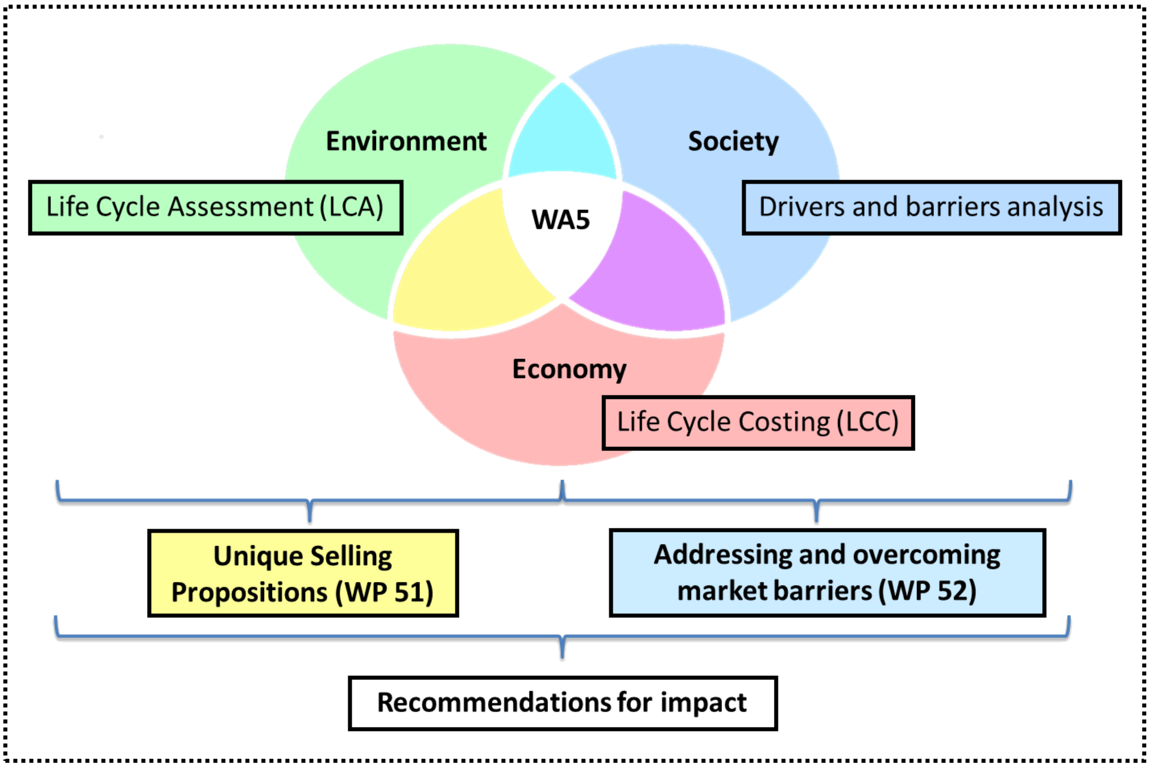
D51.2: Final guidelines for sustainability assessment of water technologies



The research leading to these results has received funding from the European Union Seventh Framework Programme (FP7/2007-2013) under Grant Agreement no. 308339 for the research project DEMEAU

Title: Final guidelines for sustainability assessment of water technologies

Summary: This report is a methodology guidelines for sustainability assessment of water treatment technologies and processes, based on the approach developed within the DEMEAU project. This approach includes environmental, economic and social aspects using Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and an analysis of drivers and barriers based on stakeholder experience. Besides methodological guidelines and recommendations for the different tools, this report also comments on the organisation of the exchange and collaboration process between the assessment team and the project partners. Finally, unique selling propositions and recommendations for impact are derived which should foster implementation and uptake of innovative technologies and processes within the water sector.

Grant agreement no:	308339
Work Package:	WP51
Deliverable number:	D51.2
Partner responsible:	KWB
Deliverable author(s):	Christian Remy (KWB), Kristina Wencki (IWW), Miranda Pieron (KWR), Anna Kounina (Quantis), Christoph Hugi (FHNW), Thomas Gross (FHNW)
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Planned delivery date:	August 31, 2015
Actual delivery date:	September 25, 2015
Dissemination level:	Public

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1 Introduction

1.1 Purpose of this document

Within the DEMEAU project, the objective of work area 5 (WA5) was the sustainability assessment to foster the market uptake of emerging water technologies in response to rising concerns about micropollutant contamination in wastewater and drinking water sources (Figure 1-1). The goal of this document is to describe the methodology of the sustainability assessment applied to different case studies in DEMEAU. Results of these sustainability assessments for the case studies can be found in deliverables D51.1[1] and D52.2[2] of the DEMEAU project.

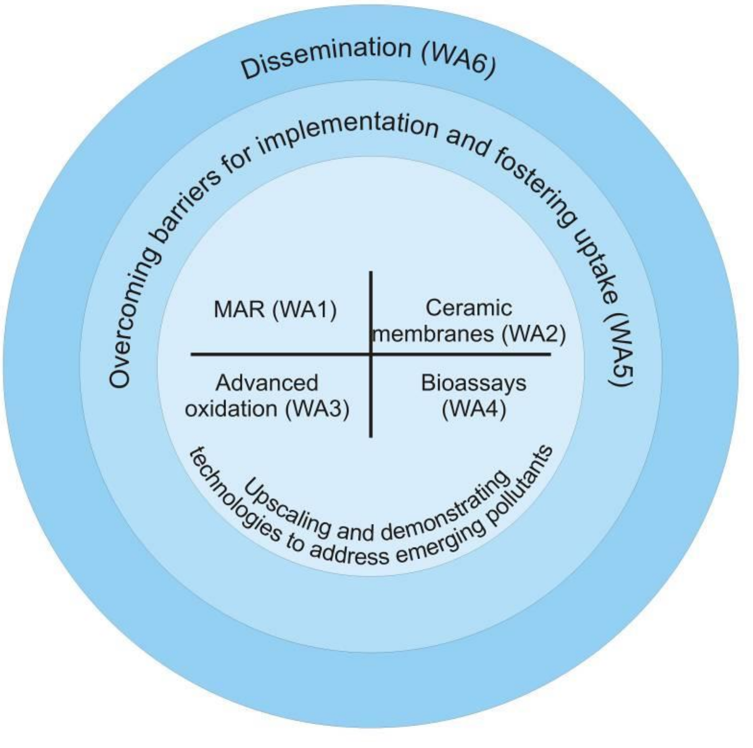

Figure 1-1: Structure of DEMEAU project and integration of WA5

1.2 Overview of DEMEAU approach to sustainability assessment

The DEMEAU approach is based on environmental and economic assessments to propose unique selling propositions of emerging water technologies and stakeholder based drivers and barriers assessments to derive recommendations to overcome market barriers. Finally, the different tools of sustainability analyses built the basis to formulate recommendations for impact in the water sector.

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[1] Remy C, Gallice A, Kounina A, Oberschelp C, Pieron M, Wencki K, Hugi C, Gross T (2015). Unique selling propositions. Deliverable 51.1 of the DEMEAU project (FP 7 framework), http://demeau-fp7.eu

[2] Gross T, Gallice A, Kounina A, Pieron M, Remy C, Wencki K, Hugi C (2015). Recommnedations for impact. Deliverable 52.2 of the DEMEAU project (FP 7 framework), http://demeau-fp7.eu

Within the course of DEMEAU, the WA5 team developed and field-tested a methodology for sustainability assessment, based on three main tools (Figure 1-2):

1) Life Cycle Assessment (LCA) for analysing environmental benefits and impacts
2) Life Cycle Costing (LCC) for analysing economic aspects
3) Drivers and barriers analysis, based on stakeholder participation

The sustainability assessment was carried out in DEMEAU for selected case studies of WA1-4 which are connected to the project consortium, and which were selected upfront to take part in the assessment. The final goal of the assessment was to formulate recommendations for impact of innovative processes and technologies from WA1-4 in the water sector which reflect unique selling propositions based on environmental and economic analyses and identified drivers and barriers.

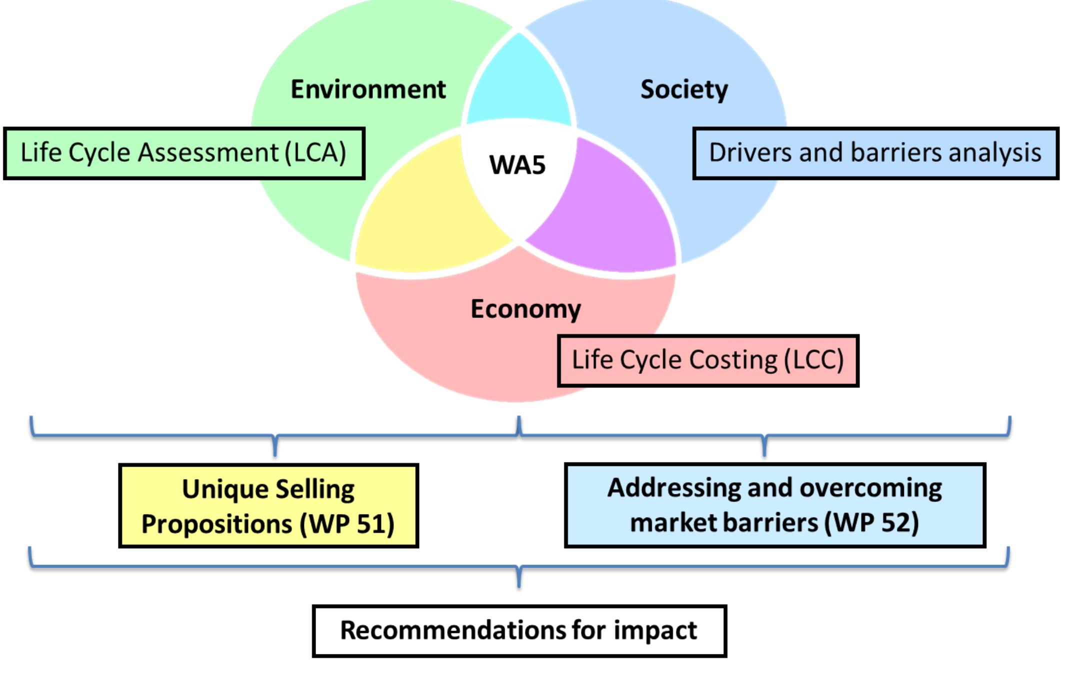

Figure 1-2: Framework for sustainability analysis in WA5

1.3 Content of this report

This methodology report is structured along the DEMEAU approach for sustainability assessment:

1) Exchange process with project partners (chapter 2)
2) Methodology of Life Cycle Assessment (chapter 3), including methodological developments on toxicity characterization of organic micropollutants (USEtox®) and water footprinting
3) Methodology of Life Cycle Costing (chapter 4)
4) Methodology for drivers and barriers analyis (chapter 5)
5) Integration of results into recommendations for impact based on these sustainability assessments (chapter 6)

Results of sustainability assessments can be found in D51.1 for LCA and LCC and D52.2 for drivers and barriers analysis and recommendations for impact.

2 Setup of exchange process with project partners

This chapter describes the setup and organisation of the exchange process between the assessment team of WA5 and the case study partners. The process was developed "on-the-go" during the project, and some important features and experiences are summarized here to facilitate the assessment and improve cooperation and exchange in similar projects.

2.1 Selecting the case studies

In a first step, suitable case studies or processes which take part in the sustainability assessment are selected. Most often, project proposals already indicate which processes or sites are to be analysed in the project, but this selection has to be specified and validated at the beginning of the study. In particular, the following aspects are important for this process:

Information of potential case study participants about the methodology, data needs and potential outcomes of the study

Potential participants need to be informed on the methods and tools which will be applied in the assessment, the type of input which will be required from their side (e.g. process data, cost data, participation in meetings, workshops, interviews), and the expected outcomes of the study. Within DEMEAU, the WA5 team already gave a presentation at the first general assembly to explain the goals of the sustainability assessment, potential outcomes, and the need for close cooperation and exchange with the project partners for this task. Following up on this presentation, an information leaflet (few PowerPoint slides, see Annex-A for examples) was sent around shortly after the general assembly to inform all potential partners again on this issue and ask for their definitive willingness to be part of this approach.

Cross-check with potential case studies if suitable data can and will be supplied

When establishing further contacts to the different partners and case study sites, it is important to cross-check with the contact persons and their organisations if suitable data can and will be supplied for the assessment. Data for LCA and especially LCC may be sensitive for technology providers or operators, and the willingness to share this data within the project and finally publish it in reports or presentations has to be confirmed. In this aspect, it is helpful to guarantee intermediate steps of cross-check and validation of input data and results with the partners before any information is published. This will increase trust and confidence in the cooperation and ease the partner's decision to offer data for the analysis.

Identification of responsible individuals to establish and maintain contact between assessment team and case study partners)

Single contact persons should be identified both from the side of the assessment team, but also from the case study sites. The responsibility of an individual person in establishing and maintaining the contact will help in channeling the communication flows (e.g. preventing multiple persons asking for comparable input at a time) and establish a trustful relationship between the assessment team and the case study partners. Ideally, existing personal contacts between project partners can be used to build upon successful cooperation in previous projects, which will ease the task to involve the case study partners in the analysis.

Validation of selection within project consortium

The final selection of case studies and partners for the sustainability analysis should be communicated to the entire consortium to be transparent in the decision process. With this step, all involved partners can check and validate the selection and approve the final list of case studies and processes to be analysed.

2.2 Defining systems, system boundaries and scenarios

Sustainability assessments require clarity of systems and their processes to be compared. Both LCA and LCC provide favourable conceptual structures to foster such a system understanding through: (i) a 'definition of goal and scope' of the systems in question, including the functions of the system and the system boundaries; and (ii) a thereupon based 'life cycle inventory' of all relevant processes within these systems.

Details of these key steps in setting up LCA and LCC models are provided in chapter 3.2 of this document. This section focuses on the exchange between LCA/LCC experts and case study partners building the basis for setting up the models.

Definition of system or process to be assessed and related system boundaries of the assessment

For all steps of the sustainability assessment, the precise definition of suitable systems and their boundaries is the first task.

Layout of the current system: This first step involves the detailed characterization of the current water treatment system and its processes under study. Usually, a flow chart of the system or process has to be provided by the case study partners, which should then be reproduced by the LCA/LCC experts in form of a flow diagram in their own layout.

Cross-check: The system layout by the LCA/LCC experts can then be used for first cross-check and validation by the case study partners, who will confirm the general layout and precise misunderstandings or false interpretations by the assessment team.

System boundaries: In comparative studies of possible future measures - such as comparison of possible new technologies against micropollutants on existing water treatment plants - individual scenarios have to be defined which represent the different options available to reach a certain purpose or function. Based on the validated system layout, the LCA/LCC experts should propose suitable system boundaries for the assessment from their perspective, taking into account all processes upstream and downstream which are relevant for the specific goals of the study. The final decision on suitable system boundaries for LCA and LCC should be taken in close cooperation with the case study partners. Experience shows that comparative studies can probably exclude those parts of the larger system that are not changed by the different options, thus limiting the amount of data that is required and the complexity of the models. However, assessment of the entire water treatment systems is often worthwhile also in comparative studies, as information of the relative importance of system changes or upgrades in comparison to the overall impact or cost of the system can be of major interest for the goal of the study. Aggregated generic models for water and wastewater treatment are also available in LCA databases if no primary data is available. Further details can be found in chapter 3.2.

Definition of scenarios in comparative studies

The appropriate scenario definitions for LCA and LCC should take into account that these scenarios are really comparable in their primary function to enable a fair and robust comparison. For this task, the precise definition of system functions is helpful to check whether all alternatives really provide the same functionality. System functions can be characterized by simple tasks (e.g. "wastewater treatment"), but should often be accompanied by a qualifier (e.g. "according to EU discharge standards XY") to specify the minimum water quality or efficiency of the process/system under study. From this definition of system function, suitable scenarios can then be derived for a comparative analysis. Finally, scenarios should be precisely described by flow diagrams and be cross-checked and validated by case study partners.

2.3 Exchanging and validating input data

Data collection

To collect process data from case study partners, a suitable format has to be defined by the assessment team based on their previous experience in similar studies. Usually, a template in the form of an excel sheet is suitable to explain the data needs for LCA and LCC based on an “ideal” set of information (see example in Annex-B). This template should be reasonably structured along the system parts as defined in the system layout, and it should contain suitable units for data collection. This template should be seen as starting point for the data exchange between case study partners and the assessment team, and can be adapted at any point during the study. Usually, a “ping-pong” iterative procedure will evolve with several rounds of feedback, questions and precision of data between the assessment experts and the data providers. Updating of process data during the course of the project with latest results of lab, pilot or full-scale trials can easily last until the very moment before the final meeting, so it is advisable to set a reasonable “deadline” for datasets to be finalized before to allow for some time to implement them into the models.

Data validation

To validate the data exchanged between several partners, it is helpful to check the transferred datasets for consistency while integrating them into the different modelling tools. This consistency check should relate to correct use of units, closing of mass balances within reasonable accuracy, and comparing selected process parameters and efficiencies to reference data or previous studies in this field. It is highly recommended to enter a final round of data validation with the case study partners before publishing final results of the assessment, as transferred data could be affected by numerical errors, wrong units, or misunderstandings in the process. Final validation of input datasets will greatly increase trust of all partners into the results of the assessment and prevent “last-minute” surprises when presenting or discussing assessment data and results. Data validation is also crucial before publishing of any data in public presentations or reports to maintain credibility of the assessment and trust between case study partners and the assessment experts.

2.4 Validation of results and quality control

If system definitions and input data have been carefully cross-checked and validated as discussed above, the final outcomes of the assessment are usually well accepted within the project consortium. Nevertheless, results and conclusions of the sustainability assessment should be presented and discussed with the relevant project partners prior to any public presentations or reports, e.g. by sending PowerPoint slides or draft reports to the case study partners ahead of publication for quality control. This last loop will increase their trust into the outcomes of the assessment and enable a cooperative and open discussion of the conclusions that are finally presented to the public. In case of diverging views on specific results or conclusions of the assessment, it is possible to discuss these aspects internally within the project consortium. Limitations of the assessment and diverging interpretation of the results should be transparently communicated in public presentations of the sustainability assessment. Usually, it will highly increase acceptance of the project outcomes if critical comments and limitations of the study are openly communicated, also identifying future needs for precision or development of the methodological approach. Taking into account the inherent complexity of technical processes and systems and the methodological difficulties of multi-dimensional evaluation, it will most certainly not decrease the impact of the assessment if critical aspects are clearly identified and made transparent in final reporting.

