Methodological framework for the sustainability assessment of MOONSHOT initiatives

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2 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 2040 to contribute to the achievement of the Flemish climate objectives. 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 economic and environmental impact. This framework should allow to estimate this 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. For the MOONSHOT program, the sustainability assessment framework is specifically focused on the economic and environmental impact. This report describes the methodological guidelines that will be used within the MOONSHOT innovation program. These methodological guidelines are also 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 tested on running MOONSHOT projects to prove its applicability. Finally, an article is published for a broad audience to explain the advantage of using the developed methodological framework.

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(D)PBP	(Discounted) Payback Period
CAPEX	Capital Expenditures
CF	Characterization Factor
CRM	Critical Raw Materials
DSP	Downstream Processing
EoL	End of Life
FTE	Full Time Equivalents
FU	Functional Unit
GHG	Greenhouse Gases
GWP	Global Warming Potential
IRR	Internal Rate of Return
KPI	Key Performance Indicator
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
MOT	Moonshot Trajectory
NPV	Net Present Value
OAT	One-at-A-Time
OPEX	Operational Expenditures
PFD	Process Flow Diagram
SA	Sensitivity Analysis
TEA	Techno-Economic Assessment
TRL	Technology Readiness Level
WACC	Weighted Average Cost of Capital

7 GLOSSARY

Allocation based on partitioning	In case of a multifunctional system, this approach means that a specific part of the burden of the system will be allocated to the defined reference flow based on a criteria such as for example mass, energy content or price.
Allocation based on substitution	Used in case of a multifunctional system. While the functional unit (FU) stays the same, an extra process is included in the system leading to a change in system boundaries. The added process represents the alternative production process that would otherwise be required to produce the by-product (or co-product). Its environmental impact is subtracted from the environmental impact of the reference flow.
Background system	The background system covers the remainder of the system for which no process-specific details are included and where the economic and environmental data is replaced by generic or average data.
Background system	The background system covers the non-core process of the system.
Break-even analysis	The break-even analysis aims at understanding what conditions, such as parameter values, need to be met to reach a certain environmental and/or economic performance. It is often used to understand how the results can develop when a range of values is considered.
Characterization factor	The multiplication factors of emissions in an impact category (for example, the global warming potential (GWP) in the climate change impact).
Climate Change impact	The potential impact of all greenhouse gas (GHG) emissions emitted during the entire lifecycle of the product or service.
Contribution analysis	A contribution analysis shows the contribution of the different life cycle stages, processes or specific inputs/outputs to the selected output indicator.
Discounted Payback Period (DPBP)	The point in time when the initial investment is paid back by the net incoming cash flows considering the time value of money.
Foreground system	This part covers the core process itself. For the foreground system, the process specific technical, economic and environmental data is included in the model.
Foreground system	The foreground system covers the core process of the system under study. This is the process for which most information is known and for which the data has the highest quality available.

Functional Unit (FU)	Quantified description of the function that a product system fulfills for use as a reference unit
Geographical scope	The location for which the assessment is performed.
GHG avoidance cost	The average cost to avoid greenhouse gas emissions over the lifetime of the product.
Impact factor	The multiplication of the amount of elementary emissions and resources (for example GHG emissions in case of climate change impact) with their corresponding characterization factors. Here it specifically represents the impact reported as environmental data for the background processes.
Intermediate product	An intermediate product is a product used to produce a final good or finished product
Internal Rate of Return (IRR)	The discount rate at which the net present value (NPV) is zero.
Levelized cost of product	The average cost per unit of product produced over the lifetime of the process.
Multifunctionality	The characteristic of a system, such as technologies or processes, to provide more than one function.
Net Present Value (NPV)	Investment criterion indicating the profitability of a project.
One-at-a-time sensitivity analysis	The one-at-a-time (OAT) sensitivity analysis, or perturbation analysis, aims at varying only one parameter at a time in the aim to identify the factors whose variation can influence most the variation of the model results, and to what extent.
Payback Period (PBP)	The point in time when the initial investment is paid back by the net incoming cash flows.
Process Flow Diagram (PFD)	It illustrates all the unit processes and their inputs and outputs within the defined system boundaries (i.e. foreground system).
Recycled content	The ratio of recycled materials (secondary materials) in the total material input flow of the foreground system.
Recycling output rate	The ratio of secondary materials after the recycling process compared to the total output flow of materials.
Recycling rate	The ratio of materials that enter the recycling process compared to the total output flow of materials.
Reference flow	A quantified amount of resource(s)/product(s) needed for a system to fulfil the function described in the functional unit
Renewable content	The ratio of renewable materials (non-fossil materials) in the total input flow of the foreground system.
Reuse rate	The ratio of materials that are being reused compared to the total output flow of materials without further processing (except for basic cleaning).
Share of renewable energy	The ratio of renewable energy compared to the total energy input.
System Boundary	Selection of which processes are inside the analysed system

System expansion	Expansion of the functional unit (FU) to also include the extra functions in case of a multifunctional system.
Temporal scope	The year for which the assessment is performed.
Total manufacturing cost	The sum of the total operational expenditures for one year.
What-if analysis	What-if analysis is a specific scenario analysis approach that allows to analyze the potential outcome of changes on the model, more specifically technological choices or changes in the system boundaries.

8 INTRODUCTION

8.1 Goal of the Methodological Framework

In the proposal phase, the word file ‘full SBO proposal’-template is used with a dedicated section on the valorization impact in which also a first assessment of the sustainability impact is included. Note that the term sustainability within the framework of the MOONSHOT refers to the economic and environmental impact. It contains both a qualitative and quantitative part for the sustainability impact. For the quantitative part both the climate change and economic impact are requested. Some sub questions are formulated to clarify what is requested exactly. The methodological guidelines presented in this report can be used by the researchers if they need inspiration on how they can approach the calculations. The goal of the quantitative sustainability impact assessment within the proposal phase is to identify the main influencing parameters and help to set initial research targets that can be used in the identification of the go/no-go milestones. The goal is not to determine the exact sustainability impact since this is not possible with the limited available resources.

When a proposal is granted and the project is executed, using the methodological framework for the sustainability assessment is obliged. The main goal of the sustainability assessment is to have a clear understanding of the potential sustainability impact of an innovation. It serves to guide researchers towards the most sustainable configuration, given the MOONSHOT context, of their development by setting clear research targets and as such help to define the technology roadmap towards implementation. The following subgoals are defined:

1) To have a substantiated estimate of the economic and climate change impacts with the aim to identify the hot-spots (i.e. understand where the impact is coming from) and with these to update research targets from the proposal phase and define the next steps towards implementation (i.e. technology roadmap and follow-up trajectory);
2) To compare the economic and climate change impact with state-of-the-art and emerging technologies;
3) To understand the contribution of a project to the specific MOT goals and KPIs;
4) To specify what is required for a successful implementation.

To guide the researchers in following the methodological framework, a semi-structured Excel template is foreseen for the first three subgoals. This template should be submitted as a deliverable at the end of the project. Mid-term a project, the first results should be discussed with the members of the advisory board/interested stakeholders and the project manager from Catalisti/Flux50. The specific goals of the discussion are (1) to discuss the updated research targets from the proposal phase and (2) to discuss follow-up trajectories with the advisory board members.

Following the methodological framework and template allows for transparency in methodological choices, the use of default values, consistency in the used decision criteria, and consistency in reporting. The guidelines in this report include information on how to conduct the assessments, depending on the MOT and technology readiness level (TRL). The methodological framework is aimed at practitioners/researchers in the execution phases of the MOONSHOT Innovation program. Dedicated instruction movies are available with guidelines on how to use and complete the Excel template.

As described in the deliverable 'State-of-the-art of sustainability assessment methodologies and methods and their fit for the evaluation of MOONSHOT initiatives', several assessment approaches exist that address the environmental and economic performance of products, processes, and services. However, there is no harmonized framework for the assessment of emerging technologies, nor for the assessment of innovation projects, that fits the goal of the methodological framework needed for MOONSHOT. Therefore, the methodological framework and template described in this report builds on available sustainability frameworks and assessment approaches and will focus on those aspects that meet the objectives of the MOONSHOT innovation program. The goal of the framework is to guide the practitioners in their analysis of emerging technologies and the identification of their research targets.

The majority of the guidelines are based on the principles of Techno-Economic Assessment (TEA) and Life cycle Assessment (LCA) as these are most fit for the MOONSHOT Innovation program. The guidelines will follow the main steps of these methodologies, however, it is important to mention that the guidelines provided in this document do not aim to provide a new standard for these existing methodologies. They aim, instead, to make use of good practices from these existing assessment methodologies to support the goal defined for the MOONSHOT Innovation program. This implies that following the methodological framework does not result in the calculation of the absolute economic and environmental impacts, nor does it have the goal to compare non-related projects to each other in terms of sustainability impact.

8.2 Moonshot Objectives

The MOONSHOT Innovation program has four main research lines defined as Moonshot Trajectories (MOTs): (1) Biobased Chemistry, (2) Circularity of Carbon in Materials, (3) Electrification & Radical Process Transformation, and (4) Energy Innovation. Within each research line, specific technical, economic, and environmental goals and key performance indicators (KPI) have been defined to support the development of more sustainable solutions. Using the methodological framework and template also allows specifying the extent to which the results from the project add to the defined goals and KPIs. An overview of the main goals and specific KPIs are provided in Table 1. For the latest overview of the specific goals and KPIs per MOT we refer to the MOONSHOT website: https://moonshotflanders.be/.

Table 1: Summary of main goals and specific goals and KPIs per MOT

MOT 1 Biobased Chemistry

Goals and KPIs focus on developing new, sustainable biobased chemical products with preferably new functionality and higher added value, considering circularity, rational use of crops, and global market potential.

1) Products and processes will be more sustainable in terms of carbon footprint and environmental impact than their fossil-based counterparts.

2) Products are based on stable, competitively priced supply chains/raw materials from the circular use of biomass and the rational use of crops.
3) End products must be able to play an important role in (future) Flemish industrial value chains and have considerable global market potential.

MOT 2 Circularity of Carbon in Materials

Goals and KPIs focus on developing recycling technologies for polyolefins and heteropolymers (with a focus on chemical recycling) and the development of chemical platforms for more easily recyclable plastics. The focus should be on CO_2 emissions reduction.

4) Recycle 70% of post-consumer volume (contaminated) polyolefins (TRL 6) by 2030, with the ambition to transform 75% of all polyolefin-type plastics at the end of their cycle of use into building blocks for new products by 2040.

5) Recycle 60% of the post-consumer volume of heteropolymers (TRL 6) by 2030, With the ambition to be able to transform 80% of all heteropolymer-type plastics (polyamides, polyurethanes, PET) at the end of their cycle of use into building blocks for new products, by 2040.
6) Develop 2 chemical platforms for more easily recyclable plastics (TRL 6) by 2030.

7) Reduction in CO_2 emissions of around 1 million tons of CO_2/year.

MOT 3 Electrification & Radical Process Transformation

Goals and KPIs focus on developing economically viable technologies that reduce CO_2 in the chemical industry, focusing on CO_2 capture, purification and utilization, and hydrogen production.

8) 60% reduction in ‘CO_2 emission/ton produced’ by the (petro)chemical industry (TRL 6) by 2035.

9) Economically profitable CO_2 capture & purification and conversion process (TRL 6) by 2025.
10) CO_2 capture and purification at point sources at €20-30/ton and for Direct Air Capture at €50-100/ton.

11) Cost-efficient (< €2.000/ton) hydrogen production at low CO_2 emissions (TRL 6) by 2025.

MOT 4 Energy Innovation

Goals and KPIs focus on developing technologies that enable to offer 80% of the total energy demand of the Flemish energy-intensive industry as sustainable energy (with a focus on CO_2 emissions reduction) in a cost-effective way.

12) CO_2 emission reduction in the order of 10 million tons CO_2/year for energy-intensive industry for the reference year 2018 in an economic cost-effective way

13) innovative technologies to provide CO_2 neutral/sustainable energy to meet the increasing energy demand (estimated at 70 TWh) of the industry (TRL 6) by 2030, followed by at least 1 innovative technology every 5 years (TRL 6).
14) innovative technologies for transport and storage of energy (TRL 6) by 2030, with at least 1 innovative technology to TRL 6 every 5 years thereafter.
15) development of a novel generation of flexibility algorithms, 3 innovative processes “designed for flexibility” and a portfolio of cross-sectoral models to ensure that +20% of the industrial energy demand is provided by flexibility by 2030.

8.3 TRL

Technology readiness level (TRL)[1] is an indicator or measurement system that allows one to assess the maturity or stage of development of the system under study, be it an individual process unit or the overall process or technology. The TRL scale, originally defined by NASA, goes from 1 to 9, with 1 being the lowest and 9 the highest. TRL 1 represents the idea when scientific research is just beginning. TRL 9 is reached when a full-scale plant is proven in an operational environment (Mankins 2009). Figure 1 below provides further details on the TRL

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[1] https://cdn1.euraxess.org/career-development/researchers/manual-scientific-entrepreneurship/major-steps/trl

scale definition that is followed for the MOONSHOT Innovation program. This is the same as the definition used by the European Commission.

Within the MOONSHOT Innovation program, projects are at an early stage of development, i.e. TRL lower than 6. The specific TRL highly influences the data availability and quality and therefore also the accuracy of the sustainability assessment that is performed. Results also need to be analyzed and interpreted accordingly, as higher uncertainties are related to lower TRLs. Moreover, assessments need to be repeated and validated once more data is available. In the methodological framework, a distinction in the requirements is made based on the TRLs. For projects within the MOONSHOT program, it should therefore be clearly defined at which TRL it is situated to correctly apply the methodological framework.

→	**TRL 1**	**TRL 2**	**TRL 3**	**TRL 4**
	Basic principles	Technology concept	Experimental proof of concept	Validation in lab

TRL 5	**TRL 6**	**TRL 7**	**TRL 8**	**TRL 9**
Validation in relevant environment	Demonstration in relevant environment	Demonstration of system prototype	System complete and qualified	System proven and operational

Figure 1: An overview of technology readiness levels (TRLs)

8.4 Report structure

The following chapters will provide detailed information on the different aspects of the methodological framework. In general, the four different phases of TEA and LCA will be followed as the main structure to build the guidelines. In addition, some more general aspects and their challenges will be highlighted. In each chapter also guidelines will be provided per TRL to support the practitioners in their assessments. The guidelines are made as such that researchers can focus only on those parts that they need more guidance in. There is no need to read the full document. In addition, researchers can focus only on the grey highlighted boxes if they quickly want to screen the specific requirements for MOONSHOT.

In each section, a general introduction is provided, as well as the specific requirements for the MOONSHOT innovation program. The specific requirements are introduced in the text using the MOONSHOT logo and are highlighted in light grey.

For each section, also a reference is made to the Excel template. Specific guidelines for the Excel template are indicated using the Excel logo and the grey highlighted text.

The first step in TEA and LCA assessment includes the definition of goal and scope. Before indicators are selected and impact calculations are initiated, the evaluator should define ‘what’ needs to be assessed. Major parts of this are the choice regarding the goal, geographical and temporal scale, functional unit, the delineation of the system boundaries, and defining the benchmark systems. These elements will be discussed in Chapter 9.

Chapter 10 will provide a more detailed description of the foreground inventory analysis. This includes first a description of what needs to be included in the process flow diagram. Next it is described how the mass and energy balance can be calculated depending on the TRL. Finally, the equipment inventory is explained.

Chapter 11 will provide information on the impact assessment. In this chapter a general introduction is provided, followed by a description of the technical, economic, environmental and combined indicators that need to be calculated.

Chapter 12 describes the interpretation phase. Once the impacts are calculated, it is important to understand how changes in parameters will influence the results. In this chapter it is described how sensitivity and uncertainty analysis can be used.

In the final chapter information is provided concerning elements that help to put the innovation in its context and define the steps required for a successful implementation.

8.5 Excel template structure

The methodological guidelines are used to complete a semi-structured Excel template. Within the methodological guidelines we refer in each section to the worksheet in the Excel template where that specific part of the guidelines can be found. In the Excel template we refer back to the methodological guidelines. In the table below we give a short overview of the different worksheets in the Excel template. Detailed guidelines on how to work in the Excel template itself, are provided in the form of instruction videos.

Table 2: Excel template worksheet overview

Worksheet name	Description
Intro	Information on the background and purpose of the Excel template, overview of the worksheets and some general agreements in the layout of the Excel template.
Dashboard results	Automated overview of the main results
Project	Project administrative information.
Technology	Description of the innovation, the benchmark technologies and the goal and scope of the sustainability assessment.
Market	Description of market information for the targeted product(s) and an overview of relevant policy documents.
Pathway definition and results	On this worksheet different pathways can be defined as well as parameters to define scenarios. This allows to quickly see the impact of changes in defined parameters on the main findings from the sustainability assessment.
Data - technical	All technical input parameters for the mass and energy balance calculations, including the references.

Data - economic	All economic input parameters for the calculations of the economic indicators, including the references.
Data - environmental	All environmental input parameters for the environmental impact calculations, including the references (mainly characterization factors).
Data - general	General information that is needed for the calculations that are not fixed values.
1. Pathway	Calculation sheet for the first pathway. This sheet contains the calculation of the mass and energy balance, the economic indicators and environmental impact. This sheet needs to be copied if multiple pathways are defined.

9 GOAL AND SCOPE DEFINITION

The goal and scope definition step makes sure that assessments are conducted consistently. It represents the first step and allows to define the research question(s), the context and boundaries of the study, and the methodological choices that will be adopted.

9.1 Goal definition

The first step in the assessment of a new technology/process is the definition of the goal of the study. A clear goal definition provides details on the type of assessment, the systems under study and the system boundaries, and helps to define methodological choices that will be discussed below. In general, the following questions should be answered when defining the goal:

1. Which are the research questions and what information do we want to obtain from the study? Or in other words, what are the reasons for carrying out the study? (the purpose);
2. What are we going to use the results for? (intended application);
3. Which is the target audience to whom the results will be communicated? (targeted audience).

1.

Given the use of the assessment framework in the context of the MOONSHOT program, here we will focus on the first question, i.e. related to the purpose of the analysis. The intended application and targeted audience are the same for all projects within the framework of the MOONSHOT. The application of the results is to support R&D, identify new technological pathways, and support the valorisation of the technology. The targeted audience is mainly the companies that will be involved in the discussions mid-term a project and Vlaio and Catalisti/Flux50 to follow-up on the projects.

It is important to consider that the goal of the study, and then the study results, should support further improvement, development and/or implementation of the system analyzed. For example, by evaluating the economic feasibility and climate change impact of a process and identifying which processes/emissions contribute the most to it, the system can be further adapted to improve its performance. Such analysis can then support the development towards the targets/objectives of the MOTs.

For the MOONSHOT innovation program, the general purpose is to compare the development with the state-of-the-art and emerging technologies, to identify the hotspots for further improvement as indicated in section 8.1 and to prove the contribution to the MOT specific goals and KPIs. It is important that this general purpose is further specified for each project. An example of a goal of a study, could be "to understand the potential environmental performance of the bio-based product compared to its fossil-based counterpart" or "to understand the economic feasibility of the bio-based product, and what processes contribute the most to it". The goal can be specified further, adding information related to, for example, the bio-based product: "does the bio-based product produced from X (example of feedstock) have a lower climate change impact compared to its fossil-based counterpart". The more specific the goal is, the more transparent and comparable the results.

Projects evaluated for the MOONSHOT program should specify in detail the goal based on the purposes described above. Examples of goals for MOONSHOT projects are listed in the table below per MOT and in order of increasing detail with reference to TRL.

Table 3: Goal examples per MOT and TRL

MOT	TRL	Examples of goal
MOT 1	1-2	"Assess the potential climate change impact of the process. Assess if the revenues can be higher than the costs. Identify the environmental hotspots in the process and identify what flows/processes contribute the most to the impact (i.e., hotspots)."
	3-6	"Assess the bio-based product its environmental and economic impact compared to its fossil carbon-based counterpart and other emerging products. Assess which processes contribute the most to its impact." "Assess the economic and environmental impact of the production of product X with the new technology/process compared to the business as usual." "Assess which technology is preferred from an environmental sustainability point of view, given the specific context."

MOT 2	1-2	”Assess the potential environmental and economic performance of the mechanical/chemical recycling process. Identify flows/processes that contribute the most to the impact (i.e., the hotspots).”
	3-6	”Assess the environmental and economic performance of the recycling process compared to its counterparts and identify which processes contribute the most to its impact. Identify the research targets that need to be met to have an environmentally and economically preferred process compared to the counterparts.” ”Assess the impact of the production of product X with the new technology/process compared to the business as usual.” “Assess the environmental impact of product X (from recycling plastics) compared to product Y (with the same functionality)?” “Assess the impact of the recycling of X kg of plastic compared to other end-of-life options.”
MOT 3	1-2	“Assess the potential climate change impact of the production of X via the new process. Assess if the revenues can be higher than the costs. Identify the processes that contribute the most to the impacts (i.e., hotspots).” “Identify the required research targets to have an environmental and economic preferred system.”
	3-6	“Assess the environmental and economic performance of the new process compared to the state-of-the-art and emerging alternatives. Identify the flows/processes that contribute the most to the impact.” “Assess the CO_2 emission reduction potential of the use of carbon capture and utilization compared to the state-of-the art.” “Assess if the CCU-based product is economically more interesting compared to the same fossil carbon-based product.”
MOT 4	1-2	“Assess the potential climate change impact of the system. Identify if the revenues can be higher than the costs. Identify the environmental hotspots, i.e. the flows/processes that contribute the most to the impact.”
	3-6	“Assess the environmental and economic performance of the new energy system compared to the state-of-the-art and emerging alternatives. Identify the flows/processes that contribute the most to the impact.”

