D3.1 Appropriate and user friendly methodologies for Risk assessment, Life Cycle Assessment, and Water Footprinting

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Abstract	This report provides the reader with an overview of assessment methodologies used within DEMOWARE and the specific features when using QMRA, QCRA, LCA, and WFP approach for the assessment of water reuse systems. For the actual application of LCA and water footprint databases and assessment software is needed. Therefore, three complementing goals shall be achieved: - To provide practitioners with the principles, methods and limitations of QMRA, QCRA, LCA and WFP - To provide LCA, WFP, RA practitioners with additional information when using the respective method for the assessment of water reuse systems. For QMRA a summary of guidelines and default values is collected from different guidelines documents (WHO, Australia, US-EPA), which allow a first simplified and thus user friendly risk estimate.

Versioning and Contribution History

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Glossary

DALY: Disability adjusted life years

LCA: Life Cycle Assessment

QMRA: Quantitative microbial risk assessment

WFP: Water footprinting

WIIX: Water Impact Index

WWTP: Wastewater treatment plant

YLL: Years of life lost

YLD: Years lived with disability

PFBA: Perfluorobutanoic acid

PFPeA: Perfluoropentanoic acid,

PFHxA: Perfluorohexanoic acid,

PFOA: Perfluorooctanoic acid,

PFHxS: Perfluorohexane sulfonate, and

PFOS: Perfllurooctane sulfonate

Executive Summary

In recent decades, significant progress has been made in the fields of sustainability research and analysis. Multiple assessment methods have been developed to cope with issues of resource depletion, water scarcity, emissions into the environment, and public health. Suitable tools for analysing these impacts on the environment and humans in a defined framework are Life Cycle Assessment (LCA) for assessing resource use and emissions on a life-cycle basis, water footprinting (WFP) for assessing water quality and quantity aspects, or quantitative microbial/chemical risk assessment (QMRA, QCRA) for assessing impacts on human health and the environment from exposure to pathogens and chemicals, respectively.

This report aims at providing the reader with an overview of assessment methodologies used within DEMOWARE and the specific features when using RA, LCA, and WFP approach for the assessment of water reuse systems. For the actual application of LCA and water footprint requires the use of specific LCA databases and assessment software. Therefore, three complementing goals shall be achieved with this report:

- To provide practitioners with the principles, methods and limitations of QMRA, QCRA, LCA and WFP
- To provide LCA, WFP, RA practitioners with additional information when using the respective method for the assessment of water reuse systems
- For QMRA, a summary of guidelines and default values is collected from different guidelines documents (WHO, Australia, US-EPA), which allow a first simplified and thus user friendly risk estimate.

This might be helpful for both new projects (where local data does not yet exist) but also for existing projects where risk based approaches are planned to be implemented. For higher tier risk assessments, the collection of local data is mandatory. In fact, one of the fundamental principles of risk-based management approaches is that there are no two identical systems and thus risk management plans will always be dependent on local information.

Within the different chapters of the report, the most important steps of each assessment method are summarized and explained. Issues of risk assessment in general, acceptable/tolerable risk, and the use of different measures for communicating risk are addressed. Moreover, a summary of default values for different exposure scenarios is provided, which allow first-tier risk estimation. A precautionary realistic worst case scenario is proposed in case that local data are lacking. Additionally, examples will be given on how to calculate risk as well as the required treatment performance to be in line with internationally accepted benchmarks. Finally, a proposition is made on how to communicate the quality of the used data and thus the credibility of the outcomes of the overall assessment.

For LCA, guidance is given on the suitable definition of goal and scope for water reuse systems, relating to function and functional unit, reference flow, system boundaries, co-products, and scenario definition. For impact assessment, a minimum set of environmental indicators is proposed based on the ReCiPe methodology. For data collection of the Life Cycle Inventory, important aspects are discussed concerning collection and validation of primary data, as well as background data coming from LCA databases. Finally, advice on impact assessment, presentation and discussion of indicator results, and interpretation of the outcomes of LCA are provided. A separate chapter discusses the emerging methods for WFP and describes two selected methods (water scarcity footprint and Water Impact Index) in their data needs and calculation principles.

1 Introduction

In recent decades, significant progress has been made in the fields of sustainability research and analysis. Multiple assessment methods have been developed to cope with issues of resource depletion, water scarcity, emissions into the environment, and public health. Suitable tools for analysing these impacts on environment and humans in a defined framework are Life Cycle Assessment (LCA) for assessing resource use and emissions on a life-cycle basis, water footprinting (WFP) for assessing water quality and quantity aspects, or quantitative microbial/chemical risk assessment (QMRA, QCRA) for assessing impacts on human health and the environment from exposure to pathogens and chemicals, respectively.

In the field of water reuse, these tools can be used to assess different options of water reuse (processes, strategies) against each other and against a situation without water reuse. Within the DEMOWARE project, these tools will be used to assess different systems of water reuse at selected sites in Europe in terms of potential environmental impacts, effects on the water cycle and on public health risk. With this information, water reuse schemes can be promoted by showing their environmental profiles and potential benefits, positive effects on the water cycle management, and acceptable risk management for the protection of public health.

The different methods differ in the spatial and temporal extension as well as in their degree and levels of implementation (Table 1-1).

Table 1-1 Overview of the different assessment methods used in DEMOWARE

	What is assessed?	Scale	Model Input	Model Output
Life Cycle Assessment (LCA)	Potential environmental impact of products or systems, often comparing scenarios with the same function	Impact assessment based on regional to global scale, general assessment	Resources and emissions during all stages of a product or system life cycle	Indicators representing potential environmental impacts (various indicators and methodologies available)
Water footprinting (WFP)	Consumptive and non-consumptive water use, including changes in water quality related to a certain product or system	Impact assessment on local, regional or global scale	Amount and quality of water withdrawals and discharge along the life cycle	WFP indicators, e.g. Water Impact Index, water footprint network indicator, virtual water
Quantitative chemical risk assessment (QCRA)	The probability of chemical agents exceeding predefined environmental or health based limit or precautionary values	local to regional	Emissions, production volumes, environmental concentrations at different endpoints, daily intake (for humans) + limit values, acceptable daily intake	Ratio between predicted environmental concentration and predicted no effect concentration (PEC/PNEC)

Quantitative microbial risk assessment (QMRA)	Probability of a specific system to deliver water of a predefined quality and the consequences of its failure to do so.	Inherently local, system specific	Exposure assessment + dose response model	Risk of infection/illness Health indicators (e.g. DALYs)

While the LCA framework is standardized for a long time (ISO 14040 2006, ISO 14044 2006) and widely used by industry and research facilities and annually updated databases ensure a common basis for assessment, water footprinting is an emerging tool where a selection of methods is under development and testing (Kounina et al. 2013), framed recently by the new ISO standard 14046 (ISO 14046 2014). In contrast to LCA, the broad use of QMRA of ensuring drinking and recycled water quality is currently practiced by a limited number of countries where its use is mandatory for drinking water supplies (e.g. NL) and water recycling schemes (e.g. AUS). Risk assessment of chemicals takes place at a wide range of international and national levels. Within REACH, new chemical products have to assess before entering the market. Within the water sector, it is the responsibility of health and environmental authorities to define risk based limit values for potentially toxic chemicals. The responsibility of the water practitioner is to ensure that the system delivers water of the required quality.

2 Goal and scope

This report aims at providing the reader with an overview of assessment methodologies used within DEMOWARE and the specific features when using RA, LCA, and WFP approach for the assessment of water reuse systems. For the case of chemical risk assessment, simplified models for chemical exposure assessment are available which can readily be used for water reuse systems (e.g. technical guidance document on risk assessment of new and existing substances (IHCP 2003), Australian guidelines for water recycling (WHO 2006,NRMMC-EPHC-AHMC 2006). However, the major challenge of quantitatively assessing chemical risks is the derivation of acceptable concentrations for currently unassessed chemicals (and mixtures) for different environmental and health endpoints and is the responsibility of the responsible health authorities. Thus, in case that no additional toxicological investigations are conducted, the presented methods will be limited to those substances for which toxicological values are available.

Moreover, the actual application of LCA and water footprint requires the use of specific LCA databases and assessment software. Therefore, three complementing goals shall be achieved with this report:

- To provide practitioners with the principles, methods and limitations of QMRA, QCRA, LCA and WFP
- To provide LCA, WFP, RA practitioners with additional information when using the respective method for the assessment of water reuse systems
- For QMRA, a summary of guidelines and default values is collected from different guidelines documents (WHO, Australia, US-EPA), which allow a first simplified and thus user friendly risk estimate.

This might be helpful for both new projects (where local data does not yet exist) but also for existing projects where risk based approaches are planned to be implemented. For higher tier risk assessments, the collection of local data is mandatory. In fact, one of the fundamental principles of risk-based management approaches is that there are no two identical systems and thus risk management plans will always be dependent on local information.

3 Appropriate methodologies on RA, LCA and WFP

3.1 Risk assessment

Risk assessment can be applied to various fields and endpoints ranging from technical and economic risks to risks for human health and various environmental compartments (soil, groundwater, surface water etc.).

Health and environmental risk assessments, regardless whether applied to chemical or microbial hazards, generally consist of the following four steps (WHO 2006, Haas 1999, IHCP 2003):

1. Hazard Identification
2. Hazard characterization/ effects assessment
3. Exposure assessment
4. Risk characterization

In hazard identification, the task is to attribute a certain hazardous feature, like "causing illness" or "genotoxicity" to a certain chemical or microbial agent. Usually, this involves research by chemists, toxicologists, epidemiologists and other relevant disciplines (Haas et al. 1999). In the following step of hazard characterization, it is investigated at which level of exposure a harmful effect can be expected. The major goal is the derivation of dose-response (or dose-effect) relationships for microbial hazards and predicted–no-effect-concentration/acceptable daily intakes for chemical substances based on toxicological testing. The third step of exposure assessment tries to model/estimate the expected concentration or dose the endpoint of interest (soil, groundwater, humans) is exposed to. Finally, in risk characterization, the relevant information is brought together and an estimation of the probability of a harmful effect caused by the exposure to a specific hazard is formulated.

In practice of water reuse, risk assessment (RA) tries to assess the probability and the consequences of the occurrence of hazardous events, which lead to the presence of a hazard (chemical or biological) in the reclaimed water. In general, RA can be conducted qualitatively, semi-quantitatively and quantitatively. The most important part in risk assessment is to get started. Risk assessment and management is an inherently iterative process aiming at implementing a proactive manner of managing both knowledge and uncertainty. Positively speaking, every time the team responsible for assessing a system is not able to give a satisfactory answer to one or all of the following questions, a new area of improvement has been identified:

1. What can happen?
2. How likely is it to happen?
3. What are the consequences?
4. How do we control/prevent it to happen?
5. How do we know that the barriers and reduction measures in place work the way we expect them to?