3 Life Cycle Assessment (LCA)

3.1 LCA for water treatment systems

As defined in ISO 14040[3] and 14044[4], Life Cycle Assessment follows a defined methodological framework to enable a systematic and comprehensive characterisation and quantification of selected potential environmental impacts, which are associated with a product or service. Using the life-cycle perspective, all relevant processes upstream and downstream of the process under study are described with substance flow models, listing all required inputs from the environment (e.g. fossil fuels, metal ores, land use) and outputs into the environment (e.g. emissions into air, water and soil). From this detailed list of input and output flows (forming the "Life Cycle Inventory") and using existing impact assessment methods (e.g. global warming potential method based on IPCC data (IPCC 2001[5], 2007)[6]), selected indicators are calculated to describe the potential environmental impact of these flows regarding specific areas of environmental concern (e.g. cumulative energy demand of fossil fuels, global warming potential, eutrophication of surface waters, or human/ecotoxicity). Using a well-defined system boundary and functional unit and assuring functional equivalency between compared options, different scenarios or processes can be compared in their indicator profiles to reveal potential environmental benefits or drawbacks and promote an informed decision making process between alternatives.

For water treatment processes, typical LCA system boundaries are defined in relation to the water flow to be treated (as input or "reference flow"). They include the treatment process itself, all direct emissions into the environment (effluent water quality which is discharged or used in the environment, direct emissions to atmosphere), and all indirect processes required to build and operate this treatment process (Figure 3-1). These indirect processes typically include production of electricity and chemicals required for water treatment, production of materials for infrastructure, and disposal of waste such as sludge or chemical residues.

[3] ISO 14040 (2006). Environmental management - Life Cycle Assessment - Principles and framework. International Standardisation Organisation, Geneva, Switzerland

[4] ISO 14044 (2006). Environmental management - Life cycle assessment - Requirements and guidelines. International Standardisation Organisation, Geneva, Switzerland

[5] IPCC (2001). Climate change 2001: The Scientific Basis. Intergovernmental Panel on Climate Change (IPCC), Cambridge University Press, Cambridge, UK

[6] IPCC (2007a). Climate change 2007: the physical science basis. In: Contribution of working group I to the fourth assessment report of the intergovernmental panel on climate change. Cambridge University Press, Cambridge, UK

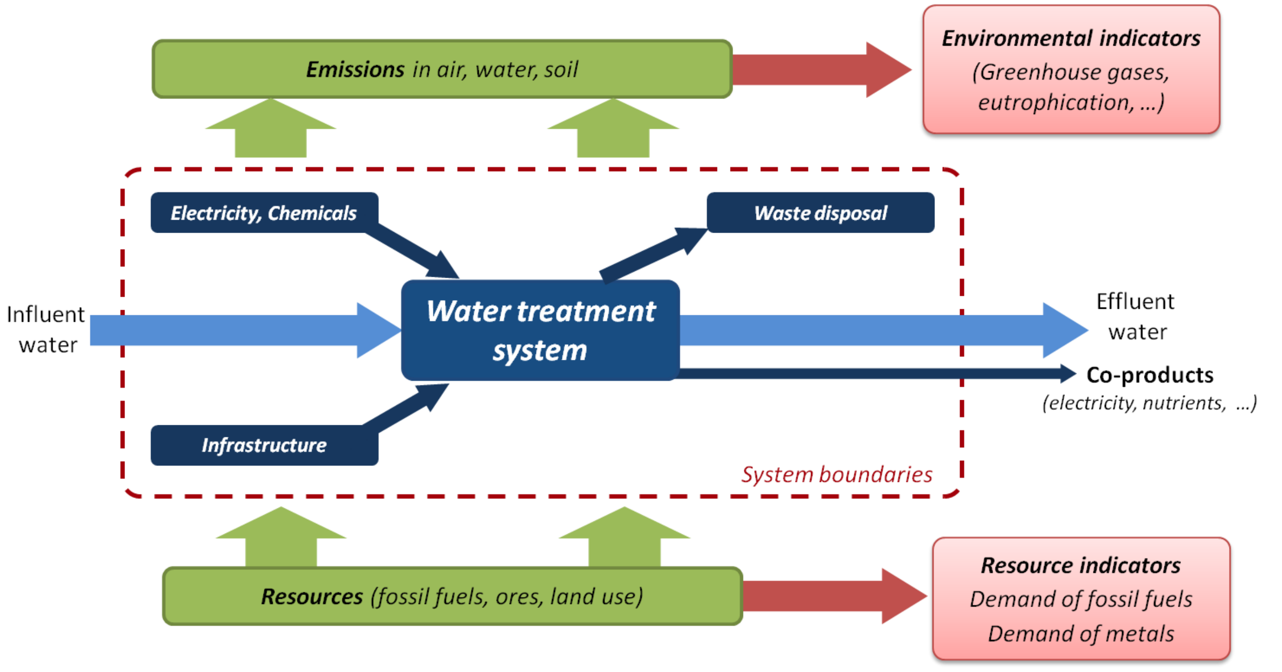

Figure 3-1: Typical system boundaries of an LCA for a water treatment system

According to ISO 14040, the execution of an LCA study involves a defined methodological approach. The ISO framework defines the working steps to be followed and how they should be documented, but it does not provide precise guidance of the specific choices that the LCA practitioner will make during the assessment (e.g. on appropriate system boundaries, functional unit, data sources etc.). Thus, the standard leaves room for the user to adapt these definitions guidelines for the LCA to the specific goal and scope of the study. However, it requires reporting of sound argumentation and reasonable justification on the choices made be by the LCA user practitioner to ensure transparency for the reader and enable an external check and validation of the study outcomes.

In detail, the standard requires four steps to be taken into account (Figure 3-2):

1. Definition of goal and scope of the LCA study
2. Collection of the data for the Life Cycle Inventory
3. Impact assessment by calculating indicators and putting them into perspective
4. Interpretation of the results and discussion on their stability towards important assumptions (sensitivity analysis) and on limitations of the study results

This process is generally seen as iterative, so that the definitions or inventory data can still be adjusted in the course of the LCA study if this will help in better fulfilling the goals of the study. If the study claims to be in full agreement with ISO14040/44 and is intended for public disclosure, a critical review by external experts is mandatory to check and validate the correct reporting of the LCA study according to ISO14040/44 requirements.

In the present report, recommendations are provided on how to set up the LCA framework for assessing drinking water and wastewater treatment processes. It is based on experience and learning from the DEMEAU project and previous studies in this field, and it should serve as methodological guideline for the LCA expert working in this field.

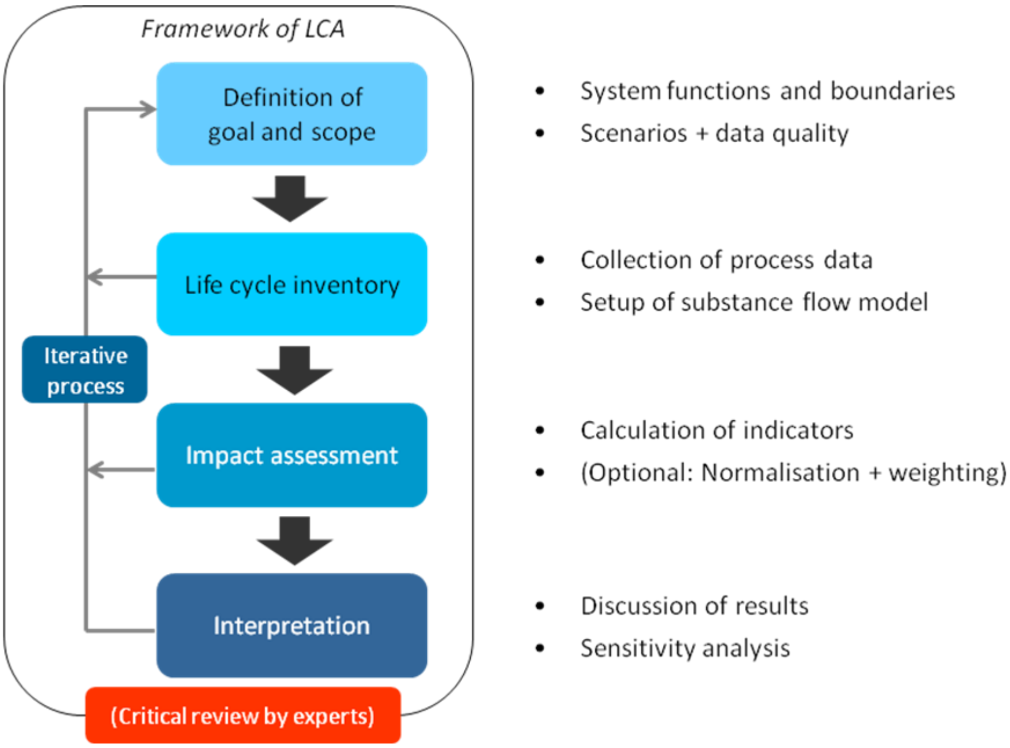

Figure 3-2: Framework of LCA according to ISO 14040/44

3.2 Goal and scope definition

Goal

The definition of a specific goal for the LCA study seems to be a redundant step at first sight, but it can provide valuable insights to formulate this goal in a most precise way. The goal will give information about the nature of the LCA study (e.g. "analysing environmental profile of process XY" or "comparing alternative treatment processes for drinking water production at site XY") and the intended use of its outcomes. LCA can be used to analyse a single process or to compare different alternatives in their environmental impacts. Assessing a single system in its environmental footprint with LCA will provide useful information about environmental "hot spots", while comparing alternatives or reference benchmarks from other studies can help in decision making by identifying advantages and drawbacks of scenarios.

Usually, the goal definition also includes potential target groups (e.g. "operators, regulators, scientists, public") for the study, so that the LCA study can reflect on the level of technical know-how and specific questions to be answered for this target group in terms of result discussion and interpretation, and also recommendations for action.

Scope

The scope of the study defines the system functions and functional unit of the LCA, the reference flow, the system boundaries, the projected or required data quality for the inventory, other assumptions and limitations, and the choice of impact categories/indicator models for the impact assessment.

System functions and functional unit

Usually, the system functions refer to the treatment of water to a specifically defined quality standard. The system function should be described precisely (e.g. "annual impact of discharge or further treatment of secondary effluent of WWTP XY") and provide a qualifier for the water quality to be reached, e.g. certain concentration limits or defined quality parameters (e.g. "suitable for groundwater recharge according to Spanish regulations").

For the functional unit, most LCA studies relate to the volume of water treated or re-used (e.g. [per m^3 of water]) provided that a defined water quality is reached after treatment[7]. It is important whether the functional unit relates to the influent of a process (e.g. [per m^3 of water from secondary clarifier]) or to the product water (e.g. [per m^3 of water produced]), as these volumes may not always correspond if the process involves water losses, for example in backwash water of filters or membrane concentrates. Other suitable alternatives for a functional unit in wastewater treatment relate to the pollutant load of the influent wastewater, which is often expressed as population equivalent (pe) according to defined pollutant loads per person and year (e.g. [per pe_{COD}*a] relating to the average load of 120 g COD/(pe*d) typically found in municipal wastewater[8]). This approach enables the comparison of different sites with different concentrations in wastewater, as the comparison will take into account the actual pollutant load to the system. The functional unit can also relate to the total operation of a system for a certain period of time (e.g. [per day, per year]), but the size of the system should be included then. In general, it is advisable to provide all necessary information in the LCA report to recalculate the LCA results to other functional units (e.g. provide data of system size (pe), water volume per year (m^3/a), or organic pollutant load (mg/L COD)), thus enabling comparability between LCA studies using different functional units.

Reference flow

The reference flow describes the influent water quality and quantity for the treatment process. The quantity of water is described by the volume to be treated (e.g. [m^3 of water]) and potentially information about treatment capacity, i.e. minimum, mean, and maximum flow rates (e.g. [m^3/s]). While the total volume information is used to calculate volume-related inputs and outputs (e.g. electricity demand in [Wh/m^3]) for system operation, flow rates can be useful to define the size of the required infrastructure in terms of hydraulic capacity (e.g. tank volumes), which may also influence efficiency of the specific units or aggregates.

For quality parameters, chemical parameters should include basic water quality data (e.g. total solids, suspended solids, chemical and biological oxygen demand, total or dissolved organic carbon, phosphorus (total P, PO_4-P), nitrogen (total N, NH_4-N)), but also specific information on relevant substances of interest (e.g. inorganic or organic micropollutants such as heavy metals, pharmaceuticals, or endocrine disruptors) and other water quality parameters which may have an influence on treatment efficiency (e.g. spectral UV adsorption at 254nm, UV transmission). If microbial water quality is relevant (e.g. when assessing options for disinfection), indicator parameters (e.g. total heterotrophic plate counts, *E. coli*, *Enterococci*) as well as specific organism groups (e.g. *Salmonella*, MS2 phages, *Giardia*, *Cryptosporidium*) can be important.

It is important to define the reference (= influent) flow as precisely as possible to enable the deduction of treatment targets for water quality parameters (e.g. 80% reduction in COD) for the different process steps. Although LCA itself will describe only mean values of effluent water quality and related resource needs over a longer timeframe (typically one year), it may also be useful to quote min-max values for influent water quality parameters, as these may influence the required treatment if certain quality standards have to be fulfilled at all times.

[7] Corominas L, Foley J, Guest JS, Hospido A, Larsen HF, Morera S, Shaw A (2013). Life cycle assessment applied to wastewater treatment: state of the art. Water Research 47 (15), 5480-92

[8] Remy C, Miehe U, Lesjean B, Bartholomäus C (2014). Comparing environmental impacts of tertiary wastewater treatment technologies for advanced phosphorus removal and disinfection with life cycle assessment. Water Science and Technology 69 (8), 1742-1750

System boundaries

The definition of adequate system boundaries can have a decisive impact both on the LCA results and conclusions, but also on the amount of time and effort to be invested into the assessment for data collection. In general, the system boundaries should include all relevant processes that are influenced by the process under study. In practice, it is useful to limit the system boundaries to those parts of the system that presumably have a major impact on the LCA results. As this fact is not always directly obvious from the beginning of the study, the system boundaries may be developed in a kind of ranking, starting with the most important processes and moving to less important ones. Naturally, the selection presented below is not valid for all LCA studies in this field, but it can give some advice on how the system boundaries may be defined based on experience in previous LCA studies of water treatment.

The system boundaries should at least include:

- The water treatment process which is to be studied
- Electricity production required for the treatment
- Production of chemicals/additives required for the treatment (e.g. $FeCl_3$, polymers, NaOH, lime, activated carbon)
- Disposal of waste in high volumes (e.g. sludge etc.)
- Treatment of side-streams (e.g. backwash water) and its effect on the treatment train and upstream or downstream processes

Depending on the specific scope of the study, it may also include:

- Storage, pumping and distribution of water to the point of use or discharge
- Production of infrastructure for major equipment (typically ponds, tanks, filters, machinery, pipe systems)
- Specialized equipment with regular replacement (e.g. UV lamps)

In most LCA studies, infrastructure has only a minor impact on the overall environmental profile due to the long lifetime of equipment (10-50 a) used in water treatment and transport. However, if a low-energy treatment system is combined with large infrastructure (e.g. pipe distribution network) it is advisable to include major parts of the infrastructure in the LCA.

To understand the process under study and the system boundary definitions of an LCA, it is recommended to draft a flow diagram of the process that will be studied and all processes that will be included or excluded from the assessment (Figure 3-3). This will help the project team to understand the system and specify the LCA definitions in terms of system boundaries.

Co-products

Some processes and systems (especially in wastewater treatment) may deliver co-products beside the primary function of water treatment (e.g. nutrients N and P, electricity). These co-products can be accounted for in LCA by subtracting the related environmental burden for the substituted product (e.g. grid electricity, production of mineral fertilizer), following the "avoided burden" approach. However, the real substitution of products may not always reflect the full substitution potential that is theoretically available: if nutrients are applied at times without explicit nutrient demand of the crops, the actual substitution of equivalent mineral fertilizer will not be 100% of the applied nutrient, but only a fraction of it (e.g. 50%) on an annual basis. Hence, careful argumentation should be provided when describing the substituted products and their annual amount with regard to effective substitution potentials.

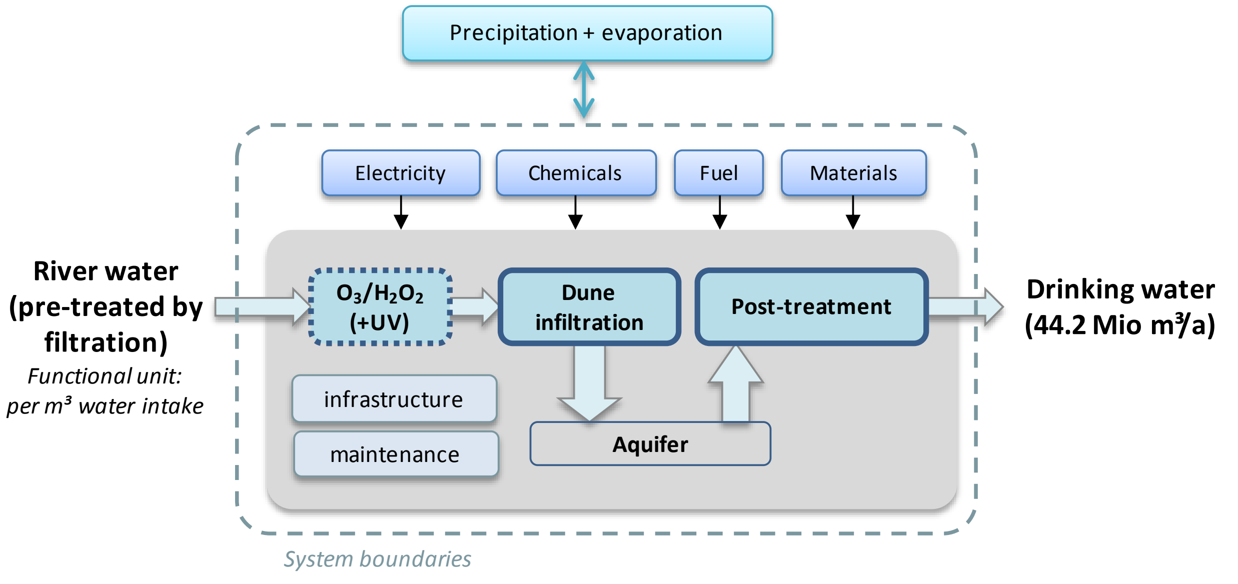

Figure 3-3: Examples of system boundaries for drinking water treatment (source: D51.1)

Scenarios

For a comparative LCA, different scenarios have to be defined which are then characterized and their potential environmental impacts are compared. The definition of scenarios should be most precise in technology terms, mentioning the technology/process to be analysed and its major features (e.g. oxidant dose, membrane pore size). For some scenarios, system boundaries may have to be adjusted if upstream or downstream effects are connected to the process (e.g. filter backwash water which is recycled to an upstream process).

While defining the scenarios, it is important to guarantee functional equivalency between compared alternatives, i.e. assure that each scenario fulfils the same primary system function as defined above. For LCA of water treatment processes, this equivalency is often related to a "minimum" water quality that has to be produced, because different treatment trains and processes will typically result in different water qualities while using different amounts of resources (e.g. electricity, chemicals). However, LCA can reflect on different water or product qualities with certain indicators, e.g. eutrophication (for nutrient emissions) or ecotoxicity (for pollutant emissions). Hence, different water quality discharged into the environment is somehow reflected in the LCA analysis, so that scenarios with different effluent water qualities can be compared in LCA if all of them deliver at least a minimum water quality defined for the system function. For drinking water processes, the product has to meet legal limits and guidelines values regulated in respective national or EU regulations.