The purpose needs to be specified in the Excel template in the worksheet ‘Technology’ under the title ‘purpose of the sustainability assessment’.

The TRL of the system under study needs to be specified in the Excel template in the worksheet ‘Technology’ under the title ‘TRL’

9.2 Scale of the system

We introduced above the concept of technology readiness level (TRL), as an indicator that “allows one to assess the maturity or stage of development of the system under study”. The stage of development can indicate whether the technology is still at lab-scale, pilot or industrial and full-scale of development. However, when assessing the environmental and economic performance of an emerging system, it is important to do so for a projected future industrial scale. The reason is twofold. On the one hand, when upscaling the technology, economies of scale apply and the process is further optimized, leading to a potentially improved performance (efficiency), lower costs and impacts. On the other hand, the technology can be compared with its mature counterpart that is already on the market and at commercial scale. Comparisons of technologies at different scales would not be consistent and would provide biased results.

To assess the technology at industrial scale, such *scale* of the system needs to be further defined. This represents the capacity of the plant/technology, such as the amount of output product generated in industrial plants, the amount of waste processed, or the total energy output. For example, in a chemical liquid phase batch process the scale of the process can be expressed based on the size of one batch expressed in Liters (100 L/500 L/ 1000 L,...). Other examples are the production of 1000 kton of biochemicals per year, or the processing of 250 kton of pre-treated waste per year in a waste-to-energy (WtE) plant. The definition of the scale/capacity of the system can be defined based on the scale of similar commercial processes, expert knowledge, market volume, capacity of main equipment. Different scales can be suitable for a process, and the analysis should be conducted according to the choice made.

Projects evaluated for the MOONSHOT program should consider evaluating their process/technology at TRL 9 and should specify the chosen scale of the system for the assessment. Upscaling procedures will be discussed in Chapter 10 to provide more details on how to scale-up low TRL data.

The capacity is indicated in the Excel template on the worksheet ‘Pathway definition and results’ in the table ‘scale’.

9.3 Functional Unit

The functional unit (FU) is a quantified description of the function that a product system fulfills. The definition of a functional unit is a key aspect, as it allows us to define for which function we are analyzing the product or service. For example, we could analyze the environmental impacts of a technology for its ability to deliver 1 kg of product X. This gives us the basis of evaluation of the environmental impacts, that will then be expressed as, for example, kg CO_2 eq./kg of product. An example of an economic impact is the cost of a specific chemical operating unit expressed per kg output. It must be noted that, environmental impacts and costs estimated based on the FU are relative indicators. For example, a potential result could be the impact of a specific chemical operating unit expressed per kg output as mentioned before. Such indicators should be distinguished from absolute indicators, such as the total cost of a specific chemical operating unit, and should be interpreted accordingly.

The definition of a FU is even more crucial when comparing different product systems. Two systems can only be compared on an equal basis, or the results would be invalid. It is imperative to avoid comparing “apples and oranges”. The FU represents therefore the comparison basis. If products have different performance characteristics, then they cannot simply be compared as product A versus product B, but need to be compared for their common ability to deliver a specific function, here defined as FU. Similarly, when comparing multiple scenarios within a project assessment, or when comparing multiple separate assessments over time, the same FU is needed to make valid comparisons.

In some cases, the exact application and/or performance is not clear yet. In such cases one can define multiple FUs to check for robustness. In other cases, several functions can be identified. For example, in a power plant, both electricity and heat can be produced or in a refinery several products are produced. This is called multifunctionality and is discussed in the next section.

Throughout the assessment, the FU provides a reference to which the inputs and outputs can be related. The FU should as much as possible be related to the ‘functions’ of a product, rather than the physical product itself (see Table 4). This way it can be ensured that properties such as the performance of the products are addressed. Examples of functional units for product systems are summarized in the table below.

Table 4: Functional Unit examples

Product system	Function	Functional unit
Power plant	Generating electricity	1 kWh of electricity generated
Hand dryer	Drying hands	1 pair of hands dried
Light bulb	Providing light	100 lumens light for 1 hour
Paint/coating	Painting/coating a surface	1 m^2 surface painted/coated
Biofuel or e-fuel	Driving a car/truck	1 km driven by a car/truck
Plastic waste	Treating plastic waste	1 kg of treated plastic waste

Biobased solvent	Serve as solvent in a chemical process	1 kg of the specific biobased solvent

Considering the above examples, if we want to compare two types of biofuels to provide the same function and therefore for their ability to fulfill 1 km driven by a car, we might need different amounts of input feedstock for the two systems. Depending on the type of feedstock and the efficiency of the process we could need, for example, 1.5 kg of biomass A compared to 1 kg biomass B to provide the same energy required for the drive. The feedstock amounts of 1.5 kg and 1 kg are the references flows of system A and system B, respectively. Such reference flows are used to estimate the mass and energy flows for the system under study.

Projects evaluated for the MOONSHOT program should define a FU which will be used in the sustainability assessment. When the characteristics, structural properties and composition are the same as the benchmark, or when little is known about the performance, for example, because it is at a low TRL, a FU based on physical characteristics should be used. Such a FU can for example be defined in terms of mass (kg product) or energy (MJ or kWh product). The table below provides examples of FU per MOT. Be aware that these are only examples, and FU should be defined based on the goal of the study and the technology analyzed.

Table 5: Functional Unit examples per MOT

MOT	Goal of the study/analysis	Examples of functional unit
MOT 1	Assess the environmental and economic performance of the bio-based product compared to its fossil carbon-based counterpart (with the same characteristics).	1 unit (kg/MJ/piece/etc.) product
MOT 2	Assess the environmental and economic performance of two recycling solutions – mechanical and chemical recycling – and identify the main hotspots.	1 tonne of post-consumer volume polyolefins/ heteropolymers.
MOT 3	Assess the impacts of production of hydrogen with the new process compared to the state of the art.	1 tonne produced hydrogen/other product.

MOT 4	Assess the impacts for the production of energy/energy storage and identify hotspots.	1 MJ energy produced, or 1 kWh of energy stored (energy storage systems).

The functional unit is defined in the Excel template on the worksheet ‘technology’ under the title ‘Functional unit (FU)’. Multiple functional units can be defined if that is required. In the calculation sheet ‘1. Pathway’, the mass and energy balance should also be calculated for the defined FU in column G. In case multiple FUs are defined, the calculations need to be done for each. For the other pathways, the same procedure needs to be followed, however, a new calculation worksheet needs to be included.

9.4 System boundaries

The system boundaries identify the unit processes that are evaluated in the assessment (what is considered and what is left out). The choice of these boundaries depends on the goal of the assessment, and in most cases also on the availability of data. To enable a fair comparison between scenarios or pathways and with the benchmark, it is crucial that the same system boundaries are used for one assessment. A visualization of the product system and the different system elements (e.g. process units, unit operations or individual unit equipment) that are included in the system boundaries is requested for the MOONSHOT innovation program.

The scope of different studies can vary from gate-to-gate to cradle-to-grave. Gate-to-gate only includes the factory gates. Cradle-to-gate is an assessment of a partial product life cycle from raw material extraction (‘cradle’) to the factory gate (i.e., before it is transported to the consumer). Cradle-to-grave is the full life cycle assessment from raw material extraction (‘cradle’) to the use phase and disposal or End-of-Life phase (‘grave’). Cradle-to-cradle is a specific kind of cradle-to-grave assessment, where the end-of-life disposal step for the product is a recycling or recovery process (Cao 2017). A graphical overview is provided in Figure 2. Note that between the post-treatment/DSP and distribution, some other processes might take place that are the same for the targeted product in the MOONSHOT project and the benchmark product.

It is important to consider that the analysis of the impacts throughout the whole life cycle (cradle-to-cradle or cradle-to-gate) allows understanding how impacts/costs are distributed through different processes, limiting potential burden shifting. When considering only a few processes and excluding the others, there is a risk of underestimating the impacts that would otherwise result from a broader assessment. Results could be biased, leading to better results because impacts are concentrated in a process that hasn’t been considered. It is therefore important to choose the system boundaries considering potential consequences.

On the other hand, the choice of the system boundaries is strictly related to the goal of the study and the chosen functional unit, and processes can be excluded if not relevant for the assessment. For example, if the goal is to estimate the climate change impact of the production of X and the FU is the production of the unit product X, the use phase and end-of-life of such product should not be considered. These processes are out of scope as the focus is on the production process. Similarly, when comparing two systems/technologies, common processes can be excluded from the assessment. Their inclusion would not add any additional information to the comparison as they would provide the same result. For example, in case the targeted product is an intermediate product, such as for example a chemical, with exactly the same chemical structure, composition, characteristics and intended application, a cradle-to-gate approach is sufficient as the rest of the value chain will be exactly the same. The choice of the system boundaries is therefore important and needs to be done consistently with the goal and scope of the study, as well as with the available data and means.

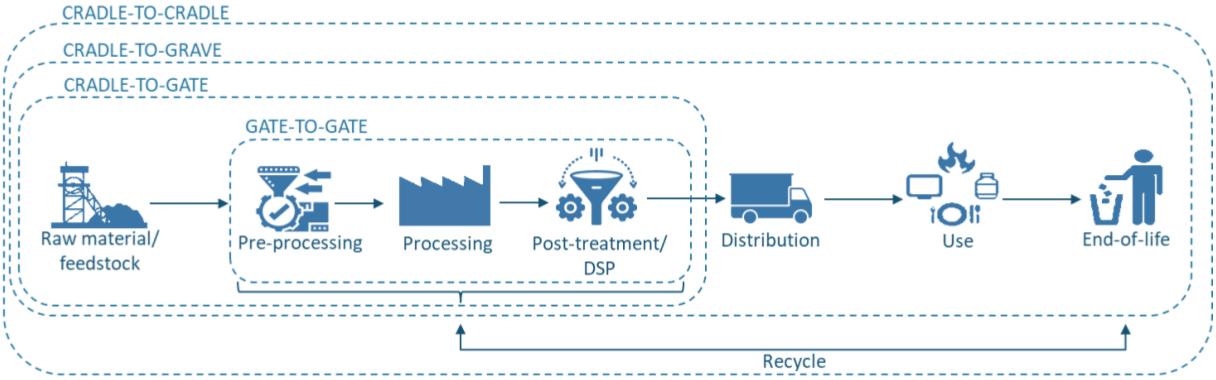

Figure 2: System boundaries

Projects evaluated for the MOONSHOT program should define their system boundaries and provide a graphical representation. Dependent on the goal of the study, there can be chosen for cradle-to-cradle or e.g. cradle-to-gate analysis. The choice should be clearly motivated.

The following table gives examples of potential system boundaries for the FUs defined above per MOT. It is important to understand that such system boundaries are only examples for the sake of the explanation. The practitioners should review their goal and FU and consistently define the system boundaries.

Table 6: System boundaries examples per MOT

MOT	Examples of functional unit	System boundaries
MOT 1	1 unit (kg/MJ/piece/etc) product	Cradle-to-gate

MOT 2	1 ton of post-consumer volume polyolefins/ heteropolymers	Gate-to-cradle
MOT 3	1 ton of petrochemical product	Cradle-to-gate
	1 ton of petrochemical product	Cradle-to-grave or cradle-to-cradle (depending on the inclusion or not of resource recovery or recycling)
MOT 4	1 MJ energy	Cradle-to-gate

System boundaries are defined in the Excel template in the worksheet ‘Technology’ under the title ‘System boundaries’. The motivation for the system boundaries selected for the project under evaluation, needs to be provided under ‘please explain choice’.

The Process Flow Diagram (PFD) that is included in the Excel template on the calculation worksheet ‘1. Pathway’ provides a visual representation of the foreground system (see section 9.6). The PFD that represents the foreground system needs to be included for each pathway. A calculation worksheet needs to be included for each defined pathway.

9.5 Multifunctionality and Allocation

Multifunctionality refers to the characteristics of systems, such as technologies/processes, to provide more than one function. Examples include a power plant, which can provide electricity, but can also provide heat (multi-output); the refining of crude oil that can provide 3 functions/products, such as naphtha, kerosene, and heavy fuel oil (multi-output) or a process that treats two different waste streams (multi-input). A graphical representation of multi-output and multi-input processes is provided in Figure 3.

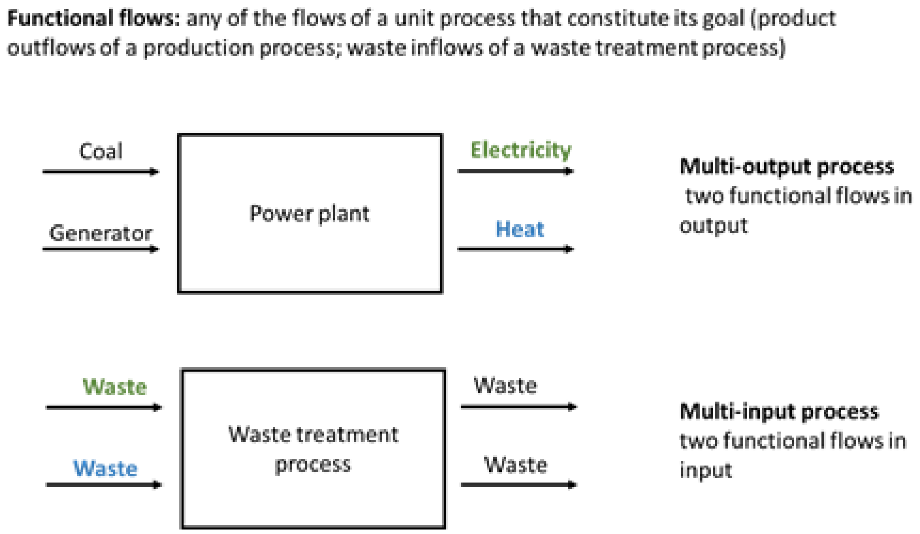
Functional flows: any of the flows of a unit process that constitute its goal (product outflows of a production process; waste inflows of a waste treatment process)

Figure 3: Multi-output and multi-input process (Figure adapted from lifecycleinitiative.org [2])

In the multi-output process, for example, different products can be produced in the process. Such products differ from waste and emissions for their characteristics:

1. Products include the main output of the process that drive production, as well as by-products that have a positive value and therefore cannot be considered as waste. For example, the waste heat produced in a power plant can be considered a by-product that, given its value, has a function in the system.
2. Waste can be defined, in simple terms, as a by-product (i.e. material or substance) that has no market value and no use after the completion of a process and can therefore be discarded (potentially at a cost). For example, the fly ash resulting from the flue gas treatment in power plants can be considered waste and disposal.
3. Emissions are substances, and often pollutants, discharged from the process to the environment (air, water, soil). Examples include emissions at the stack in power plants.

In case of multifunctional processes, such as multi-output, challenges arise on how the environmental and economic impacts of the system should be allocated to the different products (or inputs in case of multi-input systems). For example, if our FU is the production of 1 MJ of electricity, but the system delivers both electricity and heat, how much of the impacts of the power production system (the power plant and related processes) can be allocated to the production of only electricity? Which processes belong to the system under study and to the product?

Several solutions are proposed in literature to address these challenges. However, there is not one correct way that applies to all multifunctionality problems. According to the ISO 14040/14044 guidelines, solutions should be considered in a hierarchical order to minimize related uncertainties. In these guidelines we propose to either use ‘system expansion’, allocation based ‘substitution’, and allocation based on ‘partitioning’.

System expansion means that you include the extra functions in your FU. In the case of a power plant this can for example be that the FU is defined as 1 MJ of electricity and x MJ of heat produced. As shown in the figure, the co-production is also considered in the alternative/benchmark system, where two production processes are included to address the production of both products A and B. Therefore, it is important that this expansion is also done for the benchmark process.

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[2] https://www.lifecycleinitiative.org/wp-content/uploads/2013/06/Module-g-Multifunctionality-allocation-system-boundaries.pdf

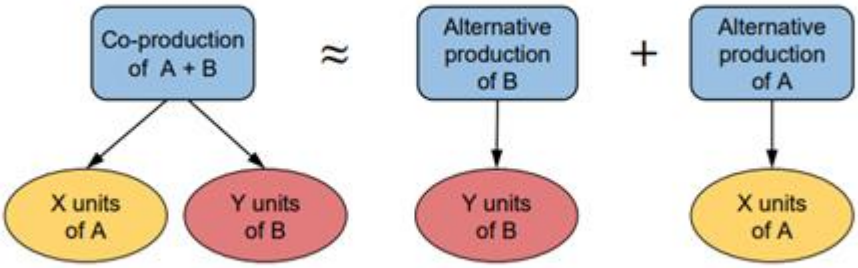

Figure 4: System expansion[3]

Allocation based on substitution means that, while the functional unit stays the same, an extra process is included in the system leading to a change in system boundaries. The added process represents the alternative production process that would otherwise be required to produce the by-product (or co-product). It is therefore included as negative process (-) and results in credits for the system (see Figure 5), meaning that the system is credited (environmental benefits/revenues) because it allows avoiding the production of that product from other sources, reducing the impacts. The reference scenario in this case (right of the figure) would only include the alternative production of the main product – in our example electricity (see figure below).

More practically, substitution is carried out by subtracting the impacts associated to the alternative production of the co-product to the impacts of the system. In the case of the power plant, the heat production as co-product allows to avoid the production of the same amount of heat from other sources/production process (such as heat production from coal), leading to savings/benefits. The overall impact for the production of electricity, would therefore be the impact/cost associated to the power plant for the production of 1 MJ electricity and x MJ heat minus the impacts/costs associated to the alternative production of x MJ of heat from coal/other sources (the source depends on location, time, etc.). For example, if we estimate the impact of the system as 20 and the impact of alternative heat production from coal as 5, then the overall impact of electricity production alone would be 20-5 =15 units (examples are simplified and numbers fictitious).

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[3] https://eplca.jrc.ec.europa.eu/uploads/ILCD-Handbook-General-guide-for-LCA-DETAILED-GUIDANCE-12March2010-ISBN-fin-v1.0-EN.pdf

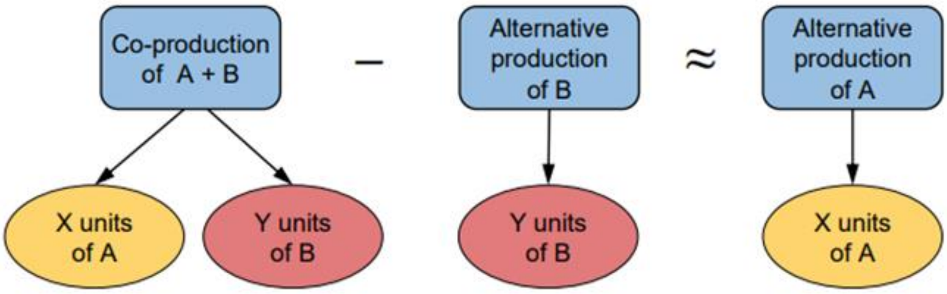

Figure 5: Allocation based on substitution[3]

Allocation based on partitioning means that part of the burden of the system will be allocated to the defined reference flow. According to the LCA ISO standards, this allocation should be as much as possible avoided. This allocation approach should be as much as possible be avoided as it relies on a choice of the practitioner, leading to uncertainties. It is therefore advised to first use system expansion or allocation based on substitution. In case allocation based on partitioning cannot be avoided, it should be done based on a physical or economic relationship. The choice for allocation needs to be clearly described. Allocation based on partitioning can be compared to a weighting approach. We assign a weight to every product based on a physical characteristic, such as mass, volume, or energy content, and the impacts/costs are allocated based on it. For example, if different beverage cans are transported together and we want to assess the impacts and costs of transporting only the coke cans, then we can divide the total impacts and costs of the transport system by the relative volume of the coke cans. Using allocation based on volume is here consistent, as the impacts of the transportation are related to the weight of the cargo. On the other hand, the choice of partitioning/weighting factor is key and should be conducted with care. For example, in case the co-products have a high volume/mass but a very low value, it would be inconsistent and unfair to allocate impacts and costs based on these physical characteristics. If we consider the mining of gold, where gold is mined as small percentage of the total amount of lower-value materials recovered, allocating based on mass would underestimate the impacts and costs associated to gold mining. In this case, allocation based on the economic value would be a preferred option.

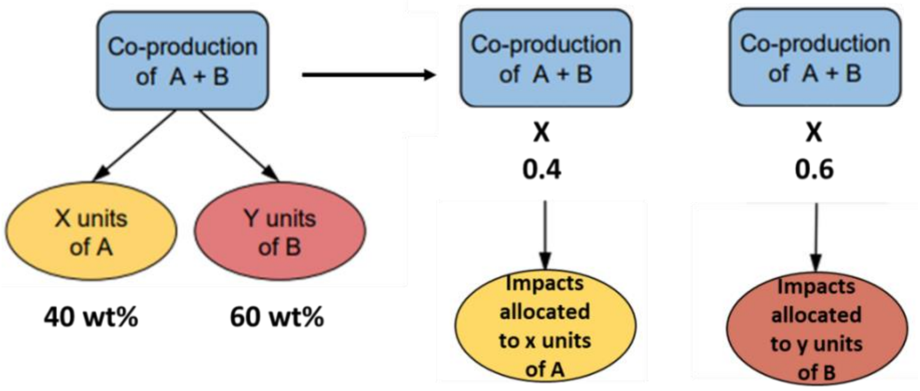

Figure 6: Allocation based on partitioning[3]

Projects evaluated for the MOONSHOT program should define the methodology that is used for the multifunctionality in case of multi-input/output systems. If possible, researchers should use system expansion. If that is not possible, researchers can use allocation based on substitution. If this is also not possible, allocation based on partitioning can be used, clearly indicating the basis for allocation.