The focus of this study lies on the assessment of risk to human health and environmental risks due to the exposure to chemical and microbial wastewater constituents. According to WHO Guidelines for the safe use of excreta, wastewater and greywater, "the most effective means of consistently ensuring safety in wastewater use is through the use of a comprehensive risk assessment and risk management approach that encompasses all steps of the process [...]"(WHO 2006), p. 16, chap. 2.6, l. 4).

The current state of the art in microbial risk assessment involves a quantitative prediction of the exposure to so-called reference pathogens and the derivation of the related risk of infection and illness, respectively. This methodology is called quantitative microbial risk assessment (QMRA).

In Europe, major contributions to the development of QMRA and RA in general have been developed within the MICRORISK (www.microrisk.com) project with special focus on drinking water supplies. Major differences between RA for drinking water systems and RA for water reuse applications can be attributed to both source water quality and the relevant routes of exposure. Table 3-1 gives an overview on differences between RA in drinking water and water reuse applications.

Table 3-1 Similarities and differences between microbial risk assessment for drinking water and water reuse systems.

Characteristic	Drinking Water	Water reuse
Exposure route	Drinking water consumption Inhalation (e.g. *legionella spp.)*	Depending on use category, generally several different routes of exposure during various steps of water reuse (pre-treatment, storage, post-treatment, distribution)
Raw water quality	Depends on water source: Protected groundwater source (usually of high microbiological quality), surface water: high variability, prediction of source water quality at a given time challenging	Low microbial and chemical quality of secondary effluent but: Quality of source water (effluent wastewater treatment) can be controlled and predicted to a certain extend
Sources of contamination	Surface water: often multiple sources of contamination, hard to identify unknown sources, microbial source tracking as a major field of research	Main sources of pollution: human and animal faeces and industrial discharges (toilet flushing, surface runoff), prior information of presence of pathogens and chemical substances exist through epidemiological and local data
Risk management approaches	Water Safety Plans, country specific approaches depending on the organisation of the water sector	Sanitation Safety Plans, Water Reuse Safety Plans (in progress)
Ingested volume	High volume (0.5-2L) intentionally ingested Unintentional inhalation	Usually small volumes unintentionally ingested (except from potable reuse applications) Exposure via other routes of exposure products (e.g. raw vegetables) possible
Type of barriers	Multiple barrier principle (source protection, treatment, network, installations in buildings), Focus on water quality control	Control measures may include treatment and non-treatment options aiming at water quality and exposure reduction, respectively.

3.1.1 Tolerable risk and health based targets

Questions of risk are related to the question whether a system keeps within tolerable boundaries or whether a system is capable of reliably producing safe drinking water under normal and incident conditions. Zero risk does not exist! Consequently, levels of risk which are considered to be safe need to be defined.

Against this background, the definition of safety is usually the responsibility of the authorities in charge; the WHO states:

"The judgement of safety — or what is a tolerable burden of disease in particular circumstances — is a matter in which society as a whole has a role to play. The final judgement as to whether the benefit resulting from the adoption of any of the health-based targets justifies the cost is for each country to decide" ((WHO 2011), p. 36).

In chapter 10 of the Stockholm Framework (Fewtrell and Bartram 2001) Hunter and Fewtrell list different standpoints, which could be used for the determination of a level of risk, which might be called acceptable. They state that a risk might be acceptable when:

- *"it falls below an arbitrary level of probability*
- *it falls below some level which is already tolerated*
- *it falls below an arbitrary defined attributable fraction of total disease burden in a community*
- *the costs of reducing the risk would exceed the costs saved*
- *the costs of reducing the risk would exceed the costs saved when the "costs of suffering" are also factored in*
- *the opportunity costs would be better spent on other, more pressing, public health problems*
- *public health professionals say it is acceptable*
- *the general public say it is acceptable (or more likely, do not say it is not)*
- *politicians say it is acceptable"*

There are many discussions running on the acceptable or tolerable level of risk, which shall not be summarized in detail at this place. If QMRA is applied, tolerable levels of risk are most often defined as tolerable additional burden of disease expressed in DALYs[1] (WHO, AUS) per person per year (pppy) or as tolerable probability of infection pppy (NL). For chemical risks, predicted no effect level and concentration are used for threshold chemicals, and tolerable additional disease probabilities for non-threshold chemicals (see section 3.1.4.2)

When it comes to the quantification of risk in water reuse systems, the operator's responsibility is to provide a satisfactory level of certainty that the system is able to produce water which is considered to be safe. Here, a tolerable level of 10^{-6} additional DALYs pppy is applied following current WHO guidelines.

3.1.2 Tiered approach of RA

RA aims at calculating the probability of illness, infection or harmful effects as the result of chemical or microbial exposure given the information of the present raw water quality, system operation and reduction measures in place. As a second step, the calculated risk is compared to the set health target. If the calculated risk lies well below the set health target, the system can be considered to be adequately safe (Petterson et al. 2006). Wastewater is usually not disinfected and microbial water quality parameters are not usually measured. The same accounts for most chemical parameters other than the ones regulated in national wastewater regulations. Thus, for new projects the data availability will usually be rare. In these cases, realistic worst case scenarios based on conservative assumptions may serve as a first approach towards risk quantification. In case the health target is not met, which will often be the case for reuse systems, additional measurements for the verification of barrier performances and implementation of further risk

[1] For additional information on the DALYs indicator please see www.who.int/healthinfo/global_burden_disease/metrics_daly/en/

reduction measures have to be gathered. Thus, RA is a tiered approach which starts with collecting the available information for first risk estimations (see Figure 1). RA can play an important role at different steps of the overall risk management circle ((Petterson et al. 2006), (Smeets 2010)).

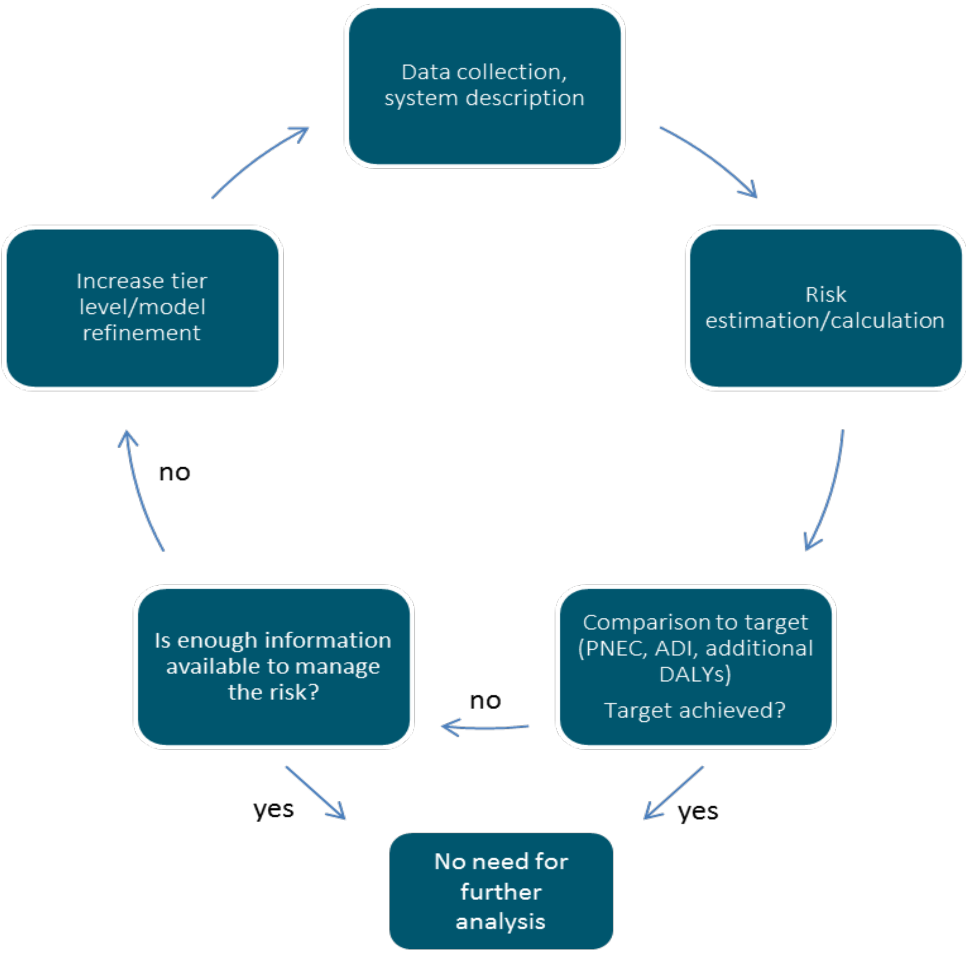


Figure 1 Tiered approach to RA (adapted from (Petterson et al. 2006))

3.1.3 Hazard identification

Municipal wastewater contains a variety of chemical and microbial hazards, ranging from viruses to bacteria and parasites to heavy metals and organic micropollutants. The following section gives an overview of hazards present in municipal wastewater as well as specific aspects when dealing with the assessment of pathogens and chemical substances, respectively.

3.1.3.1 Microbial hazards and reference pathogens in municipal wastewater

The presence of pathogenic microorganisms in municipal wastewater depends on the general health status of the local population. The higher the prevalence of a certain illness within the population the more likely it is that the illness causing pathogens might be found in the wastewater. However, not all of the pathogens present in wastewater are equally likely to be relevant for water reuse schemes. Table 3-2 gives an overview of viral, bacterial and protozoan pathogens potentially found in wastewater according to WHO (2006). Due to the high number of pathogens usually so-called indicator organisms are used to assess the hygienic quality. For QMRA so-called reference pathogens or index organisms are used to calculate the microbial risk. These are real pathogens, which represent the larger groups of viruses, bacteria and protozoa. The most frequently used reference pathogens are Rotaviruses, *Campylobacter* and Cryptosporidium parvum. An overview of indicator organisms and reference pathogens measured in wastewater is given in Table 3-3.