Data quality

In general, input data quality is decisive for the validity and representativeness of the LCA results. For a valid and meaningful LCA study, the best achievable data quality should be targeted with respect to the goals of the study. However, data availability is often a limiting factor for the LCA. The following hierarchy lists potential data sources and qualities in a qualitative ranking:

1) Existing full-scale plants at the site
2) Pilot tests with industrial-scale units, using the original feed water quality
3) Small pilot tests with original feed water quality

4) Lab-scale tests with original feed water quality
5) Data from pilot/lab tests with simulated/feed water quality
6) Data from comparable studies at other sites or from literature

As LCA studies often investigate future options for water treatment ("prospective LCA"), full-scale data is often not available for all processes, especially if different technology options are compared that are still to be developed or optimized. Upscaling process data from pilot or lab-scale trials is often used for prospective LCA studies, but certain aspects have to be carefully addressed in this case (see below in Life Cycle Inventory/Collection of primary data). If data gaps are identified during the study, LCA data may be complemented with available data from comparable studies or literature, taking into account the effect of different feed water qualities on process design and performance and required treatment efficiency. In any case, transparency on the data quality used for the LCA should be high, so that the target groups of the LCA can make their own judgement on validity and representativeness of the LCA outcomes.

Assumptions and limitations

If assumptions are taken in the definition part of the LCA, they should be clearly explained and properly justified. This affects e.g. the exclusion of certain system parts from the system boundaries ("infrastructure is excluded from this LCA"), the crediting of co-products, or the filling of gaps in required process data with literature data. Likewise, obvious limitations of the LCA study should be communicated in a transparent way, so that the reader can clearly identify these limitations and include them in the interpretation (e.g. "heavy metals are excluded from the assessment of ecotoxicity").

Choice of impact assessment methods

The ISO standard provides no clear guidance on the choice of LCA impact assessment methods and indicators. A number of different systems for impact assessment have been developed in different locations, and many of them are used in practice for LCA impact assessment. However, this guideline will propose a minimum set of indicators that can be used for LCA assessment of water treatment processes. The choice is made with regard to most important environmental impacts of water treatment previously identified in LCA studies in this field, and also wide-spread application of the indicators in the LCA community. This guideline proposes a set of 11 indicators at mid-point level (i.e. in the middle of the cause-effect-chain), which are all related to a specific impact category (Table 3-1). End-point indicators which aggregate the environmental effects towards a certain area of protection (e.g. human health, ecosystem) are not recommended here, as they increase the uncertainty in modelling and lower the transparency of the results (see also chapter 3.4).

For the DEMEAU project, new aspects of impact assessment modelling have been tested and introduced in relation to the environmental impact of organic micropollutants (a focus area of DEMEAU technologies) and also to aspects of water footprinting. For this purpose, DEMEAU developed characterization factors for selected organic micropollutants towards their potential effect on human and ecotoxicity. In addition, a water scarcity footprint was calculated for selected case studies where direct water losses through evaporation (i.e. in groundwater recharge ponds for open infiltration) occur. Both methodological aspects are discussed below in chapter 3.2.1 and 3.2.2.

Table 3-1: Proposed set of LCA indicators for impact assessment

Impact category	Indicator	Unit	Contributing substances
Consumption of energy resources	Cumulative energy demand of fossil resources[9]	[MJ]	Hard coal, lignite, natural gas, crude oil
	Cumulative energy demand of nuclear resources[6]	[MJ]	Uranium
Climate change	Global warming potential (100a)[10]	[kg CO_2-eq]	CO_2 (fossil), N_2O, CH_4
Acidification	Terrestrial acidification potential (100 a)[7]	[kg SO_2-eq]	SO_2, NO_x, NH_3
Eutrophication	Freshwater eutrophication potential[7]	[kg P-eq]	P species in water
	Marine eutrophication potential[7]	[kg N-eq]	N species in water
Particulate matter	Particulate matter formation[7]	[kg PM_{10}-eq]	Fine dust (PM10)
Human toxicity	Human toxicity (non-cancer)[11]	[CTU_h]	Inorganic and organic toxic substances
	Human toxicity (cancer)[8]	[CTU_h]	
Ecotoxicity	Freshwater ecotoxicity[8]	[CTU_e]	Inorganic and organic toxic substances
Water scarcity	Water scarcity footprint[12]	[m^3-eq]	Water consumption

[9] VDI (2012). VDI guideline 4600: 2012-01: Cumulative energy demand - Terms, definitions, methods of calculation. Beuth Verlag, Berlin, Germany

[10] Goedkoop MJ, Heijungs R, Huijbregts MAJ, De Schryver A, Struijs J, Van Zelm R (2009). ReCiPe 2008, A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level; First edition Report I: Characterization. http://www.lcia-recipe.net

[11] Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts MAJ, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, van de Meent D, Hauschild MZ (2008). USEtox-the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. International Journal of Life Cycle Assessment 13 (7), 532-546

3.2.1 New characterization factors of selected organic micropollutants for human and ecotoxicity calculated with the USEtox® model

As one of the goals of the DEMEAU project was to assess the micropollutant removal efficiency of different technologies, the impacts of effluent water release on aquatic ecosystems as well as on humans who ingest treated drinking water or freshwater fish are key to quantify and understand.

These impacts were quantified in this project by the indicators freshwater ecotoxicity, human toxicity (cancer), and human toxicity (non-cancer) listed in Table 3-1. These indicators were assessed with the model USEtox[13], a scientific consensus and reference model for human toxicity and freshwater aquatic ecotoxicity. It is developed within the Life Cycle Initiative led by the UNEP/SETAC life cycle initiative, recognized as a state-of-the-art model by the European Commission (JRC-IES 2011[14]) and recommended in the Product/Organization Environmental Footprint guidelines (European Commission 2013[15]). USEtox allows modelling the cause-effect chain starting from the substance emission into air, water or soil and ultimately leading to impacts on ecosystems or human health.

In the European market, over 100'000 different chemicals are used and emitted[16], which makes a comprehensive assessment of toxic impact very data intensive. The USEtox model can currently screen about 3'000 chemicals in a published database, including for example pesticides, pharmaceuticals, and cosmetics.

In the DEMEAU project, a set of eleven substances were monitored to test the removal efficiency of selected technologies for emerging organic micropollutants. Among these eleven substances, six had previously not been covered in the USEtox database: bezafibrate, carbamazepine, diclofenac, iopromide, metoprolol and sulfamethoxazole. Hence, new characterization factors (CFs) for these substances were developed based on a literature review of physico-chemical and (eco)toxicity data, as well as updated CFs of other substances if additional toxicity data is available (as for the cancer effect of phenazone which is not accounted for in the USEtox database).

Physico-chemical data were derived from the chemical estimation programme EPI Suite™ version 4.0[17] for the USEtox fate calculations. This suite of physical/chemical property and environmental fate estimation programs is developed by the US EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC) and provides both experimental and modelled physic-chemical data. Experimental data is favoured when available. Ecotoxicity data relies on a literature review[18], where EC_{50} values are collected for each substance for freshwater organisms covering algae, crustacean and

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[12] Pfister S, Koehler A, Hellweg S (2009). Assessing the Environmental Impacts of Freshwater Consumption in LCA. Environmental Science & Technology 43 (11), 4098-4104

[13] Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts MAJ, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, van de Meent D, Hauschild MZ (2008). USEtox-the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. International Journal of Life Cycle Assessment 13 (7), 532-546

[14] JRC-IES (2011). ILCD handbook - recommendations for Life Cycle Impact Assessment in the European context. European Union report. 1–159

[15] European Commission (2013a). Commission recommendation on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations. Off J Eur Union 56:1–216

[16] Higgins T, Sachdev JA, Engleman S (2010). Toxic chemicals: risk prevention through use reduction

[17] US EPA (2012). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.10. United States Environmental Protection Agency, Washington, DC, USA

[18] Personal communication with Dr. Cornelia Kienle in DEMEAU, Swiss Centre for Applied Ecotoxicology

fish trophic levels leading to various endpoints such as luminescence inhibition, immobilisation or mortality. Mammalian toxicity data is used to extrapolate to human toxicity effect. LD_{50} and LC_{50} can be found for inhalation and ingestion data in literature, mainly for rats and mice. Then the minimal value is selected for the extrapolation to humans as conservative estimates. Final EC_{50} value (geometric mean across different trophic levels of freshwater organisms) and human ED_{50} values for cancer and non-cancer effects through inhalation and ingestion are calculated according to the procedure described in the USEtox User Guide[19]. Table 3-2 presents the developed characterization factors for human toxicity and freshwater ecotoxicity. Physico-chemical and (eco)toxicity USEtox input parameters are specified in Annex-D.

Table 3-2: Developed characterization factors (CFs) for human toxicity and freshwater ecotoxicity

CAS	Substance name	Human toxicity CF for emissions into freshwater [$CTU_h/kg_{emitted}$]			Freshwater ecotoxicity CF for emissions into freshwater [$CTU_e/kg_{emitted}$]
		Cancer	Non-cancer	Total	
41859-67-0	Bezafibrate	0.00E+00	1.83E-05	1.83E-05	1.27E+03
298-46-4	Carbamazepine	0.00E+00	2.22E-06	2.22E-06	7.63E+02
15307-86-5	Diclofenac	0.00E+00	1.86E-04	1.86E-04	1.91E+03
73334-07-3	Iopromide	0.00E+00	2.34E-07	2.34E-07	2.40E+01
51384-51-1	Metoprolol	0.00E+00	6.31E-07	6.31E-07	4.49E+03
60-80-0	Phenazone (Antipyrine)	3.64E-08	3.88E-07	4.24E-07	5.16E+01
723-46-6	Sulfamethoxazole	0.00E+00	4.64E-07	4.64E-07	4.68E+03

For comparison and validation, toxicity factors of all monitored substances including both developed and existing characterization factors (per kg substance emitted) are compared with organic substances covered in the USEtox database. Figure 3-4 presents the characterization factor of the monitored substances compared to more than 3'000 substances covered in USEtox. Monitored substances cover a wide range of toxicity, most toxic substance on human health (non-cancer) effect being diclofenac and the most toxic on aquatic ecotoxicity being sulfamethoxazole. These developed characterization factors were used to calculate the human toxicity and freshwater aquatic toxicity impact results shown and interpreted in deliverable D51.1.

These characterization factors have been integrated in the update version of the USEtox database at the release of USEtox2.0 in September 2015.

[19] Huijbregts M, Hauschild M, Jolliet O, Margni M, McKone T, Rosenbaum RK , van de Meent D (2010). USEtoxTM User manual. USEtoxTM team publication. 1–23. www.usetox.org

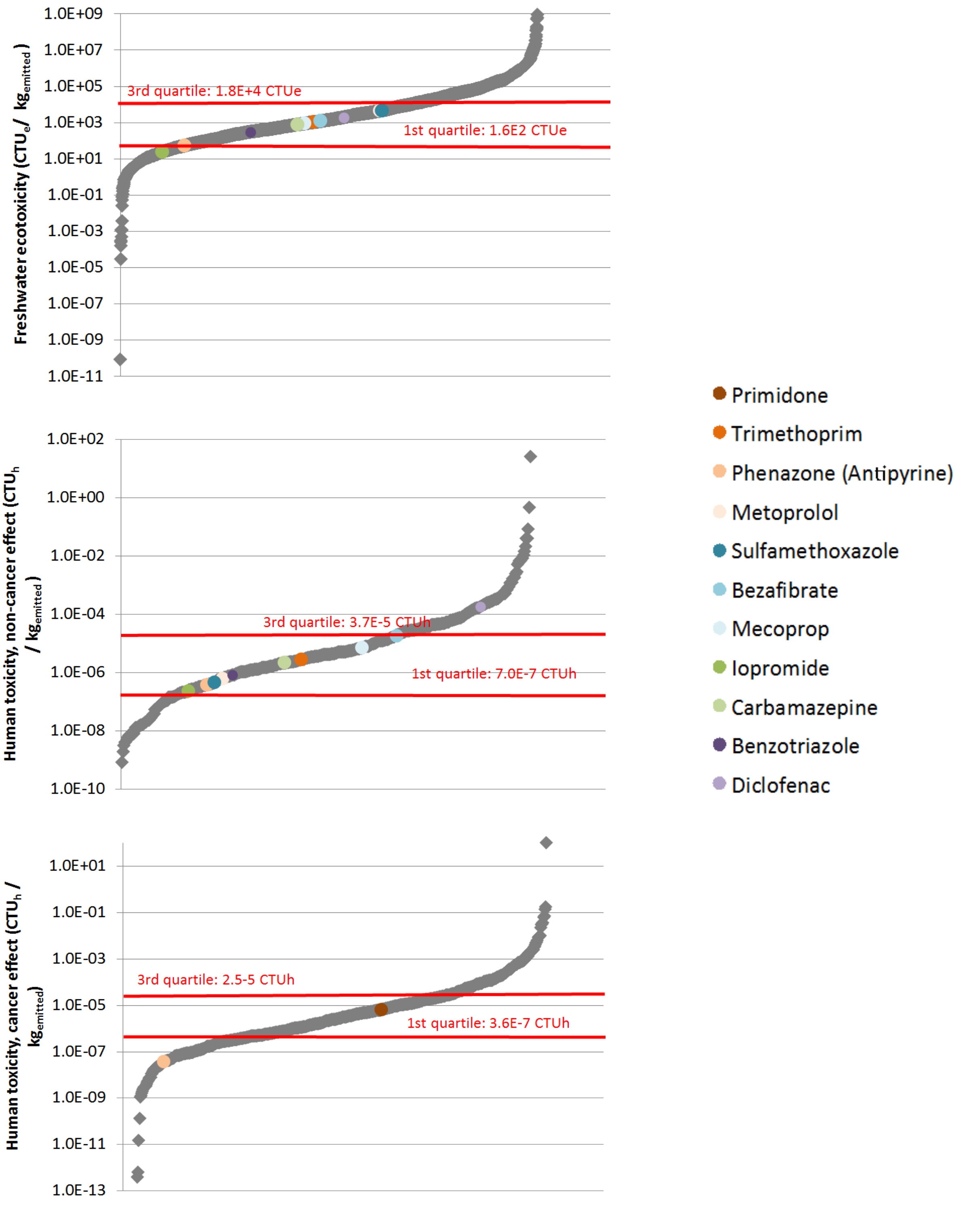


Figure 3-4: Characterization factors of monitored substances (coloured dots) vs. substances covered in USEtox (grey dots) for freshwater ecotoxicity (upper panel), human toxicity non-cancer (middle panel), and human toxicity cancer (lower panel)

3.2.2 Water footprinting: calculation of water scarcity footprint

In general, a water footprint (WFP) is a set of methods that assesses quantitative and qualitative impacts of water withdrawal and discharge, as well as emissions into water or air that affect water quality. In line with the life cycle perspective of LCA, WFP accounts for qualitative and quantitative impacts throughout the system under study and related upstream and downstream processes. WFP has recently been standardized in a new ISO standard (ISO 14046[20]) aligned on the ISO 14040/14044 standards, where basic requirements have been formulated towards a methodological framework for WFP. Currently, many different methods for WFP are used in the scientific community with different focus and purposes (see review of methods addressing water scarcity[21]), and new methods are still being developed.

According to ISO 14046, a comprehensive water footprint shall be expressed as a water footprint profile which encompasses:

1) **Water availability footprint:** this WFP assessment method accounts for reduced water availability through consumption and degradative use, addressing also water quality aspects of water withdrawal and release on available water resources

   OR: Water scarcity footprint: this footprint is defined as a water availability footprint that considers only water quantity (no quality aspects)

2) **Water degradation footprint:** this assessment provides the contribution of a product, process or organization to potential environmental impacts related to water quality (e.g. aquatic eutrophication, aquatic acidification, aquatic ecotoxicity, thermal pollution)

Besides the ISO-based WFP methods, other approaches exist to assess the impact related to water scarcity and degradation such a the volumetric approach of the Water Footprint Network[22].

WFP results reflect a specific set of impacts related to water that can be used by stakeholders interested in these specific issues. However, to keep a global perspective across all existing impact indicators, the water availability/scarcity footprint should be integrated with other “conventional” impact indicators of LCA, where water degradation footprint being usually already accounted.

For LCA studies in the field of water and wastewater treatment, water footprinting has only been applied in few case studies[23,24] using different methodologies. Within DEMEAU, a simple water scarcity footprint (WSF) methodology is tested for selected case studies to develop an understanding of the meaning of WSF for water treatment processes, and to test available methodologies on the inventory data that has been collected. For water inventory data of consumed water for the background processes, extracts from the Quantis database[25] have been used which describe a water

[20] ISO 14046 (2014). Environmental Management - Water Footprint - Principles, Requirements and Guidelines. Inernational Standardisation Organisation, Geneva, Switzerland

[21] Kounina A, Margni M, Bayart JB, Boulay AM, Berger M, Bulle C, Frischknecht R, Koehler A, Milà I Canals L, Motoshita M, Núñez M, Peters G, Pfister S, Ridoutt B, Van Zelm R, Verones F , Humbert S (2013). Review of methods addressing freshwater use in life cycle inventory and impact assessment. International Journal of Life Cycle Assessment 18 (3), 707-721

[22] Hoekstra AY, Chapagain AK, Aldaya MM, Mekonnen MM (2011). The Water Footprint Assessment Manual: Setting the Global Standard. Water Footprint Network, Enschede, NL

[23] Shao L, Chen GQ (2013). Water footprint assessment for wastewater treatment: Method, indicator, and application. Environmental Science and Technology 47 (14), 7787-7794

[24] Risch E, Loubet P, Núñez M, Roux P (2014). How environmentally significant is water consumption during wastewater treatment?: Application of recent developments in LCA to WWT technologies used at 3 contrasted geographical locations. Water Research 57 20-30

[25] Quantis (2011). http://www.quantis-intl.com/waterdatabase/software.php. Lausanne, Switzerland

inventory for all background processes such as electricity or chemicals production. In DEMEAU, the water degradation footprint was already estimated through the indicators for human toxicity, freshwater ecotoxicity, and freshwater eutrophication. These default indicators are complemented with a water scarcity footprint, chosen because of its simplicity of calculation, the limited amount of data that is required for the impact assessment, and to test the applicability and usefulness of this indicator method for water treatment systems.

Water scarcity footprint (WSF)

A water scarcity footprint can be calculated by multiplying the direct and indirect water consumption of a process or scenario with the related water scarcity index (WSI). For this case study, the following data has to be collected:

- Direct water consumption of the process (e.g. evaporation, export in food) based on a local water balance [e.g. m^3 per functional unit]
- Indirect water consumption of the background processes (e.g. for electricity production). This information is extracted from Quantis database and is also incorporated in the latest version of the ecoinvent database v3.1[26]
- Water scarcity indices (0.1-1) from Pfister et al. (2009)[27] which are also publically available as a layer in GoogleEarth[28] in a 0.5°/0.5° gridcell scale (Figure 3-5). National average WSI in country-scale are available as excel-file.