In case of multiple output or input systems, the methodology selected for multifunctionality needs to be indicated in the worksheet ‘Technology’ under the title ‘Multifunctionality – methodological choice’ in the Excel template.

9.6 Background and Foreground system

As indicated in the previous section, in principle the system under study covers the whole lifecycle from cradle-to-cradle. However, this does not mean that each step of the system is included with all its process-specific details. Therefore, the system is divided in the foreground and background system. The foreground system covers the core process itself, where most information is known and the data with the highest quality will be available. For the foreground system, the process specific technical, economic and environmental data is included. The background system covers the remainder of the system. For this system no process-specific details are included, however, the economic and environmental data is replaced by generic or average data (see section 9.9 for more information on data types). Referring to Figure 2 above, the foreground system could be the gate-to-gate system, while the background system could be the cradle-to-gate and gate-to-cradle system. Some examples of foreground and background system can be found in the Table below.

Table 7: Examples foreground and background system

Example	Foreground system	Background system
Chemical recycling plant for plastic packaging	Chemical recycling plant with detailed description of mass and energy use.	The energy production process, e.g. wind turbines, to produce the energy used in the chemical recycling plant. The environmental impact for electricity production using a wind turbine can be retrieved from a database.
CO_2 conversion process to produce methanol	CO_2 conversion process with detailed description of mass and energy use	CO_2 capture plant. An average price for CO_2 can be

		considered that represents the upstream steps.

Based on the TRL of the new process, the background and foreground system can differ. For example, at a low TRL, the foreground system can be limited to the processing itself, while at a higher TRL, pre-processing and post-processing will also be part of the foreground system. The choice of what to include as foreground and background system depends on the goal of the study as well as on how strong the contribution of a process is to the sustainability impact and uncertainty. The difference between the background and foreground system is important for the required data quality, which will be discussed in more detail in Section 9.9.

Projects evaluated for the MOONSHOT program should divide the system within the defined system boundaries into a background and foreground system. The foreground system should be visualized in the PFD.

The foreground system needs to be visualized in the process flow diagram (PFD) that is included in the Excel template in the calculation worksheet '1. Pathway'. It should also be clear in the process description provided on the worksheet 'Technology' what the foreground system entails. In case multiple pathways are defined, a calculation sheet needs to be provided for each.

9.7 Temporal and geographical scope

The definition of the temporal and geographical scope are key concepts for consistent assessments, as the location and time when the technology will be implemented can influence the inventory and consequently the impacts. The environmental and economic performance of a product system/technology could differ significantly if implemented in different locations or in different years. For example, if electricity is produced in Norway or Poland, the resulting environmental impacts for the production of 1 MJ (FU) will be substantially different due to the energy mix adopted in the two countries (Norway uses a very renewable energy mix, while Poland still relies more on coal). Similarly, if we consider the production of 1 MJ of electricity in Poland today, it will potentially not have the same impact in 20 years. Policies and technological development would ideally lead to a higher renewable share in the energy mix.

It is important to make sure that the temporal (year) and geographical (location) scope of the data used to represent both background and foreground processes is harmonized, to avoid mismatches and inconsistent results. The harmonization should also be conducted with the benchmark system for comparison.

Projects evaluated for the MOONSHOT program should specify the location and time of implementation of the system under study. Based on these specifications, relevant data can be collected from databases/literature. In the framework of the MOONSHOT innovation program, the standard location is Flanders, and the timeframe is the current year (i.e., assume that you would implement your innovation now. In case the location or timeframe is different, this should be clearly indicated.

The temporal and geographical scope needs to be indicated in the Excel template in the worksheet 'Technology' under the titles 'Geographical scope' and 'Temporal scope'. The default values are the current year and Flanders for respectively the temporal and geographical scope. An explanation needs to be added in case these standard values are not used.

9.8 Benchmark systems

To be able to conclude if a process is desired from a sustainability point of view, it needs to be compared with a benchmark. This benchmark is either the conventional, best-in class technology that is currently in place and that could be replaced by the new process or is an emerging technology with the same aim.

To enable comparison, it is key that the benchmark system is defined with the same system boundaries and functional unit as the system of the new process or product. In case of a pure comparative assessment, the system boundaries for the assessment can be limited to the processes which vary between the benchmark and new process system. For example, a new production process for methanol is assessed. The produced methanol will have the exact same downstream processes, use phase and end-of-life phase as methanol produced in the conventional way. In this case, the benchmark system of the assessment will be the conventional production process of methanol. The downstream process, use phase, and end-of-life phase can be left outside the system boundaries. One needs to take in mind that such a comparative assessment only allows to compare the specific process and cannot be used to make any claims on the sustainability of methanol itself as part of its lifecycle is disregarded.

The benchmark technology should be selected in such a way, that it provides the most likely alternative for the new product or process. The developments within the MOONSHOT Program are still at low TRL and therefore the market introduction is only expected by 2040. Comparison with emerging technologies is as a consequence key. Comparison with conventional processes under the current conditions, is not relevant as we expect that these conditions will change in the future. This means that if the new product or process is modelled as it would be produced in the future, this should also be done for the benchmark technology. For the future, the background system might change and this needs to be accounted for. For example, if the future electricity mix is assumed to be completely renewable, this should be assumed for both the new process system and the benchmark system. If the time horizon defined in the goal is in the future, improvements need to be included for all systems. The exact impact of these changes on the conventional system might be difficult to estimate. In that case it needs to at least be described in a qualitative way and the results need to be interpreted with the potential changes in mind.

Projects evaluated for the MOONSHOT program should define the benchmark technology or system with the same system boundaries and functional unit. Potential future developments and changes in the benchmark system, needs to be included in the assessment.

In the Excel template the benchmark systems should be described on the worksheet ‘Technology’ under the title ‘Benchmark technologies’. In column B, the name of the benchmark process should be provided. Column C gives an indication of the TRL of the benchmark system. A description of the system is provided in columns D-F. Finally, columns G-J contain the positioning of the new technology under study compared to the defined benchmark process. Note that multiple benchmark processes can be added.

9.9 Data Availability and Quality

9.9.1 Data Availability

To calculate the required indicators, the necessary data must first be collected. The necessary data consists of both technical, economic and environmental data. With technical data, we mean all sorts of data related to the physical properties of the process (e.g. input mass), process characteristics (e.g. yield). In conclusion, it comprises all data required to make a mass and energy balance. Economic data relates to the prices of inputs, price indices or scale exponents. Environmental effect data specifies the effect of specific emissions and resources on specific environmental impact categories, for example the greenhouse gas effect of 1 kg methane, expressed in kg $CO_{2\text{-equivalents}}$. The data collection of the foreground system represents a substantial part of the work required to assess technologies and will be discussed in detail for the different TRLs.

The TRL of a technology gives an indication of which data can be collected directly (i.e. primary data) and which need to be completed by secondary data (i.e., non process specific data). The higher the TRL of a technology, the more data can be collected directly. The different types of data are explained below.

9.9.1.1 Primary Data

Primary data are process-specific and obtained from the known process or directly from partners within the supply chain. Examples are measured input flows or energy efficiencies, laboratory process data, product prices from suppliers, technology patent data of the respective process, etc.

9.9.1.2 Secondary Data

Average data is data reflecting industry averages that is available in sources like databases and published literature. The average data must be representative for the datapoint in the project. Average data is generally used for background processes. Examples are average product or equipment prices from databases, average flue gas content of a CO_2 source, etc.

Estimated data is calculated based on primary and average data. It has not been measured from existing processes but is calculated to reflect a typical scenario. Primary and average data are used under specific assumptions to estimate unknown process parameters. This type of data is especially important when a project at early TRL is simulated at commercial scale. Examples are simulated process data based on similar processes, calculating energy demand based on reaction enthalpies, scaling a process, capital cost estimations, data from process engineering models etc.

9.9.2 Data Quality

To assess data quality, Weidema and Wesnæs (1996) proposed a matrix, called Pedigree matrix, based on five indicators. The matrix uses a score from 1 to 5 for each indicator. The lower the score, the higher the quality. The main indicators used are:

1) Reliability of the data: is the data verified by measurements or based on assumptions or (non)-qualified (expert) estimates?
2) Completeness of the data: does the data come from a representative sample of data points or does it cover one point estimate (f.e. conversion yield of one experiment versus the average conversion yield over a large range of experiments)?
3) Temporal correlation of the data: does the age of the data corresponds with the time horizon of the project (f.e. water price 2000 vs water price 2030)?
4) Geographic correlation of the data: is the data representative for the region of the project (f.e. characterization factor for the Chinese electricity mix vs the Belgian electricity mix)?
5) Technological correlation: how close does the data cover the exact process (average global recyclability rate of a metal compared to a products-specific metal recyclability rate)

The indicators and scores for each are provided in the matrix in Annex B – Pedigree Matrix. The matrix can be used to have an overall idea of the quality of the data used and where improvements might be required. It is important to be transparent in the quality of the data used. For those parameters that have a high impact on the sustainability results, it is important to collect high-quality data. For parameters that have less impact on the sustainability results, time and costs to collect more reliable data might be saved. Identifying the most important parameters is explained in Chapter 12, and can only be done after the first iteration of the assessment.

For the MOONSHOT innovation program, the researchers need to indicate for each parameter the data source and type. Note that the number of the data type indicates where the data is coming from as a general category.

1. Primary data from experiments
2. Secondary data from literature or simulations for similar technology, time and region
3. Secondary data from literature or simulations for different technology, time or region
4. Expert estimate received for project
5. Own assumption
6. Default value from template

A sensitivity analysis (see Chapter 12) should be performed to evaluate the influence of each input parameter on the output indicators. It is important to assess and improve the data quality as much as possible for parameters with high uncertainty and sensitivity.

The data source needs to be included for each parameter in column F under ‘indicative value’ of the worksheets ‘Data – technical’, ‘Data – economic’ and ‘Data – environmental’ in the Excel template. The sources need to be included in the notes and mentioned between square brackets. It is advised that the value found in the different sources is mentioned in the notes to keep track of the data found and to define the value ranges in column G. In column H of the same worksheet the data type needs to be indicated under ‘Data type’. The dropdown list should be used.

10 FOREGROUND INVENTORY ANALYSIS

10.1 Process Flow Diagram

To define the different processes within the system boundaries, a process flow diagram (PFD) can be drafted. The PFD illustrates all the unit processes and their inputs and outputs within the defined system boundaries. As the whole system includes an enormous amount of unit processes, the PFD usually only covers the foreground system. The main inputs that are identified on the PFD are feedstock (e.g., biomass, fossil fuel, …), chemicals (e.g., solvents, catalysts, …), utilities (e.g., electricity, water, …) and other materials (e.g., packaging, …). Inputs required for, for example maintenance and transport, can also be included. Equipment is usually not identified on the PFD. The main outputs identified on the PFD are products, emissions and waste. Non-physical inputs, such as human labor or investments, are not included in the PFD. Figure 7 provides a simplified version of a PFD with only one unit process.

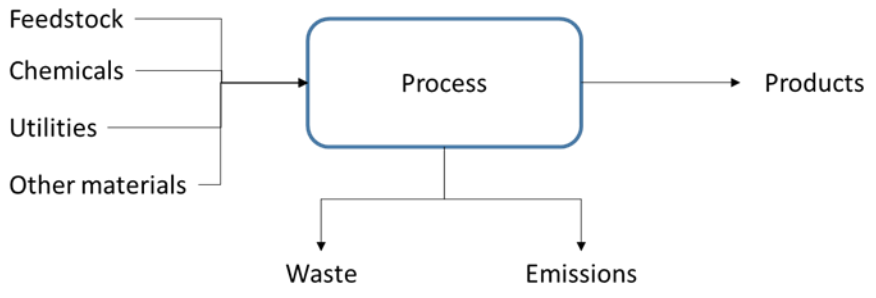

Figure 7: Simplified PFD

The PFD should include as much information as is available to identify the individual inputs and outputs and these need to be specific per unit process. For example, it is preferred to add the names of individual chemicals on a PFD instead of one input arrow stating 'chemicals'. However, this level of detail can vary with the TRL. The PFD can include quantitative numbers on the input and output flows based on the mass and energy balance calculations (see section 10.2), but can also be purely qualitative. Figure 8 provides an example of a more extended PFD, including the main results of the mass and energy balance calculations, for an algae biorefinery plant.

To be able to assess the economic and environmental impact of a new process and product, and to be able to compare it with a conventional benchmark, the technology should be assessed as if it were already mature. This means that the results of the assessment should state the impact of the technology at TRL 9. As all MOONSHOT innovations are still on a lower TRL, scaling up is key. For the PFD, this means that for each of the unit processes, the question needs to be asked 'how will this process be performed in an industrial setting, being at TRL 9'. For example, a process can still be a batch process in a laboratory environment at TRL 3-4, but can be assumed to be a continuous process in an industrial environment on TRL 9. To scale-up the laboratory unit processes to mature unit processes on TRL 9, Table 8 can be used.

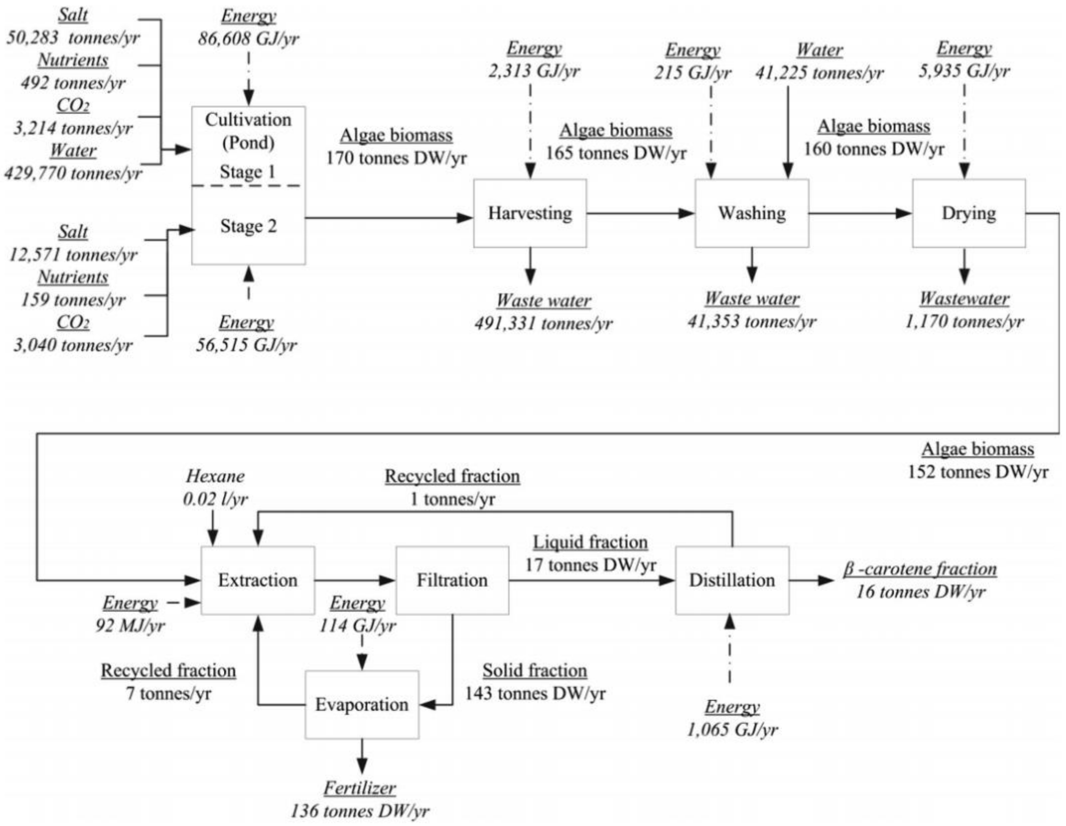

Figure 8: Example of a PFD with mass and energy balance (Thomassen, Egiguren Vila et al. 2016)

Table 8: Scale-up unit processes from TRL 3-4 to TRL 9 (Piccinno, Hischier et al. 2016)

TRL 3-4 unit process	TRL 9 unit process
Reaction under heating	Heated liquid batch reaction on an insulated batch reactor with an in-tank stirrer
Mixing (magnetic stirrer), Dispersing	In-tank stirring
Blending, mixing (viscous solution), homogenizing (all types), dispersing	Rotor-stator type homogenizer
Pestling in mortar, Grinding/milling, other particle size reduction	Grinding
Filtration (e.g., membrane, reverse osmosis, dialysis), sieving, centrifugation/cyclonic separation, other solid-liquid separation	Filtration/centrifugation
Distillation (rotary evaporation)	Evaporation
Vacuum drying, drying, rotary evaporation	(Oven) drying/vaporization
(Manual) transferring of liquids	Pumping

Waste disposal	Pre-treatment (case specific), solvent recycling (distillation or filtration), byproduct isolation
Normally not included in laboratory process	Heat recovery through heat exchangers

Projects evaluated for the MOONSHOT program should include a qualitative PFD with the main unit processes, inputs and outputs included in the foreground system. Below the requirements per TRL are provided.

The PFD should be included in the Excel template on the calculation worksheet ‘1. Pathway’ for the first pathway. In case multiple pathways are defined, a calculation worksheet needs to be included for each.

10.1.1 TRL 1-2

At low TRL, the foreground system can be limited to one core unit process. Other important pre-processing or post-processing processes can be added as a black-box. While it is important to identify the inputs and outputs as specific as possible, at low TRL, this might not always be feasible. In this case, a general term such as ‘catalyst’, ‘energy’, ‘chemical’ can be used. Moreover, simplifications are allowed by, for example, considering main inputs and outputs and neglecting minor flows. This should be done with the help of experts, and the implications of such choices should be considered and discussed.

Projects evaluated for the MOONSHOT program situated on TRL 1-2 should include a qualitative PFD with the main unit processes, inputs and outputs, but general terms are allowed.

10.1.2 TRL 3-4

At TRL 3-4, the technology has been tested in a laboratory environment. Therefore, the PFD of the process itself should contain the specific inputs and outputs instead of the general terms used at TRL 1-2. For the pre-processing and post-processing processes, these general terms are still allowed.

Projects evaluated for the MOONSHOT program situated on TRL 3-4 should include a qualitative PFD with specified inputs and outputs for the main unit processes. General terms are allowed for the pre-processing and post-processing steps.

10.1.3 TRL 5-6

In TRL 5-6, the technology has been validated or demonstrated in a relevant environment. More specific information on the foreground process is therefore available. Besides information on the unit process, inputs and output flows of the main process, also specific information needs to be gathered for the inputs and outputs of the pre-processing and post-processing processes. Each of these unit processes, input and output flows, should be identified as was it at TRL 9. If the included processes are still lab-scale processes, Table 8 can still be used.

Projects evaluated for the MOONSHOT program situated on TRL 5-6 should include a PFD with specified inputs and outputs for all main unit processes, including the pre- and post-processing steps.

10.2 Mass and Energy Balance

The mass and energy balance is the base for almost all quantitative sustainability indicators. This mass and energy balance gives an overview of all inputs and outputs required for the product or process, within the defined foreground system boundaries[4]. Collecting the data for the mass and energy balance is a time-intensive job as the quality of the data needs to be safeguarded. More information on data availability and quality can be found in section 9.9.

As a part of the foreground inventory analysis, the mass and energy balance will include all physical inputs and outputs for the foreground system. It is important that the mass of the input flows equals the mass of the output flows in the mass balance. The mass and energy balance needs to be calculated for each unit process as well as for the whole process system to allow for proper comparison. This also allows to identify how each unit process will contribute to the sustainability impact. Data on the background system, i.e., data on for example the production process to produce a raw material or the electricity that enters the system under study, does not need to be part of this mass and energy balance, and will be added in the Impact assessment directly as costs, revenues or environmental impacts. This will be discussed in detail in Chapter 4.

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[4] If the mass and energy balance covers the entire life cycle, including both foreground and background processes, it is also called the life cycle inventory (LCI). In the LCI, a full overview of all primary resources and emissions required for the specific product or function is provided.

The mass and energy balance needs to be calculated as if the processes are at TRL 9. The level of detail of the mass and energy balance calculations, depends on the TRL and the data availability. At low TRL, one will have to use proxies and theoretical relationships as data from e.g. experiments is still limited. To scale-up the process, in general two main strategies can be followed. First, if the process resembles a process which is already at a commercial scale, being TRL 9, this mature process can be used as a proxy. Second, if no proxy process is available, the process could be scaled to a mature scale following certain relationships as described below. Both scale-up procedures should always be done with assistance from technical experts and scale-up assumptions (for example, linear extrapolation of energy consumption) should always be stated. Also, the Product Environmental Footprint (PEF) category rules[5] can provide a source of information if general data is missing. The PEF category rules provide specific guidelines for a certain product or sector on what assumptions could be made to obtain the mass and energy balance, as required to calculate their environmental impact. It also contains default data on for example transport scenarios or end-of-life scenarios.

To increase the transparency and allow for sensitivity and uncertainty analysis, it is important that all assumptions are clearly indicated in the template and that there is a dynamic link with all further calculations. In the template separate worksheets are foreseen for the input data and the calculations.

Projects evaluated for the MOONSHOT program should include a mass and energy balance, including a quantitative overview of all physical inputs, outputs and equipment capacities within the foreground system boundaries. References to how the data was upscaled to TRL 9, need to be provided. Specific guidelines per TRL are provided below.

The mass and energy balance should be calculated in the Excel template on the calculation worksheet ‘1. Pathway’ for the first pathway. The mass and energy balance calculation is done based on the input data from the worksheet ‘Data – technical’ and the parameters defined on the worksheet ‘Pathway definition and results’. The calculation worksheet needs to be copied for each pathway if multiple pathways are defined. For each unit process, the mass and energy that enters and results should be calculated.