Table 3-2: overview of selected viral, bacterial and protozoan pathogens found in wastewater (WHO 2006, chap. 2.7.1)

Agent	Disease
Viruses	
Adenovirus	Respiratory disease, eye infections
Astrovirus	Gastroenteritis
Calicivirus	Gastroenteritis
Coronavirus	Gastroenteritis
Coxsackievirus A and B	Herpangina, aseptic meningitis, respiratory illness, fever, paralysis, respiratory, heart and kidney disease
Echovirus	Fever, rash, respiratory and heard disease, aseptic meningitis
Enterovirus	Gastroenteritis, various
Hepatitis A and E	Infectious hepatitis
Norovirus	Gastroenteritis
Parvovirus	Gastroenteritis
Poliovirus	Paralysis, aseptic meningitis
Reovirus	Not clearly established
Rotavirus	Gastroenteritis
Bacteria	
Campylobacter jejuni	Gastroenteritis, long-term sequelae (e.g. arthritis)
Escherichia Coli	Gastroenteritis
EHEC	Bloody diarrhea, haemolytic-uraemic syndrome (HUS)
Leptospira spp.	Leptospirosis
Salmonella	Salmonellosis, Gastroenteritis, diarrhea, long-term sequelae (e.g. arthritis)
Shigella	Shigellosis (dysentery), long-term sequelae (e.g. arthritis)
Vibrio cholera	Cholera
Yersinia enterocolitica	Yersiniosis, Gastroenteritis, long-term sequelae (e.g. arthritis)
Protozoa	
Cryptosporidium parvum	Cryptosporidiosis, diarrhea, fever
Giardia intestinalis	Giardiasis

Table 3-3: Overview of measured ranges of pathogens in different sources of water and human faeces ((WHO 2011), chap.7)

Microbe	Number per gram faeces	Number per litre in untreated wastewater	Number per litre in raw water
Faecal coliforms	10^7 (mostly non-pathogenic)	10^6-10^{10}	100-100000
Campylobacter spp.	10^6	100-10^6	100-10000
Enteroviruses	10^6	1-100	0.01-10
Rotaviruses	10^9	50-5000	0.01-100
Cryptosporidium parvum	10^7	1-10000	0-1000
Giardia intestinalis	10^7	1-10000	0-1000

3.1.3.2 Chemical hazards in municipal wastewater

Chemical hazards in municipal wastewater consist of a wide range of naturally occurring or synthetic organic and inorganic chemicals. Examples of different groups of chemicals are summarized in Table 3-4. The numerous groups of chemicals include even more single compounds, substances and ions. Each of them might have specific effects on certain environmental compartments, species and human health, alone or in combination with other chemicals substances. The high amount of different substances (and transformation products), potential effects and different exposed species and compartments are one of the major challenges and sources of uncertainty regarding the risk assessment of chemicals for water reuse systems.

Table 3-4: Selection of major groups of chemicals in municipals wastewater (Khan 2010)

Chemical	Origin	Examples
Heavy metals	drinking water and drinking water pipes, gutters and surface runoff, diverse industrial discharges,	Cd, Hg, Pb, Cu, Zn, As, Cr, Ni
Synthetic industrial chemicals	Final or intermediate industrial products, depends on catchment area and local industry	dyes, PAHs, solvents, heat stabilizers, epoxy resins, bleaching chemicals
Volatile organic compounds	Industrials solvents	TCE; cDCE, VC
Algae toxins	Cyanobacteria (e.g. growth in open storage reservoirs)	microcyctins, nodularins, cylindrospermopsin and saxitoxins
Pesticides	Stormwater, illegal disposal, fruit, insect repellents etc.	Groups: herbicides, insecticides, fungicides Substances: Diuron, Terbutryne, Dicofol, Cybutryne

Disinfection by products	Formed during disinfection, reaction between disinfection agent and other water constituents	THM, chlorinated organic substances, bromate, NDMA
Radionuclides	Natural background/runoff, medical and industrial usage	Ra, Rn, U, Th
Pharmaceuticals	Excretion by people as well as direct disposal of unused products	Antibiotics, Beta-blockers, X-ray contrast media
Natural steroid hormones	Excretion by people	Oestradiol, oestrone, testosterone
Antiseptics	Broad range of cosmetic and medical products	Triclosan, Triclocarban
Perfluorochemicals	Water resistant surfaces (clothes, cookware), firefighting foams	PFBA, PFPeA, PFHxA, PFOA, PFHxS, PFOS
Nanoparticles	Cosmetics, medicine, pharmaceuticals, Industry	TiO, ZnO
Nutrients	Organic and inorganic N and P sources	N, P
Salinity/Salts	drinking water, seawater seepage, households	Mg^{2+}, Cl^{-}, Ca^{2+}, SO_4^{-}, Na^{+}, K^{+}, B^{-}

3.1.4 Hazard characterization

The major task in hazard characterization is the determination of the properties of a chemical or microbial hazard. It involves the determination of the environmental behaviour, physical-chemical properties as well as the derivation of dose response relationships. For microbial risk, a functional relation is derived between the number of organisms ingested and the probability of infection (Haas et al. 1999). For chemicals, acceptable concentrations or no-effect concentration are derived from toxicological testing. Depending on the quality and quantity of toxicological data, uncertainty/safety factors are applied to the outcomes of the respective toxicological tests (IHCP 2003). Distinctions are made between health and environmental endpoints. While for humans health doses in terms of so-called acceptable daily intakes (ADI) are derived, the values for environmental endpoints usually are expressed as concentrations. These so-called predicted-no effect concentrations (PNECs) are formulated for different environmental compartments, e.g. $PNEC_{soil}$, $PNEC_{groundwater}$. However, back calculated form the ADI, PNECs can also be formulated for human health issues where exposure via the environment might occur, like e.g. $PNEC_{human}$ for soil or food concentrations of certain chemicals (IHCP 2003).

3.1.4.1 Dose response relations in microbial risk assessment

A major limitation of QMRA is that dose-response relations are just known for a limited number of pathogens. The most commonly used relationships between dose and the probability of infection are based either an exponential or Beta Poisson models. Other approaches exist using e.g. confluent hypergeometrical functional relations for Norovirus proposed by (Teunis et al. 2008). The dose response parameters of the most frequently used reference pathogens are shown in Table 3-5.

Table 3-5 dose response-models for selected reference pathogens

Exponential(k), Beta-Poisson parameters (N_{50}, α)				
Pathogen	k (r=1/k)	N_{50}	α	a, β References
Campylobacter		896	0.145	(Haas et al. 1999), (WHO 2006)
Giardia	50.23			(Haas et al. 1999), (Rose et al. 1991)
Rotavirus		6.27	0.2531	(Haas et al. 1999), (WHO 2006)
Cryptosporidium parvum	238			(Haas et al. 1999)

3.1.4.2 Dose response relation in chemical risk assessment

For health risk assessment of toxic chemicals, a distinction is made between chemicals with and without threshold level, as well as between acute and chronic toxic effects.

For non-threshold chemicals, negative effects are always possible regardless of their concentrations because, often, linear relationships between exposure and risk are assumed for these groups of chemicals, e.g. many carcinogens (van Leeuwen and van Vermeire 2007). For these groups of chemicals, risk is expressed as the probability of additional disease (e.g. cancer) cases occurring, e.g. one in a million or 1/100.000.

In the case of threshold chemicals, it is assumed that negative effects will not occur given that a particular concentration is not exceeded. Both the existence and non- existence of such threshold values are possible unverifiable assumptions (Asano et al. 2007).

A major limitation of chemical risk assessment of complex matrices, like e.g. treated wastewater, is the lack of scientifically derived PNEC values for a large number of chemical constituents for different environmental endpoints. The assessment of mixtures of chemical substances is another source of uncertainty where there is definitely a need for further research and development.

3.1.5 Exposure assessment

Exposure assessment aims at quantifying the amount or dose of a certain hazard to which the population or environmental endpoint of interest is exposed to. Exposure assessment can roughly be divided into two parts:

1. Modelling of the water quality the population is exposure to, accounting for raw water quality and the barriers (treatment steps, health protection measures etc.) being in place.
2. Application of relevant exposure scenarios (ingestion, inhalation, dermal absorption etc.) depending on the local situation and the properties of the specific hazard to be assessed.

A major difference between microbial and chemical exposure assessment is that pathogens are single particles and that already single pathogens might be able to cause illness. This means that already short periods of a malfunctioning treatment step might have direct health impacts.

In contrast, in chemical risk exposure assessment usually concentrations are modelled and acute toxicity caused by a short term failure of a treatment steps seems rather unlikely. Moreover, for risk estimation of chemicals other exposure routes (like food consumption) have to be considered as well. Usually, only 10% of the acceptable daily intake of a chemical is regarded as tolerable for drinking water consumption.

Risk assessment does not require complicated modelling in general. If worst case assumptions already reveal that risk falls below tolerable levels, no further modelling has to be done. (Khan 2010) summarized different levels of modelling approaches:

Level 0: Hazard detection and failure modes identification

Level 1: 'Worst case approach'

Level 2: Quasi-worst case and plausible upper bounds

Level 3: Best estimates and central values

Level 4: Probabilistic risk assessment, single risk curve

Level 5: Probabilistic risk analysis, multiple risk curves.

3.1.5.1 Modelling of water quality

In water reuse, different treatment technologies are used to achieve the required water quality. In QMRA, the treatment performance of every individual treatment process has to be assessed and its performance validated. In countries where QMRA is mandatory (e.g. Australia, Netherlands), usually direct pathogen measurements are limited to raw water samples, whereas treatment performance is verified and monitored using indicator organisms. The performance of a specific treatment step is inherently site-specific and depends on various factors, like influent water quality, pre-treatment, system specifics, control engineering, and maintenance. Table 3-6 summarizes a review of the performance of different treatment steps. If no other data is available, the lower values may be used for a first precautionary assessment. A professional planning, engineering and construction has to be seen as a prerequisite. This table will not replace validation and verification monitoring but rather gives the information at hand for a first estimation of the treatment performance of the system. Similar reviews can be found in ((WHO 2011), chap. 7) and (WHO 2006), chap. 5).