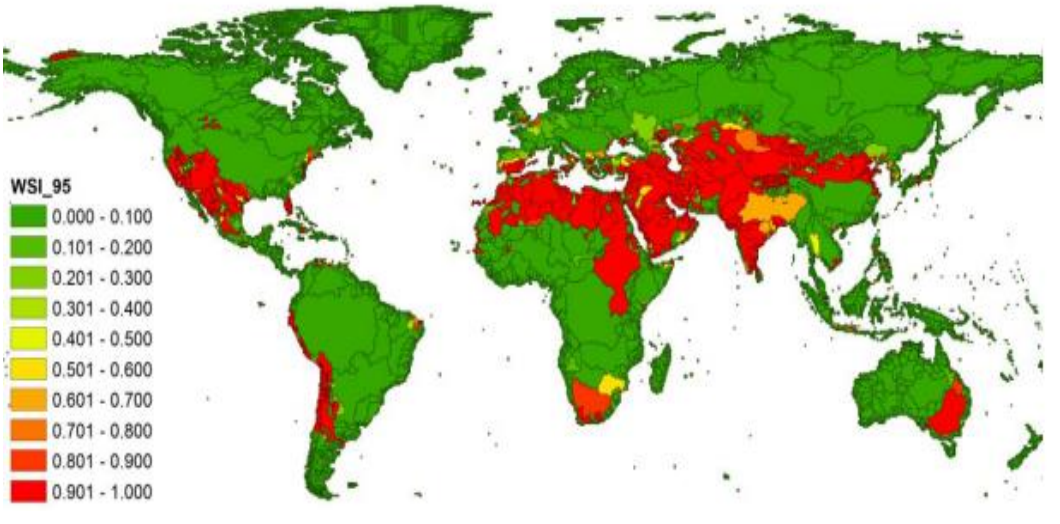


Figure 3-5: World map of water scarcity index[24]

Multiplying the water consumption data with the respective WSI gives a water scarcity footprint in m^3-eq. For background processes such as electricity or chemicals production, national or European average WSI can be used to reflect average conditions in these countries. Summing up all direct and indirect contributions gives the total water scarcity footprint of the system. An example of how to calculate a water scarcity footprint is described below.

[26] Ecoinvent (2014). Ecoinvent data v3.1, ecoinvent reports No. 1-26, Swiss Center for Life Cycle Inventories, www.ecoinvent.org. Dübendorf, Switzerland

[27] Pfister S, Koehler A, Hellweg S (2009). Assessing the Environmental Impacts of Freshwater Consumption in LCA. Environmental Science & Technology 43 (11), 4098-4104

[28] http://www.ifu.ethz.ch/ESD/downloads/EI99plus

Illustrative example of calculating a water scarcity footprint (WSF)

Water system:	Open infiltration pond for groundwater recharge

Simplified inventory

Input data:	Water evaporation from open groundwater pond: 1'000 m^3/a
	Electricity for pumping: 10'000 kWh/a
	Excavation for pond construction: 10'000 m^3 (lifetime: 40 a)

Addition information

Indirect water use:	Electricity production consumes 100 L/kWh
	Excavation consumes 400 L/m^3 (data from Quantis database)
Water Scarcity Index:	Taken from the Google Earth layer provided by Pfister et al. (2009)
	WSI = 0.7 (local at site, i.e. high water scarcity)
	WSI = 0.3 (country mix, for electricity production and excavation)

Calculation of WSF

WSF (direct):	1'000 m^3/a* 0.7 = 700 m^3-eq/a	(evaporation)
WSF (indirect):	10'000 kWh/a * 0.1 m^3/kwh * 0.3 = 300 m^3-eq/a	(electricity)
	10'000 m^3/40a * 0.4 m^3/m^3 * 0.3 = 30 m^3-eq/a	(excavation)
WSF (total):	700 + 300 + 30 = 1'030 m^3-eq/a	

Results and interpretation

The water scarcity footprint of this groundwater pond is 1'040 m^3-eq/a, with 700 m^3-eq/a of direct water losses in evaporation and 330 m^3-eq/a for indirect water losses due to electricity generation and excavation. This footprint has to be taken into account when evaluating the water scarcity footprint of the groundwater recharge facility.

3.3 Life Cycle Inventory (LCI)

For the Life Cycle Inventory, both primary data (= process data of the water treatment process, water quality data) and background data (= datasets for background processes such as electricity production) are required. In general, primary data has to be collected by the LCA practitioner from the information available from the site, whereas background data is taken from LCA databases with the help of specific software. Background data can be extracted from dedicated LCA databases.

Collection of primary data

Primary data for the LCA relates to all relevant data of the water treatment process. This data can be divided into three sub-groups: a) data on water quantity (volume) and water quality improvements, i.e. treatment efficiency; b) process data on required electricity, chemicals, and infrastructure; and c) data on waste quantity and quality. Collection of this data should follow a systematic approach, e.g. using an excel-based template, which lists all relevant data required for the LCA. Collected data should represent the mean operating conditions of the treatment process over the respective time-frame of the LCA, e.g. operation during one year. Hence, primary data from lab, pilot or full-scale installations should be processed to reach most representative mean data for the system.

A typical dataset for inventory data of a water treatment process contains information on water influent and effluent volume and quality, electricity and chemicals required, and waste flows such as sludge or backwash water (example in Figure 3-6 for a DEMEAU case study of ultrafiltration). Water quality data can often be directly transferred from lab/pilot studies to represent full-scale plants. Likewise, operating parameters such as chemical dosing or waste streams (volume of backwash water, sludge amount) may be transferred directly from pilot to full-scale design, but this transfer has to be carefully justified. For chemical dosing, it is highly important to report the actual chemical formula of the chemical dose (e.g. g Al or g polyaluminium chloride $Al_5(OH)_3Cl_2$) and the respective concentration of the chemical in the applied product (e.g. $FeCl_3$ (40% in H_2O)) (Table 3-3).

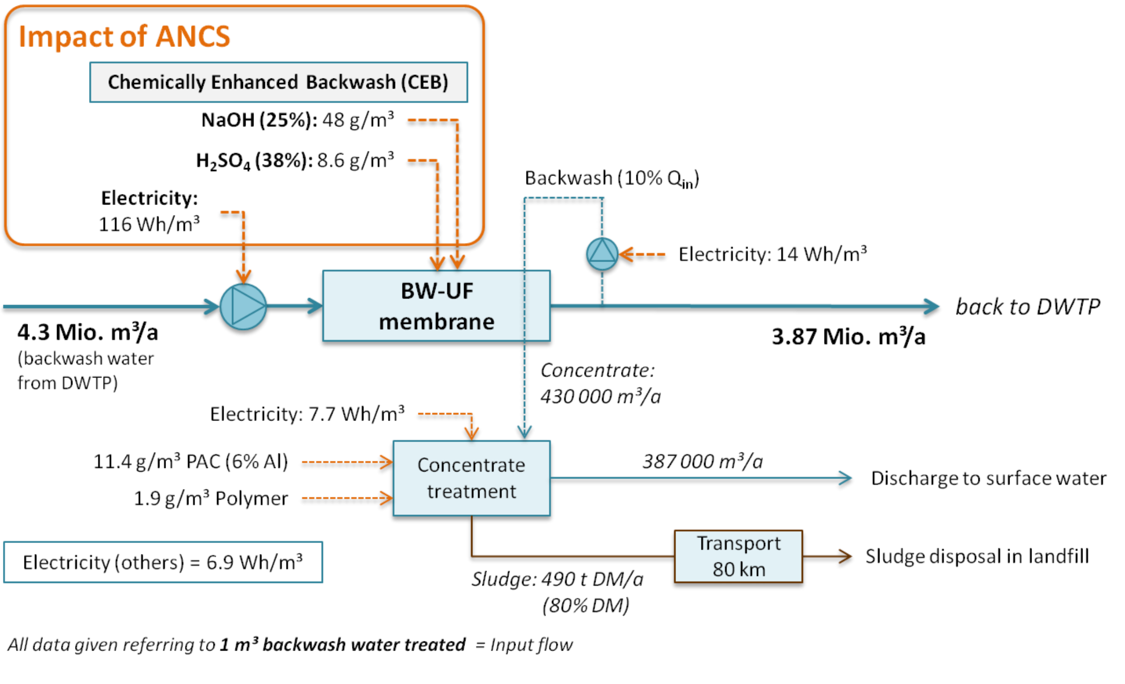


Figure 3-6: Life Cycle Inventory for operation of ultrafiltration plant for backwash water treatment (source: D51.1)

For electricity as one of the most important inputs to water treatment processes, upscaling from lab or pilot installations to full-scale has to be based on detailed engineering, as electricity demand of small aggregates and pilot installations is often not optimised and does not represent the actual electricity demand of the full-scale process. In case of water pumping, pressure head (e.g. for water lifting) or required feed pressure (e.g. transmembrane pressure for membranes) can be used to estimate full-scale electricity demand, using a rule-by-thumb of 5 Wh/m^3 for each m of water head (or 50 Wh/m^3 for 1 bar of feed pressure). For other electricity consumers (e.g. ozone generators, UV systems), applied doses can be recalculated to electricity demand using literature information (e.g. 10-15 kWh/kg O_3 generation) or supplier data.

Validation of transferred primary data by case study partners

The validation and cross-check of transferred primary data with data suppliers (e.g. site operators, external partners or companies) is a decisive task in data collection to ensure high input data quality for the LCA study and increase trust of internal and external partners in the LCA outcomes. Therefore, it is highly recommended to summarize the collected data in a suitable format which can be directly used as input for the LCA model and to send this data to the respective partners for final validation. In this way, transferred data can be cross-checked by the respective experts for potential errors introduced during data transfer and recalculation, e.g. relating to simple number errors, wrong physical units or transfer between physical units, or misunderstanding of process data or layout by the LCA practitioner. Bilateral data validation usually requires some time and effort of all participants, but this step leads to a final dataset which is accepted by all partners and can thus provide high quality results in LCA impact assessment.

Background data

Background data for the LCA describes the inventories of background processes such as electricity production, chemicals production, or production and transport of materials for infrastructure. These datasets can be extracted from LCA databases, with the ecoinvent v2.2 database[29] being one of the most widely used databases publically available. These databases can be accessed and evaluated with the help of specific LCA software (e.g. UMBERTO, GaBi, SIMAPRO, Quantis Suite, OpenLCA, etc.).

When using background datasets, the LCA practioner has to choose the most representative available dataset for the specific LCA study, especially considering the location of the case study. For electricity production, local supply mixes are available for each European country at medium voltage, which is mostly used for industrial processes such as water treatment plants. For production of chemicals and materials, country-based datasets are often not available in the database, so that these processes have to be described by datasets relating to average European or even global data. If no dataset is available for a chemical or material, its production can be approximated by comparable materials (e.g. using HDPE dataset for other plastic materials) or by precursor products (e.g. acrylonitrile as precursor of acrylamide and also polyacrylamide) (Table 3-3).

All required materials for infrastructure have to be scaled to an annual basis to be comparable to operational efforts. Therefore, material demand for plant construction is divided by the assumed technical lifetime of the respective aggregate or building. Typical lifetimes assumed for infrastructure of water treatment are 30-50 a for tanks, pipes and buildings and 10-15 a for machinery, aggregates and pumps. Specific aggregates with regular replacement (e.g. membranes, UV lamps) have dedicated expected lifetimes which have to be defined in cooperation with the site operators and the suppliers.

For transport of chemicals or materials, road transport by truck is usually assumed from the production site to the water treatment plant. Transport distances can be estimated based on local

[29] Ecoinvent (2010). Ecoinvent data v2.2, ecoinvent reports No. 1-26, Swiss Center for Life Cycle Inventories, www.ecoinvent.org. Dübendorf, Switzerland

information about location of potential suppliers. Usually, specifically manufactured materials and chemicals are transported over longer distance (e.g. HDPE pipes, $FeCl_3$ solution) with estimates ranging from 200-600 km, while heavy materials such as concrete, sand or gravel are produced more locally (20-50 km). However, these estimates can be adjusted based on the local setting of the case study and available information.

Table 3-3: Exemplary list of typical chemicals used for water treatment and related LCA datasets from Ecoinvent[30]

Chemical	Concentration	Related dataset of Ecoinvent database
$FeCl_3$	40%	Iron (III) chloride, 40% in H_2O, at plant [CH]
Polyaluminium-chloride	10% as Al	Mixing of Al_2O_3 (190 kg) and HCl (220 kg, 30%) before conditioning, using 30 kWh electricity and 192 kWh heat
Polymer	100%	Acrylonitrile from Sohio process, at plant [RER] (53 kg acrylonitrile are hydrolysed into 71 kg acrylamide)
H_2SO_4	37.5%	Sulphuric acid, liquid, at plant [RER]
HCl	30%	Hydrochloric acid, 30% in H_2O, at plant [RER]
Citric acid	100%	For 1000 kg citric acid: fermentation of 4750 kg molasse, separation and purification using 960 kg H_2SO_4 (37%), 128 kg HCl (30%), 1000 kg limestone, 3000 kWh electricity, 71.4 GJ heat, and 600 m^3 water
NaOH	50%	Sodium hydroxide, 50% in H_2O, production mix, at plant [RER]
NaOCl	15% as Cl	Sodium hypochlorite, 15% in H_2O, at plant [RER]
MEM-X	4% (as tenside)	For tenside: fatty alcohol sulphate, petrochemical, at plant [RER]

Disposal of construction materials or waste flows (e.g. organic or inorganic sludge) can be described with selected LCA datasets for disposal pathways. However, datasets are not available for all disposal routes for all types of materials or waste flows. It is recommended to include waste disposal at least for all waste with is routinely produced at the treatment process, also using most suitable datasets for approximation if no specific dataset is available. Disposal of construction materials often has only minor impacts on the overall environmental profile of water treatment processes, as infrastructure in

[30] Remy C (2013). Life Cycle Assessment and Life Cycle Costing of tertiary treatment schemes. Kompetenzzentrum Wasser Berlin, Berlin, Germany gGmbH, www.kompetenzwasser.de/Abschlussberichte-des-Projektes-OXE.572.0.html

general has a minor contribution to the total impacts compared to operational use of chemicals or electricity[31,32,33].

3.4 Life Cycle Impact Assessment (LCIA)

For impact assessment in LCA, results of midpoint indicators should be reported for all scenarios. Typically, column charts or bar charts are used which present the absolute indicator scores related to the functional unit (e.g. kg CO_2-eq/m^3 water) (Figure 3-7). For contribution analysis, the indicator score and chart should be divided into most important processes and contributors (e.g. electricity demand, chemicals, infrastructure, direct emissions during operation, etc.). It can be helpful to further sub-divide the contributions in different process stages (e.g. ozonation, filtration, UV disinfection) to allow the reader to track the differences between scenarios to the features of the different processes in comparison.

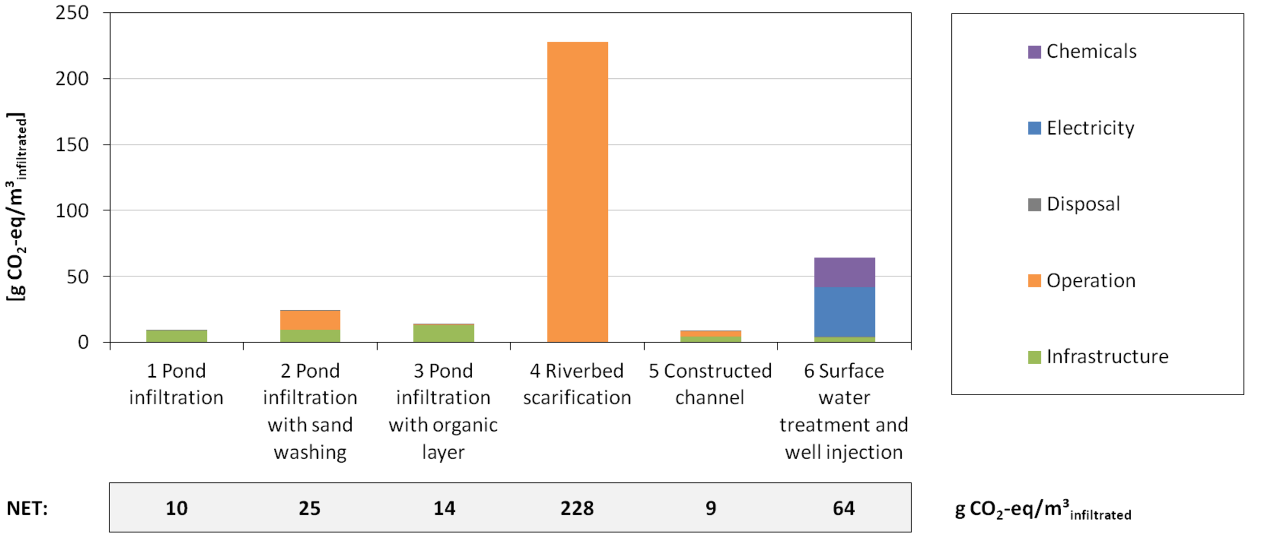


Figure 3-7: Global warming potential per m^3 infiltrated water for different scenarios for groundwater recharge (D51.1)

For an overview of all LCA results, different LCA indicators cannot be easily displayed in absolute scores together in one chart as they all relate to specific units of impact (e.g. CO_2-eq, MJ, P-eq). However, a suitable way to show the complete picture for all impact categories is a relative chart, where all scenarios are evaluated in % in relation to the scenario with the highest score in this impact category (= 100%). In this way, comparative LCA results can be presented in a single diagram showing all indicator results and the relation between the different scenarios (Figure 3-8).