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[5] https://ec.europa.eu/environment/eussd/smgp/PEFCR_OEFSR_en.htm

10.2.1 TRL 1-2

At TRL 1-2, no experimental data is available yet and data is therefore based on literature, expert input or assumptions.

To calculate the mass balance, stoichiometry can be used. The feedstock and reactants of each process can then be scaled-up linearly to TRL 9. In general, the mass flows are underestimated when the stoichiometric relationship is used as no excess of reactants, nor side reactions are assumed. This can therefore be seen as the most optimal case.

To obtain the product quantity, the process yield is important. This can differ over different TRLs. If a proxy technology is available, the yield of this proxy technology can be used. If no proxy technology is available, the yield should be discussed with technical experts. Often a reaction conversion of 100% is assumed at TRL 1-2.

The solvent and catalyst quantity should be discussed with experts. For solvents, the relative amount used is usually higher in a laboratory environment, unless an exact concentration is required.

For energy demand, thermodynamic simulations can be done based on generic input data or literature values. The minimum energy demand for the reaction can be calculated based on the change in the enthalpy at standard conditions for thermochemical conversions. For electrochemical and biological conversions, the change in Gibbs free energy can be used (Langhorst, McCord et al. 2022). In case of exothermic reactions, the excess heat is waste heat, unless specified otherwise.

For separation, one can assume that perfect separation will take place. In addition, one can assume that recycling is possible, however, this needs to be discussed with technical experts. At TRL 1-2 the energy use for separation can be excluded.

10.2.2 TRL 3-4

From TRL 3 on, the first data from lab experiments is available and should be used. Following the guidelines below, these can be further upscaled to TRL 9.

The feedstock and reactants of each process can be scaled-up linearly from TRL 3-4 to TRL 9, because these are used in stoichiometric quantities in a laboratory environment. For processes where one reactant was used in excess, also linear scale-up should be applied if this excess is required to ensure the conversion takes fully place (Piccinno, Hischier et al. 2016).

To obtain the product quantity, the process yield is important. This can differ over different TRLs. If a proxy technology is available, the yield of this proxy technology can be used. If no proxy technology is available, the yield of the laboratory process can be used, however, this should be discussed with technical experts. From the laboratory experiments also information on temperature, pressure, selectivity, productivity, residence time, pH, voltage, current density and faradaic efficiency are available.

For solvents, the relative amount used is usually higher in a laboratory environment. These should therefore be scaled up using a 20% reduction (solvent use TRL 9= 20% solvent use TRL 3-4) (Picinno et al., 2016). However, when an exact concentration is required, the solvent use at TRL 9 should be equal to the solvent use at TRL 3-4. This should be discussed with experts. Solvent recycling can be included in TRL 9 and also the energy consumption for solvent recycling should be included in that case.

The catalysts are often used in small amounts, but should be included in the mass balance, with a linear scale-up. Recycling, including its energy use, can be included based on expert opinion if this is feasible on TRL 9.

For electrochemical conversions, the energy demand for the reaction can now be calculated based on the applied voltage and current density. The energy demand for the reactor can in other cases be calculated using the heat capacity of the reaction medium, the temperature difference and the enthalpy of the reaction (i.e. considering the reaction conditions). For the calculation of heating energy, stirring energy, homogenizing energy, grinding energy, filtration and centrifugation energy, distillation energy, drying energy, pumping energy, the recommendations from Picinno et al. (2016) can be consulted. An overview of the guidelines provided in the paper is included in Annex A – Upscaling. Energy demand for cooling is still ignored. In case of excess heat this is either waste heat or is included in the FU. Energy integration across the different unit processes should not yet be included. Considering that this energy integration might be an important aspect, one can make estimations about this based on expert input.

For separation, one can include the first estimates of the mass and energy flows if available. However, the results for separation at laboratory scale are often not representative for a large scale and therefore need to be used with caution. In a sensitivity analyses one can still look at the scenario with perfect separation and recycling as the most optimal case. In case the composition of the flow and their properties are known, an estimate of the energy requirement and separation efficiency can be made using a software package like Aspen or ChemCAD. Otherwise, the change in enthalpy can be used as a proxy for the minimum energy demand. At these TRL, also recycling can be considered if a reasonable purge ratio is included. Roh, Bardow et al. (2020) suggest estimating the energy demand based on the energy needed for pressurizing vapor feed streams.

10.2.3 TRL 5-6

At TRL 5-6, the technology has been validated or demonstrated in a relevant environment. Compared to TRL 1-4, more specific information will be available to update the previous calculations. At this TRL, also cooling should be included as well as estimations on energy integration. Here software packages like Aspen or ChemCAD can be used. To scale-up, the same framework as for lower TRLs can be used. For data that is still missing, mainly related to long-term effects, sensitivity analysis should still be performed to identify the potential impact.

10.3 Equipment inventory and other inputs

The equipment inventory will provide an overview of the required unit processes for the foreground system, for example pumps, reactors, or centrifuges. For each unit, the required capacity for the process will be calculated based on the scale of the process as selected in the goal and scope definition step. If available, the minimum and maximum possible capacities should be considered.

Besides the equipment, also data on the area of land use, transport requirements (e.g., indicate where the inputs are sourced from) and required personnel for the process needs to be added.

Projects evaluated for the MOONSHOT program should include an equipment inventory of all unit processes and the required capacity within the foreground system boundaries. In addition, from TRL 3 on, the amount of land use (m²), transport requirements (ton*km) and required personnel (full time equivalents (FTE)) needs to be estimated, while this is optional at TRL 1-2.

The equipment inventory needs to be included in the Excel template in the Pathway worksheets. On the worksheet ‘Data - technical’, the input data to calculate the land use, transport requirements and personnel needs should be added.

An indication of the minimum and maximum size of individual equipment is also included in the worksheet ‘Data - technical’. Using this information and the indicated scale on the ‘Pathway definition and results’ worksheet, allows to calculate the required number of equipments for each step of the value chain.

11 IMPACT ASSESSMENT

11.1 General

Different performance indicators can be calculated to compare emerging technologies. Within Chapter 4 it is explained which performance indicators should be used. However, it is important to be aware that calculating these performance indicators is data intensive and the quality of the results depends on the quality of the input data (“trash in gives trash out”). Furthermore, additional uncertainty is introduced due to the additional calculations. For example, greenhouse gas (GHG) avoidance cost is a comprehensive and widely used indicator, but also one of the most data-intensive measures as it needs both GHG reduction and economic indicators, leading to high uncertainties (Roh, Bardow et al. 2020). The complexity level of the indicators can vary widely.

To increase the transparency and allow for sensitivity and uncertainty analysis, it is important that all assumptions are clearly indicated in the template and that there is a dynamic link with all further calculations. In the template a separate worksheet is foreseen for the input data and the calculations.

An overview of performance indicators that are required for the MOONSHOT innovation program is provided in Table 9. The indicators are structured based on four categories: (1) technical, (2) economic, (3) environmental, and (4) combined. The next sections describe how each of these performance indicators can be calculated.

The input data needs to be included in the Excel template on the different data worksheet.

Table 9: Performance indicators for MOONSHOT

Category	Indicator
Technical	Recycled content
	Renewable content
	Reuse rate
	Recycling rate
	Recycling output rate
	Share of renewable energy
Economic	Total manufacturing cost
	Levelized cost of product
	Net present value

	(Discounted) Payback Period
	Internal rate of return
Environmental	Climate change
Combined	GHG avoidance cost

11.2 Technical Indicators

The technical indicators relate to the mass and energy balance and can be linked to circularity topics. For the MOONSHOT program, the following indicators are relevant: recycled content, renewable content, reuse rate, recycling rate, recycling output rate and the share of renewable energy.

11.2.1 Recycled content

The recycled content provides the ratio of recycled materials (secondary materials) in the total material input flow of the foreground system.

$$Recycled\ content = \frac{Mass_{secundary\ input}\ [kg]}{Mass_{total\ input}[kg]} \qquad [1]$$

11.2.2 Renewable content

The renewable content provides the ratio of renewable materials (non-fossil materials) in the total input flow of the foreground system. Note that energy is excluded from this indicator.

$$Renewable\ content = \frac{Mass_{renewable\ input}\ [kg]}{Mass_{total\ input}[kg]}$$

[2]

11.2.3 Reuse rate

The reuse rate provides the ratio of materials that can be reused compared to the total output flow of materials without further processing (except for basic cleaning). The reuse rate is often expressed for a specific product, such as plastic packaging.

$$Reuse\ rate = \frac{Mass_{reusable\ materials}\ [kg]}{Mass_{total\ output}[kg]}$$

[3]

11.2.4 Recycling rate

The recycling rate provides the ratio of materials that can be recycled compared to the total output flow of materials. The recycling rate is often expressed for a specific product, such as plastic packaging.

$$Recycling\ rate = \frac{Mass_{materials\ going\ to\ recycling}\ [kg]}{Mass_{total\ output}[kg]} \qquad [4]$$

11.2.5 Recycling output rate

The recycling output rate provides the ratio of secondary materials after the recycling process compared to the total output flow of materials. The difference between the recycling rate and the recycling output rate is that the losses in material in the recycling process itself are taken into account in the recycling output rate, but not in the recycling rate. The recycling output rate is often expressed for a specific product, such as plastic packaging.

$$Recycling\ output\ rate = \frac{Mass_{materials\ after\ recycling}\ [kg]}{Mass_{total\ output}[kg]}$$

[5]

11.2.6 Share of renewable energy

The share of renewable energy provides the ratio of renewable energy compared to the total energy input. The following energy sources are considered to be renewable: solar, wind, geothermal, hydro, tidal and biomass. If renewable energy is included and additional energy storage is required (for example, through power-to-gas), this should also be included in the system boundaries. Furthermore, renewable energy availability needs to be discussed in the frame of the temporal and geographical context defined for the study.

$$Share\ of\ renewable\ energy = \frac{Energy\ input_{renewable}\ [MJ]}{Energy\ input_{total}\ [MJ]} \qquad [6]$$

Projects evaluated for the MOONSHOT program MOT 1 bio-based chemistry should calculate at least the renewable content. Projects evaluated for the MOONSHOT program MOT 2 Circularity of Carbon in Materials should calculate at least the recycling rate, the recycling output rate and the recycled content. If not equal to zero, it is recommended to also provide the reuse rate. Projects evaluated for the MOONSHOT program MOT 3 electrification & radical process transformation and MOT 4 energy innovation should calculate at least the share of renewable energy.

11.3 Economic Indicators

Economic indicators are used to gain insight in the cost structure and/or economic feasibility of a technology. Depending on the goal of the study, one can focus on the costs only or also include the benefits and calculate profitability indicators. In the next sections it is first described how the intermediate indicators capital expenditures, operational expenditures and revenues can be estimated. Next the cost of goods manufactured, levelized cost of product, minimum selling price and the different profitability indicators are explained. The economic indicators need to be calculated for the system under study and not for the identified benchmark system(s). For the benchmark system, market prices or information from literature or databases can be used as will be explained in Chapter 12.

11.3.1 Capital Expenditures (CAPEX)

The total capital investment is the total amount of money needed for the plant and manufacturing facilities (i.e. fixed capital investment) plus the amount of money required as working capital needed to operate the facilities (Peters, Timmerhaus et al. 1968). The fixed capital investment is further subdivided in the direct costs known as manufacturing fixed-capital investment and the indirect cost known as nonmanufacturing fixed-capital investment. For the definitions, we follow Peters, Timmerhaus et al. (1968).

The direct cost includes the money needed for the installed process equipment as well as the components needed to have it in operation such as site preparation, piping, instruments, insulation, foundations, and auxiliary facilities. The purchased equipment needs to be estimated and the other costs are often calculated using ratios based on the purchased equipment cost.

The indirect costs are for example construction overhead, administrative and other offices, supervision expenses, engineering expenses, contractors' fees, miscellaneous construction costs, and contingencies. These costs can be estimated as a ratio of the direct costs.

The working capital consists of money invested in raw materials and supplies or (semi)finished products in stock, accounts receivable, cash kept on hand, accounts and taxes payable. The ratio of working capital depends on the company, but most companies use 10 to 20% of the total capital investment. In case the products produced are dependent on the season, this can be 50% (Peters, Timmerhaus et al. 1968).

Several methodologies are available in literature to estimate Capital Expenditures. Below the ones that can be used for the MOONSHOT program are described.

Preferably, a specific quote from a supplier is used. However, at low TRL insufficient information on the process is available to receive this quote.

In case a similar process is available for which the cost is known, an order-of-magnitude estimation can be done using the six-tenth rule. This is especially interesting to use at TRL1-2. The uncertainty range using this methodology is around 30-50% (Towler and Sinnott 2021). The six-tenth rule uses a cost exponent to scale the cost of a process up or down compared to the reference process. On average this cost exponent is 0.6, however, for some processes or unit operations, specific cost exponents are available that should be used. The formula that can be used to apply the six-tenth rule is provided in equation [7] below.

$$Capital\ cost\ new\ plant = \\ Capital\ cost\ previously\ constructed\ plant\ (\frac{Capacity\ new\ plant}{Capacity\ previously\ constructed\ plant})^{0.6}$$

[7]

Most of the costs that are available from previously constructed plants are from a different year and, therefore, need to be corrected using a cost index such as the Chemical Engineering Plant Cost Index (CEPCI). The CEPCI is used to adjust process plant construction costs from one period to another. For the order-of-magnitude estimate, the capital cost calculated for the new plant using the six-tenth rule, needs to be corrected using the CEPCI. The CEPCI should not be used for prices that are older than 10 years. Even for prices older than 5 years it is not recommended to use the CEPCI. An overview of the CEPCI value since 2013 is provided in the table below. The formula to use is provided in equation [8].

At TRL 3-4 when the major equipment needs are known, the Lang factor method can be used to estimate the CAPEX. The Lang factors are based on the general type of the plant, i.e. solid processing plant, solid-fluid processing plant or fluid processing plant. The accuracy of this method is between -20% and +40% (Peters, Timmerhaus et al. 2003). The delivered-equipment cost needs to be multiplied by the lang factor to get the fixed-capital investment cost. The lang factors are respectively 4, 4.3 and 5 for the solid, solid-fluid and fluid processing plant (Peters, Timmerhaus et al. 2003).

Table 10: CEPCI values

Year	Value
2014	576.1
2015	556.8
2016	541.7
2017	567.5
2018	603.1
2019	607.5
2020	596.2
2021	708
2022	816

$$Present\ cost = original\ cost\ \left(\frac{CEPCI\ present\ year}{CEPCI\ year\ original\ cost}\right) \quad [8]$$

An alternative for the Lang factors is the use of ratio factors. This method estimates the fixed-capital investment and total capital investment by adding the elements of the capital investment as a ratio of the delivered-equipment cost. The accuracy is estimated between ±20 and 30% (Peters, Timmerhaus et al. 1968). This approach is preferred over the use of the Lang factors as one can also leave out elements that are not necessary. For example, in case yard improvements are not required. In case the price for purchase equipment does not include delivery, Peters, Timmerhaus et al. (1968) advise to add a cost of 10% of the purchased equipment cost. Working capital is estimated as 15% of the total capital investment to determine the ratios. An overview of the ratio factors per plant type is provided in Table 11. An example of the use of these ratio factors would be the cost of a batch reactor for chemical synthesis without installation cost. To add installation cost, this reactor cost can be multiplied with a factor 147%

Table 11: Ratio factors for estimating capital investment items based on delivered-equipment cost (Peters, Timmerhaus et al. 2003)

Plant type	Solid	Solid-Fluid	Fluid
Fixed capital Investment			
Direct costs			
Purchased equipment delivered	100	100	100
Purchased equipment installation	45	39	47
Instrumentation and controls	18	26	36
Piping	16	31	68
Electrical systems	10	10	11
Buildings	25	29	18
Yard improvements	15	12	10
Service facilities	40	55	70
Indirect costs			
Engineering and supervision	33	32	33
Construction expenses	39	34	41
Legal expenses	4	4	4
Contractor's fee	17	19	22
Contingency	35	37	44
Working capital			
Working capital	70	75	89

From TRL 5 on the unit cost estimate approach is advised for the main equipment. The purchased equipment cost is based on quotations from suppliers and other costs are estimated based on unit cost (e.g., employee hours, material amounts required, etc.). Missing data can be estimated based on the previously described approaches.

For the MOONSHOT innovation program, the capital investments need to be estimated. In case quotes from suppliers are available, this is preferred. Otherwise, an order-of-magnitude estimate can be made at TRL 1-2. For TRL 3-4 an estimate using the ratio factors is preferred over the Lang factors. For TRL 5 and higher, quotations from companies should be available for at least part of the equipment.

The CEPCI can be used to adjust historical process plant construction costs to the most recent period for which the CEPCI is available.

In the Excel template the CAPEX for the first pathway needs to be calculated on the calculation worksheet ‘1. Pathway’ in the table related to the economic calculations. The first part of the table is reserved for the investments. The calculation of the CAPEX should be done for each unit process and should consider the required capacity that is calculated in the technical part. To calculate the CAPEX, input data from either the worksheet ‘Data – economic’ or ‘Data – general’ can be used. On the worksheet ‘Data – economic’ the lang factors and ratio factors are provided under ‘general capital cost’. The CEPCI values are provided in the Excel template on the worksheet ‘Data – general’. In case multiple pathways are defined, the calculation worksheets need to be provided for each.

11.3.2 Operational Expenditures (OPEX)

OPEX refers to the recurring costs that necessarily emerge from the maintenance and operation of a process. These costs are calculated on a yearly basis. The OPEX can be broken down into a couple of cost elements such as labor, operations, maintenance, insurance, tax, energy and material flows. The OPEX can be divided into fixed and variable costs. Fixed costs are independent of the amount of product produced. Examples are insurance, property taxes, and labor. Variable costs are directly related to the amount of produced product. Examples of variable costs are raw materials, energy, and utilities. Below for each it is described how these can be included in the assessment.

11.3.2.1 Labor

To calculate the labor costs, one should have an idea about the amount of labor needed, the type of labor needed (e.g., plant managers, lab managers, lab technician, clerks and secretaries, etc.), and the costs of these different labor types. As a general rule of thumb, Peters, Timmerhaus et al. (2003) indicate that for chemical processes operating labor amounts to 10% to 20% of the total product cost. The authors also published a table in which typical operating labor requirements are mentioned for different types of equipment (see Table 12). The values in this table can be used as a proxy to estimate the labor requirements. Labor costs will highly depend on location. For Belgium the average hourly labor cost was 41.6 in 2021[6]. The latter value will also be used as default value in the Excel template.

Table 12: Estimation of labor requirement per process equipment type (Peters, Timmerhaus et al. 2003)

Equipment type	Workers/unit/shift
Blowers and compressors	0.1-0.2
Centrifugal separator	0.25-0.5
Crystallizer, mechanical	0.16
Dryer: rotary and tray	0.5
Dryer: spray	1

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[6] https://ec.europa.eu/eurostat/web/labour-market/labour-costs/database

Evaporator	0.25
Filter: vacuum	0.125-0.25
Filter: plate and frame	1
Filter: rotary and belt	0.1
Heat exchangers	0.1
Process vessels, towers (incl. auxiliary pumps and exchangers)	0.2-0.5
Reactor: batch	1
Reactor: continuous	0.5

In addition to the labor requirements for operating, also labor requirements for laboratory tests are necessary. These are estimated as 10% to 20% of the operating labor cost. Labor costs for supervision and clerical assistance are estimated as 15% of the cost for operating labor and are independent of the actual operation.

In case the labor requirement from another plant is taken as a reference, one needs to take into account that labor often does not scale linearly with production capacity. Peters, Timmerhaus et al. (2003) indicate that a power of the capacity ratio of 0.2 can be used to estimate the relationship between labor requirement and production rate.

11.3.2.2 Maintenance and Repair

Costs for maintenance and repair are often calculated as a ratio of the fixed capital investment costs. A range of 2% to 10% is reported, however, is highly dependent on the type of installation. Researchers should consider using a higher ratio for the maintenance and repair factor in case the system is more complicated or working outside normal operating conditions. In the Excel template a default value of 5% is included, however, this can be increased to 10% if required.

11.3.2.3 Insurance

A default value of 1% of the fixed-capital investment per year is included in the Excel template.

11.3.2.4 Taxes

In Belgium the corporate tax rate amounts to 25%[7] and is included as a default value in the Excel template.

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[7] https://tradingeconomics.com/country-list/corporate-tax-rate?continent=europe

11.3.2.5 Overhead costs

The plant overhead costs are costs required for the routine plant services that are not directly related to the production. For chemical plants these costs can be estimated as a percentage between 50 and 70 of the total expenses for operating labor, supervision and maintenance (Peters, Timmerhaus et al. 2003).

11.3.2.6 Energy and material flows

In general, it is important to consider a cost or revenue for each flow that enters or leaves the system. Free flows in general do not exist as there will almost always be a cost linked to the flow that needs to be included in the assessment. For example, an upstream production cost, a downstream treatment cost, a transportation cost, a handling cost on site or an opportunity cost. The flows are calculated in the mass and energy balance as explained in section 10.2.

Prices for raw materials (feedstock, catalyst, solvents, etc.) can be obtained via primary suppliers, or via secondary sources such as databases or literature. Information from primary suppliers is always preferred. An overview of databases is provided in Table 13. Peters, Timmerhaus et al. (2003) indicate that the raw material costs for chemical plants is in general 10% to 60% of the total product cost.

Energy prices depend on multiple factors such as the location of production (e.g., on-site or from the grid), the energy source (e.g., renewable or non-renewable) and the operation of the system (e.g. flexible production). Information on prices can be found in publicly available databases such as Eurostat (Energy database) for both natural gas and electricity, for different periods in time. A default value for electricity and natural gas is provided in the Excel template. Note that this is an average, annual price. In case of flexible systems, the volatile electricity price should be included in the model.