Table 3-6 Review of the treatment efficiency in LUR (log unit reduction) of different wastewater treatment options ((NRMMC-EPHC-AHMC 2006), WHO 2006)

Treatment	Viruses (including adenovirus, rotavirus and enterovirus)	Phage (viral indicators)	E. Coli	Bacterial pathogens (including *Campylobacter*)	Clostridium perfringens	Protozoa		Helminth eggs
						Giardia	Crypto	
Primary Treatment	0-0.1	0-1	0-0.5	0-0.5	0-0.5	0.5-1	0-0.5	0-2
Secondary treatment	0.5-2	0.5-2.5	1-3	1-3	0.5-1	0.5-1.5	0.5-1	0-2
Dual media filtration	0.5-3	0.5-4	0-1	0-1	0-1	1.5-2.5	1.5-2.5	2-3
Membrane filtration	2.5-6	3-6	3.5-6	3.5-6	>6	>6	>6	>6

Reverse osmosis	>6	>6	>6	>6	>6	>6	>6	>6
Lagoon storage	1-4	1-4	1-5	1-5	N/A	3-4	N/A	1.5->3
Chlorination	1-3	0-2.5	2-6	2-6	1-2	0.5-1.5	0-0.5	0-1
Ozonation	3-6	2-6	2-6	2-6	0-0.5	N/A	N/A	N/A
UV radiation	>1 (Adenovirus) >3 (Enterovirus, Hepatitis A)	3-6	2->4	2->4	N/A	>3	>3	N/A
Wetlands (surface flow)		1.5-2	1.5-2.5	1.5-2.5	1.5	0.5-1.5	0.5-1	0-2
Wetland (subsurface flow)		1.5-2	0.5-3	0.5-3	1-3	1.5-2	0.5-1	

In addition to wastewater treatment, non-treatment control measures may reduce the probability of infection. These include mainly measures of exposure prevention, e.g.:

- Crop restriction for consumer protection
- Restriction of irrigation periods (e.g. irrigation just during the night)
- Irrigation technologies with low aerosol formation (particle removal might be necessary beforehand)
- Setback distances
- Use of natural pathogen die-off
- Protective hedges
- Protective gear
- Hygiene procedures

In (WHO 2006) attempts are made to allocate additional log units to these kind of non-treatment options (see (WHO 2006), chap. 5). At this early stage and lower tier risk assessment, for which this report is intended, it is recommended to focus on the technical systems, first.

For modelling of chemical substances, a summary like in Table 3-6 is not reasonable due to the large number of chemicals substances, local boundary conditions and use categories. However, Table 3-7 gives an overview of a selection of technologies, which can be used to reduce concentrations of broad categories of chemical constituents of municipal wastewater. In general, the same conceptual approach is used as for microbial hazards.

Table 3-7: Selection of available treatment technologies (not exhaustive) for additional wastewater treatment.

	Ozonation	Chlorine	Membrane processes MF	UF	NF	RO[7]	Rapid sand filtration	Precipitation/Floccula-tion	Micro screening	Polishing pond	Biological activated fil-ter	Adsorption on acti-vated carbon
Nutrients (N, P)			(x)[2]	(x)[2]	x	x	(x)[4]	x	(x)[4]	x	x	x[6]
Heavy met-als						x		x				
Organics and micropollu-tants	x	(x)			x	x					x	x
Ions and sa-linity					x[7]	x						

[1] Removal depends on pore size and operating parameters
[2] In combination with bioreactor
[3] Removal depends on filter media and operating parameters
[4] Particular fixed nutrients
[5] Removal depends on operating parameters
[6] Organic compounds
[7] strongly dependent on size and charge

3.1.5.2 Scenarios for direct human exposure

Depending on local conditions, exposure to reclaimed water might happen over several pathways.

3.1.5.2.1 Ingestion

For water reuse systems ingestion might be the most important route of exposure to microbial and chemical substances. In QMRA, the number of pathogens to which the population of interest is exposed is estimated based on the modelled water quality. Assumptions have to be made for:

a. the volume of ingested water per exposure event
b. the number of exposure events per time period (usually per year)

For water reuse application, different scenarios and groups of people have to be considered. If no local information is available Table 3-8 may serve as orientation.

Since in QCRA chronic effects should be considered as well, some additional factors have to be accounted for (Khan 2010).

$$Intake\left[\frac{mg}{kg * d}\right] = \frac{C_W * IR * EF * ED}{BW * AT}$$

CW = hazard concentration in water
IR = ingestion rate [L/d]
EF = Exposure frequency [d/year]
ED = Exposure duration [years]
BW = body weight [kg]
AT = averaging time (over which exposure is averaged [d])

Table 3-8 Assumptions for exposure assessment for different use categories based on international guidelines ((WHO 2006),(NRMMC-EPHC-AHMC 2006))

Use categories	Reuse in agriculture		Potable reuse		Urban irrigation		Other uses
	Restricted	Unrestricted (commercial)	Direct	Indirect	Public	Private	Toilet flushing
Number of exposure events per year	100	70 (lettuce) 140 (other raw produce)	365	365	50	90	1100
Volume of water ingested per exposure event [ml]	0.1-1	5 (lettuce) 1 (other raw produce)	1000	1000	1	0.1-1(routine) 100 (accidental)	0.01
Route of exposure	Ingestion						

3.1.5.2.2 Exposure to volatile compounds

Chemical exposure to volatile compounds can be calculated as follows (Khan 2010):

$$Intake\left[\frac{mg}{kg * d}\right] = \frac{C_A * IR * ET * EF * ED}{BW * AT}$$

CA = hazard concentration in air
IR = ingestion rate [L/d]
EF = Exposure frequency [d/year]
ET = Exposure time [h/d]
ED = Exposure duration [years]
BW = body weight [kg]
AT = averaging time (over which exposure is averaged [d])

3.1.5.2.3 Dermal absorption

Chemical exposure via dermal absorption can be estimated by (Khan 2010):

$$DAD\left[\frac{mg}{kg * d}\right] = \frac{DA_{event} * EV * ED * EF * SA}{BW * AT}$$

DA_{event} = absorbed dose per event [mg/cm²/event]
EV = event frequency [events/day]
EF = Exposure frequency [d/year]
SA = skin area available to contact [cm²]
BW = body weight [kg]
AT = averaging time (over which exposure is averaged [d])

3.1.5.3 Scenarios for environmental endpoints and human exposure via the environment

Environmental exposure assessment and human exposure via the environmental are conducted for chemical substances. For a first tier basic estimation of local predicted environmental concentration (PEC_{local}), it is referred to the European Union Technical Guidance document on risk assessment. For the special case of managed aquifer recharge, the Australian Guidelines for Water Recycling offer simplified model assumptions which can readily be used. Table 3-9 gives an overview on relevant environmental endpoints, references proposed for basic modelling as well as processes and assumptions being considered in the respective approaches.

Table 3-9: Overview of different environmental endpoints

Compartment	Guidance document	Processes considered	Assumptions
(agricultural) Soil	(IHCP 2003)	Biodegradation, volatilisation, leaching, (derived from K_{OW}, K_H), atmospheric deposition	Annual loads applied once a year, averaged over 30 and 180 days for environmental and human health
Groundwater	(IHCP 2003)	Biodegradation, volatilisation, leaching,	$Soil_{porewater}$ concentration = groundwater concentration
Surface water	(IHCP 2003)	Partitioning, Dilution	WWTP effluent concentration, substance specific partitioning, dilution of 10 (if no other information available)
Managed Aquifer recharge	(NRMMC-EPHC-NHMRC 2009)	Adsorption, biodegradation, retardation	first-order exponential decay, distinction between aerobic and anaerobic conditions Sorption is expressed by K_{OC} and K_D, L/kg distribution coefficient for linear isotherm

3.1.6 Risk Characterization

Risk characterization brings together the information gathered during hazard assessment and exposure assessment in order to formulate an estimation of the type, magnitude and probability of the present risk.

3.1.6.1 Risk characterization in QMRA

In QMRA risk is usually expressed as probability of infection or in terms of the DALY indicator. The latter one will be introduced in the following section.

3.1.6.1.1 DALY calculation

An infection of a certain pathogen may lead to several different health outcomes (e.g. 1 day diarrhoea, 10 day diarrhoea, long term sequelae, death). Infections of the same pathogen will not lead to any symptoms in some cases (asymptomatic infection) while in other cases they will lead to severe illness or death. Moreover, some pathogens will preferably infect people of a certain age group, like Rotavirus does for children. For DALY calculation, the distribution of the different health outcomes caused by a specific pathogen are weighted between 0 (perfect health) and 1 (death) and summed up. Table 3-10 gives a summary of the average amount of DALYs per case of disease of widely used reference pathogens.

Table 3-10 Average values for DALY calculations for typical reference pathogens ((WHO 2006), (Mara and Sleigh 2010))

Reference pathogen	DALYs per case of disease	Disease risk pppy equivalent to 1µDALY pppy	Disease/ infection ratio	Tolerable infection risk pppy
Campylobacter[a]	$4.6\cdot10^{-3}$	$2.2\cdot10^{-4}$	0.7	$3.1*10^{-4}$
Cryptosporidium[a]	$1.5\cdot10^{-3}$	$6.7\cdot10^{-4}$	0.3	$2.2*10^{-3}$
Norovirus[b]	$9\cdot10^{-4}$	$1.1\cdot10^{-3}$	0.8	$1.3*10^{-3}$
Rotavirus[a]	$1.4\cdot10^{-2}$	$7.1\cdot10^{-5}$	0.05	$1.4*10^{-3}$

[a](WHO 2006), [b] (Mara and Sleigh 2010),

3.1.6.1.2 Inverse risk calculation for different use categories

The WHO as well as the Australian guidelines for water recycling apply a tolerable risk level of 1 additional µDALY pppy. Using this tolerable risk level and applying a conservative estimate of rotaviruses and other pathogens concentrations in untreated wastewater, the required log reduction in water treatment as well as the tolerable number of pathogens per litre in recycled water can be calculated for being in line with existing WHO standards. If exposed to high volumes of water this calculation results in extremely low target concentrations for virus particles in water. For drinking water supplies, a tolerable level of approximately 1 virus/100000L is calculated. Such low values equal an operational zero and are hardly detectable by current monitoring practices. Instead, other sources of evidence have to be used to deduce a level of certainty which is considered acceptable. LRU (log reduction units) are used to assess the treatment performance of each treatment step. Figure 2 to Figure 4 illustrate the dependencies between the number of exposure events per year, the average ingested volume of water and the required log reduction which is necessary to achieve the limit of 1 additional µDALY pppy for rotavirus, cryptostoridium and *campylobacter*, respectively. A conservative estimation of 5000 virus particles, 10000 oocysts and 1000000 bacteria per L of raw wastewater was used for the calculation.