[31] Lundie S, Peters GM, Beavis PC (2004). Life Cycle Assessment for Sustainable Metropolitan Water Systems Planning. Environmental Science & Technology 38 (13), 3465-3473

[32] Lassaux S, Renzoni R, Germain A (2007). Life Cycle Assessment of Water from the Pumping Station to the Wastewater Treatment Plant. International Journal of Life Cycle Assessment 12 (2), 118-126

[33] Remy C, Jekel M (2012). Energy analysis of conventional and source-separation systems for urban wastewater management using Life Cycle Assessment. Water Science and Technology 65 (1), 22-29

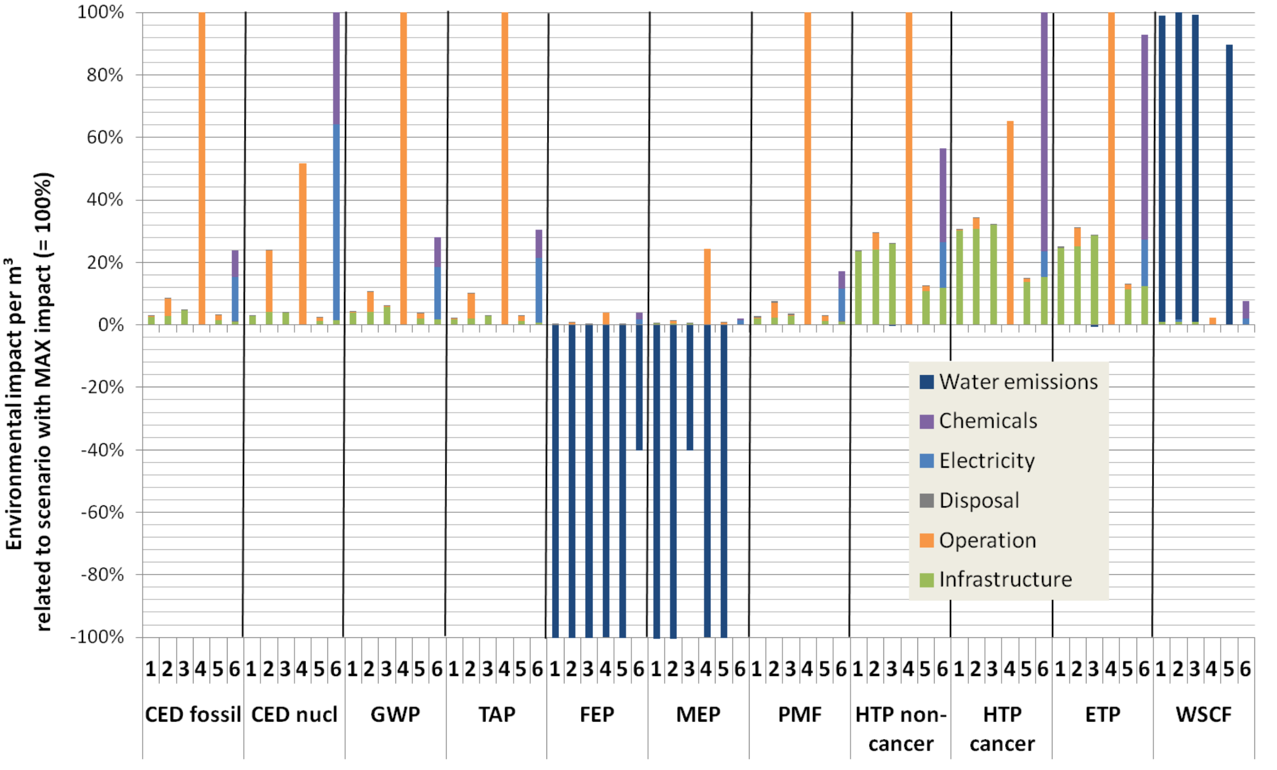


Figure 3-8: LCA results for 11 environmental indicators of six scenarios for groundwater recharge (D51.1)

In a further step, LCA indicator values may be normalised to the total environmental impact of an average person per year. Normalisation data is available for EU27 population, based on resource and emission inventories for the entire EU27 and respective LCA indicator scores. If LCA indicator results are normalized, they can provide information of the magnitude of contribution from the water treatment process under study in relation to the total environmental footprint of society. However, normalisation is not applied within the DEMEAU LCA framework, as the focus is on comparing different options for water treatment and not their contribution to the total environmental impacts in society.

Apart from normalisation, further aggregation of LCA indicators towards end-point based scores or single indicators is not recommended here. While end-point methods introduce further uncertainty by modelling the cause-effect chain towards the final end-point, aggregation of LCA results into single indicators requires subjective weighting of the impact categories against each other. If weighting and aggregation is applied, it is highly recommended to report LCA indicator results also at the midpoint level to allow a transparent assessment of the individual indicator results prior to discussing the aggregated scores. Instead of reporting end-point indicators as final results to relevant stakeholders, the DEMEAU team has opted for an approach based on economic and environmental 'unique selling propositions' which at mid-point levels allows pin-pointing specific environmental benefits and trade-offs (see also section 6.3).

3.5 Interpretation

The interpretation of the LCA study should deliver a short summary and discussion of the major conclusions from the LCA study. All phases of the LCA can be addressed in the discussion. For interpretation of LCA indicator results, a comprehensive reflection should be made on the entire LCA study and its limitations towards fulfilling the projected goal. In particular, the following questions can be addressed:

- What data quality could be reached for the LCA input data? Is the data quality sufficient for the projected goal of the study? Where might be limitations in terms of representativeness? Are there known uncertainties in up-scaling from lab/pilot scale to full-scale operation?
- Are the results stable against variation in input data? For this purpose, sensitivity analysis can be employed which varies important input data or assumptions (e.g. treatment efficiency, dosing of chemicals) and shows the influence of these variations on the outcomes of a comparative LCA
- Can the results be transferred to other cases? What are the main influencing factors (e.g. in terms of influent water quality) for the performance of the treatment process?
- What recommendations can be given based on the conclusions from this LCA study?

The interpretation should reflect the fact that the indicator results are based on a relative approach, that they indicate potential environmental effects, and that they do not predict actual impacts on category endpoints, the exceeding of thresholds or safety margins, or give information on associated risks.

4 Life Cycle Costing (LCC)

4.1 Methodological framework

Comparing costs can be done either for a static point in time or – in a more sophisticated way – over a certain timeframe in the past or in the future. Life Cycle Costing (LCC) is one example of the latter category that is often referred to in dynamic cost calculations. Sometimes the time horizon of such calculations is fixed by simplifying means. But as the name already suggests, the timeframe of LCC should actually cover the whole life cycle of the technology from production over use until disposal. This is a main difference to the Total Cost of Ownership (TCO) approach that describes only the costs occurring in the operating and removal phase. TCO can therefore be seen as a part of the life cycle cost model that aims to include all costs (and revenues) from a "cradle-to-grave-perspective". In combination with a Life Cycle Assessment (LCA) that investigates the environmental impacts of a product or service (Chapter 3), and the analysis of drivers and barriers (Chapter 5), LCC can serve to address the economic dimension of sustainability.

In contrast to Life Cycle Assessment, Life Cycle Costing does not follow a defined methodological framework. Nonetheless there are several guidelines trying to enable a systematic collection and calculation of costs associated with certain products, services or measures. One possible approach for performing a LCC analysis for water and wastewater treatment processes based on experience and learning from the DEMEAU project will be described on the following pages. In analogy to LCA, four steps can be distinguished for the iterative process of a LCC:

1) Definition of goal and scope of the LCC study
2) Collection of cost data
3) Definition of key parameters and calculation
4) Presentation and interpretation of results including discussion on their stability towards important assumptions (sensitivity analysis) and on limitations of the study results

4.2 Goal and scope definition

Defining the goal and scope of LCC is an important step although most of the decisions should be already made in defining the specific goal and scope of the LCA. Nevertheless, it is worthwhile doing it to keep in mind what the LCC is supposed to be done for.

Within DEMEAU the LCC is used in the context of a cost comparison calculation which is a common way to compare the costs of options in order to identify the "best investment". As the target group of the cost assessment consists of decision makers in operating companies or utilities, the decision rule for the cost comparison in LCC is very simple: "prefer the option with the lowest costs".

The options of the cost comparisons in DEMEAU are several innovative technologies for micropollutant removal that are compared to conventional alternatives in order to find their unique selling propositions. This means that different scenarios have to be defined for the LCC. Even if there are already some scenarios given by LCA (see chapter 2.2), there might be more scenarios required for the LCC, for example, if different financing modes are available within a single scenario (e. g. contracting, leasing). Differentiating these options may easily be done by adding letters to the scenarios defined in the LCA (e. g. splitting scenario 1 into scenario 1a and 1b).

Using a well-defined system boundary and functional unit is a crucial factor for LCC as well as LCA. In general, system boundaries for LCC may be defined easiest according to cost accounting by the case study partners. But in order to assure consistency in results and facilitate the combined interpretation of LCA and LCC results, system boundary and functional unit of LCC should preferably be chosen in alignment with those of the LCA. For water treatment processes, costs are therefore usually calculated in relation to the influent flow (e.g. [EUR/m^3_{Qin}]) or effluent flow (e. g. [EUR/$m^3_{treated}$]) of the process over the lifetime. Nevertheless, it is also imaginable to choose other functional units as long as they are consistent with the units used for LCA (see chapter 3.2).

4.3 Data collection

For calculating life cycle costs it is necessary to collect all costs occurring in each phase (setup, operating, and removal) of the water treatment process´ lifetime. Revenues occurring from e.g. waste disposals or appearing as residual value of infrastructure after the considered time frame have to be included in the calculation as "negative costs" as well. In general, this cost information is collected best as real costs directly from the site owners. Missing data has to be derived from literature or estimated by expert consultation or educated guess which is regularly associated with high uncertainty, limited data quality, validity and representativeness of LCC results from the beginning. In order to ensure a high quality of results, real cost data should therefore be targeted at first. Concerning the issues of data quality, assumptions and limitations in LCA and LCC, and validation of transferred primary data by case study partners, the reader is referred to chapters 3.2 and 3.3.

In order to facilitate the data collection process for the process owners and to ensure that all relevant costs will be collected, two major considerations were made within data collection for LCC in DEMEAU project:

Identification of main cost drivers

At a first stage main cost drivers of technology implementation were identified. Having an overview of all major cost categories relevant for water treatment systems helps to collect all cost data in a structured way and limit the efforts of data collection to those costs that presumably have major impacts on life cycle costs in the end. A list of the six main cost drivers identified for DEMEAU´s technologies is presented in the table below (Table 4-1).

This list may be not valid for all LCC studies in this field, but it can give some idea of costs required to perform a detailed LCC in order to design an excel-based template, which lists all necessary data required for LCC to be used for the following collection of cost data.

Table 4-1: Main cost drivers for water treatment systems

Category	Examples in this category
Assets	real estate, technical equipment and machines, factory and office equipment, intangible assets, etc.
Personnel	salaries and wages, internal training costs, etc.
Material	energy, raw materials, operating supplies, waste disposal, etc.
Services	expertise/consultancy, costs of project entity, external substituting services (e. g. maintenance, inspection, cleaning, analyses), etc.
Financing	capital acquisition costs, capital interests, fees (e. g. water abstraction charges), administrative charges, etc.
Taxes and dues	value added taxes, local business taxes, corporate taxes, compensation payments for failures, etc.

Collection of cost data

Based on this first assessment cost, data should be collected. While collecting the life cycle cost inventory in the categories described above, two major cost categories should be distinguished from the beginning in order to facilitate further calculations: capital expenditure (CAPEX) and operational expenditure (OPEX).

CAPEX includes all initial and follow-up payments for acquiring assets, fixing problems with existing assets, preparing assets to be used in business and costs for property (e. g. Figure 4-1). The biggest part of CAPEX usually is already spent even before a new measure is operational. But it is also necessary to consider reinvestments for each part of the system after its lifetime ends, so that the whole system can be used longer than its original lifetime. By doing this, it is also possible to compare life cycle costs of technologies or measures with deviating lifetimes by choosing the least common multiple of both lifetimes as time horizon for the analysis. From a theoretical point of view the reinvestment can be just as high as the investment at the beginning of the project adjusted to inflation. As water treatment and networks are usually strongly associated with high long-term investments, capital expenditure has a major impact on the overall life cycle costs. It should therefore be carefully collected and/or transferred from pilot to full-scale plant together with the case study partners involved in order to reach most accurate results and increase trust of internal and external partners in the LCC outcomes (see chapter 3.3).

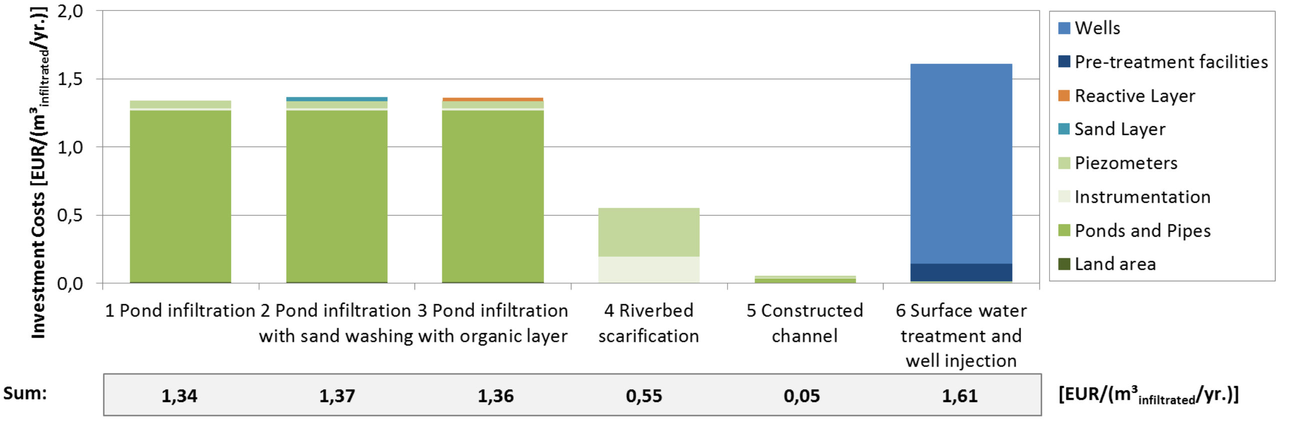


Figure 4-1: CAPEX per system capacity for managed aquifer recharge scenarios in a DEMEAU case study (source: D51.1)

In contrast, OPEX are the ongoing costs for a measure (e. g. Figure 4-2). They include all kinds of payments for supplies and raw materials, maintenance and repair, administration, insurance, salary and wages, fuel and electricity and so on, that occur on a regular basis (e. g. annually). Relevant operational cost data is all expenses directly induced by technology operation as well as all overhead costs linkable to that. As the allocation of overhead costs is strongly depending on a company´s internal accountancy system, overhead costs are always associated with uncertainty and should therefore be added with precaution. If operational costs have to be transferred from pilot to full-scale implementation, then this should be done in close collaboration with process engineers and LCA practitioners for ensuring that the full-scale costs are adjusted to take into account missing optimisations of e. g. energy demand at lab or pilot installations in an appropriate way (see chapter 3.3). Thus, it might be helpful in some cases to collect specific costs [EUR/unit] information additionally or instead of absolute cost information for operational expenditure.

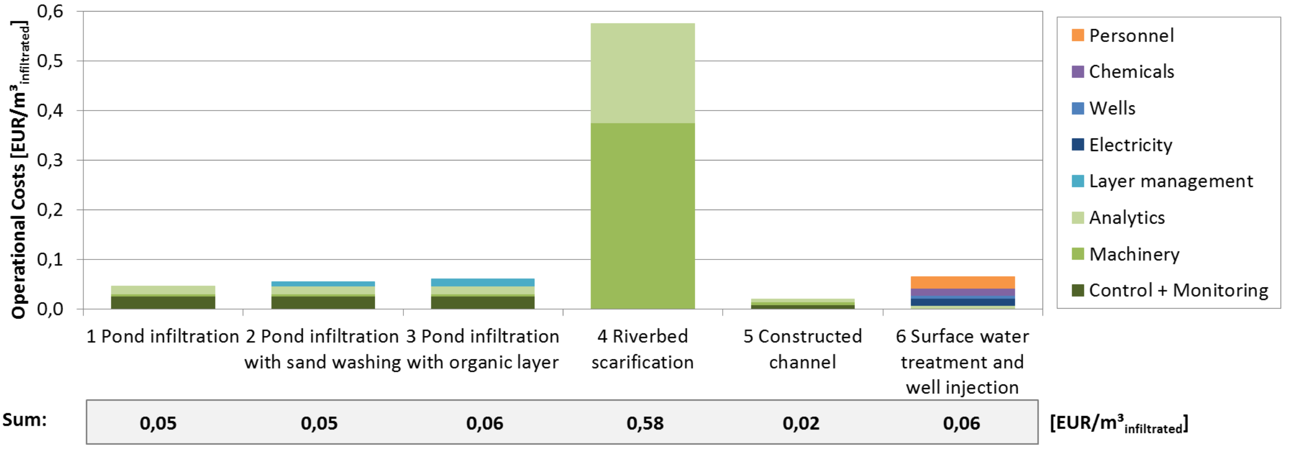


Figure 4-2: OPEX per m³ infiltrated water for managed aquifer recharge scenarios in a DEMEAU case study (source: D51.1)

If costs are only available in foreign currencies they should be converted into the currency chosen for calculation using the mean exchange rate of the base year of the calculation. For example in a DEMEAU case study conducted at a WWTP in Switzerland most of the costs had to be converted using the mean exchange rate of Euro versus the Swiss franc in 2013 (1 EUR = 1.2311 CHF) according to the European Central Bank[34]. If there are no real costs available and prices have to be derived from literature theses should be corrected in order to account for deviations in time but also location. Here, the Chemical Engineering Plant Cost Index[35] (CEPCI) can help to adjust historic prices with regard to inflation and price increases. To obtain current prices, the outdated price is divided by the CEPCI of the corresponding year and multiplied by the target year.

Besides all this cost data, there is some general information needed, including information on the cycle structure (service life years for setup phase, operating phase and removal phase) and the system´s performance (e. g. water inflow/outflow per year, utilisation rates). As far as these are not already covered by Life Cycle Inventory, general data has to be gathered in this stage of the assessment process as well.

4.4 Definition of key parameters and calculation

Besides the input cost data, the most decisive parameters for the calculation of life cycle costs are the assumptions for life cycle duration, the discounting rate and the inflation rates.

Life cycle duration

Within LCC costs are accounted for each period over the whole lifetime for each measure. Usually each of these periods is considered to equal a year. The life cycle duration should be defined in accordance with the economic lifetime of the system that is supposed to equal the technical lifetime as a general rule. For water treatment systems in general, a life cycle of 30 years is often assumed, but this estimate has to be proved case by case. Regarding Managed Aquifer Recharge (MAR), for instance, quite shorter lifetimes of the systems (3-18 years) have to be assumed according to the local experts. In order to enable comparisons of life cycle costs with a conventional treatment system in the end,

[34] ECB (2014). Statistical data warehouse. Europen Central Bank, Frankfurt am Main, Germany, http://sdw.ecb.europa.eu/quickview.do?SERIES_KEY=120.EXR.A.CHF.EUR.SP00.A

[35] Vatavuk WM (2002). Updating the Cost Index. In: Chemical Engineering, Issue 1, p. 62-70

LCC should always be calculated for harmonized project durations which can be defined as least common multiple of all systems lifetimes. If the lifetime of a whole system or some technical equipment ends before this harmonized project duration is reached, reinvestments that would have to be made in practice have to be reflected in the calculation as well. In DEMEAU a 'cash flow oriented' approach was chosen for this issue which means that reinvestments are considered in their full amount in the period they occur and seized in total by the discounting factor of this period of the life cycle. This is a major difference to LCA, where e.g. the material demand for plant construction is divided by the assumed technical lifetime of the system (= assuming a time-independent mean material demand for each year), but the cash-flow oriented approach is a more accurate approach to cost calculations and economic impacts from the operators perspective. For some parts of the system (e. g. buildings) that are expected to last longer than the assumed system lifetime, this has, of course, to be done in an opposite way. In this case there will be a residual value left at the end of the system life cycle that has to be subtracted from the accumulated costs over lifetime.

Discount rate

Commonly future costs are given a lower weight than costs today. The rationale behind this is simply that the further in the future costs will occur, the lower the weight aligned to it in an LCC perspective. This method is called "discounting". Since in dynamic cost comparisons costs are accounted for multiple periods, all costs need to be discounted. Now the nature of discounting implies an exponential growing discount factor. Defining this discount factor is not an easy task and can vary between applications and countries. Therefore, it is indispensable to check the influence of the discounting rate on results in sensitivity analyses.