It is important to consider price fluctuations. These are highly dependent on the specific market conditions and need to be clearly described. Also, future availability of the sources might be a risk and needs to be considered in the assessment. In general, one needs to make sure that the assumed prices are in line with the temporal and geographical defined scope. To evaluate for the impact of changing prices, we refer to Chapter 12.

11.3.2.7 Others

In addition to the operational costs mentioned above, also costs for operational supplies, patents and royalties and rent can be included. Also, general expenses for administrative costs, distribution and marketing costs and research and development costs can be included in the analysis. However, these are all excluded in the Excel template for the MOONSHOT Program.

11.3.3 Revenues

Both the sales price and market volumes are important to understand the economic feasibility of a certain process.

At low TRL, the sales price can be estimated based on the price of a benchmark product if it has the same application and performance or on the production costs (including both CAPEX and OPEX) and addition of a profit margin. In the Excel template a standard profit margin of 5% is included. In case the benchmark products do not have the same application or performance, the potential selling price should include a correction for the performance. Market volumes can be based on the market volumes of benchmark products. In case location and targeted application highly impacts the price and market growth rates, this should be considered. Prices can be obtained from databases such as listed in Table 13.

Table 13: Databases 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
CatCost	Cost estimation tool for pre-commercial catalysts	Open access

In the template developed for the MOONSHOT program, default values are included for most of the operational costs. These default values should be used. In case these are not relevant for the specific process under study, an explanation needs to be added and the default value can be replaced in the template.

For the costs related to the inputs such as feedstock, solvents and catalysts, a list is provided for the most common types, however, missing data needs to be completed based on primary input from suppliers or secondary sources such as literature or databases.

In the Excel template, the default values for the general operational costs are included on the worksheet ‘Data – economic’. On the same worksheet, the default value for the profit margin can be found under ‘Revenues’.

11.3.4 Cost Indicators

11.3.4.1 Total Manufacturing Cost

The total manufacturing cost is the sum of the total OPEX for one year. This means the sum of the direct costs related to e.g., raw materials and energy as well as indirect costs related to e.g. maintenance and labour as well as overhead costs. For the MOONSHOT program we will assume that there are no raw materials in stock at the end of the year.

11.3.4.2 Levelized Cost Of Product

The levelized cost of product is calculated by dividing the sum of all the costs over the lifetime by the sum of the product produced over the lifetime. Since the innovations that are developed within the MOONSHOT Program are still at low TRL, the operational costs, as well as the product amounts that is produced, is assumed to be constant over the lifetime. Therefore, the levelized cost of product can be calculated by dividing the sum of the annualized CAPEX and total OPEX by the amount of the targeted product that is produced in one year.

The annualized CAPEX can be calculated via equation [9]. with i the discount rate for which the weighted average cost of capital (WACC) is used and n the lifetime of the installation. For the MOONSHOT Program, the default value for the WACC is set to 8%.

$$Annualized\ CAPEX\ installation = \frac{CAPEX\ installation}{\frac{1-(1+i)^{-n}}{i}} \quad [9]$$

11.3.5 Profit Indicators

Profit indicators are most often used by companies to make investment decisions. These indicators show if and how much money can be earned based on the investment. However, at low TRL these are not the most important indicators. Due to uncertainty in the input data, at low TRL the question is not so much what the exact economic feasibility is, but to identify the parameters that influence the economic feasibility most. Therefore, the interpretation of the profit indicators can best be done via an uncertainty and sensitivity analysis as explained in Chapter 12.

11.3.5.1 Net Present Value (NPV)

The net present value (NPV) is an investment criterion indicating the profitability of a project using Eq. [10], where T is the life span of the investment, CF_n the difference between revenues and costs in year n, I_0 the initial investment in year 0, and i the discount rate (Van Dael, Kuppens et al. 2015). The NPV compares the amount of money invested in a project today to the present value of the future cash receipts from the investment. The NPV needs to be positive for a project to be considered as interesting from an economic point of view.

$$NPV = \sum_{n=1}^{T} \frac{CF_n}{(1+i)^n} - I_0 \qquad [10]$$

For the discount rate, often the weighted average cost of capital (WACC) is used. The WACC is the average after-tax cost of capital including both own equity and debt. A default value of 8% is included in the template. For the life span of the investment a default value of 15 years is included. In case the lifetime of certain equipment is shorter, a reinvestment should be included in the calculations.

11.3.5.2 (Discounted) Payback period (D)PBP

The payback period is defined as the point in time when the initial investment is paid back by the net incoming cash flows. The simple payback time that does not include the time value of money, is calculated by dividing the CAPEX by the yearly cash flow (note that the cash flow needs to be positive). The discounted payback period is similar, however, considers the time value of money.

The shorter the (D)PBP the more attractive the investment is. It needs to be shorter than the expected plant lifetime.

11.3.5.3 Internal Rate of Return (IRR)

The IRR is the discount rate at which the NPV is zero. For an IRR to be attractive for an investor it must be higher than the return rate that can be generated in lower risk markets or investments than the project. For innovative processes such as envisioned for the MOONSHOT program, an IRR above 25% is recommended as target. As the IRR does not give any insights in the absolute profit, it is recommended to use the IRR combined with the NPV. In general, the NPV is preferred to compare different alternatives.

In the template developed for the MOONSHOT program, the profit indicators are automatically calculated if CAPEX, OPEX and revenues (in case of profit indicators) are included. The default value for the WACC is set to 8% and the project lifetime to 15 years. Linear depreciation should be included for the tax calculations using the expected technical lifetime of the equipment or the project lifetime in case the technical lifetime is longer than the project lifetime. The calculations of the taxes themselves are automatically included in the Excel template.

The cost indicators need to be added based on the calculated mass and energy balance and costs.

The default values for the WACC and the project lifetime are added on the worksheet 'Data – economic' in the Excel template. The calculation of the cost indicators should be added in the table 'Results' under the economic calculation table on the calculation worksheet '1. Pathway'. In the same results table, the profit indicators will be calculated. These will be automatically calculated based on the included CAPEX, OPEX and revenues.

11.4 Environmental Indicators

Environmental indicators allow quantifying the exchanges between the system and the environment and translating them into environmental impacts. In a life cycle approach, environmental indicators can consider both emissions and credits to the environment, depending on the approach used to address multifunctionality (see section 2.5). Credits are related to avoided impacts due to the avoided production of energy and/or materials, or from carbon storage. The estimation of environmental credits is considered when using the allocation method based on substitution (section 2.5). Emissions are considered as positive contributions to the environmental impacts (as they increase the impact), while credits are accounted as negative contributions (negative value), as they are subtracted to the total impact. Environmental impacts are then estimated as net result.

Different environmental impacts can be estimated, including impacts to different environmental targets, such as air, water and soil. The choice of which impacts to address depends greatly on the goal of the study (see Chapter 9), as it defines what research question we need to answer and with which indicators. As stated in section 2.4, a cradle-to-cradle approach is assumed with some exemptions (section 9.4). This will determine which impacts need to be assessed.

In the following section(s), the estimation of selected environmental impacts is explained. For the MOONSHOT program the focus is now on climate change. An important aspect in the calculation is related to the availability of data and the use or not of an LCA software (such as Gabi, SimaPro, OpenLCA) and database by the practitioner. Regarding the data, in the lifecycle of the product we can differentiate between direct emissions, such as CO_2 emissions from a process under study, and indirect emissions, associated to the production of, for example, input flows (solvents, electricity) that are not directly analyzed. The former (direct emissions) are associated to the foreground system (see section 2.6). Indirect emissions are associated to the upstream and downstream processes included in the background system. To give an example, direct emissions are the scope 1 emissions as defined by the Greenhouse Gas Protocol. They include the emissions of combustion processes or chemical production that are under the control of the company – in this case that are under analysis in the project. Indirect emissions, instead are the scope 2 and scope 3 emissions, and therefore emissions associated to the production of energy (electricity, heat, fuels) and materials used in the processes under study.

If the practitioner does not have access to an LCA software and database:

- Impacts associated with the direct emissions from the foreground system, such as emissions from the process under study, can be estimated based on the mass balances and following the calculation steps described below.
- Impacts associated with indirect emissions from upstream and downstream processes, such as the production of input materials/energy flows, or the treatment of waste streams, can be estimated using background processes. Such processes can be found in databases (see Table 14 for examples). Based on these background processes, that provide a complete inventory of inputs and outputs, the impact of upstream and downstream processes can easily be estimated. In the Excel template we provide impact factors for the most common material and energy flows, such as solvents, electricity, etc. These impact factors provide the sum of all characterized emissions in the cradle-to-gate production of a respective input (solvent, electricity). The impact factors can be used directly in the estimation of impacts from the system under study by multiplying the amount of each flow (for example an amount of solvent needed in the process) with the corresponding impact factor (impact/unit of input). For a correct estimation of the impacts, it is key to make sure that units are aligned.

Below, a description of how to estimate climate change impacts considering both direct and indirect emissions is provided.

If the practitioner or the project consortium have access to an LCA software such as SimaPro or Gabi, these can be used to model the system and obtain impacts for both foreground and background processes. One can also make use of open-source software like OpenLCA and Activity browser. Note that the latter two are open source, but that the database might still require a license.

Table 14: Databases for environmental assessments

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, transport and disposal 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[8]
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[9]	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
ESU World Food	LCI database for food	Licence required
LC-Inventories.ch		Licence required

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[8] 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)

[9] 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

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

11.4.1 Climate change

The climate change impact category represents the potential impact of all greenhouse gas (GHG) emissions emitted during the entire lifecycle of the product or service (Finkbeiner, 2009). The Kyoto Protocol defines six greenhouse gases: CO_2, CH_4, N_2O, HFC, PFC and SF_6.

Direct emissions

Direct GHG emissions, emitted in the foreground system, should have been identified in the foreground inventory analysis and should be visible on the PFD. To quantify how much each of these emissions contribute to climate change, they need to be multiplied with a characterization factor (CF), also called the Global Warming Potential (GWP) in case of climate change impact. The GWP provides the potential impact of each greenhouse gas relative to the GWP of CO_2, which is used as reference. The potential climate change impact is therefore expressed in terms of kg CO_2-equivalent [kg CO_2 eq.]. The use of a common unit, CO_2-equivalents, allows making the effect of different GHGs on climate change comparable. To estimate their CO_2 equivalent potential, the actual mass of a gas, such as CH_4 or N_2O, is multiplied with the global warming potential (GWP) factor for that specific gas (Galli et al. 2012). The GWPs of the six GHG are summarized in Table 15.

A key point to consider in the estimation of the climate change impact of a system is the distinction between biogenic and non-biogenic/fossil carbon emissions. The difference is related to the distinction made by the IPCC (Intergovernmental Panel on Climate Change) between the slow carbon cycle (associated to fossil carbon) and the short carbon cycle (associated to bioenergy systems). In bioenergy systems, carbon is sequestered from the atmosphere during, for example biomass growth and released to the atmosphere at the end of life of the biomass (during incineration/degradation). As the cycle is short, the balance between carbon in the atmosphere and carbon in biomass is assumed to be maintained (storage of CO_2 emissions in biomass = -1 [kg CO2 eq.] as the biomass is taking it away from the atmosphere, CO_2 emissions from the degradation/combustion of the same biomass = +1 [kg $CO_{2\,eq}$.] because it is an input to the atmosphere) leading to a net of 0. Given this distinction, emissions associated to biogenic carbon are accounted as neutral with a GWP = 0 (see Table 13). On the other hand, CO_2 emissions from fossil carbon, such as CO_2 emissions from the combustion of coal/natural gas, have a characterization factor of 1 and therefore an impact on the atmosphere. Characterization factors for both biogenic and fossil carbon emissions are included in Table 13.

Table 15 can then be used to estimate the impact on climate change of the direct emissions in the foreground system.

Table 15: GWP for GHGs based on Kyoto Protocol[10,11] in kg CO_2 eq./kg substance

Substance	AR5 (2014)
CO_2 (fossil-origin)	1
CO_2 (biogenic)	0
CH_4 (fossil-origin)	28
CH_4 non-fossil origin	28
N_2O	265
HCFC-141b	782
HFC-134a	1300
HCFC-22	1760
HCFC-142b	1980
CFC-11	4660
CFC-12	10200
SF_6	23500

Overall, for direct emissions from foreground processes, such as emissions occurring during the processing of materials, combustion processes, etc., the impacts are calculated from the CFs listed in the table above. In particular, the impact is obtained by:

- Multiplying the total mass of each gas emitted (per functional unit) with the global warming potential (GWP] associated to that specific gas. Unit of resulting characterized emissions will be [kg CO_2 eq.];
- Summing all characterized emissions. These emissions can be either emissions (burdens) or credits (benefits).

Indirect emissions

To quantify the impact on climate change of indirect emissions associated, for example, to the production of the inputs (electricity, solvents), impact factors for the most common inputs are provided in the Excel template. These impact factors provide the sum of all emissions in the cradle-to-gate production of a respective input, such as electricity, multiplied with their corresponding GWPs (i.e., CFs), as provided in Table 15. Also, for waste

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[10] https://pre-sustainability.com/articles/updated-carbon-footprint-calculation-factors/

[11] https://www.ercevolution.energy/ipcc-sixth-assessment-report/

streams, impact factors are provided, covering the cumulative climate change impact of all emissions occurring during the waste management processes.

The impact associated to the amount of input required is therefore estimated by multiplying the amount of input with the impact factors associated to its production in the time and location considered. For example, if a process requires 1 MJ of electricity, this amount will be multiplied with the aggregated impact associated to the production process of electricity in Flanders in the year 2025. Such impact will be expressed as kg CO_2/kWh. When multiplying flow quantities and aggregated impacts, make sure that the units kWh * kgCO_2eq/kWh are consistent (and not kWh with MJ). Conversion errors can really change the results. Besides the common impact factors provided in the Excel template, also larger databases exist. If the project consortium has access to software such as SimaPro or Gabi, these can be used to obtain impact factors for the inputs and waste. In case software would be used, it is important to use the GWP for the greenhouse gases as indicated in Table 15.

The procedure to convert the mass and energy balance as shown in the PFD into their corresponding climate change impacts is provided in Figure 9 and further explained in the bullet points below. Also include the impacts for transport and equipment if available.

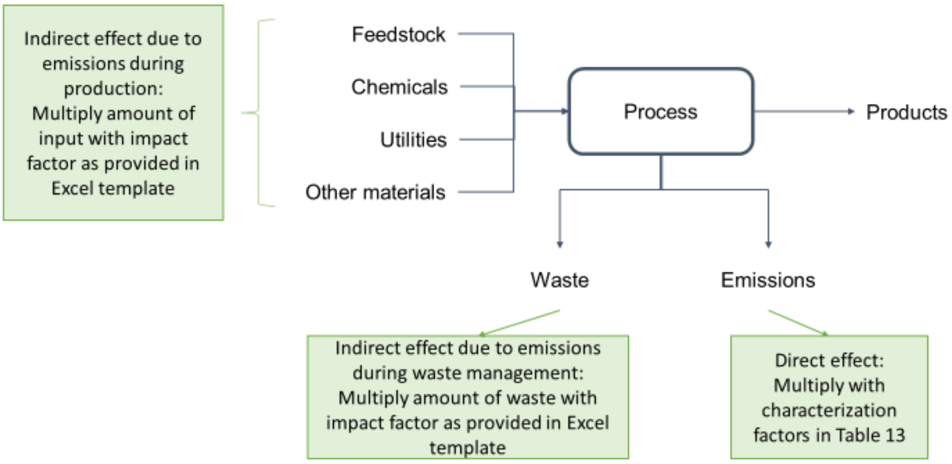


Figure 9: Procedure to convert mass and energy balance to the environmental impacts

As explained above, credits can also be estimated if the allocation approach based on substitution approach is used to take into account multifunctionality (see section 9.5). Credits are related to avoided impacts due to the avoided production of energy and/or materials, or from carbon storage. To estimate credits related to the avoided production of energy/materials, the same approach adopted for the impact estimation of inputs (based on background processes) is used. When considering the recovery of materials and energy, the credits associated to their avoided production can be estimated by multiplying the amount of input with the impact factors associated to its production in the time and location considered. Differently from the impacts, though, such value is given a negative sign and eventually subtracted from the total impact.

Following the distinction made above on fossil and biogenic carbon emissions, further considerations need to be made related to the carbon stored in products. If we assume that biogenic carbon emissions are neutral given their short cycle (storage = -1, emissions = +1, leading to a net of 0), the carbon stored in products made with renewable/bio-based materials and that is not emitted as biogenic CO_2 emissions, is accounted as credit (-1). Therefore, to estimate credits associated to carbon storage, instead, a negative value is given to the GWP for CO_2 emissions (GWP_{CO2} = -1). For fossil carbon stored in products, instead, a GWP = 0 is assumed, as fossil CO_2 emissions will have an impact once emitted.

As a last step, all impacts on climate change are summed up. As credits have a negative sign, their value is subtracted, giving the net climate change impact (impact + (-) credit, as the credit has a negative value). The total impact on climate change needs to be expressed per FU.

The procedure that is described above should preferably also be used to estimate the climate change impact of the defined benchmark system(s). For the systems to be comparable, the calculation approaches need to be considered for both background and foreground processes. If the calculation approaches and the underlying assumptions are not harmonized, this will influence the accuracy of the conclusions taken. At the same time, collecting the required information on the benchmark processes takes a lot of time and therefore the following guidelines are followed for the MOONSHOT program. At TRL 1-2 the climate change impact that is available in databases or in literature can be used to compare with. From TRL 3-4 on, the impact calculation needs to be harmonized if the practitioner or the project consortium have access to an LCA software, and the process is available in the databases. If software is not available, the climate change impact that is available in databases or in literature can be used. For TRL 5-6 the calculations always need to be harmonized.

Projects evaluated for the MOONSHOT program should include the estimation of the climate change impact for both the system under study and the defined benchmark processes. The calculation of the impact needs to be done in the Excel template for the system under study. For the benchmark system, information from literature or databases can be used. For a correct estimation of the impacts, it is key to make sure that units are aligned.

The input values are included in the Excel template on the worksheet ‘Data – environmental’. On this worksheet also default values for some characterization and impact factors are provided for some parameters. Using the input values, the environmental impact for the first pathway is calculated on the calculation worksheet ‘1. Pathway’ in the environmental table. For each defined pathway, a separate calculation worksheet needs to be foreseen.

11.4.2 GHG emission reduction potential

The GHG emission reduction potential refers to the difference in the net climate change impact between the system under study and the benchmark system (another technology or the same under different conditions). Such indicator allows to estimate the potential climate benefits associated to the adoption of the system compared to the benchmark for the fulfilment of the functional unit. The emission reduction potential can be estimated by subtracting the net (considering both impacts and credits, if applicable) climate change impact [kg CO_2 eq.] of the system under study to the climate change impact [kg CO_2 eq.] of the benchmark system. If the result is a positive value, it represents the CO_2 avoidance/emission reduction potential of the system (as the benchmark would have higher impacts).

11.4.3 Other environmental impacts

The current version of the methodological framework is limited to the quantification of climate change impact. This choice is based on the objectives of the MOONSHOT program focused on reducing carbon emissions and related climate change impact, as well as the higher complexity that would be introduced if other impacts would need to be estimated manually. Nevertheless, it is important to note that the consideration of climate change impacts only could lead to burden shifting. By only taking into account GHG emissions, the assessment does not take into account the environmental impacts that would occur due to other emissions, such as emissions to water, soil, etc. Such emissions and related impacts could occur, for example, in different processes along the life cycle of the system under study, highlighting other hotspots. By not addressing them, results are biased, to a certain extent, by such assessment choice made.

To address this limitation, the methodological framework will further be adapted based on the feedback from stakeholders. Moreover, in the Excel template, a color code from the Green metrics tool is included to give an indication on the hazardousness of the solvents. A color-code is included for the catalyst material used based on the critical raw materials list. More information on both aspects is included in Chapter 13. In the Excel template a section is foreseen where other environmental impacts can be discussed in a qualitative way. The idea is to give an indication of the potential implication to support technology development while keeping the quantitative assessment simple.

Projects evaluated for the MOONSHOT program can include a qualitative description of other expected environmental impacts that are not captured by the quantification of the climate change impact.

For the solvents a color code is provided in the Excel template based on the hazardousness of the solvent. The color code is based on the categories defined in the Green metrics toolkit.

For the (catalyst) materials that are used, a color code is provided in the Excel template based on the list of critical raw materials.

In the Excel template a qualitative description of other environmental impacts than climate change can be included on the worksheet ‘Pathway definition and results’ under the title ‘other environmental impacts than climate change’.

A color code is provided for the selected solvents on the worksheet ‘Data – environmental’ in column D. A green color indicates that the solvent is recommended, an orange color means that it might be problematic, and a red color indicates the solvent is hazardous. The solvents are selected using the dropdown list on the worksheet ‘Data – economic’ in column D.

For the (catalyst) material a color-code is added in the Excel template on the worksheet ‘Data – economic’ in column D where the (catalyst) material can be selected using a dropdown list. A red color indicates that the selected material is one of the critical raw materials on the list of the European Commission. A green color indicates that it is not on the list.

11.5 Combined Indicators

Combined indicators integrate the economic as well as the environmental indicator results.

11.5.1 GHG avoidance cost

The GHG avoidance cost or also referred to as the abatement cost, is calculated by dividing the NPV times -1 by the GHG emission reduction potential over the project lifetime. The GHG avoidance cost is expressed as €/ton CO_{2eq} avoided. This measure helps to identify the most cost-effective strategy to reduce GHG emissions.