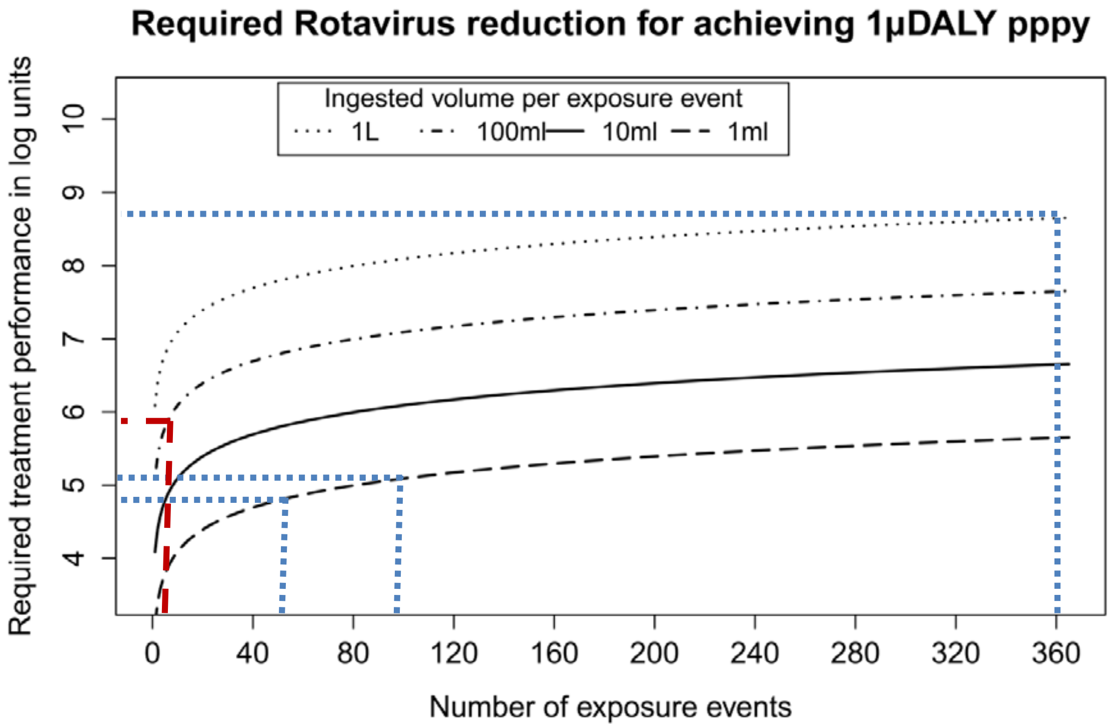


Figure 2 Required log reduction of Rotaviruses in order to achieve the WHO benchmark of 1 additional µDALY pppy. A raw water quality of 5000 Rotaviruses per litre is assumed. Blue line scenarios from right to left (drinking water, restricted irrigation (farmers), public irrigation). The red line represents a 1 time accidental spill and the ingestion of 100 ml.

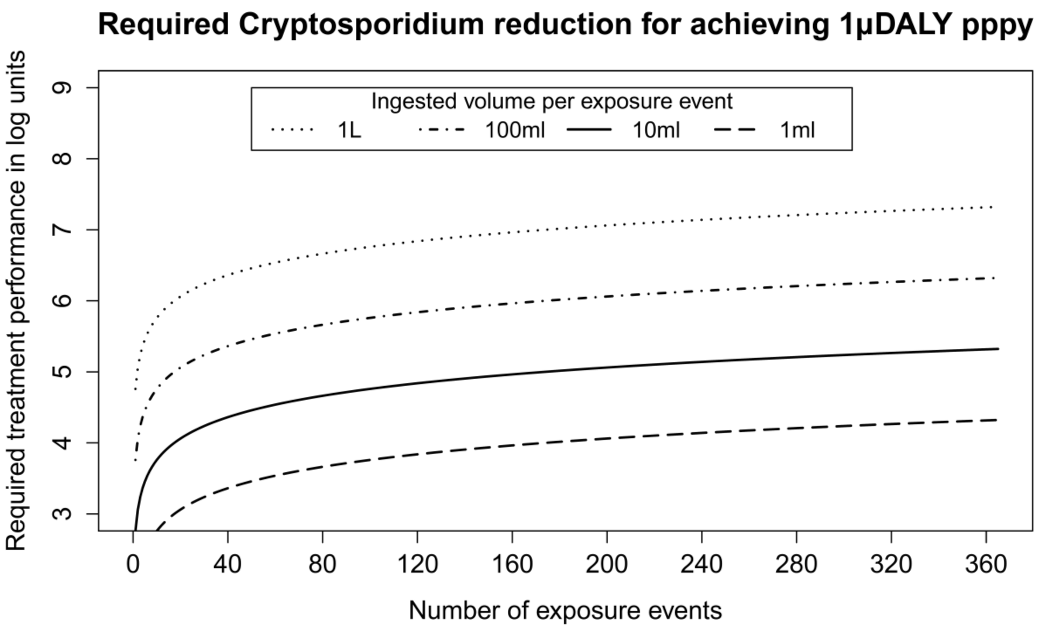


Figure 3 Required log reduction of Cryptosporidium parvum in order to achieve the WHO benchmark of 1 additional µDALY pppy. A raw water quality of 10000 oocysts per litre is assumed.

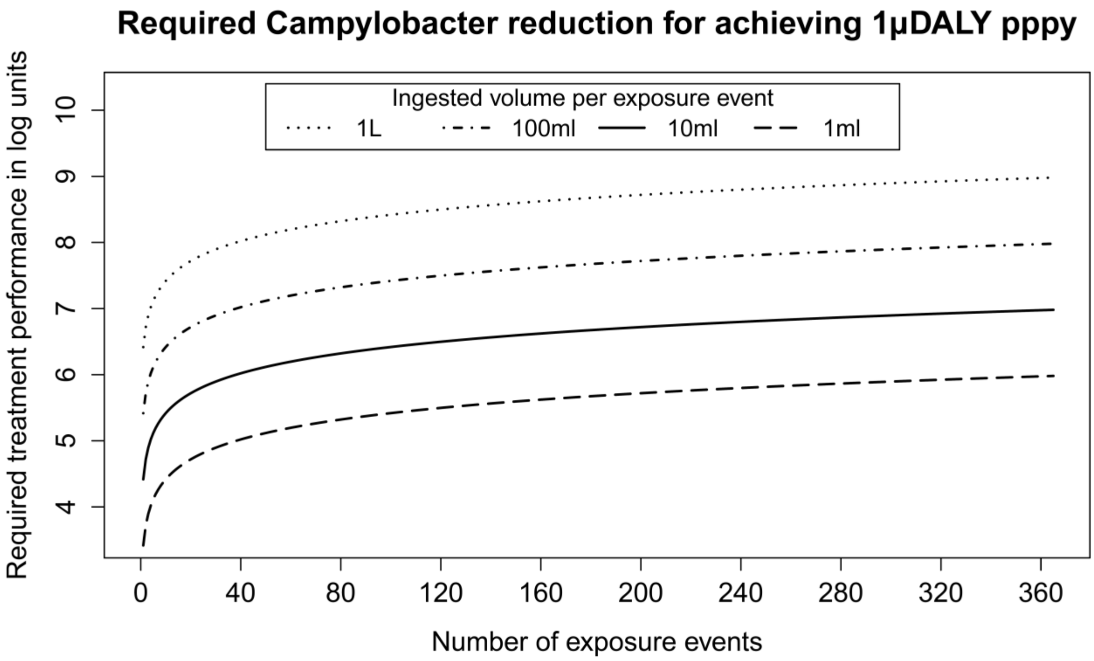


Figure 4 Required log reduction of *Campylobacter* in order to achieve the WHO benchmark of 1 additional µDALY pppy. A raw water quality of 1000000 bacteria per litre is assumed.

3.1.6.2 Risk characterization in QCRA

In quantitative chemical risk assessment, risk is expressed by comparing modelled or estimated exposure to the tolerable or acceptable effect levels/concentrations (ADI, PNECs). Thereby, risk quotients (RQ) or risk characterisation ratios (RCR) are calculated for each single endpoint. RQ/RCR > 1 indicate that given the current state of knowledge, risk is above acceptable levels and reduction measures should be implemented or that the model has to be refined. RQ < 0.1 is often defined as area of negligible risk (van Leeuwen and van Vermeire 2007).

Uncertainties within risk estimates can be made transparent in several ways. After Jager et al. cited in (van Leeuwen and van Vermeire 2007) risk and related uncertainties can be expressed as illustrated in Figure 5.

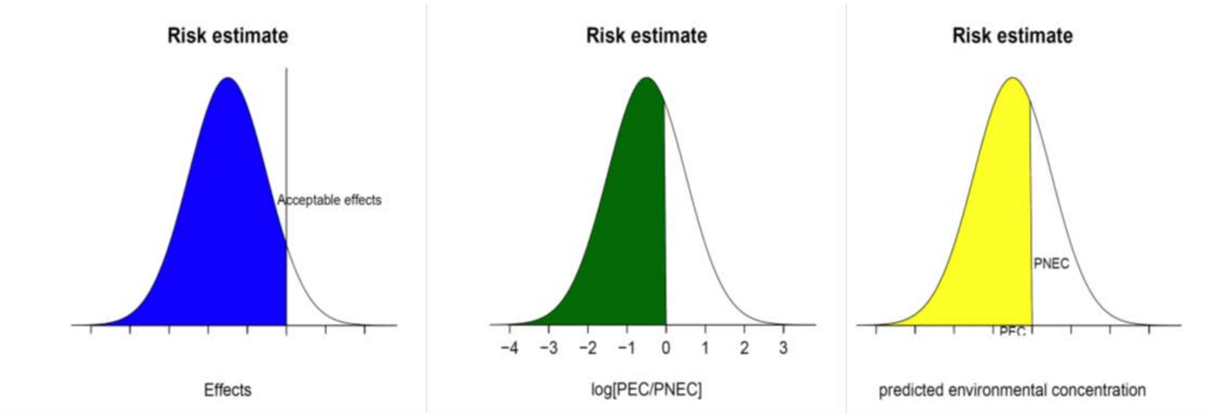


Figure 5: Options for illustrating risk and uncertainty in risk characterization(van Leeuwen and van Vermeire 2007)

3.1.6.3 Uncertainties and internal quality audits

A crucial part of any risk assessment is an at least qualitative assessment of present uncertainties. Approaches on how to identify knowledge and data gaps and how to communicate them can be found in (EFSA 2006), (WHO-IPCS 2008) or US-EPA (2008; 2011). Although those guidelines refer to the exposure of chemicals, the methods are applicable to microbial exposures as well.

Moreover, a critical (self) audit/assessment should be conducted. This audit is not only useful for a transparent communication of results thus serving as a basis for discussion, but also reveals areas of potential improvement/knowledge gaps, which is a key objective of any risk assessment.

For the present simplified and user friendly approach, which is based on a realistic worst case scenario focus should be on the quality of data and assumptions.

A simple scoring system may be applied to the different assumptions made for raw water quality, treatment performance, exposure assumptions etc.

Table 3-11: Scoring system for a critical self-assessment of the data quality of a risk assessment study.

Data Quality	Score (out of 5)
Local, long term, validated and representative data available	5
Local measurements + peer-reviewed literature + expert knowledge	4
Literature Review + expert knowledge	3
Expert knowledge or literature review	2
Educated guess	1
Uneducated guess	0

3.1.7 Proposed approach for simplified assessment

3.1.7.1 Simplified microbial risk estimation

The following procedure is proposed for a fist risk estimate (example see box on page 22):

Step 1: Define the context of the assessment

Catchment, wastewater treatment, storage, post treatment, use category, reference pathogens

Step 2: Define water quality, treatment performance and exposure scenarios

As the endpoint of QMRA is human health, conservative values for model parameters and variables are recommended which represent a realistic worst case scenario. Any modifications to this approach have to be supported by local investigations or other scientific evidence or prior knowledge of the system.