In accordance with German frameworks on dynamic cost calculations for water treatment systems[36], the initial discount rate for all case studies in DEMEAU was assumed to be3 % per year. Afterwards, this assumption was tested against higher discount rates (5% and 7% per year) within sensitivity analyses in order to prove the stability of results.

Inflation rate

Since costs are accounted for multiple periods, also involving costs in future periods, reasonable assumptions regarding future cost increases or decreases as well as inflation need to be taken into consideration. Therefore the costs in future periods defined on the basis of today's price levels need to be multiplied with the so-called inflation factor. Assuming e.g. today to be the basis, the costs of each following period must be multiplied with the inflation factor, which is depending on the period t of the analysis and the assumed inflation rate. Estimations of cost increases are regularly based on experienced data arising from comparable activities of the past. If no comparable data is available reasonable assumptions have to be made. But as it is very difficult to rate the current price level to identify short-term trends, and to consider economies of scale or inflationary influences within the trend extrapolation, the impact of different inflation rates on the results has to be checked carefully in sensitivity analyses afterwards.

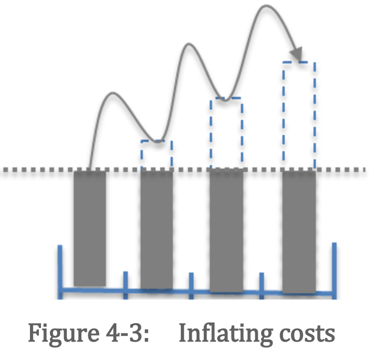


Figure 4-3: Inflating costs

In DEMEAU all life cycle costs were initially calculated without inflation. In sensitivity analyses the results were then again tested on their stability by inflating costs for energy, operating supplies, personnel and external services with inflation rates from 1-3% per year.

[36] LAWA (2012). Leitlinien zur Durchführung dynamischer Kostenvergleichsrechnungen (KVR-Leitlinien) (Guidelines for dynamic comparative cost methods). 8th Edition. German Working Group on water issues of the Federal States and the Federal Government, Hennef, Germany.

Net Present Value (NPV)

Based on these assumptions on costs and key parameters life cycle costs of each technology were finally calculated by summing up all inflated and discounted costs of each period over the defined time horizon. The result of this calculation is a figure describing the total discounted costs over a certain lifetime, also known as 'Net Present Value (NPV)' of the investment. Based on this figure, several other indicators (e. g. annual amount of annuity, break-even analysis per investment) can be calculated as well.

4.5 Presentation of results

Presenting the investment costs per system capacity (Figure 4-1) and operational costs per year (Figure 4-2) as presented above can serve as basis for a first validation check with site owners as well as part of the presentation of input data for calculation. In order to highlight cost drivers in infrastructure and operating costs the most important process stages or contributors should be made visible here. This is even more valuable if a LCA is performed as well, since figures that are aligned to each other can easier be compared and transferred into a final result.

Final results of the life cycle costing can generally be presented in several ways, such as absolute figures as NPV trend line over time (Figure 4-4: Net present value (NPV) of managed aquifer recharge scenarios over time in a DEMEAU case study (discount rate: 3%, no inflation) (source: D51.1)), in relation to the influent flow (e.g. [EUR/$m^3{}_{Qin}$]) or effluent flow (e. g. [EUR/$m^3{}_{treated}$]) of the process (Figure 4-5) or as cumulated values over time (Figure 4-6).

Showing the NPV over time can be done best by using trend charts showing the absolute value of NPV [Mio. EUR] in relation to time [yrs.] (see Figure 4-4). In this way of presenting, break-even-points of investments and reinvestments in infrastructure become clearly visible.

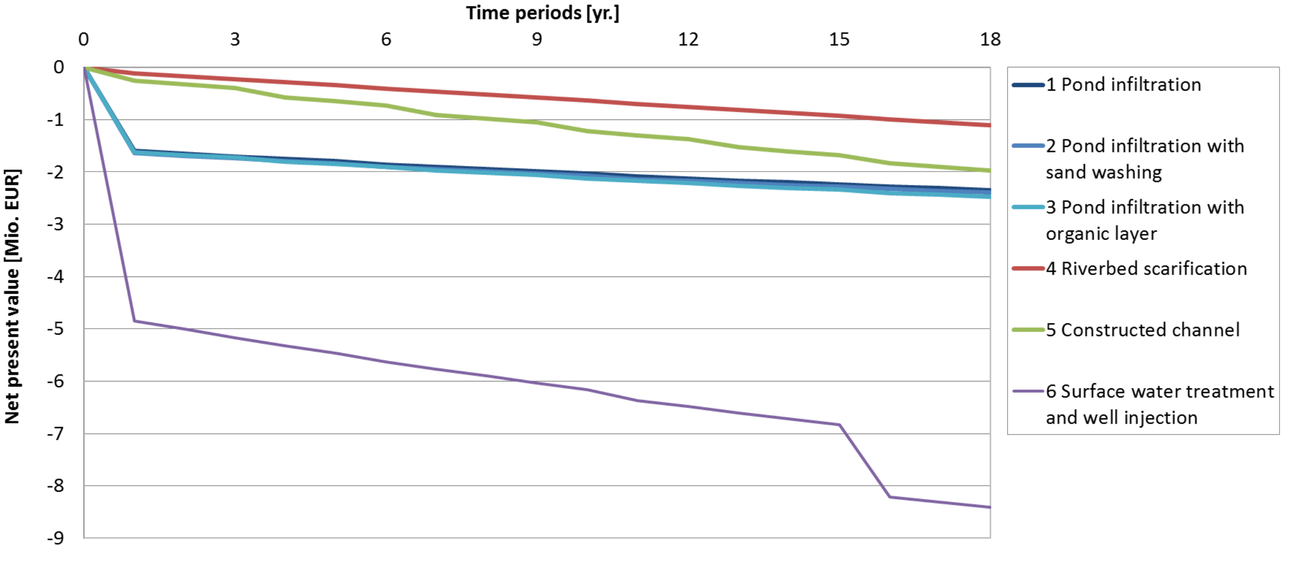
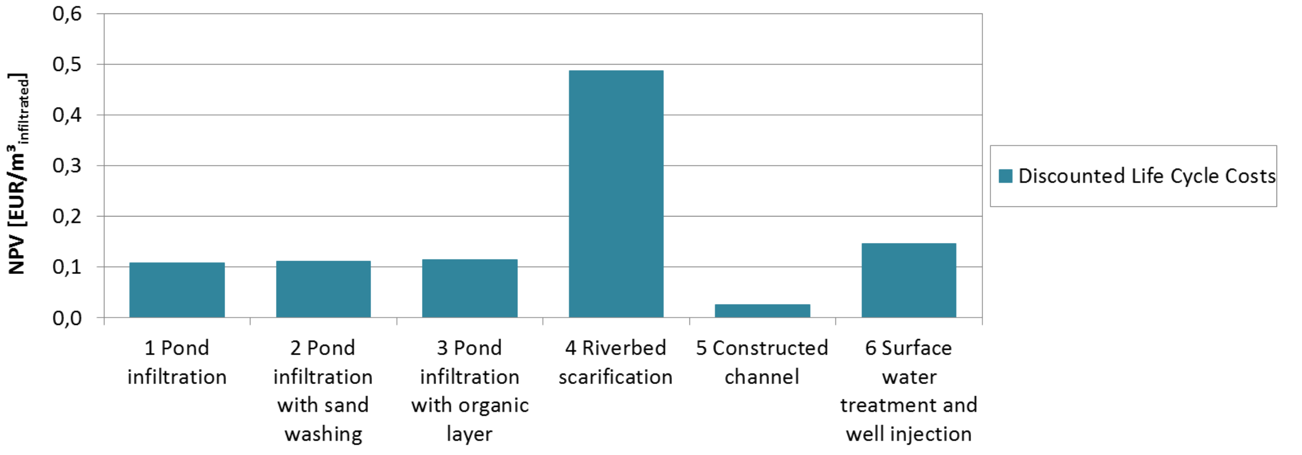


Figure 4-4: Net present value (NPV) of managed aquifer recharge scenarios over time in a DEMEAU case study (discount rate: 3%, no inflation) (source: D51.1)

If several different scenarios were assessed within LCC it is also worthwhile to present the NPV of all cases in a comparative figure (Figure 4-5) which enables the site partner to identify the cheapest solution in cost comparison easily. The figures should therefore be all calculated in the same unit (e. g. per m^3 influent flow (e.g. [EUR/m^3Qin]) or effluent flow (e. g. [EUR/m^3treated]) over life time. Other units (e. g. [EUR/p.e.]) can also be used, but as these are probably less intuitive, these types of values were not calculated within DEMEAU.



Sum:	**0,11**	**0,11**	**0,11**	**0,49**	**0,03**	**0,15**	**[EUR/m$^3_{infiltrated}$]**

Figure 4-5: Net present value (NPV) per m^3 infiltrated water of managed aquifer recharge scenarios in a DEMEAU case study (discount rate: 3%, no inflation) (source: D51.1)

In cases where a break-even-analysis is required, the illustration of the cumulative NPV over time (Figure 4-6) can be a very useful figure in order to highlight the period in time, when the investment amortizes. Here, the current value of investment is presented as a sum of all discounted costs and earnings up to this point in time. Whenever the sum reaches the value 0, the investment will have paid off (break-even-points of costs and savings (BEP 1, BEP 2)). It is surely not to mention that this kind of illustration is only reasonable for investments where high costs savings are expected to take place over time such as for instance Automated Net Control Systems (ANCS).

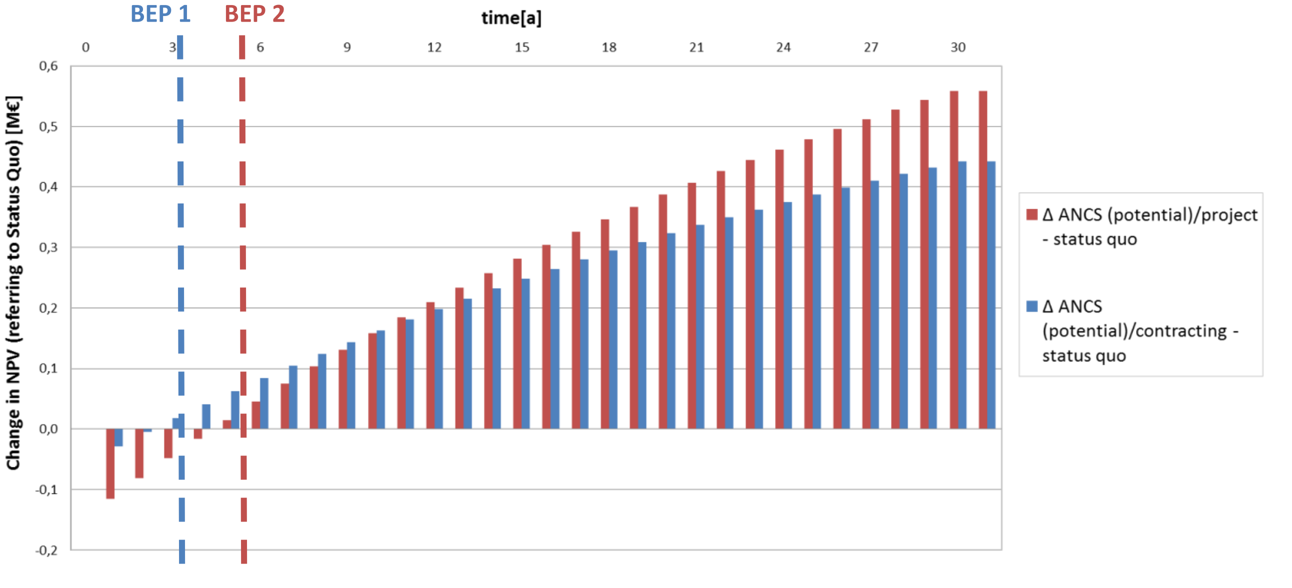


Figure 4-6: Change in net present value (NPV) (referring to *status quo*) of two 'potential' ANCS scenarios in a DEMEAU case study in Germany with break-even-points BEP1 and BEP2 (source: D51.1)

As well as in LCA, results of LCC require interpretations. This can be taken care of by a short summary and discussion of the major conclusions (incl. all limitations). Questions to be answered in sensitivity analyses and conclusions should be closely related to those answered in the respective parts of the LCA (see chapter 3.5) and will therefore not be repeated here again.

5 Analysis of drivers and barriers with stakeholder participation

5.1 Theoretical background

This chapter provides a short introduction to the theoretical background of the social drivers and barriers analysis with stakeholder participation.

5.1.1 Socio-technical system's perspective

Water systems can be regarded as large systems of complex interactions and processes in a physical network of natural and engineered water structures. However, an essential component influencing the functioning of such large systems is the more intangible social side of it, encompassing for example stakeholders' interests, designers' guiding principles, governing policy rules and regulations[37,38]. Because of this, such systems are also known as 'socio-technical systems'.

Socio-technological systems tend to evolve continuously towards a stable state, in which the various components of the system are carefully balanced. Establishing change in such a context thus means that the system needs to be destabilised, requiring a certain momentum. Generally, large systems will allow incremental change to take place that does not threaten the established system interconnections[31]. However, the uptake of innovative water technologies could also mean that a more radical change is needed, requiring a bigger force to unbalance the system and lead it towards a new synergetic status quo. This process of transition is where barriers need to be overcome for successful implementation of innovative practices. This is especially the case in the water sector, since water and wastewater services are closely connected to people's health and environmental protection. Thus, this sector is naturally more conservative towards innovation and uptake of new technologies, as reliability and continuous operation with predictable costs are of highest priority for the responsible stakeholders, such as operators and regulators.

Considering these socio-cultural systems on a less abstract level, they can be perceived as networks of stakeholders, interacting with water structures and technologies. Regarding uptake of innovations, Jeffrey and Seaton emphasized the importance of the extent to which stakeholders are willing and able to absorb, accept and utilize innovations[39]. They called this the stakeholders' "receptivity to innovations". Furthermore, Wejnert concluded from her extended review of theories on the diffusion of innovations that there are two major components that influence innovation implementation next to the characteristics of the innovation itself[40]. The first component involves the actors that influence the probability of adoption of an innovation such as developers, end users, technology promoters, SMEs (Small and Medium-sized Enterprises), researchers etc. The second component includes actors influencing the adoption environment such as the public opinion, current trends, policies and regulations, including regulators, non-governmental organizations (NGOs), etc.

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[37] Hughes T (1987). The evolution of large technological systems. In: The Social Construction of Technological Systems (Bijker, Hughes, Pinch, eds). Cambridge, USA: MIT Press

[38] De Graa, R (2009). Innovations in urban water management to reduce the vulnerability of cities. Feasibility, case studies and governance. PhD Dissertation. Delft University of Technology, Delft

[39] Jeffrey P, Seaton, RAF (2004). A Conceptual Model of "Receptivity" Applied to the Design and Deployment of Water Policy Mechanisms. Environmental Sciences 1:277–300

[40] Wejnert B (2002). Integrating models of diffusion of innovations: A Conceptual Framework. Annual Review of Sociology 28:297–326

5.1.2 Distinguishing multiple system levels

Rip and Kemp developed a multi-level perspective, providing an analytical framework to study processes on and interactions between various system levels of large socio-technical systems as described above[41]. In this project, to identify drivers and barriers to successful uptake and implementation of the four DEMEAU technologies, an adapted version of their basic framework (developed by Brown et al.[42]) will be applied. They identified four analytical system levels of institutional capacity, also addressing the stakeholder constituencies of Jeffrey and Seaton[33] and Wejnert[34]:

- Barriers on the contextual level: e.g. regarding enabling policies, regulations and incentives, and/or impact on the system's context (environment, health, etc.).
- Barriers on the inter-organisational level: e.g. regarding relationships, agreements and consultative networks among stakeholders that are needed to cooperatively promote technology implementation.
- Barriers on the intra-organisational level: e.g. regarding organizational culture, procedures and resources within organisations for technology implementation.
- Barriers on the individual level: e.g. regarding relevant knowledge, skills and motivation of involved individuals.

5.1.3 Distinguishing multiple stages of innovation

Uptake and implementation of innovative technology is not an isolated activity. It depends on other activities throughout the so-called innovation cycle. This cycle represents the route from market demand and/or innovative idea to actual launching of the resulting innovative technology. In the various stages of this innovation cycle multiple stakeholders are required to get from idea to design, through piloting towards a full-scale implementation. Each stakeholder has his/her own view on the process and his/her own perspective on (expected) drivers and barriers within the innovation cycle. Therefore, implementation drivers and barriers should not only be studied on the various analytical social levels, but also from the different stakeholder perspectives, with respect to their role in the multiple stages of the innovation cycle.

5.2 Conceptual framework applied in DEMEAU

Based on the existing insights described in the previous section, a conceptual framework was established for this research. First an overview of this framework is presented, followed by the operationalization of the various concepts for WA5.

5.2.1 Overview

Combining the insights on the multiple analytical levels for assessing a social system's institutional capacity (e.g. for uptake and implementation of innovative technology), the subsequent innovation stages, and the fact that perceived drivers and barriers vary among stakeholders, a conceptual framework was established as schematically depicted in Figure 5-1. The figure only shows two stakeholders (X and Y) who are involved in the development and implementation of an innovative micropollutant removal technique, but more stakeholders (e.g. U, V and W) could be involved. Furthermore, the figure shows the four analytical system levels of Brown et al[36] in which drivers and

[41] Rip A, Kemp R (1989). Technological change. Human choice and climate change (S R, Malone E, eds). Battelle Press, Columbus, Ohio, USA

[42] Brown R, Mouritz M, Taylor A (2006). Institutional capacity. In: Australian Runoff Quality: A Guide to Water Sensitive Urban Design (Wong T, ed). Engineers Australia, Canberra, Australia

barriers could manifest themselves: the individual, intra-organisational, inter-organisational and contextual level. Also the subsequent stages of innovation (collectively representing an 'innovation cycle') are shown in the figure. They have been operationalized for this project on technologies for micropollutant removal and screening from water, presented in Table 5-1.

