidelines.

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ANNEX A - SUSTAINABILITY METHODOLOGIES, TOOLS AND INDICATORS

This deliverable was started with making an overview of different sustainability methodologies/methods, tools and indicators. From this overview, the most relevant methodologies/methods, tools and indicators in the framework of the MOONSHOT program were selected. The table below provides an overview of all methodologies/methods, tools and indicators listed. Note that this table is not complete and that more methodologies/methods, tools and indicators exist.

	Methodologies/Methods	Guidelines for the method	Tools for the method	Indicators for the method
Environmental assessments	Life Cycle Analysis (LCA)	ISO	Ecolizer	ReCiPe/PEF indicator set
		Product Environmental Footprint (PEF)	Global CO_2 initiative tool	Carbon footprint
		Global CO_2 initiative guidelines	Environmental input-output tables	Water footprint
		JRC technical report: the plastics LCA method	Simapro	Ecological footprint
		LiSET (matrix mapping) or screening LCA	Gabi	Cumulative Exergy Extracted from the natural Environment (CEENE)
		Prospective LCA/ex-ante LCA/Anticipatory LCA/streamlined LCA	Umberto	Cumulative Energy Demand (CED)
		ERPA matrix	Brightway	Land use indicators (direct and indirect)
		MECO method	One Click LCA	

	LIME2	Open LCA	
		EASETECH	
		SESAME for energy systems	
		XPrize/LEIF template	
		IF template for proposals	
Input-Output Analysis (IOA)			
Environmental impact assessment	Finnveden & Moberg, 2005		Environmental impacts
Strategic Environmental Assessment	Dir. 2001/42/EC		Use of natural resources
Environmental Auditing	ISO 14001		
Ecological footprint (as method)			Area used
Environmental risk Assessment (chemicals)		Fate, exposure and effect assessments	
Quantitative risk Assessment (accidents)		Probability assessment and effect assessment	

Economic assessments	Cost-Benefit Analysis (CBA)	Handbook chemical engineering	Matches	Net present value, minimum selling price, internal rate of return, payback period, present value
	Life Cycle Costing (LCC)	Book Hunkeler et al., 2008. Environmental LCC	One Click LCA (construction sector)	Life cycle cost
			Life Cycle Vision (construction sector)	Total cost of ownership
			D-LCC	
			BridgeLCC (construction sector)	
			Open LCA	
			Gabi	
	IOA			
Criticality analysis	Geopolitical supply risk	Gemechu et al. (2016, 2017)	GeoPolRisk	
		European Commission (2014, 2017)		
	Economic Scarcity Potential (ESP)			
Technical	Material flow analysis/substance flow analysis	Brunner and Rechberger, 2004	STAN, eSankey	All sorts of circularity indicators: recycling rate, recovery rate, ...

Total Material Requirement (TMR) - focus on society/nation	Finnveden & Moberg, 2005		Stocks (changes in)
Material Intensity Per Unit Service (MIPS) - focus on product/service			Direct Material Input
			Direct Material Consumption
			Total inputs
			Total outputs
Energy analysis			Cumulative energy demand
Exergy analysis			Cumulative exergy demand
Emergy analysis			Cumulative emergy demand
Mass and energy balance		Aspen-Plus	Energy consumption/ energy efficiency
		ChemCAD	Waste production
			Green chemistry metrics such as atom economy, carbon economy, percentage yield, reaction mass efficiency, effective mass efficiency, E-factor, ...
			% (non)renewable energy
			E factor/ Environmental Quotient (EQ)

				MLI (mass loss indices)
				ELI (Energy loss index)
				Mass index S^{-1}
				Material efficiency
				Raw material consumption
Integrated assessments	TEA	Engineering toolbox	Global CO_2 Initiative tool	Cost per energy consumption
		Global CO_2 Initiative guidelines		
		Book chapter Van Dael et al. 2015		
		Catcost		
	ETEA	Thomassen et al., 2019	BASF eco-efficiency toolbox	Eco-efficiency
	TSA	Faber, Mangin and Sick, 2021 (Global CO_2 Initiative)	SeeBalance (BASF)	Sustainable value
	LCSA		AgBalance (BASF) - farming	Cost per ton CO_2 avoided
	Material flow cost accounting			
	Eco-efficiency assessment	ISO 14045:2012		Eco-efficiency

		BASF eco-efficiency analysis method		
Uncertainty, sensitivity and risk analysis	Uncertainty analysis		Monte Carlo analysis	Probability distributions for results
	Sensitivity analysis		Oracle Crystal Ball	Sensitivity Index
			@risk	Sensitivity Ratio
	(Multiple) Scenario analysis		DOE - factor-based approach	
			Other scenario development methods	
Aggregation	Multi-criteria decision analysis (MCDA)	Van Schoubroeck et al., 2021	MCDA Index Tool	
			Diviz	
			Packages in R, Matlab, Python, ...	
			PriEsT (specific for AHP)	
			Decisionarium	
			DESDEO	
			ASMO	
Cir cul			Impact	

			C2C	
			Circulytics	
			Circularity calculator	
			Circularity check	
			Madaster circularity indicator	
			Circular IQ	
			CTI	
			PRP	