Using the default values provided in the different tables of this report, conservative values which lead to an precautionary risk estimate mean:

- pathogen concentration in raw wastewater (high),
- treatment efficiency (low),
- ingested volume (high)
- number of exposure events per year (high)

Step 3: Risk calculation

- Calculate probability of infection per exposure event
- Calculate probability of infection per year

- Apply disease per infection ratio and severity factor for DALY calculation

Step 4: Re-check quality of data and information to assess quality of the present assessment

3.1.7.2 Simplified chemical risk estimation

For a simplified and user friendly assessment, it is assumed that no additional toxicological tests are performed and PNEC values are available.

Step 1: Define goal and scope of chemical risk assessment (endpoint, chemicals, use category)

Step 2: Collect quality standards and existing PNEC values for the endpoint of interest in existing databases and scientific literature.

Step 3: Collect information of concentrations to be expected in reclaimed water (local measurement literature review and expert knowledge)

Step 4: Estimate environmental or human exposure according to existing estimation models using conservative assumptions (see section 3.1.5

Step 5: Compare estimated exposure levels to collected quality standards.

RQ > 1	→ unacceptable risk →increase tier level/r risk reduction measure necessary
0.1 < RQ < 1	→ increase tier level/ risk reduction measured to be considered
RQ < 0.1	→ negligible risk → no further analysis required

Step 1: Define the context of the assessment

System description and problem formulation:

Describe the system including catchment, wastewater treatment, reuse category, reference pathogens

Step 2: Define water quality, treatment performance and exposure scenarios

a. **Raw water quality:**

Direct measurements of real pathogens are preferred, for a precautionary first estimate the higher values for raw wastewater of Table 3-3 may be applied.

Example:

- *5000 rotavirus particles / L*

b. **Allocate log reduction potential to each individual treatment step**

Direct validation by monitoring of microbial indicators recommended. For a first and precautionary estimate the lower values of Table 3-5 may be used.

Example for virus reduction:

- *Primary treatment 0 log*
- *Secondary treatment: 0.5 log*
- *Dual media filtration: 0.5 log*
- *Chlorine disinfection (depends on 'ct'- value): precautionary assumption 1 log*

c. **Define exposure scenarios based on use category**

If no further information is available for a first precautionary estimation the higher values in Table 3-4 may be used.

Example for restricted irrigation:

- *1ml per exposure event and*
- *100 exposure events per year*

Step 3: Risk calculation

Risk is calculated by combining the expected dose/exposure event with the dose response models outlined in Table 3-2. Then, risk per person per year (pppy) is calculated.

a. Option 1: compare calculated probability to tolerable probability (e.g. 10^{-4} pppy)
b. Option 2: multiply probability with pathogen specific value for DALYs per case of disease (Table 3-6) and compare to WHO benchmark of 10^{-6} additional DALYs pppy

Example:

P (Infection | exposure 1ml, raw water (5000 RV/L), treatment (2 log) = 0.027 per exposure event

P (infection | 100 exposure events per year) = 1 – (1- P (per exposure event))^{100} = 0.94 pppy

➔ *Approx. 395 µDALYs pppy → risk reduction necessary*

Step 4: Assess quality of data and assumptions

Apply scoring points for each model input for assessing quality of results

Example: Raw water quality:	*Literature reviews + expert knowledge*	→	*3 out of 5*
Performance of primary treatment:	*Literature review + expert knowledge*	→	*3 out of 5*
Performance of secondary treatment:	*Expert knowledge*	→	*2 out of 5*
Dual media filtration:	*Expert knowledge, measurements, review*	→	*4 out of 5*
Chlorine disinfection:	*Validated local data, long term*	→	*5 out of 5*
Exposure assumptions:	*Educated guess*	→	*1 out of 5*
	Total score		*18 out of 30*
	Confidence in results		60%

3.2 Life Cycle Assessment

Life Cycle Assessment as defined in ISO 14040/44 ((ISO 14040 2006, ISO 14044 2006)) follows a methodological framework to enable a systematic and comprehensive characterisation and quantification of selected environmental impacts which are associated with a product or service. Using the life-cycle perspective, all relevant processes upstream and downstream of the system under study are described with input-output 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"), 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/eco-toxicity). 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, a typical LCA framework includes the water flow to be treated (as input or "reference flow"), the treatment process itself and 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 which are required to build and operate this treatment process (Figure 6). 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.

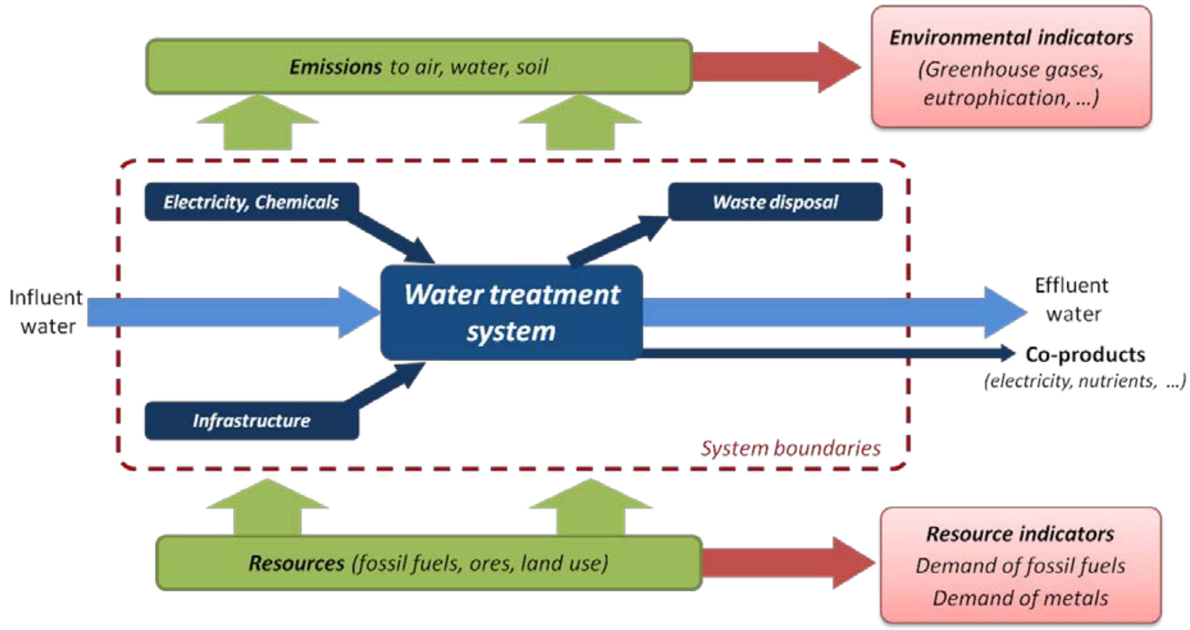


Figure 6 Typical system boundaries of an LCA for a water treatment system

According to ISO 14040, the execution of an LCA study involves a defined set of steps that can be followed. 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 the definitions 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 the LCA user 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 (Figure 7):

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.

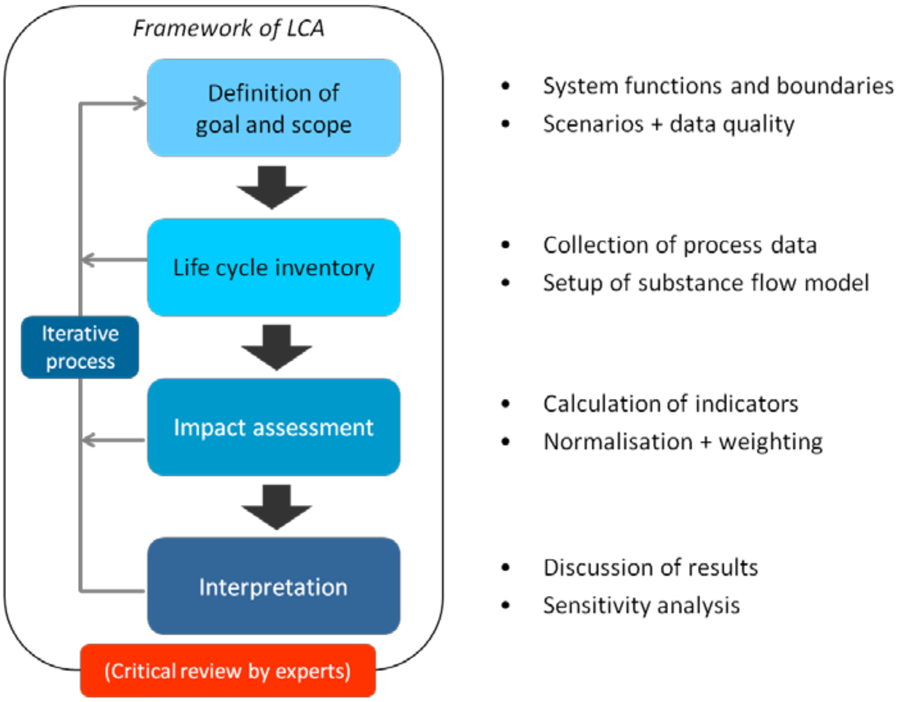


Figure 7 Framework of LCA according to ISO 14040/44

In practice, carrying out a full LCA study can be a laborious task and requires considerable expertise of the LCA practitioner. A meaningful definition of system boundaries and functional unit and equivalent scenarios for comparative studies are a prerequisite for an LCA which should compare different technological options or processes in their environmental impacts. Data collection can be a difficult task, requiring precise definitions of what is needed from the operators of the plant, careful up-scaling and transfer of lab/pilot results to projected full-scale plants, and realistic integration into full-plant concepts or systems. Data cross-check and validation with partners is a necessity to end up with valid datasets which are agreed upon in the project team to increase trust and understanding of LCA outcomes. Finally, choice of LCA indicators and further processing of results towards normalisation or aggregation needs some advice for the non-expert, so that LCA results are meaningful but still understandable for non-experts and can be used as decision support without taking final responsibility from the stakeholders.

Hence, this report introduces a simplified approach for LCA of water treatment systems, focussing on LCA of water reuse systems for different purposes. For all necessary steps in LCA, guidance is provided on how to implement a first simplified LCA with reasonable efforts. Therefore, the report describes all required steps of ISO14040/44 for a complete LCA of water reuse systems and gives detailed advice on how to approach them from a methodological point of view. However, as the LCA standard provides only a framework for this task, the described aspects should be seen as "user-friendly" guidance and may be adapted according to the specific goal and scope of the study at any time, provided that reasonable justification is given alongside.