11.5.2 Energy use per ton of GHG avoidance

The energy use of the innovation per ton of avoided CO2eq is calculated by dividing the total energy use of the system under study by the GHG emission reduction potential. This metric is calculated as energy is a scarce resource in Belgium.

12 INTERPRETATION

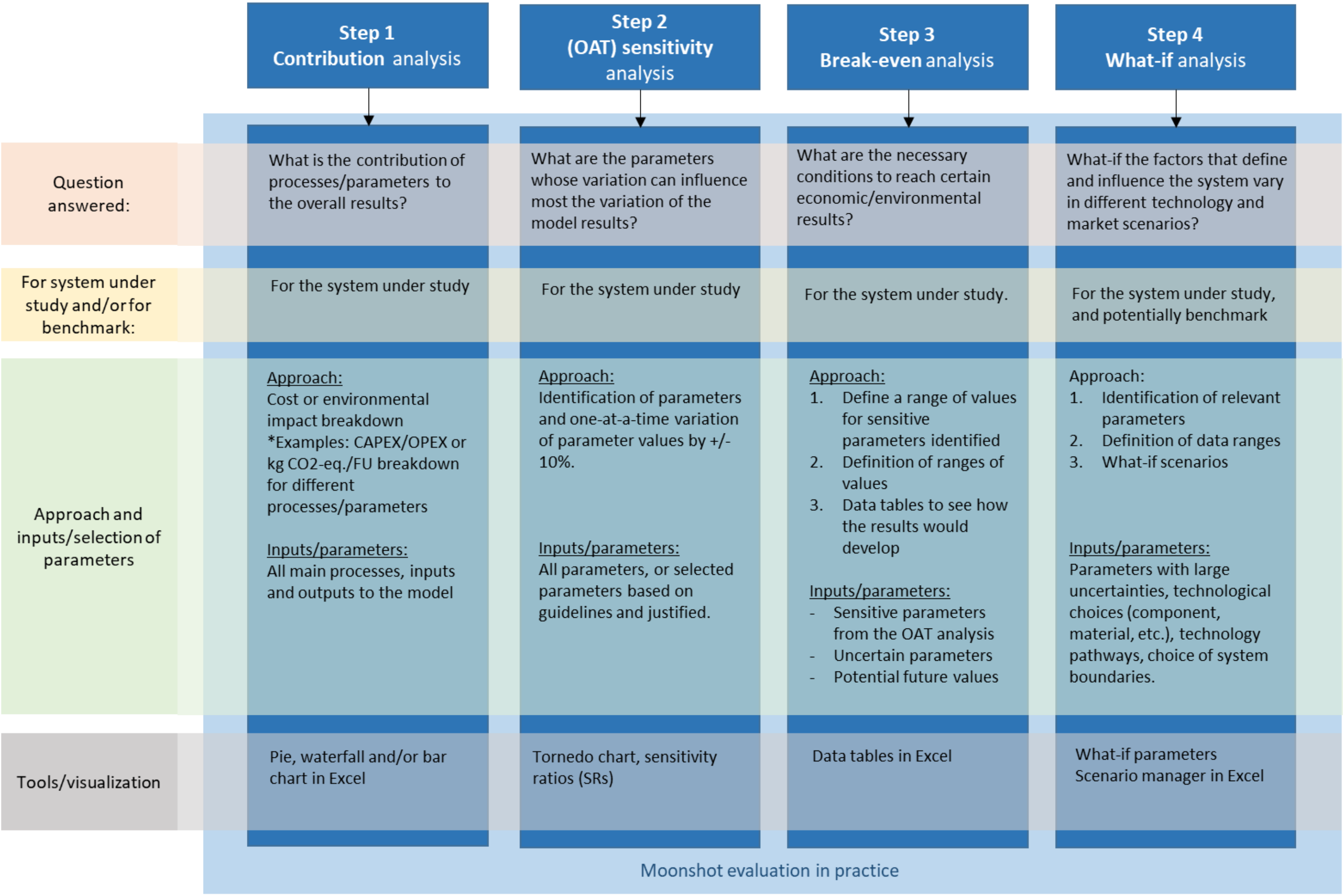
12.1 Introduction

The interpretation phase is the most important part of the sustainability assessment, and even more at low TRL. It helps to identify those parameters/processes that have the highest impact on the results, and to quantify the potential variability and uncertainty of the results. Based on these analyses, research and data quality targets can be set for those parameters that have more influence on the results, and further iterations of the assessment can be conducted to obtain more robust results. Moreover, in the interpretation phase, the information provided by the results is checked and evaluated to provide recommendations and conclusions.

Of specific concern in early-stage assessments are the different uncertainties that arise due to the limited knowledge and data on the technologies/processes and input parameters, modeling and design choices, as well as the potential variability of inputs due to, for example, the spatial and temporal context of implementation and assessment. Performing uncertainty and sensitivity analyses to address such uncertainties allows to make more reliable conclusions as the robustness of the results is identified. Moreover, it allows to better support technology development by providing more useful and valid results.

Typically, uncertainty and sensitivity analyses are performed to deal with the uncertainty surrounding the data and to identify the most influential parameters within the study. Although closely related, uncertainty and sensitivity analysis are two different disciplines. Uncertainty analysis assesses the uncertainty in model outputs that derives from uncertainty in inputs. When assessing emerging technologies in early development stages (i.e., at low TRL), uncertainties in input values and costs are often substantial. These uncertainties should be analyzed and reported to provide a robust understanding to decision-makers and reduce risks (Brun, Kühni et al. 2002). Sensitivity analysis assesses the effects of the variation of inputs, and therefore the importance of the inputs, on the total variation in analysis outcomes. In layman terms, uncertainty analysis covers the reliability of the input parameters and their impact on the results, while sensitivity covers the importance (i.e. contribution) of the input parameters for the results. Within the assessment's interpretation phase, priority should be given to the parameters that are characterized by high uncertainty and high sensitivity. For those parameters one needs to find high quality data. This effort to search for high quality data is less crucial for parameters that do not have a high impact on the sustainability results. We assume that the baseline assumptions are made with the best information available at that time. Comparing the results with other available sources is recommended to check the initial assumptions and get a good idea of how reliable these are.

Sensitivity analysis is here considered as a valuable step in the early-stage assessment of projects. In the following sections, different approaches for sensitivity analysis will be explained and guidelines on how to perform them are provided. Figure 10 provides a schematic overview. Each approach has a specific application and goal that will be highlighted. The sensitivity analysis should include a 'basic' uncertainty analysis where the researchers consider the most uncertain parameters within the sensitivity analysis. An extensive uncertainty analysis is not required in the framework of the MOONSHOT program. Moreover, given the goal of performing the sensitivity and uncertainty analysis, this is not required for the benchmark system. The values found or calculated for the benchmark system are used to define the research targets for the process under study as explained in the next sections.



	Step 1 **Contribution** analysis	**Step 2** **(OAT) sensitivity** analysis	**Step 3** **Break-even** analysis	**Step 4** **What-if** analysis
Question answered:	What is the contribution of processes/parameters to the overall results?	What are the parameters whose variation can influence most the variation of the model results?	What are the necessary conditions to reach certain economic/environmental results?	What-if the factors that define and influence the system vary in different technology and market scenarios?
For system under study and/or for benchmark:	For the system under study	For the system under study	For the system under study.	For the system under study, and potentially benchmark
Approach and inputs/selection of parameters	Approach: Cost or environmental impact breakdown *Examples: CAPEX/OPEX or kg CO2-eq./FU breakdown for different processes/parameters Inputs/parameters: All main processes, inputs and outputs to the model	Approach: Identification of parameters and one-at-a-time variation of parameter values by +/- 10%. Inputs/parameters: All parameters, or selected parameters based on guidelines and justified.	Approach: 1. Define a range of values for sensitive parameters identified 2. Definition of ranges of values 3. Data tables to see how the results would develop Inputs/parameters: - Sensitive parameters from the OAT analysis - Uncertain parameters - Potential future values	Approach: 1. Identification of relevant parameters 2. Definition of data ranges 3. What-if scenarios Inputs/parameters: Parameters with large uncertainties, technological choices (component, material, etc.), technology pathways, choice of system boundaries.
Tools/visualization	Pie, waterfall and/or bar chart in Excel	Tornedo chart, sensitivity ratios (SRs)	Data tables in Excel	What-if parameters Scenario manager in Excel

Figure 10. Overview of interpretation methodologies

12.2 Contribution analysis

The most basic form of a sensitivity analysis is called a contribution analysis. For projects at low TRL, it is useful to identify where the opportunities and bottlenecks within the product value chain are situated. A contribution analysis gives insights into the processes and activities in the value chain that have a major or minor contribution to the calculated indicators such as costs, emissions, etc. A contribution analysis shows the contribution of the different life cycle stages, processes or specific inputs/outputs to the different output indicators, e.g. the distribution of emissions between raw material, catalyst, and electricity needs, or the distribution of capital and operational costs to visualize the impact of the different cost components on the overall economic indicator. These contributions are often visualized by a pie, waterfall or bar chart, depicting the relative contributions of the processes to the indicators. An example of a pie and waterfall chart is provided in Figure 11 and Figure 12 respectively. Bar charts can be useful to compare the processes in the MOONSHOT project under different scenarios or pathways. An example of such a bar chart is provided in Figure 13.

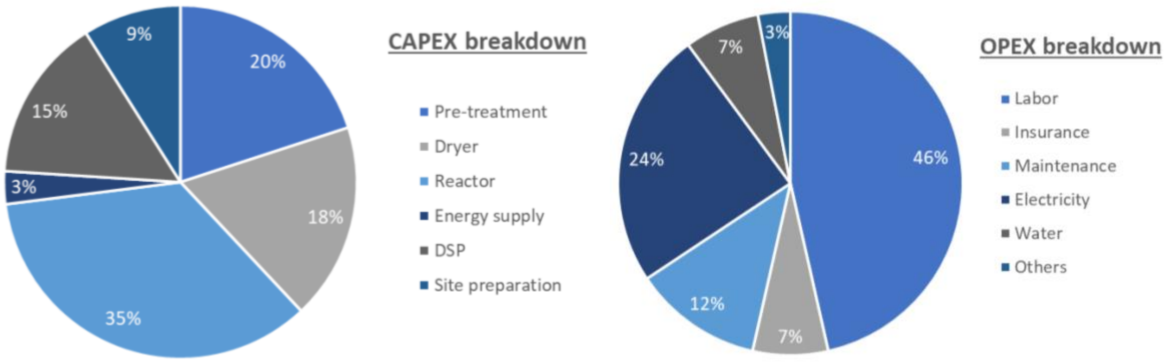


Figure 11. Example of a pie chart to visualize the cost breakdown

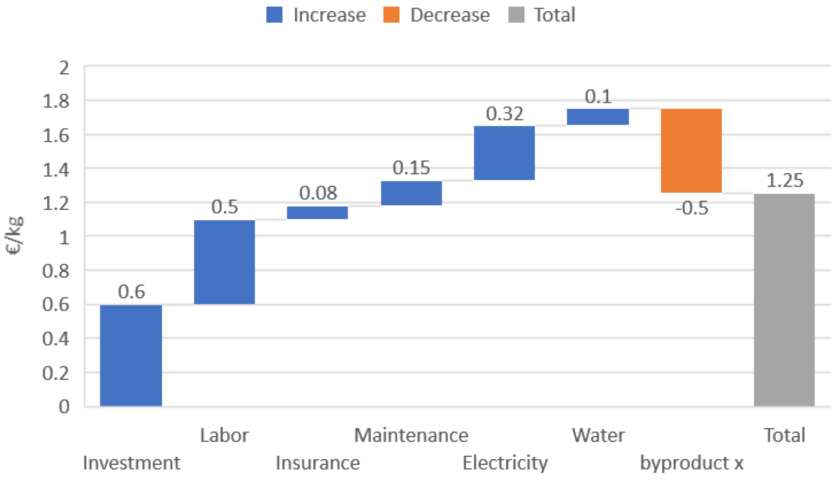


Figure 12. Example of a waterfall chart to visualize the levelized cost of product breakdown

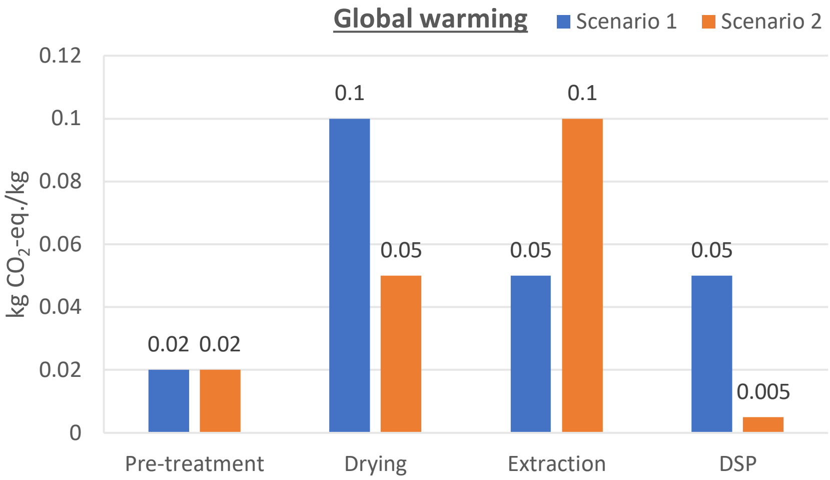


Figure 13. Example of a bar chart to visualize the environmental impact breakdown for scenario comparison

Projects evaluated for the MOONSHOT program should include a contribution analysis for both the economic and environmental impacts. This analysis should be visualized by a pie, waterfall or bar chart. The contribution analysis only needs to be made for the system under study and not for the benchmark processes.

In the Excel template, the contribution analysis should be included on the calculation worksheet ‘1. Pathway’ under the title ‘contribution analysis’ for the first pathway. For the other pathways, the same is valid, however, a new calculation worksheet needs to be included.

12.3 One-at-a-time (OAT) sensitivity analysis

The one-at-a-time (OAT) sensitivity analysis (SA), or perturbation analysis, aims at varying only one parameter at a time (as the name says) to identify the factors whose variation can influence most the variation of the model results, and to what extent. This is performed by changing the values of parameters of a small increment and decrement, usually +/- 10%. The OAT sensitivity analysis should be applied to all model parameters, to understand which factors have the higher influence on the model results. However, specific parameters can be selected if well justified. For example, if the value of a parameter was defined based on a set of assumptions, the analysis can be performed to see the potential influence of the assumptions on the model results. Other parameters that can be addressed are the ones with the highest contribution to the results. However, parameters with the highest contribution are not necessarily the most sensitive ones.

A OAT sensitivity analysis can be performed by creating a Tornado Chart using e.g. Oracle Crystal Ball. This is an example of a (licensed) spreadsheet-based software. The Tornado Chart tool shows how sensitive the output indicator is to each input parameter separately, as they change over their predefined ranges (see Figure 14). In the framework of the MOONSHOT Program, a range with +/- 10% of the base value can be used. The longer a bar, the more sensitive the parameter is to variations in the input parameter.

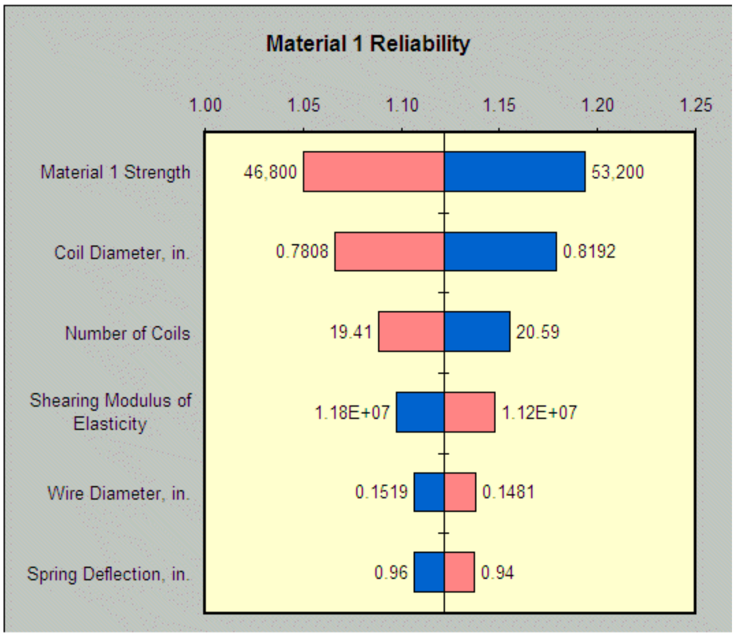


Figure 14. Example Tornado Chart from the software Oracle Crystal Ball.

If the software is not available, sensitivity ratios (SR) can be used to build a similar Tornado chart or to estimate (in %) how much the parameter (i.e. input) influences the results (i.e. output), and how much variation of the model result is expected for a certain variation of the parameter value. Sensitivity ratios are calculated using the formula indicated in equation [11]. A SR of 1 means that a 10% variation of the model results can be expected for a 10 % variation of the parameter value considered. The higher the SR, the more sensitive the output is to a change in the input parameter.

$$SR = \frac{\frac{\Delta result}{initial\ result}}{\frac{\Delta parameter}{initial\ parameter}} \qquad [11]$$

Projects evaluated for the MOONSHOT program should include a one-at-the-time sensitivity analysis. The choice of parameters to address should allow to test the effect of the variation of (at least) the parameters that are most uncertain or dependent on assumptions/simplifications. A +/- 10% variation of the parameter values should be considered. The calculations should always be done directly in the provided Excel template. The impact of changing an input parameter (of which the value is considered as uncertain) on the output indicator should be quantified either by a Tornado chart or sensitivity ratios (SRs).

In the Excel template the analysis needs to be included in the calculation worksheet '1. Pathway' under the title 'one-at-a-time sensitivity analysis' for the first pathway. The template uses separate input worksheet, i.e., data sheets, with all the parameters that need to be directly linked to the calculations on the calculation worksheet. A separate calculation worksheet needs to be foreseen for each defined pathway.

12.4 Scenario analysis

Scenario analysis is commonly used to address uncertainties and assess the influences of choices on the model results. Types of uncertainties include:

- Parameter uncertainties, related to the values associated to the parameters as a result of limited knowledge and upscaling efforts;
- Uncertainties related to choices made to define the technology: choices of components, materials, inputs, outputs, treatment processes, etc.;
- Uncertainties related to temporal and geographical scope, that can affect the background system (for example, the market prices, energy mix).

Among the scenario analysis approaches, the **break-even and what-if analyses** allow to address these uncertainties and/or choices, and to explore and analyse possible future developments of the technology. In both approaches, scenarios are developed to define the parameters to address and assess the influence on the model results.

In this framework, we aim to understand how the results – environmental and/or economic performance – would vary with the variation of:

- Parameter values, for paramaters that have a high sensitivity on the results (see OAT sensitivty) or that are highly uncertain (due to for example the lack of knowledge on the process, or the upscaling method applied), etc. In the break-even analysis it is identified how the results change when the parameter values change over a certain range.
- Technology choices: components, materials, types of technology used. How are the results influenced by e.g. including an alkaline or PEM electrolyser or if the catalyst material is changed. These are examples of a what-if analysis. Since the model is dynamic, one can also look at how these technology choices would impact the conclusions from the varying parameter values for which the break-even analysis is used.

- Choices of system boundaries (include or exclude a process, such as transport or a pre-treatment step). Note that the system boundaries should always be consistent between the system under study and the benchmark. If scenario analysis is used to address variations in system boundaries, it should be done for both systems.

The scenarios do not aim to predict the future, but to assess potential future alternatives of the system under study. The goal is, therefore, not to give an absolute result for the performance of the technology, but rather to provide a range of results depending on the scenarios addressed that can show, in a transparent way, influence of assumptions, choices, lack of data and potential technological developments.

To build scenarios, the following three main steps can be followed:

1. Identification of critical/relevant parameters. These are the parameters with significant influence on the results. The ones that depend on choices (selection of components, materials, etc.), uncertain/variable (for example in time) parameters, definition of system boundaries. The selection of the parameters should be done for both foreground and background systems.
    - For the foreground system, parameters to address can be identified based on:
        i. (preliminary) sensitivity analysis, identifying the most influencing parameters, e.g. OAT sensitivity analysis;
        ii. parameters for which there is a large uncertainty (technology choices – components, materials, unknown processes/parameters, parameters that could be subject to variation in time, etc.). Examples include the choice of inputs (material, catalyst, etc.), components, etc.;
        iii. expert opinion on how the technology could develop, what are potential technology choices/alternatives, design options, etc. (parameters that could be optimized with technology development, etc.).
    - For the background system, parameters to address can be identified based on:
        i. The external/exogenous parameters that are relevant for the system and that are, for example, expected to change in time or are highly uncertain. Common examples include the background energy system and market prices. In general the choice of the background parameters should be done with the help of stakeholders and should analyze potential political, economic, social, technological, environmental and legal parameters that could influence the technology.
        ii. Results of the contribution and sensitivity analyses. For example, if the energy consumption has a high contribution to the overall result and/or is a sensitive parameter, the background energy mix would be a parameter to address.
2. Definition of values for all parameters for the temporal scope selected and for an industrial scale. The values need to reflect how the parameter would look like, what potential alternatives could be used (technology choices, materials, etc.). And choices can also be based on MOT objectives.