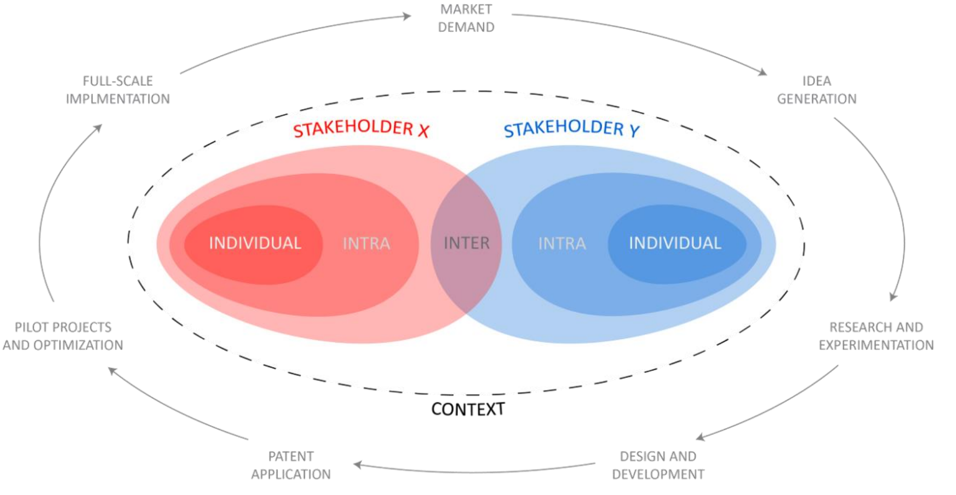


Figure 5-1: Schematic overview of the conceptual framework

Table 5-1: Operationalization of innovation cycle for innovative technologies regarding (optimized) screening and removal of micropollutants in water resources

Innovation stage	Description
Identifying market needs	Investigation of the needs that exist for technologies related to micropollutant removal. Sometimes innovation is driven by demand (from water utilities as end users – innovation pull), and sometimes innovation is driven by technological possibilities (discoveries at SME's or research institutes – innovation push).
Idea generation	When problems or opportunities have been made explicit, ideas on possible solutions are generated.
Research and experimentation	Research is done (e.g. existing alternative technologies, boundary conditions of system) and first ideas and (partial) solutions are being tested.
Design and development	Based on the first research a design is made that addresses the identified problems around emerging compounds/micropollutants.
Patent application	The developer of the innovative technology applies for a patent to secure rights of intellectual property.
Pilot projects and tests	Pilot projects are set up to test the design. This could be done in a laboratory setting, or in a real-life setting at a potential end user (drinking water or waste water treatment plant).
Technology optimization	Based on the results of the pilot tests (parameters of the technology, boundary conditions, fit in existing processes and procedures) the design has to be optimized.
Up-scaling to full scale operation	After the test and optimization phase the innovative technology should be scaled up, in order to be implemented on full-scale at the water utility.
Policy & guideline development	Before implementation can take place, the innovation needs to be embedded in existing (or sometimes new) policies and guidelines. Waste- and drinking water treatment are governed by rules and regulations for health and environmental protection.
Authorization, legal regulation	Because of the bounding regulations the water utility often needs permission from local authorities to implement the novel solution. During this procedure the innovation is measured against regulations.
Full-scale implementation	Full-scale implementation can take place at the water utility (being the 'launching customer') when the innovative technology on micropollutant removal is finished and authorized.

A multi-step methodology was developed for this assessment of drivers and barriers to development and implementation of the innovative technologies in the DEMEAU project, based on the conceptual framework as presented in section 5.1:

Step 1: Preliminary inventory of stakeholders and barriers (Aug - Sep 2013)

Step 2: Selection of case studies and stakeholders (Oct - Nov 2013)

Step 3: Drivers and barriers assessment survey (Dec 2013 - Jan 2014)

Step 4: In-depth drivers and barriers assessment workshops/interviews (Sep 2014 – Jul 2015)

Step 1: Preliminary analysis of stakeholders and barriers and desk research

In order to make the conceptual framework as presented in paragraph 5.1.4 applicable for innovative technologies in the field of micropollutant screening and removal, a preliminary inventory of stakeholders and barriers was done among the leaders of Work Areas 1 to 4.

A short online survey was distributed among the Work Area leaders, asking the following questions:

- Which stakeholders play a role in relation to the technology/implementation cases in your Work Area? Please provide their (organization's) name and describe their role with regard to the technology.
- From your perspective, which barriers for uptake or implementation of the technology could you identify (at this moment or in potential future situations)?
- Are you aware of any scientific publications (journal articles, research reports, etc.) on implementation barriers regarding this technology? Which ones?

The responses have been used to identify stakeholders in the selected case studies, to do a literature search/desk study on previously identified drivers and barriers, and to combine all information in a first inventory of categories of implementation drivers and barriers in the selected cases. The result is shown in Table 5-2 .

Table 5-2: Operationalization of the four analytical levels for the case studies on innovations in the field of micropollutant removal

Analytical level	Individual	Intra-organizational	Inter-organizational	Contextual
Relevant aspects:	• Knowledge • Skills • Motivation	• Organizational culture • Financial means • Best practices/ experience • Compatibility • Alternative technologies	• Contact/ cooperation • Role clarity • Past collaborative experiences • Distribution of resources • Shared goals and (world)views	• Public opinion • Landscape/ environmental impact • Health risks • Policies and regulations • Involvement of authorities • Political context

This initial inventory among the leaders of work areas 1 to 4 has shown that the following (types of) stakeholder play a major role in innovation in this context:

- Developer (small-medium enterprises, research institutes, consultants, etc.)
- Policy maker/regulator (local, regional national and international governing authorities)
- End user (waste- or drinking water utilities)

Step 2: Selection of case studies and stakeholders

Based on the information from the initial inventory (step 1), supplemented with inputs from the designated case study contact persons, relevant stakeholders have been selected for each case study. The selection covered stakeholders from the each of the stakeholder groups:

- Developers: e.g. SMEs, research institutes, consultants
- Policy makers/regulators: local, regional and (inter)national authorities
- End users: Waste- or drinking water utilities

A list was compiled with contact details of representatives from all relevant stakeholders per case study. This list was used for the subsequent steps of the drivers and barriers analysis.

Step 3: Drivers and barriers assessment survey

The preliminary barriers inventory among the leaders of work areas 1 to 4, combined with insights on implementation drivers and barriers from technology-specific literature have served as the basis for an online survey. Using surveys to obtain input from a very diverse group of stakeholders on four different technologies allowed a structured analysis of drivers and barriers across cases.

The survey – translated into the native languages of the respondents (identified in step 2) – consisted of four main parts, covering the four analytical levels of the conceptual framework. The respondents were asked to indicate in which stages of the innovation cycle (as operationalized in Table 5-1) they played a role, and to which degree (not, some, much, very much) the relevant aspects (Table 5-2) on the four analytical levels have served as enabling factors (implementation drivers) and/or constraining factors (implementation barriers) from their perspective. Open text fields were included for each innovation stage and each enabling or constraining aspect, allowing the respondents to elaborate on their ratings.

The results on stakeholder involvement throughout the innovation processes and the degree to which drivers and barriers were perceived within the defined categories have been visualized according to the example in Figure 5-2 and Figure 5-3. The complete results, including specific information on perceived drivers and barriers from the open text fields, have been reported in Deliverable 52.1.

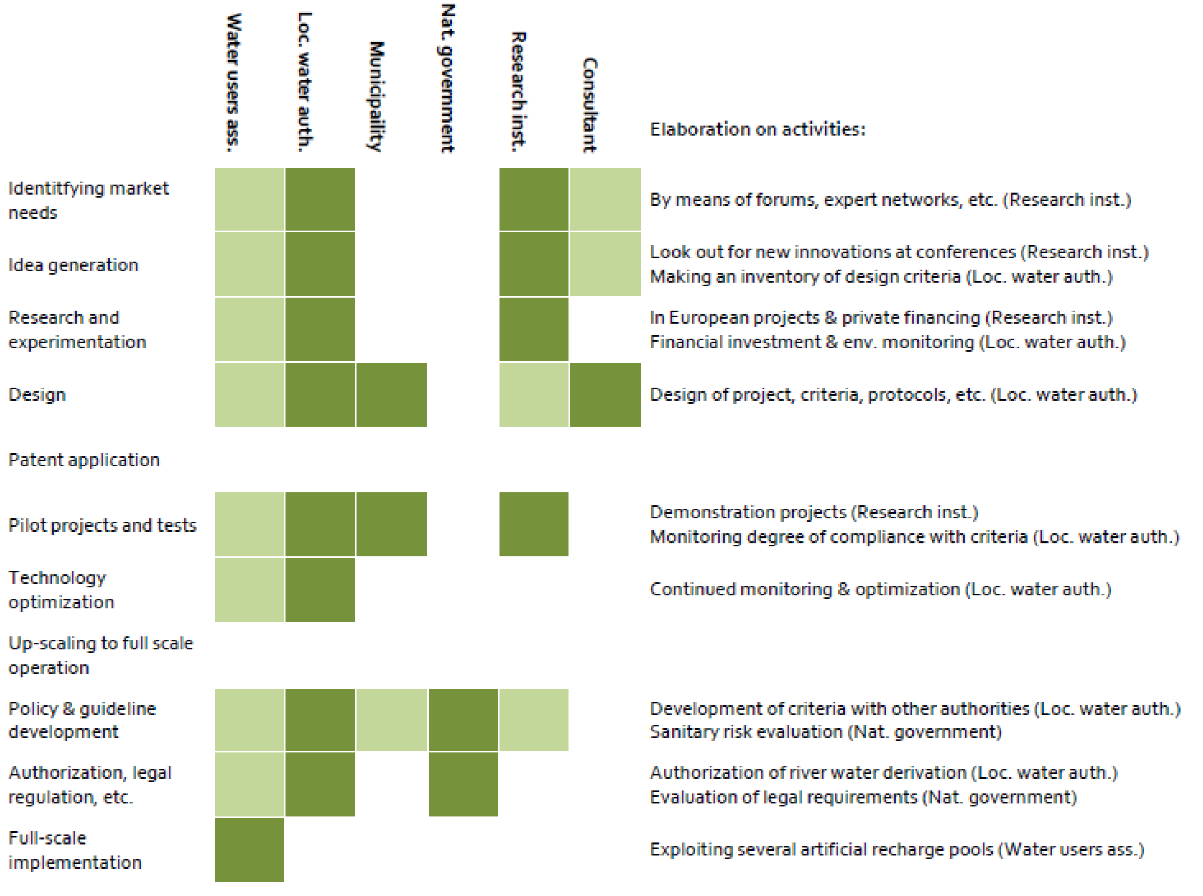


Figure 5-2: Example: Overview of the stakeholder involvement in the innovation cycle

(Dark green: as indicated by respective stakeholder, light green: as indicated by other stakeholders)

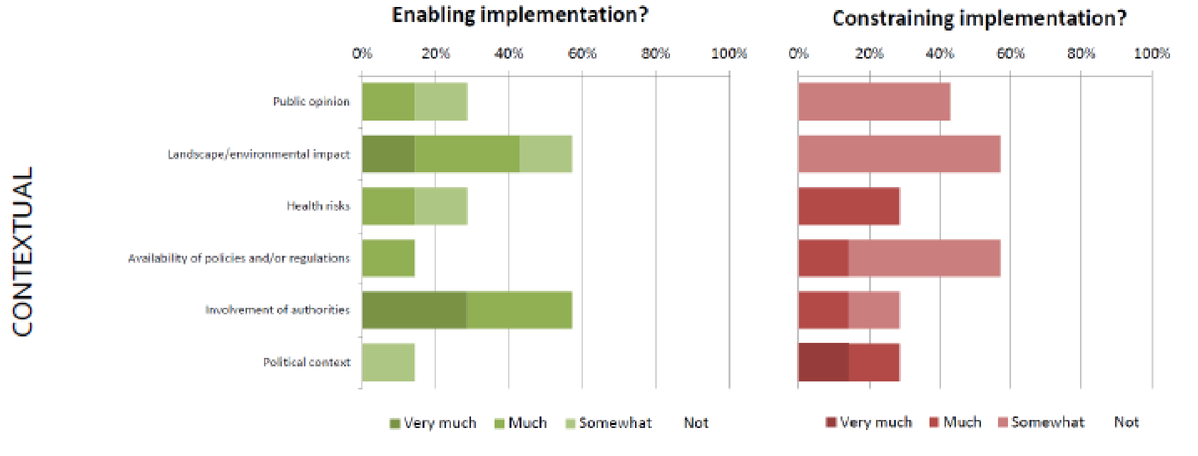


Figure 5-3: Example: Overview of degree to which aspects are perceived as drivers or barriers

Step 4: In-depth drivers and barriers assessment workshops/interviews

The activities in step 4 aimed to validate the survey results and to formulate recommendations for the various involved stakeholder groups to overcome the identified barriers. This was done by means of an interactive workshop for the cases within Work Areas 1 and 2, as they organized utility events of which these workshops could be part. Since such events were not planned in this stage of the project for the cases in Work Areas 3 and 4 it was decided to cover the workshop contents in a series of stakeholder interviews.

The workshop served two main aims (example of programme in Table 5-3):

1. **Validation of initial results –** Presentation of environmental (LCA), economic (LCC) and social (drivers and barriers assessment up to step 3) highlights for the cases that had been studied by work area 5 in collaboration with the other respective work areas 1-4. Participants were asked to vote 'agree' or 'disagree' to a set of statements that presented the most interesting outcomes, in order to validate and elaborate the first results.
2. **Overcoming challenges of implementation** – Identifying the most important barriers from the perspectives of various stakeholder groups present at the workshop, complemented with their expectations of themselves and the other stakeholder groups to overcome them (using Table 5-4 printed on big poster format). At the end of the workshops the groups presented their 'perspectives' and confronted each other with their expectations, which in turn were translated into recommendations and possible interventions (example in Figure 5-4, divided into main categories of major barriers).

Table 5-3: Example of workshop programme

Time	Activity
12:00 – 12:15	**Presentation of WA5 results (interactive)** • Participants react on results of WA5 (moderation: *<u>Miranda Pieron</u>*) • Presentation of the dynamic activity
12:15 – 13:00	**Stakeholders working groups** • Working groups (science, administration and utilities) are asked to formulate expectations and recommendations with regards to successful MAR implementation among the various involved stakeholders - Brainstorm (moderated by group representative): Please identify (from your own perspective) barriers that need to be overcome for successful MAR implementation. Please consider the different 'levels' (individual, organizational, inter-organizational, contextual) - Exercise (moderated by group representative): Please select the five barriers (from your brainstorm results) that are most difficult to handle because action is required from multiple stakeholders. Write those barriers in the first column of the table. Then, for each barrier, fill out the other three columns with expectations you have/which actions are required from each of the stakeholder groups. • Representative of each group summarises their findings to be presented in the plenary session
13:00 – 13:45	**Plenary session** • 8' presentation findings and conclusion for each GROUP A / B / C • Open discussion to translate outcomes to recommendations and solutions for further MAR application. o Participants are asked to react on the barriers and 'required actions' they've heard from other groups, reflect on similarities and differences we've heard, and together we try to come to a set of recommendations for successful MAR implementation. • Closure of the session • Moderation: *<u>Marta Hernández</u>*, Miranda Pieron, Thomas Gross, Christian Remy)

Table 5-4: Example of table that stakeholder groups were asked to fill in during interactive workshop (printed on big poster format, filled in with sticky notes)

	What are the most important barriers that the group encounters in relation to implementation of MAR?	How can you (or MAR and water operators in general) contribute to overcome this barrier?	What is required from the scientific community to overcome this barrier?	What is required from the administration / regulators to overcome this barrier?
1				
2				
3				
4				
5				

	BARRIERS	REQUIRED FROM SCIENTIFIC COMMUNITY	REQUIRED FROM ADMINISTRATION	REQUIRED FROM OPERATORS
		• Establishment of MAR communities, with special attention to the science-policy interface: exchange of knowledge, local options and consequences • Cooperate on realistic guidelines and regulations that consider the health and environmental effects in a measurable way • Willingness to communicate with each other, openness, transparancy		
TECHNOLOGICAL	• Well clogging • Lack of maintenance protocols • Quality of infiltration water • Effects on ecotoxicology of groundwater are unknown	• Model clogging effects and find solutions • Translate experiences from other countries to local projects • Stop solving problems that already have been solved somewhere else • Determine the boundary condtions under which MAR is an effective solution.	• Make existing technological questions explicit	• Make plants/playgrounds available for pilots and tests
REGULATORY	• Regulators still see too many risks • Regulation are inflexible • Conservative attitude of regulators • Regulation does not (yet) include the variety of water qualities (incl recycled water) • Lack of health and environmental parameters • Complex communication among various administrative levels	• Define health and environmental parameters to be able to make MAR practices measurable • Listing priority substances to monitor. • Dissemination to and coordination with regulators	• Aim for regulations that are locally adaptable • Inlcude measurable parameters (also of emerging pollutants) in regulations that allow measurement of the effects on water quality (instead of being strict on the inflow water) • Consider water quality on basin level • Don't come up with new regulations, but improve existing ones • Improve communication among adm. levels • Adapt EU regulations to local circumstances	• Be transparent: show results, provide test data, real costs, reasons for failure, etc. to look jointly for solutions • Participate in discussions (especially local discussions regarding specific solutions) • Don't just 'assume' that regulations are and will always be a barrier.
FINANCIAL	• MAR competes with other water related solutions • High costs for pre-treatment of (recycled) water for well injection • Open question of who pays the bill • Viability of solution is questioned	• Conduct and communicate Lifecycle Costing and Lifecyle assessments to clarify the 'choices' and longer term effects	• Aim for public funding on a longer term (avoid limited subdidies) • Integrate costs of water reclamation in water bill (to allow for higher investments) • Consider also the (partly qualitative) savings done by reclaiming water • Extending exploitation period (for operators), redistribution of costs • Not "coffee for all" (refers to autonomous regions)	• Contribute financially to development and maintenance of technology and regulations (is already done by some) • Invest in tertiary treatment (which enables infiltration of cleaner water)
SOIAL	• Conservative attitude of consumers • Lack of dissemination on local level	• Communicate findings (in understandable language) outside scientific community	• Start public dialogue about MAR, including various stakeholders	

Figure 5-4: Example outcome of interactive stakeholder workshop

6 Integration of results from LCA, LCC, and stakeholder analysis into recommendations for impact

This chapter describes the integration of results from LCA, LCC and drivers and barriers analyses applied to different case studies into recommendations for impact in the water sector. The principle aim of these capacity building documents is a dissemination of research findings beyond the scientific community including for the scope of this work the following stakeholder groups: public authorities and policy making, scientific community and technology developers, and utilities. The presented structured format could also be applicable for the dissemination of other sustainability assessments in the water sector and other fields and is thus briefly described in this chapter.

The 'recommendations for impacts' documents developed during the DEMEAU project have the following structure, which is described in the sections below:

- Technology brief in relation to micropollutants (section 6.1)
- Case studies introduction (section 6.2)
- Environmental and economic unique selling propositions (section 6.3)
- Stakeholder specific recommendations for market uptake

6.1 Technology brief in relation to micropollutants

This section contains a short description of the technology and its relevance for the removal or detection of organic micropollutants – the main target of the technologies studied in DEMEAU. It is written in a non-technical form with references to detailed information by the relevant technology work areas and literature. Preparation of this section as all other sections was in consultation with technology specialists of the respective work areas. Care was taken to avoid repetitions from specific 'technology brochures' developed by WA6 during the DEMEAU project, thus ideally the recommendations described here could be used in conjunction with these 'technology brochures'.

6.2 Case studies introduction

The work of WA5 was based on case studies conducted during the DEMEAU project. These case studies are introduced to provide links to the actual application of the technologies. Apart from case studies analysed by WA5 also other case studies conducted during the DEMEAU project by respective WAs are introduced to provide a wider picture of application areas.