3.2.1 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. "comparing alternative treatment processes for water reuse at site XY" or "comparing different strategies with and without water reuse on a greenfield site") and the intended use of its outcomes. The LCA method is suitable for comparison of different alternatives, but also for assessing a single system in its environmental footprint. While the latter will provide useful information about environmental hot spots of a single option, the comparison of different scenarios or even benchmarks from other studies enables the reader to judge and evaluate the environmental profile of a specific process in relation to other alternatives.

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. "treatment of secondary effluent of WWTP XY to reach the standards of use for agricultural purposes as defined in guidelines XY") and provide a qualifier for the water quality to be reached, e.g. certain concentration limits or defined quality parameters in microbial indicators. It can also be related to a minimum removal rate (e.g. "a minimum 4log removal of indicator bacteria E. coli as MPN/100mL").

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. 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 for re-use), as these volumes may not always correspond if the process involves water losses, for example by backwashing filters or membranes. 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). 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]).

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]), potentially extended with information about minimum, mean, and maximum flow rates (e.g. [m^3/s]) of the process. 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 capacity (e.g. tank volumes), which may also influence efficiency of the specific units or aggregates.

For quality parameters, chemical and microbial quality will both be important in LCA studies of water reuse applications. Chemical parameters should include basic water quality data (e.g. concentration of total solids, suspended solids, chemical and biological oxygen demand, total or dissolved organic carbon, phosphorus (total, PO_4-P), nitrogen (total, NH_4-N)), but also specific information on relevant substances (e.g. concentration of inorganic or organic micropollutants such as heavy metals, pharmaceuticals) and other water quality parameters which may have an influence on treatment efficiency (e.g. spectral UV adsorption at 254nm, UV transmission). Microbial parameters should include indicator parameters and organisms (e.g. total heterotrophic plate counts, E. coli, Enterococci), but also specific organism groups (e.g. Salmonella, MS2 phages, Giardia, Cryptosporidium).

It is important to define the reference (= influent) flow as precise as possible to enable the deduction of treatment targets for water quality parameters (e.g. 80% reduction in TS, 4log removal in E.coli) 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.

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. 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 train 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 up-stream 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
- Production of infrastructure for major equipment (typically 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 (10-50a) 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 into the LCA study.

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 8). This will help the project team to understand the system and precise the LCA definitions in terms of system boundaries.

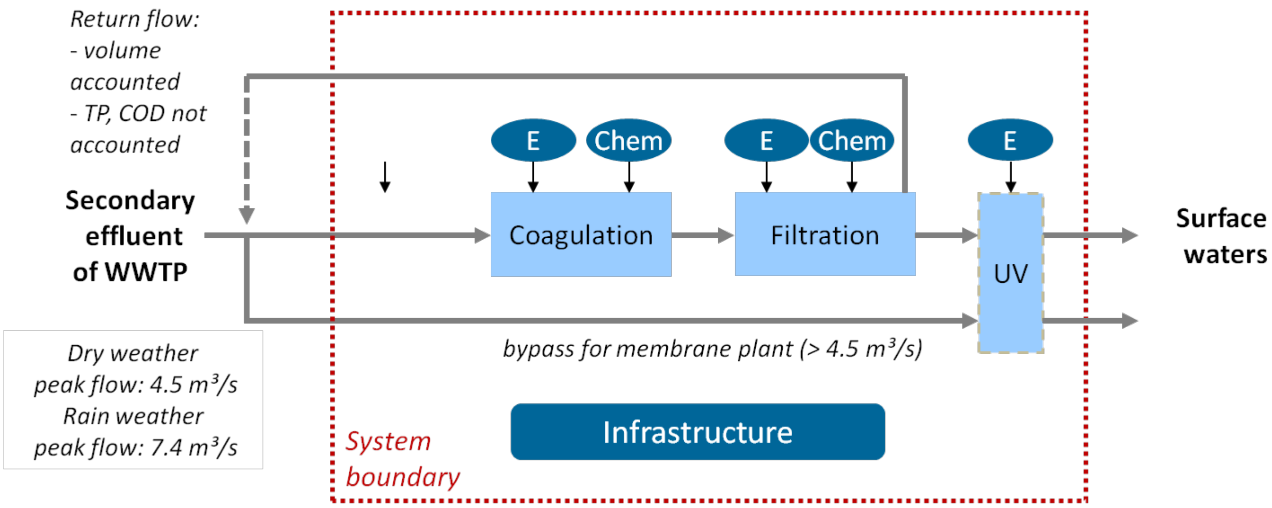


Figure 8 Examples of system boundaries for tertiary treatment of wastewater treatment plant (WWTP) effluent ((Remy et al. 2014))

Co-products

Another important part of the system boundaries relates to potential products or co-products that the system delivers. This substitution of original products (e.g. water for irrigation, nutrients N and P, electricity) can be accounted for in LCA by subtracting the related environmental burden for the substituted product (e.g. grid electricity for pumping of groundwater, 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 with reused water at times without explicit nutrient demand of the crops, the actual substitution of mineral fertilizer will not be 100% of the applied nutrient, but only a fraction of it (e.g. 50%) on an annual basis. The same holds true for water, if the amount of water applied exceeds the actual demand of the crops. Hence, careful argumentation should be provided when describing the substituted products and their annual amount with regard to effective substitution potentials.

Scenarios

For comparative LCA, different scenarios have to be defined which are then characterized and compared in their potential environmental impacts. The definition of scenarios should be most precise in technology terms, mentioning the technology/process to be analysed and its major features (e.g. UV dose, membrane pore size, ...). For some scenarios, system boundaries may have to be precised 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. each scenario fulfills the same 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 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. This holds also true for microbial parameters, where minimum targets for certain bacteria (e.g. <100 E. coli/100 mL) define minimum disinfection needs.

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 hierachy 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, full-scale data is often not available, especially if different technology options are compared. 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").

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 widespread application of the indicators in the LCA community. This guideline proposes a set of 9 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 3-12). 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.

Table 3-12 Proposed set of LCA indicators for impact assessment

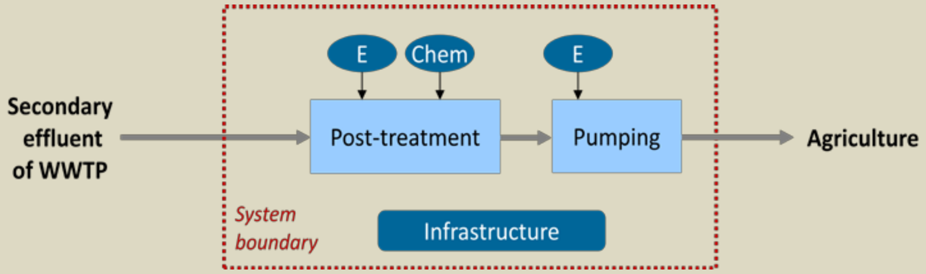
Impact category	Indicator	Unit	Contributing substances	Source
Use of energy resources	Cumulative energy demand of fossil resources	[MJ]	Hard coal, lignite, natural gas, crude oil	1)
	Cumulative energy demand of nuclear resources	[MJ]	Uranium	1)
Climate change	Global warming potential (100a)	[kg CO_2-eq]	CO_2 (fossil), N_2O, CH_4	2)
Acidification	Terrestrial acidification potential (100a)	[kg SO_2-eq]	SO_2, NO_x, NH_3	2)
Eutrophication	Freshwater eutrophication potential	[kg P-eq]	Total P, PO_4-P, org. P	2)
	Marine eutrophication potential	[kg N-eq]	Total N, NH_4-N, NO_3-N, org. N	2)
Ecotoxicity	Freshwater ecotoxicity	[CTU_e]	Inorganic and organic toxic substances	3)
Human toxicity	Human toxicity (non-cancer)	[CTU_h]	Inorganic and organic toxic substances	3)
	Human toxicity (cancer)	[CTU_h]	Inorganic and organic toxic substances	3)

1) (VDI 2012) 2) (Goedkoop et al. 2009) without long-term emissions 3) (Rosenbaum et al. 2008)

Examples of goal and scope definition for an LCA of water reuse systems

(data not representative, for method demonstration only!)

Goal of LCA study:	compare different alternatives of water reuse for an existing WWTP site to inform the operators on environmental benefits of reuse for different purposes
System functions:	reuse of WWTP effluent to meet standard for restricted irrigation (<10^3 E. coli/100 mL), including post-treatment and pumping of water to agricultural fields
Functional unit:	1 m^3 of treated wastewater to agricultural reuse
Reference flow:	annual flow of 1 Mio. m^3 of secondary effluent from WWTP, max. flow capacity of 200 L/s, with effluent quality of 1 mg/L TP, 10 mg/L TN and 10^6 E.coli/100 mL
System boundaries:	starting from secondary effluent of WWTP, including post-treatment and pumping to the field



Co-products:	water and nutrients that are delivered to agriculture, accounting for 100% of water, 50% of TP and 30% of TN delivered by water reuse
Scenarios:	1) post-treatment by UV (400 J/m^2) + pumping in 10 km pipeline 2) post-treatment by chemical disinfection (peracetic acid, 10 mg/L) + pumping in 10 km pipeline
Data quality:	pilot trials of UV plant and chemical disinfection using real secondary effluent from existing WWTP, preliminary engineering of processes and pipeline
Assumptions:	Infrastructure will be simplified (UV lamps and reactor, storage of chemical disinfectant and reaction tank, pumps and pipeline), nutrients will replace mineral P/N fertilizer production, and field emissions of fertilizer application are not included
Indicators:	1) Cumulative energy demand (fossil) 2) Global warming potential 3) Eutrophication of freshwaters

3.2.2 Life Cycle Inventory

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.

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 quality, electricity and chemicals required, and waste flows such as sludge or backwash water (Figure 9). 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) and the respective concentration of the chemical (e.g. $FeCl_3$ (40%)).