2. It is often a challenge to identify the ranges of potential values for the selected input parameters at early TRL (Thomassen, Van Dael et al. 2019). Therefore, some rules of thumb have been introduced:
    - Data ranges that reflect the technology application in different conditions/scenarios, based on expert judgement
        - For the foreground system, data ranges can reflect alternative future conditions. For example, the efficiency of a process that can vary based on technology development and optimization between 0.25 and 0.35.
        - For background energy systems, data ranges could represent the context, such as different temporal conditions. For example, if the scenario analysis addresses the variation of the background electricity mix between 2025 and 2040, the values for the input parameters in the table for the What-If analysis would be retrieved from impact factors/prices associated to the background processes for the production of the two electricity mixes. If an LCA software is available, databases can be used to calculate the impact factors. In the Excel template, the impact factor for forecasted variations of the Belgian electricity mix has been included.
        - When not available, optimistic, realistic and pessimistic scenarios are defined based on the level of uncertainty. The approach of Brun, Kühni et al. (2002) makes a choice between three classes of relative uncertainty: “accurately known parameters (class 1: relative uncertainty 5 percent), moderately inaccurate known parameters (class 2: relative uncertainty 20 percent), and very poorly known parameters (class 3: relative uncertainty 50 percent)”. If an estimation of the uncertainty can be made based on this approach, it is recommended to use this. Otherwise a general variation of 10% can be used. The indicator calculations are repeated for the selected ‘what-if’ input parameters and new results for the output indicators will show the expected changes in environmental and economic sustainability impacts.
3. Building of scenarios as combination of the parameters and potential values/assumptions. A consistency check needs to be performed to verify the feasibilty of the scenarios.

In the next subsection the break-even and what-if analysis are respectively explained.

12.4.1 Break-even analysis

The break-even analysis aims at understanding what conditions, such as parameter values, need to be met to reach a certain environmental and/or economic performance. It is often used to understand how the results can develop when a range of values is considered. This type of analysis, referred to as break-even analysis in the work of Langhorst, McCord et al. (2022), is very useful if the goal is to set specific research targets. For example, identify the value at which an economic indicator such as the NPV becomes positive or that the levelized cost of product is below a certain value. This value can for example be the current market price of the targeted product or the current market price including a green premium if that seems acceptable. If the target is based on the climate change impact, the target can be set based on the climate change impact found or calculated for the benchmark system. In particular, the break-even analysis can be applied for parameters that have a high contribution to the economic and environmental impact, or a high sensitivity based on the OAT sensitivity analysis.

In Excel, Data Tables from the What-If analysis tool can be used for this purpose. Data Tables can be used to calculate an indicator by varying the value of the selected input parameter over a predefined range. Data Tables can vary the value of maximum two parameters at the same time and keep the assumptions for the other parameters the same. A more detailed description of how to use Data Tables in Excel can be found in Annex C – What-if analysis.

Projects evaluated for the MOONSHOT program should include a break-even analysis, using 'data tables' in Excel, for parameters that have a high contribution to the economic and environmental impact. The three steps mentioned above should be used to:

1. Identify relevant parameters. These can be based on the contribution and OAT sensitivity analyses, definition of parameters with large uncertainties, and expert opinions.
2. Define data ranges. At lower TRL (<5) when no data on minimum and maximum input values are available, the researcher can use the approach defined by Brun, Kühni et al. (2002) or a general variation of 10%. However, when moving to higher TRL (>5), data ranges (such as maximum and minimum input values) should be selected from in-house research, literature, companies, or experts.
3. Build scenarios using data tables in the Excel template.

Projects should also include an analysis to address the implementation of the technology in a future point in time (here defined as 2040). Examples of values to address include electricity mix and market prices.

The above-described Excel feature to perform a break-even analysis using Data tables is described in more detail in Annex C – What-if analysis.

In the Excel template the analysis needs to be included in the calculation worksheet '1. Pathway' under the title 'Scenario analysis' for pathway 1. The template uses separate input worksheet, i.e., data sheets. The data on these sheets need to be directly linked to the calculations on the calculation worksheet to make the model dynamic (i.e., when the input parameters change, also the output needs to dynamically change).

12.4.2 What-if analysis

What-if analysis is a specific scenario analysis approach that allows to analyze the potential outcome of changes on the model. What-if analysis can provide a clear picture of how an output might change as a result of varying one, or multiple parameters (van der Spek, Fout et al. 2020). Table 16 provides an example of the input and output of a What-if analysis.

3.

Table 16. "What if" analysis example

	Input parameter x		Output indicator y
What if …	x = value 1 (most optimistic)	Then …	y = value 3
	x = value 2 (most pessimistic)		y = value 4
	…		…

In this framework, what-if analysis builds on the results of the break-even analysis to assess:

- The influence of the variation of paramater values on the technology design. Some of the combinations addressed in the break-even analysis might not be technically feasible based on the current definition of the system. How does the system need to change (technology design, components, materials, etc.) if that value should be reached?
- Other potential technology choices: components, materials, etc,. The analysis of other technology choices could be driven by, for example, the lack of knowledge on the exact configurations, or the uncertainty on which kind of materials will be used.
- Choices of system boundaries (see above).

Note that if in the technology choices the core process of the value chain or multiple unit processes across the value chain would change, i.e., a fundamental change to the PFD, this is defined as a new **pathway**. Examples include shifting from an electrochemical to a thermochemical installation or considering different chemical recycling processes.

What-if scenarios can be defined in the Excel template using defined what-if parameters. In addition, the What-if analysis tool in Excel gives you the option to work with 'Scenario Manager'. Scenario manager is useful when you want to define different scenarios, that are each described by multiple input parameters that accept a certain value for that scenario (e.g. the most optimistic, realistic and pessimistic scenario). More information on Scenario Manager is provided in Annex C – What-if analysis.

Projects evaluated for the MOONSHOT program should include a what-if scenario analysis. These should always be done directly in the provided Excel template.

The three steps mentioned above should be used to:

1. Identify relevant parameters. These can be based on the contribution and OAT sensitivity analyses, definition of parameters with large uncertainties, design options,...
2. Define data ranges/parameter choices. Technology and system boundary choices can be included using the ‘what-if’-parameters. These should be dynamically coupled to the calculations using e.g. if-functions in Excel. The technology options and system boundary choices are made based on own developments, expert input or literature data.
3. Build scenarios using what-if parameters and optionally the scenario manager tool in the Excel template.

The above-described Excel feature Scenario manager is described in more detail in Annex C – What-if analysis.

In the Excel template the analysis needs to be included in the calculation worksheet ‘1. Pathway’ under the title ‘Scenario analysis’ for the first pathway. The template uses separate input worksheet, i.e., data sheets. The data on these sheets need to be directly linked to the calculations on the calculation worksheet to make the model dynamic (i.e., when the input parameters change, also the output needs to dynamically change). In case fundamental changes to the PFD need to be addressed, resulting in new pathways, a separate calculation worksheet should be used in the Excel template.

12.5 Comparison with benchmark and setting research targets

Previous sections related mostly to subgoal 1 “to have a substantiated estimate of the economic and climate change impacts with the aim to identify the hot-spots”. Also, a comparison with the state-of-the-art is necessary within the MOONSHOT context, relating to the second subgoal defined as “to compare the economic and climate change impact with state-of-the-art and emerging technologies”. Therefore, the calculated indicator values should be compared to the benchmark process. Considering that the benchmark process is not modeled in the same level of detail as the system under study, one needs to take this into account for the interpretation of the results. It is therefore important to not just have a direct comparison between the calculated impacts for the system under study and the value found or calculated for the benchmark system. A comparison needs to be done based on the results of the sensitivity and basic uncertainty analysis and only serves as a guidance for the technology roadmap. The economic indicators calculated can be compared with, for example, the market value (i.e., current and future market prices), potentially including a price premium. The environmental impacts can be compared with the climate change impact found for the benchmark system using the approach as described in section 11.4. Based on this comparison and considering the insights from the sensitivity analysis one can define research targets that need to be met. In addition, the benchmark comparison needs to be paired with further insights gained from the elements that are more related to the broader context as described in chapter 13. This allows to provide an answer to the fourth subgoal “To specify what is required for a successful implementation”. In the end, the researcher should have an idea under which real-life circumstances the project can be upscaled to a viable market process/product.

13 CONTEXT

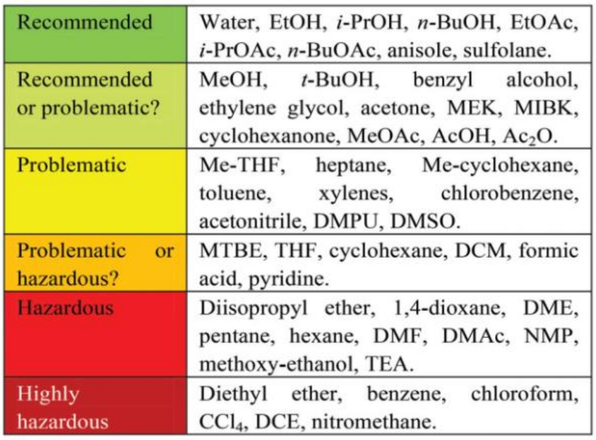
13.1 Energy

The Path 2050[12] study aims to provide cost-optimal transition pathways toward achieving an almost carbon-neutral Belgium by 2050. To achieve this ambitious goal, the development of renewable energy and related infrastructure becomes a top priority, as well as the renovation of the building stock. The findings of this study indicate, expanding the offshore wind and solar energy will play a crucial role in reaching climate neutrality. Furthermore, the development of nuclear SMR can play a crucial role from 2045 onwards. As intermediate goals by 2030, investments in infrastructure such as high-voltage grids, development of carbon capture technologies and ambitious policies for buildings can play an important role.

These global trends indicate the scarcity of renewable energy in Flanders and at the same time many of the innovations are highly energy intensive. Therefore, a clear discussion needs to be included in the projects on the energy use and how the innovations support the above-described goals or compete with other technologies for this energy. At the same time, new innovations can help in allowing to include more renewable energy on the grid by providing flexibility services. These also need to be clearly described.

13.2 Green metrics for solvents

In the green metrics toolkit from the CHEM21 project, solvents are divided in several categories based on their hazardousness. For the MOONSHOT program the categories are combined in three groups: 1) recommended, 2) problematic and 3) hazardous. The figure below gives an overview of the categories as defined in the green metrics toolkit.



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, formic acid, 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 15. Solvent categories from green metrics tool (McElroy, Constantinou et al. 2015)

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[12] https://perspective2050.energyville.be/key-takeaways

A color code is provided for the selected solvents on the worksheet ‘Data – environmental’ in column D. A green color indicates that the solvent is recommended, an orange color means that it might be problematic, and a red color indicates the solvent is hazardous. The solvents are selected using the dropdown list on the worksheet ‘Data – economic’ in column D.

13.3 Critical Raw Materials (CRM)

Due to increasing global population and industrialization, the pressure on resources increases. Therefore, the European Commission launched the Raw Materials Initiative. The main goal is to secure raw materials for the EU. One of the actions within this initiative is to publish a list of critical raw materials (CRM). The CRM are defined based on the security of supply and economic importance. In the figure below, the red dots represent the critical raw materials.

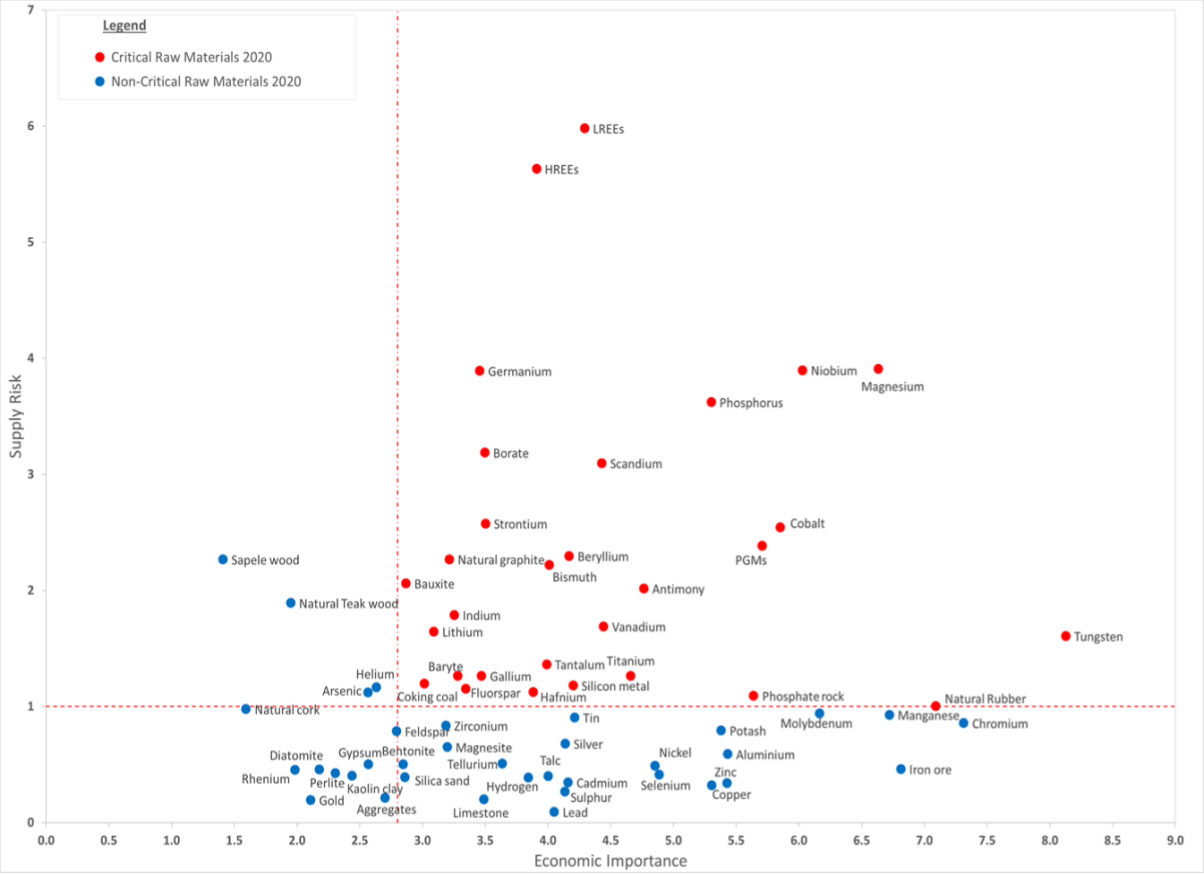

Figure 16. Critical raw materials list[13]

For the (catalyst) material a color code is added in the Excel template on the worksheet 'Data – economic' in column D where the (catalyst) material can be selected using a dropdown list. A red color indicates that the selected material is one of the critical raw materials on the list of the European Commission. A green color indicates that it is not on the list of critical raw materials.

13.4 Relevant regulations and policy measures

Depending on the specific MOT and project, different regulations and policy measures will be relevant. The table below provide some examples of European and Belgian and Flemish policy measures that might be relevant for the MOONSHOT projects.

Table 17. Relevant regulations and policy measures

Legislation	Link
RED	More information
ETS	More information
EU taxonomy	More information See also section 13.4.1
Green Deal	More information
Net-zero industry act	More information
REACH	More information
REPowerEU	More information
Electricity market design	More information
Circular Economy Action Plan	More information
European Strategy for Plastics in a Circular Economy	More information
Packaging and packaging waste directive	More information
Waste Framework Directive	More information
Vlaams Energie- en Klimaatplan 2021-2030	More information

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[13] https://rmis.jrc.ec.europa.eu/uploads/CRM_2020_Report_Final.pdf

VLAREM	More information

13.4.1 EU taxonomy

The EU Taxonomy, developed by the European Commission, is a “green classification system” to identify/evaluate sustainable economic activities for investment purposes. The EU Taxonomy aims to eventually enable change and support the transition towards sustainability.

The Taxonomy Regulation entered into force on 12 July 2020 and defines six environmental objectives:

1. Climate change mitigation;
2. Climate change adaptation;
3. The sustainable use and protection of water and marine resources;
4. The transition to a circular economy;
5. Pollution prevention and control;
6. The protection and restoration of biodiversity and ecosystems.

It also sets out four conditions that an economic activity has to meet to be recognized as Taxonomy-aligned:

- Making a substantial contribution to at least one environmental objective;
- Doing no significant harm to any other environmental objective;
- Complying with minimum social safeguards;
- Complying with the technical screening criteria.

Technical screening criteria are defined by the European Commission to determine under what conditions the economic activities can be considered as environmentally sustainable and as doing no significant harm (DNSH). Following the EU Taxonomy, the technical screening criteria for the six objectives define metrics and thresholds to define the environmental performance of the economic activities. For all activities contributing to climate mitigation, the technical screening criteria include:

- The activity, its description and the NACE code
- The reason why they contribute to climate mitigation, and the metrics and thresholds that can be used to determine the actual mitigation
- The criteria that need to be taken into account to avoid significant harm to the environment. For each of the objectives DNSH (2-6), the criteria are described with reference to EU regulations and potential thresholds (for example, for pollution prevention and control, emissions to air need to meet the thresholds for the BAT in the sector).

Further information on the EU taxonomy and the technical screening criteria can be found at the following links:

- https://ec.europa.eu/sustainable-finance-taxonomy/
- https://finance.ec.europa.eu/system/files/2020-03/200309-sustainable-finance-teg-final-report-taxonomy_en.pdf
- https://finance.ec.europa.eu/sustainable-finance/tools-and-standards/eu-taxonomy-sustainable-activities_en

13.5 Circularity principles

A circular economy aims to maximize the functionality of materials and minimize the input of primary materials and output of waste and emissions. There are multiple strategies to transition to a more circular economy. Several frameworks regarding circularity principles have been developed in the past For instance, Saidani et al., 2020 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.

Quantitative circularity assessments are often based on material flow analysis (MFA), expressing results in masses of materials or (mass) percentages of the total amount of assessed materials, water and energy flows.

It is also important to maximize functional lifetime of products, minimize primary material requirements, enable optimal repairability and maintain the quality of products in the recycling process (avoid downcycling). Ecodesign or design-for-circularity can provide important insights to already include circularity in the design stage of a new product or technology.

Technical indicators that cover circularity indicators such as the recycling and reuse rate need to be included in the Excel template on the worksheet ‘1. Pathway’ for the first pathway. A separate calculation worksheet needs to be foreseen for each defined pathway.

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15 ANNEX A – UPSCALING

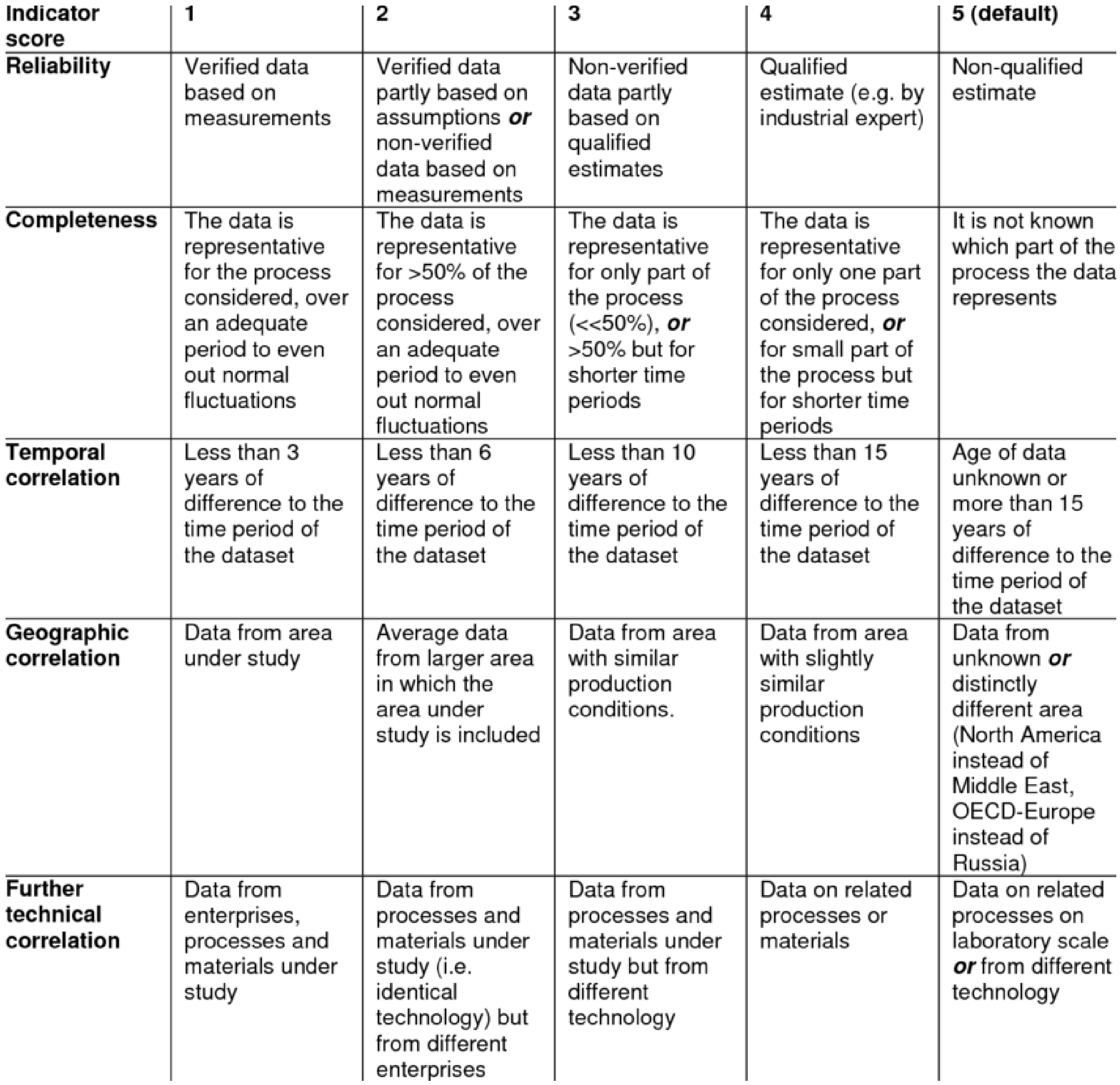
Below a summary of the upscaling guidelines of Piccinno, Hischier et al. (2016) are provided. We refer to the original publication for all details.