6.3 Environmental and economic unique selling propositions

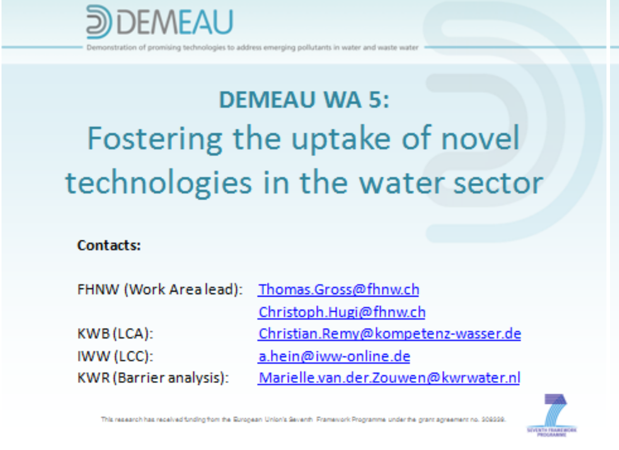
Environmental and economic footprints of technologies against micropollutants together with their relevant application areas built the basis to formulate unique selling propositions (USPs) for each technology group (WA1-4) studied in DEMEAU. This approach permitted a transparent and concise communication of key messages based on LCA and LCC assessments at mid-point level to different stakeholders while avoiding aggregation into end-point indicators (also see chapter 3.4). Thus, specific strengths and weaknesses of each technology can be highlighted and can help defining targets of future research with regard to improving environmental and economic performance. Unique selling propositions of technologies studied in DEMEAU are described in deliverable 'Unique selling propositions' (D51.1), where also results from LCA and LCC case studies are presented in detail. This section of the 'recommendations for impact' documents contains the following sub-sections:

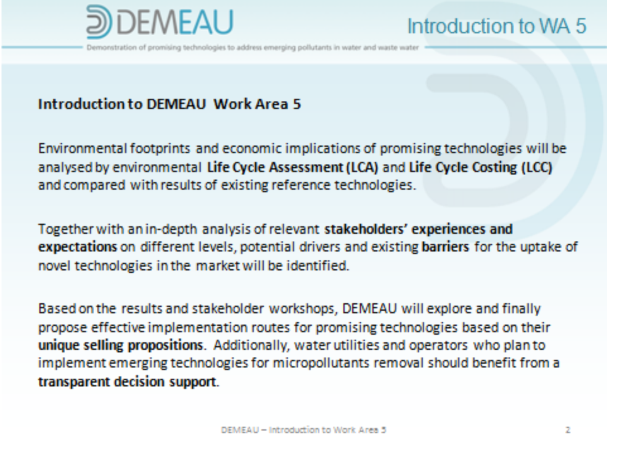
- **Methods of lifecycle-based environmental and economic assessments:** A brief introduction to LCA and LCC for a general audience with references to this document, where LCA and LCC methodologies are discussed in the preceding chapters 3 and 4, respectively.
- **Key application areas:** All technologies studied in DEMEAU fulfill various functions and are not limited to the removal of micropollutants only. This sub-section provided an overview of application areas in the water sector.
- **LCA and LCC results:** Results from LCA and LCC analyses are summarized briefly with reference to the full analyses provided in 'Unique selling propositions' (Remy et al. 2015).
- **Unique selling propositions:** USPs are provided in a table and should distinguish the technologies based on their application areas and environmental and economic footprints based on results from case studies.

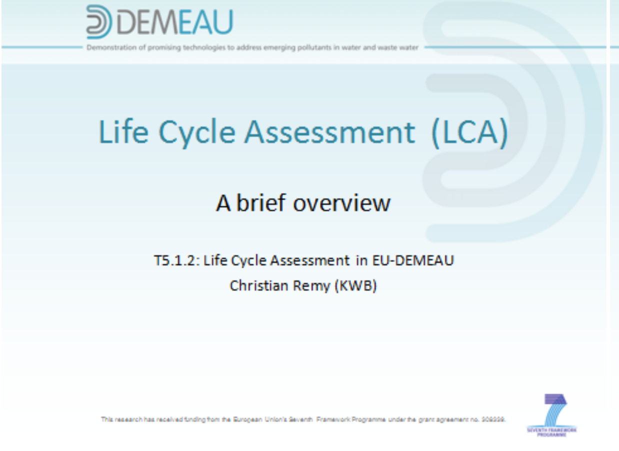
6.4 Stakeholder specific recommendations for market uptake

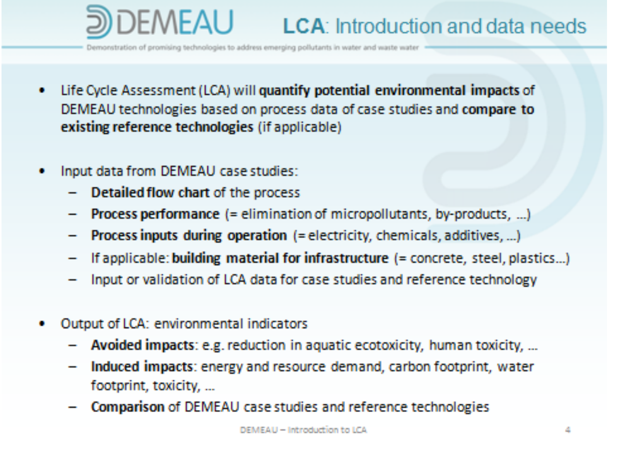
Stakeholder specific recommendations were formulated considering the results from the drivers and barriers analyses (described in chapter 5 of this document) and complemented by insights from LCA and LCC analyses, where appropriate. Special consideration was given to expectations by different stakeholder groups from other stakeholder groups. The review process involving selected case study partners and researchers of the DEMEAU consortium of the respective technology work areas helped to assure that recommendations are realistic and remained close to the actual application of the technologies. The final 'recommendations for impact' documents have been made available as PDF files on the DEMEAU homepage (http://demeau-fp7.eu) and therewith build a dissemination route for research findings of sustainability assessments.

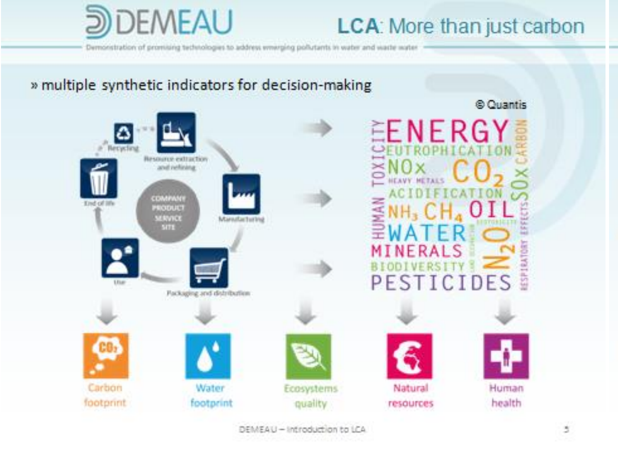
Annex-A Introductory information leaflet for project partners and case study leaders on sustainability assessment within DEMEAU WP5

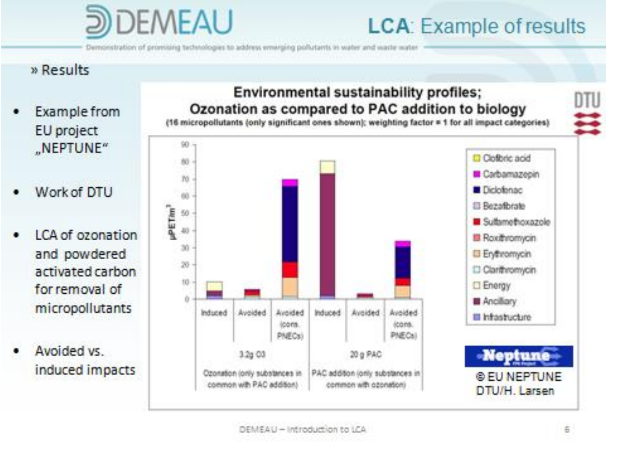












Life Cycle Costing (LCC)

A brief overview

T5.1.3: Life Cycle Costing in EU-DEMEAU

Andreas Hein (IWW)

This research has received funding from the European Union's Seventh Framework Programme under the grant agreement no. 308339.

LCC: Introduction and data needs

- Life Cycle Costing (LCC) will **assess all costs related to a product or service over the entire life cycle**, from production over use until disposal – especially for products that have long life times and/or high maintenance, use or disposal costs
- In combination with a Life Cycle Assessment (LCA) that investigates the environmental impact of a product or service, **LCC can serve to address the economic dimension of sustainability**
- LCC is an instrument to support decision making at utility level

- **Input** data from DEMEAU case studies
  - General requirements (investment project: performance per unit; service life [years] for setup phase, operating phase and removal phase, discounting rates)
  - Cost drivers (personnel cost, material, services, assets, financing, taxes & dues)
- **Output** from LCC:
  - Cash values of life cycle costs
  - Annual amounts of annuity
  - Break-even analysis per investment
  - Sensitivity checks
  - Comparisons at harmonized project durations (if more than one alternative will be assessed in a case study)
  - Decision support for "best investment"

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LCC: Cost over entire life cycle

Trade-off between setup costs and follow-up costs

LCC-assessment helps to find the "best" cost relationship taking into account the time of financial flows over service life years. It includes all costs related to individual life phases (setup, operating, removal).

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Barrier analysis

A brief overview

T5.2.1: Enabling and constraining factors for a successful technology implementation in EU-DEMEAU

Marielle van der Zouwen (KWR)

This research has received funding from the European Union's Seventh Framework Programme under the grant agreement no. 308339.

Barrier analysis: Introduction and data needs

- The analysis on implementation barriers will systematically **identify the incentives contributing to the (un)successful uptake and implementation** of DEMEAU technologies based on **qualitative data** from interviews and expert meetings with stakeholders.

- During interviews and expert meetings with stakeholders from DEMEAU case studies implementation barriers at different levels will be addressed:
  - **Policy and regulatory level**: experiences on the enabling and/or constraining character of national and EU policies in the DEMEAU cases
  - **Inter-organisational level**: experiences on the agreements, relationships, consultative networks that are needed to cooperatively promote technology implementation
  - **Intra-organisational level**: experiences on the cultures and resources within organizations for technology implementation
  - **Individual level**: experiences on technical knowledge, skills, expertise, the way in which individuals operate within the workplace and personal characteristics that enable or constrain technology implementation

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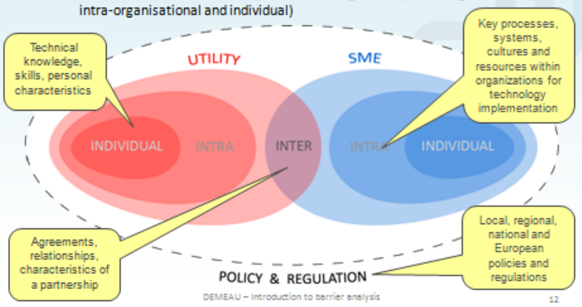
Barrier analysis: Output overview

Output of implementation barriers analysis:

- Identification of challenges for technology implementation in the DEMEAU cases at four different levels (policies and regulations, inter-organisational, intra-organisational and individual)



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Annex-B Data collection template for LCA

OPERATIONAL DATA: mean data to represent annual operation				
Inputs of the processes	Material	Quantity	Unit	Remarks
electricity per sub-process	electricity (process 1)		[kWh/d, kWh/m³, ...]	
	electricity (process 2)		[kWh/d, kWh/m³, ...]	
	...		...	
chemicals per sub-process	chemical 1 (process 1)		[g/m³, kg/d, ...]	incl. concentration [e.g. FeCl3 40%]
	chemical 2 (process 1)		[g/m³, kg/d, ...]	incl. concentration [e.g. FeCl3 40%]
	chemical 3 (process 2)		[g/m³, kg/d, ...]	incl. concentration [e.g. FeCl3 40%]
	...		...	
other inputs (additives, fuels, materials, ...)	input 1 (process 1)		[g/m³, kg/d, ...]	incl. concentration [e.g. FeCl3 40%]
(if data is available)	input 2 (process 2)		[g/m³, kg/d, ...]	incl. concentration [e.g. FeCl3 40%]
	...		...	
Outputs of the processes	Material	Quantity	Unit	Remarks
Materials	Sludge		[kg/d]	SS concentration? Quality? Disposal route?
	Backwash waters		[m³/d]	or % of inflow
	...		...	
Other specific emissions (if applicable)	Substance 1		[kg/d]	e.g. gases,
	Substance 2		[kg/d]	
	...		...	
Influent quality (long-term mean values)	Parameter	Value	Unit	Remarks
Basic parameters (as available)	pH		[-]	
	Alkalinity		[mg/L CaCO3]	or other units
	Turbidity		[NTU]	
	Suspended solids		[mg/L SS]	
	COD or DOC		[mg/L COD or DOC]	
	Phosphorus species		[mg/L TP]	or other species
	Nitrogen species		[mg/L TN]	or other species
	...		...	
Organic micropollutants (as available)	as defined in DEMEAU list of substances		[µg/L]	
(long-term mean values)			[µg/L]	
			[µg/L]	
Effluent quality (long-term mean values)	Parameter	Value	Unit	Remarks
Basic parameters (as available)	pH		[-]	
	Alkalinity		[mg/L CaCO3]	
	Turbidity		[NTU]	or % removal
	Suspended solids		[mg/L SS]	or % removal
	COD or DOC		[mg/L COD or DOC]	or % removal
	Phosphorus species		[mg/L TP]	or % removal
	Nitrogen species		[mg/L TN]	or % removal
	...		...	
Organic micropollutants (as available)	as defined in DEMEAU list of substances		[µg/L]	or % removal
			[µg/L]	or % removal
			[µg/L]	or % removal
INFRASTRUCTURE DATA (either specific weights if known, or size of major equipment)				
Building materials	Excavation		[m³]	if applicable
	Concrete		[m³ or kg]	tanks, buildings, ...
	Sand		[kg]	
	Reinforcing steel		[kg]	tanks, buildings, ...
	Steel low-alloyed		[kg]	equipment, building,
	Stainless steel		[kg]	equipment, pipes
	Cast iron		[kg]	pumps, pipes, ...
	Copper		[kg]	
	Polyethylene		[kg]	pipes, equipment, ...
	Polypropylene		[kg]	pipes, equipment, ...
	PVC		[kg]	pipes, equipment, ...
	...		...	
Replacement parts	Membrane modules		[pc]	incl. average lifetime and material composition
	UV lamps		[pc]	incl. average lifetime and material composition

Annex-C Data collection template for LCC

COSTS yearly cost data to represent annual cost for setup, operation and removal over lifetime of the investment	Material	Quantity per year of service life	Unit	Remarks
Personnel costs	Salaries and wages		EUR	
	Social security costs		EUR	
	Training costs (internal)		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Materials	Energy consumption		kWh	
	Costrate		EUR/kWh	
	Energy costs		EUR	
	Raw materials		EUR	
	Operating supplies		EUR	
	Working materials		EUR	
	Wastes		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Services	Expertise, consultancy		EUR	
	Training costs (external)		EUR	
	Cost of project entity		EUR	
	Insurances		EUR	
	(External) subsituting services for failure		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Assets	Real estate		EUR	
	Infrastructure		EUR	
	Technical equipment and machines		EUR	
	Factory and office equipment		EUR	
	Intagible and financial assets		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Financing	Interests		EUR	
	Fees		EUR	
	administrative charges for financing		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Taxes and dues	Value added tax		EUR	
	Local business tax		EUR	
	Coporate tax		EUR	
	Compensation payments for failure		EUR	
	Other		EUR	
	TOTAL		**EUR**	
Additional investment information		Quantity per year	Unit	Remarks
Performance per unit			-	technological alternatives must have
Service of life years	setup phase		years	
	operating phase		years	
	removal phase		years	
Discounting rates	discount factor(s)		%	over time, may change during LCC
	cost increases		%	over time, may change during LCC
	cost decreases		%	over time, may change during LCC
...	to be added if needed for specific cases			
GENERAL REMARKS				
- all cost data will be defined in close collaboration with the case study partner				
- allocation of overheads and indirect costs are important				
- partner should be able to provide a solid cost accounting incl. Keying experiences				
- LCC focuses payments-in and payments-out to be discounted				

Annex-D Input data for USEtox® model to calculate new characterization factors for selected organic micropollutants

Table 6-1: Physico-chemical, ecotoxicological and human toxicological input data for USEtox for 7 monitored substances (NEG = neglected)

CAS	Name	Molecular weight	K_{OW}	K_{OC}	P_{vap25}	Sol_{25}	k_{degA}	k_{degW}
		g.mol-1	*-*	*L.kg-1*	*Pa*	*mg.L-1*	*s-1*	*s-1*
41859-67-0	Bezafibrate	3.62E+02	1.78E+04	4.14E+02	8.15E-09	1.22E+00	3.02E-05	1.30E-07
298-46-4	Carbamazepine	2.36E+02	2.82E+02	1.33E+03	1.17E-05	1.12E+02	6.08E-05	2.10E-07
15307-86-5	Diclofenac	2.96E+02	3.24E+04	4.58E+02	8.19E-06	2.37E+00	1.23E-04	2.10E-07
73334-07-3	Iopromide	7.91E+02	8.91E-03	1.00E+01	2.12E-26	2.38E+01	4.86E-05	1.30E-07
51384-51-1	Metoprolol	2.67E+02	7.59E+01	1.14E+02	3.84E-05	1.69E+04	1.10E-04	2.00E-07
60-80-0	Phenazone (Antipyrine)	1.88E+02	2.40E+00	1.31E+02	3.72E-02	5.19E+04	2.40E-05	5.30E-07
723-46-6	Sulfamethoxazole	2.53E+02	7.76E+00	2.58E+02	1.74E-05	6.10E+02	1.51E-04	2.10E-07

Name	k_{degSd}	k_{degSl}	Average $\log_{EC50}$	$ED50_{inh,noncanc}$	$ED50_{ing,noncanc}$	$ED50_{inh,canc}$	$ED50_{ing,canc}$
	s-1	*s-1*	*mg.L-1*	*kg.lifetime-1*	*kg.lifetime-1*	*kg.lifetime-1*	*kg.lifetime-1*
Bezafibrate	1.44E-08	6.50E-08	1.33E+00	2.78E+01	2.78E+01	NEG	NEG
Carbamazepine	2.33E-08	1.05E-07	1.40E+00	2.03E+01	2.03E+01	NEG	NEG
Diclofenac	2.33E-08	1.05E-07	1.01E+00	3.38E+00	3.38E+00	NEG	NEG
Iopromide	1.44E-08	6.50E-08	3.06E+00	2.43E+02	2.43E+02	NEG	NEG
Metoprolol	2.22E-08	1.00E-07	6.61E-01	6.96E+01	6.96E+01	NEG	NEG
Phenazone	5.89E-08	2.65E-07	2.26E+00	5.04E+01	5.04E+01	5.37E+02	5.37E+02
Sulfamethoxazole	2.33E-08	1.05E-07	6.26E-01	8.85E+01	8.85E+01	NEG	NEG