Table 18. Upscaling guidelines (Piccinno, Hischier et al. 2016)

Step	Description/Calculation
Inputs	
Reactants	Use stoichiometric amounts (same as lab protocol)
Solvents	Reduce 20% compared to lab scale Reduce amount by recycling rate where possible and include energy inputs for recycling process
Catalysts	Design recycling process where possible
Heating	$Q_{react(1000\ l)} = \frac{\left(C_p * m_{mix} + 3.303 \frac{W}{K} * t\right) * (T_r - 298.15\ \text{K})}{0.75}$
Stirring	$E_{stir(1000\ l)} = 0.0180\ \text{m}^5\text{s}^{-3} * \rho_{mix} * t$
Homogenizing	$E_{hom(1000\ l)} = 15.47\ \text{m}^5\text{s}^{-3} * \rho_{mix} * t$
Grinding	8-16 kWh/ton depending on size and material
Filtration	1-10 kWh/ton dry material depending on grain size
Centrifugation	Slightly higher than for filtration.
Distillation	$Q_{dist} = \frac{C_p * m_{mix} * (T_{boil} - T_0) + \Delta H_{vap} * m_{dist} * (1.2 * R_{min} + 1)}{\eta_{heat} - 0.1}$
Drying	$Q_{dry} = \frac{C_{p,liq} * m_{liq} * (T_{boil} - T_0) + \Delta H_{vap} * m_{vap}}{0.8}$
Liquid transfer (pumping)	$E_{pump} = 55 \frac{\text{J}}{\text{kg}} * m$
Other processes	Use data/values from similar existing processes or machineries
Outputs	
Reaction mixture	Output containing target compound, serves as input for subsequent step.
Product/yield	Base the yield on value of similar process or use lab yield
By-product	System expansion or Allocation
Waste – solvent	Options: recycling, incineration on site or to hazardous waste incineration plant.
Waste – other	Options: hazardous waste incineration plant or 'regular' waste treatment if not contaminated.
Wastewater	Options: recycling, wastewater treatment or if contaminated to hazardous waste incineration plant.
Emissions (direct)	Include direct emissions and estimates
Waste heat	Include simple heat recovery through heat exchangers

16 ANNEX B – PEDIGREE MATRIX

Pedigree matrix from ecoinvent 3.0



Indicator score	1	2	3	4	5 (default)
Reliability	Verified data based on measurements	Verified data partly based on assumptions ***or*** non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate
Completeness	The data is representative for the process considered, over an adequate period to even out normal fluctuations	The data is representative for >50% of the process considered, over an adequate period to even out normal fluctuations	The data is representative for only part of the process (<<50%), ***or*** >50% but for shorter time periods	The data is representative for only one part of the process considered, ***or*** for small part of the process but for shorter time periods	It is not known which part of the process the data represents
Temporal correlation	Less than 3 years of difference to the time period of the dataset	Less than 6 years of difference to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographic correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions.	Data from area with slightly similar production conditions	Data from unknown ***or*** distinctly different area (North America instead of Middle East, OECD-Europe instead of Russia)
Further technical correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study (i.e. identical technology) but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials	Data on related processes on laboratory scale ***or*** from different technology

17 ANNEX C – WHAT-IF ANALYSIS

A What-If Analysis in Excel: a practical guide for ‘Scenario Manager’ and ‘Data table’ is provided below.

Scenario manager*

Scenario manager is useful when you want to change some input variables simultaneously (i.e., a scenario), and determine the results. The following steps should be followed in Excel:

Step 1: Go to tab “Data”

Step 2: Go to “Forecast”

Step 3: Click on “What-If Analysis”

Step 4: Select “Scenario Manager” and click on “Add…”

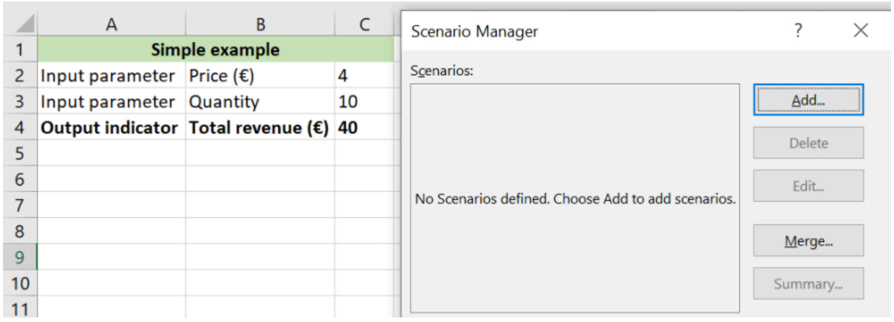
Step 5: Define your scenario: add a scenario name (e.g., ‘optimistic scenario’). Select for the “changing cells” the Excel cells that contain input values (e.g., ‘price’ and ‘quantity’) that you want to change in your scenarios. Explain in Comment what the scenario entails. Click on ‘ok’ when all information is filled out.

Step 6: Define your scenario values. For every scenario you create, click on ‘add’. Click on ‘ok’ when done.

Step 7: Continue creating other scenarios.

Step 8: Click on “summary” to create an additional sheet with an overview of all scenarios. This summary is easy for scenario comparison. The ‘changing cells’ are not labeled. If you want to label them, you need to do that manually. Note that the summary table is not dynamic. This means if you change anything in your data, you need to re-run the “summary”.

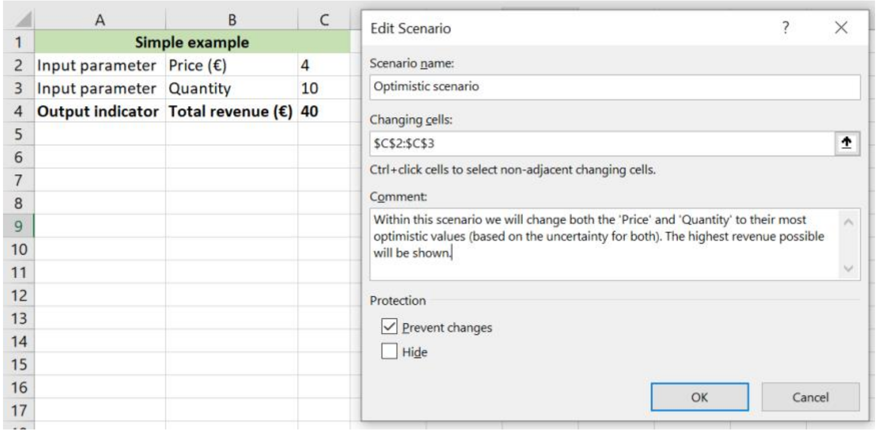
An illustrative example on how to use Scenario Manager is provided below with screenshots.



	A	B	C
1	**Simple example**		
2	Input parameter	Price (€)	4
3	Input parameter	Quantity	10
4	**Output indicator**	**Total revenue (€)**	**40**

No Scenarios defined. Choose Add to add scenarios.

Step 1 – Step 4. Open Scenario Manager and add new scenarios.



	A	B	C
1	**Simple example**		
2	Input parameter	Price (€)	4
3	Input parameter	Quantity	10
4	**Output indicator**	**Total revenue (€)**	**40**

Edit Scenario

Scenario name: Optimistic scenario

Changing cells: $C$2:$C$3

Ctrl+click cells to select non-adjacent changing cells.

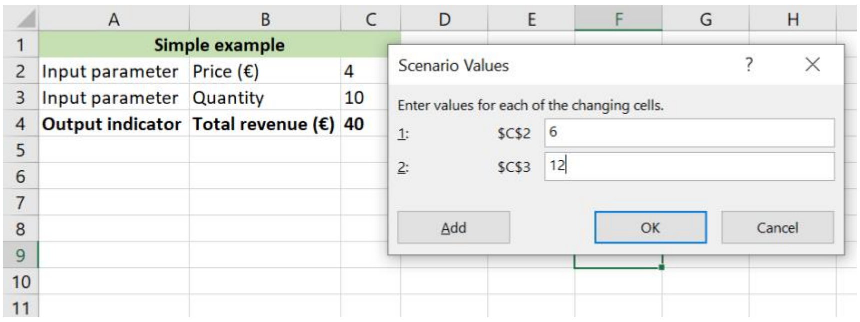
Comment: Within this scenario we will change both the 'Price' and 'Quantity' to their most optimistic values (based on the uncertainty for both). The highest revenue possible will be shown.

Protection

☑ Prevent changes

☐ Hide

Step 5. Define the first scenario.



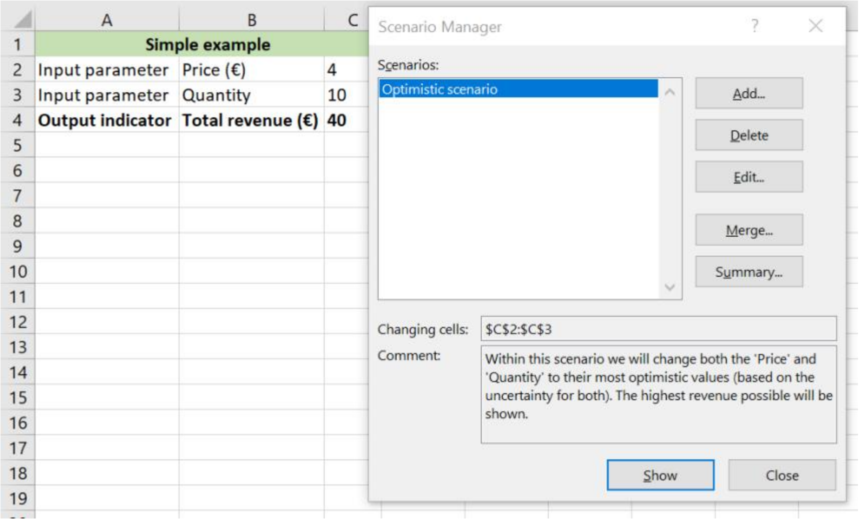
Scenario Values

Enter values for each of the changing cells.

1: $C$2 6

2: $C$3 12

Step 6. Define the scenario values.



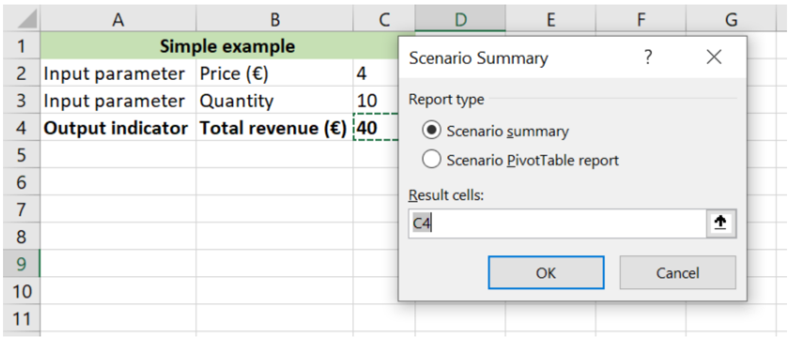
Scenario Manager

Scenarios: Optimistic scenario

Changing cells: $C$2:$C$3

Comment: Within this scenario we will change both the 'Price' and 'Quantity' to their most optimistic values (based on the uncertainty for both). The highest revenue possible will be shown.

Step 7. You can add other scenarios and/or click on 'summary' to get an overview of the results of the created scenarios



	A	B	C
1	**Simple example**		
2	Input parameter	Price (€)	4
3	Input parameter	Quantity	10
4	**Output indicator**	**Total revenue (€)**	**40**

Scenario Summary

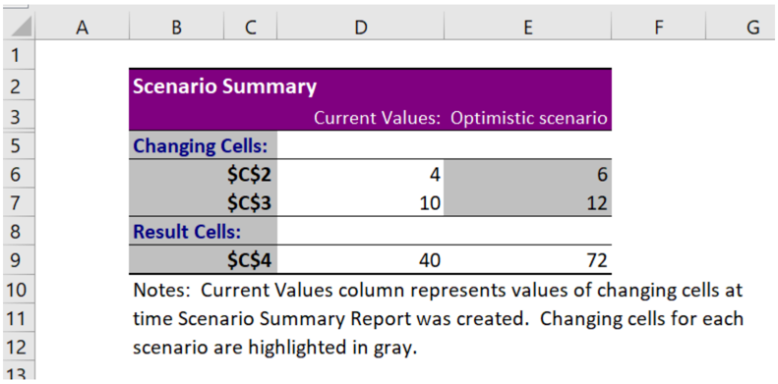
Report type

● Scenario summary

○ Scenario PivotTable report

Result cells: C4

Step 8. Define the ‘Result cells’ in the ‘Scenario Summary’. When you click on ‘OK’ a separate sheet appears with the results (see next screenshot).



Scenario Summary

	Current Values:	Optimistic scenario
Changing Cells:		
$C$2	4	6
$C$3	10	12
Result Cells:		
$C$4	40	72

Notes: Current Values column represents values of changing cells at time Scenario Summary Report was created. Changing cells for each scenario are highlighted in gray.

Step 8 (bis). An overview of the additional sheet created with an overview of the scenarios

Data tables*

Data tables are useful when you want to change one or two input parameters simultaneously and determine the results. The following steps should be followed in Excel to derive a two-parameter data table:

Step 1: Link an empty cell in the Excel to your original formula of the output indicator. Make sure you have enough empty columns to the right and empty rows below to accommodate your parameter values.

Step 2: Type one set of input values below the formula, in the same column. A heading describing the selected input parameter can be added for clarity.

Step 3: Enter the other set of input values to the right of the formula, in the same row. A heading describing the selected input parameter can be added for clarity.

Step 4: Select the entire data table range including the formula, the row and column of the input values, and the cells in which the calculated output values will appear.

Step 5: Go to tab “Data”

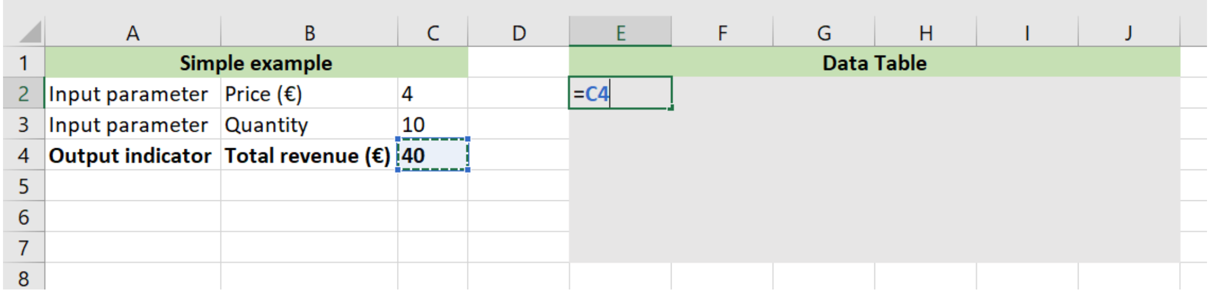
Step 6: Go to “Forecast”

Step 7: Click on “What-If Analysis”

Step 8: Select “Data Table”

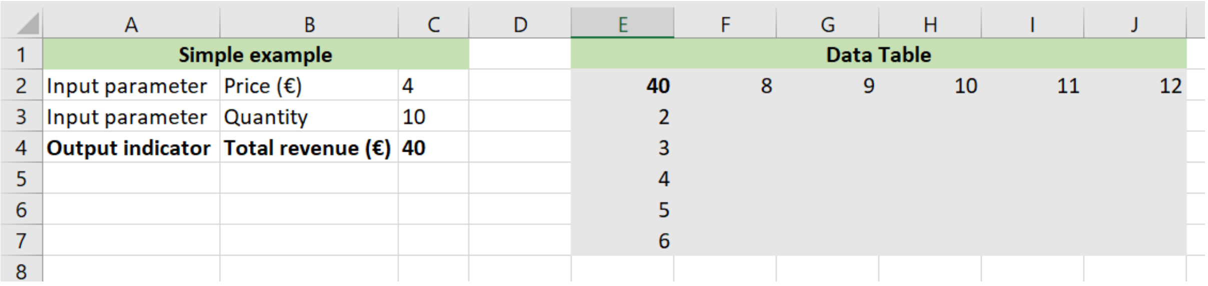
Step 9: In the “Row input cell” box, enter the reference to the original input cell for the parameter values in the row. In the “Column input cell” box, enter the reference to the original input cell for the variable values in the column. Click “OK”. Note that it is important that the value of the input parameter that is varied, is on the same worksheet as the Data Table. A link from the input worksheet to the input parameter on the worksheet where the Data Table is calculated, can be added to keep the dynamic calculations.

An illustrative example on how to create a data table is provided below with screenshots.



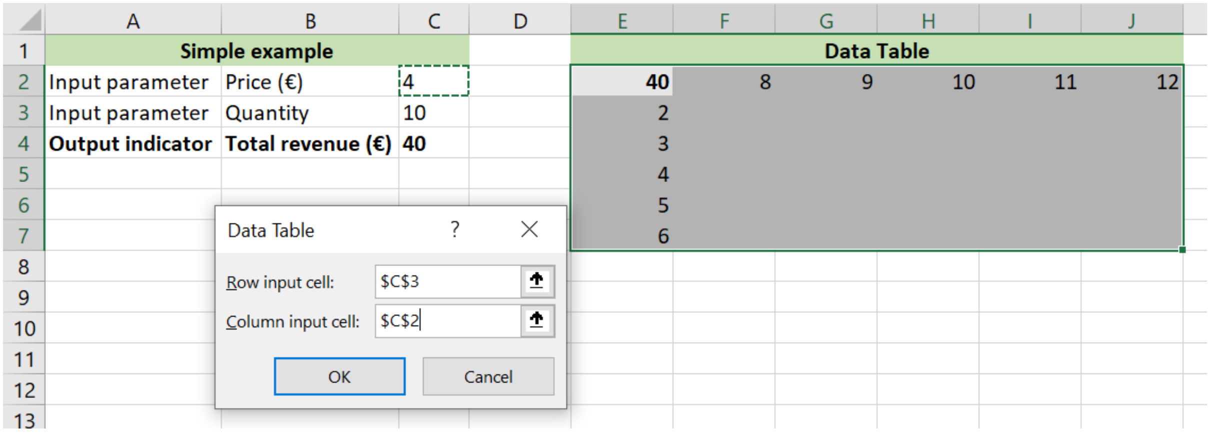
	A	B	C	D	E	F	G	H	I	J
1	**Simple example**				**Data Table**					
2	Input parameter	Price (€)	4		=C4					
3	Input parameter	Quantity	10							
4	**Output indicator**	**Total revenue (€)**	**40**							
5										
6										
7										
8										

Step 1. Link an empty cell in the Excel to the original formula of the output indicator.



	A	B	C	D	E	F	G	H	I	J
1	**Simple example**				**Data Table**					
2	Input parameter	Price (€)	4		**40**	8	9	10	11	12
3	Input parameter	Quantity	10		2					
4	**Output indicator**	**Total revenue (€)**	**40**		3					
5					4					
6					5					
7					6					
8										

Step 2 – Step 3. Insert the set of input values you want to investigate in the column and row, below and next to the linked cell.



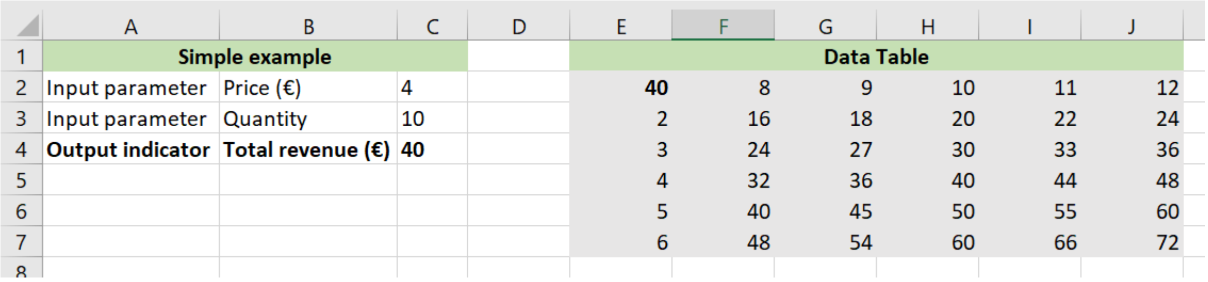
	A	B	C	D	E	F	G	H	I	J
1	**Simple example**				**Data Table**					
2	Input parameter	Price (€)	4		**40**	8	9	10	11	12
3	Input parameter	Quantity	10		2					
4	**Output indicator**	**Total revenue (€)**	**40**		3					
5					4					
6					5					
7					6					
8										
9										
10										
11										
12										
13										

Data Table

Row input cell: $C$3

Column input cell: $C$2

Step 4 – Step 9. select the entire data table and create a ‘Data Table’. In this example, row 2 contains the values of the quantity input parameter and the column E of the price input parameter. For the Data Table, this means that the original value of the price input parameter needs to be linked to the Column input cell since the value will change over the columns. For the same reason the original value of the quantity input parameter needs to be linked to the Row input cell.



	A	B	C	D	E	F	G	H	I	J
1	**Simple example**				**Data Table**					
2	Input parameter	Price (€)	4		**40**	8	9	10	11	12
3	Input parameter	Quantity	10		2	16	18	20	22	24
4	**Output indicator**	**Total revenue (€)**	**40**		3	24	27	30	33	36
5					4	32	36	40	44	48
6					5	40	45	50	55	60
7					6	48	54	60	66	72
8										

The result of the Data Table is now calculated. The results can be visualized using graphs or with conditional formatting a heat map can be obtained.

*More information on how to use Scenario Manager and Data Tables can be found on the support.microsoft.com website.

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