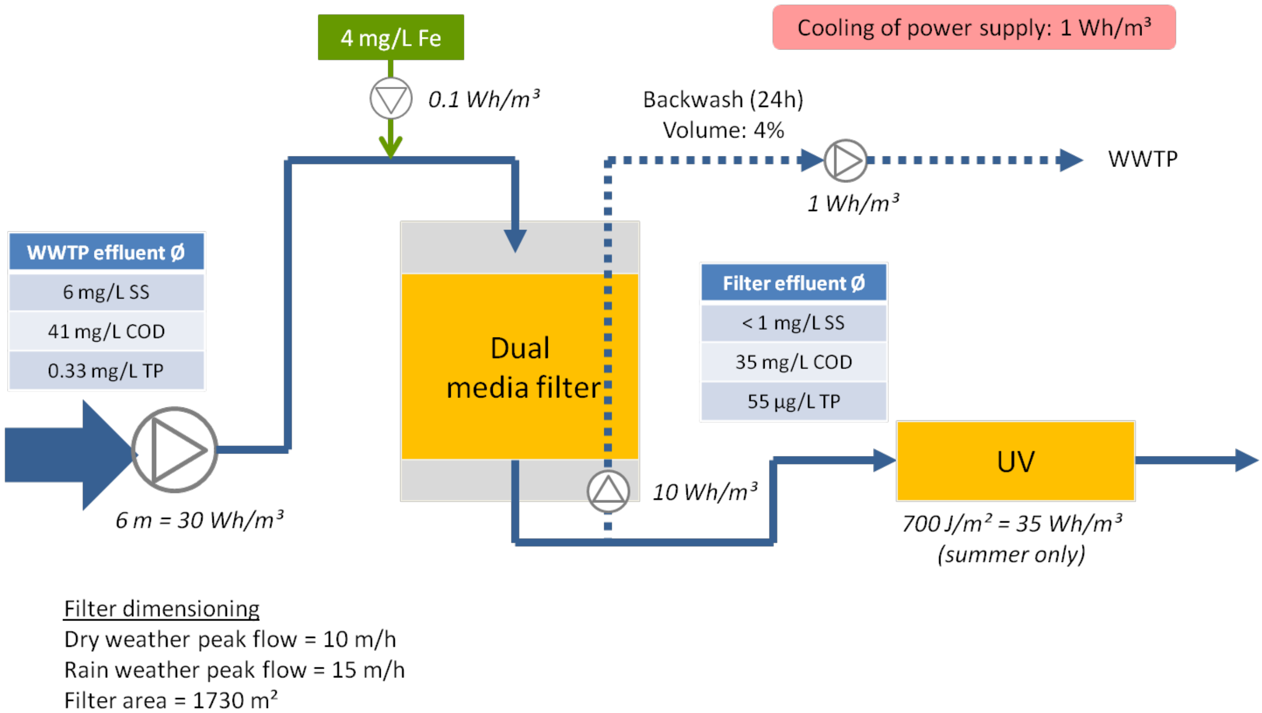


Figure 9 Life Cycle Inventory for operation of coagulation + dual media filter + UV for tertiary wastewater treatment (adapted from (Remy 2013))

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/m³ for each m of water head (or 50 Wh/m³ 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 primary data

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 in the LCA outcomes. Therefore, it is highly recommended to summarize the collected data in a suitable format which can be directly used 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 partners 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 time and effort of all participants, but this step leads to a dataset which is accepted by all partners and can thus be used in high quality for 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 database ((Ecoinvent 2010)) 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).

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. use HDPE dataset for other plastic materials) or by precursor products (e.g. acrylonitrile as precursor of acrylamide and also polyacrylamide) (Table 3-13).

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/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 information about location of potential suppliers. Usually, specifically manufactured materials and chemicals are transported over longer distance (e.g. HDPE pipes, FeCl3 solution) with estimates ranging from 200-600km, while heavy materials such as concrete, sand or gravel are produced more locally (20-50km). However, these estimates can be adjusted based on the local setting of the case study and available information.

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 general has a minor contribution to the total impacts compared to operational use of chemicals or electricity.

Table 3-13 Exemplary list of typical chemicals used for water treatment and related LCA datasets from Ecoinvent (adapted from (Remy 2013))

Chemical	Concentration	Related dataset of Ecoinvent database (Ecoinvent 2010)
$FeCl_3$	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 (220kg, 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 sulfate, petrochemical, at plant [RER]

Examples of Life Cycle Inventory for an LCA of water reuse systems

(data is not representative, for method demonstration only!)

Operational data:	1) UV system: 50 Wh/m³, disinfection of 4log for E. coli
	2) Chemical disinfection: 10 mg/L peracetic acid (= 15 mg/L acetic acid (80%) and 5 mg/L H_2O_2 (30%)), dosing pump and mixer: 10 Wh/m³, disinfection of 3log for E. coli
	3) Pumping in 10 km pipeline: 2 bar pressure head = 100 Wh/m³
Infrastructure data:	1) UV system: 50 UV lamps (each 4 kg, lifetime: 3a), reactor of 2000 kg stainless steel (lifetime: 30a)
	2) Chemical disinfection: storage tank of 3000 kg PE (lifetime: 20a), dosing pump of 10 kg cast iron (lifetime: 15a), mixer of 10 kg stainless steel (lifetime: 10a), reactor tank of 1000 kg PE (lifetime: 20a)
	3) Pump of 200 kg cast iron (lifetime: 15a), pipeline of 10km (DN200, PE) using 100,000 kg PE (lifetime: 40a).
	Transport distances: chemicals 600 km by truck, materials 300 km by truck
Background data:	Electricity = supply mix of Germany (2010)
(ecoinvent)	Acetic acid = acetic acid production [EU mix]
	H_2O_2 = H_2O_2 production [EU mix]
	UV lamps = UV lamp construction [EU mix]
	Stainless steel = chromium steel 18/8 [EU mix]
	PE = HDPE [EU mix], including extrusion for pipes [EU]
	Cast iron = cast iron from scrap (50%) [EU mix]

3.2.3 Impact assessment

For impact assessment in LCA, results of midpoint indicators should be reported for all scenarios of the LCA. 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/m³ water). For contribution analysis, the indicator score and chart should be divided into most important processes and contributors (e.g. electricity demand, chemicals, infrastructure, and direct emissions into water or atmosphere). 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 10).

Different LCA indicators cannot be 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 an overview of all indicator results 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.

In a further step, LCA indicator results can 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. For water treatment processes, normalisation typically yields in a relatively low contribution to energy demand and related greenhouse gas emissions, while water quality aspects such as eutrophication or aquatic ecotoxicity have a higher contribution (Figure 11). This effect is rather obvious, because water treatment requires only a minor share of the total energy demand in society, but it directly affects water quality discharged into the environment. Normalisation tends to underline the main function of water treatment which relates to protecting receiving surface waters from negative impacts due to nutrients or pollutants. Hence, efficiency measures in energy/resource demand should never compromise effluent quality of the process.

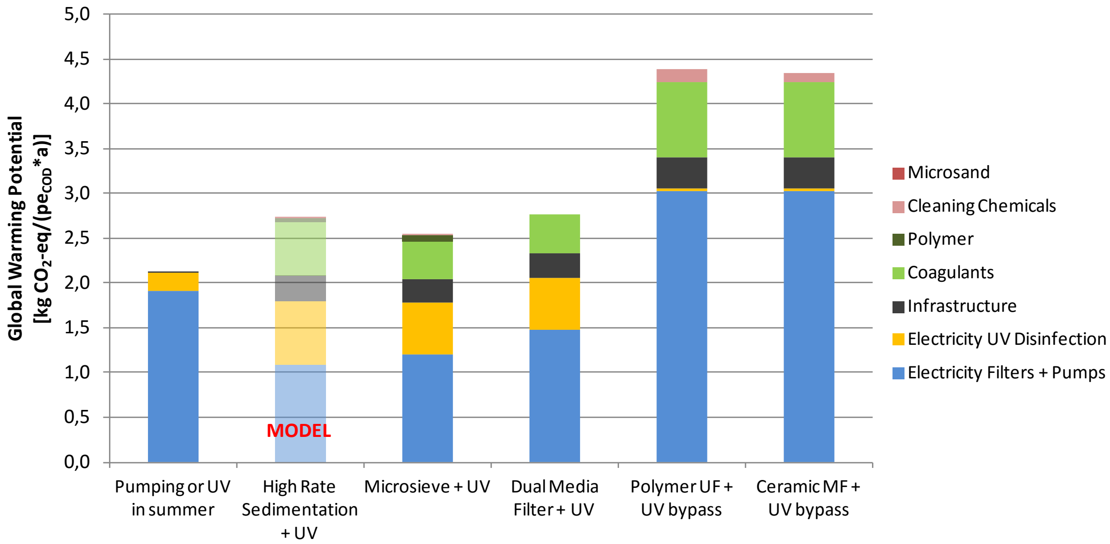


Figure 10 Global warming potential for tertiary wastewater treatment (adapted from (Remy 2013))

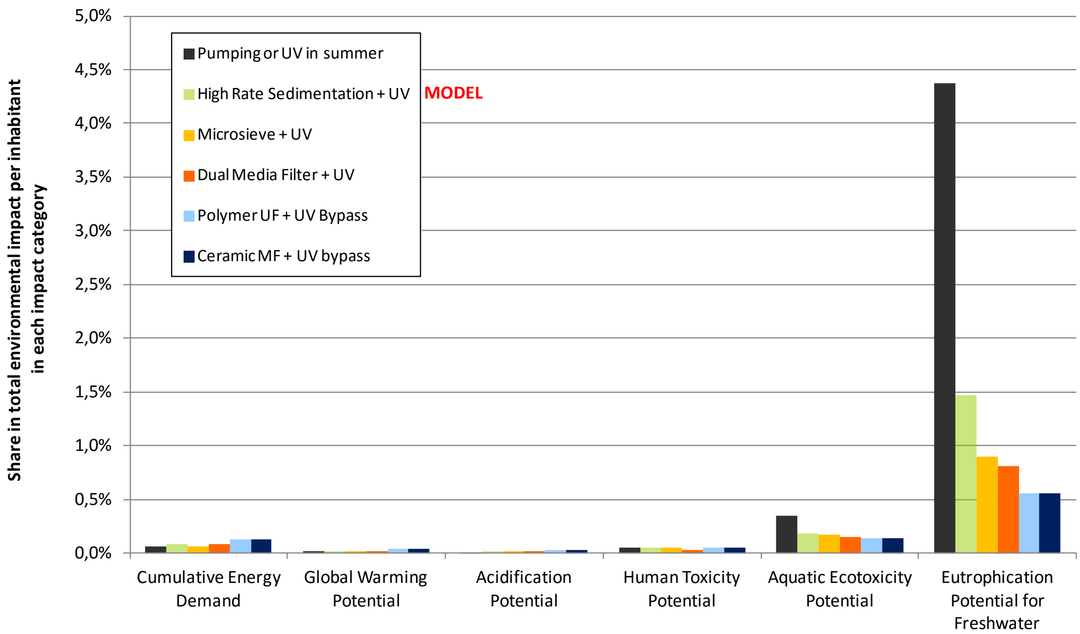


Figure 11 Normalisation of environmental indicators: contribution of tertiary wastewater treatment to total environmental impacts in EU 27 (2000) (adapted from (Remy 2013))

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.

3.2.4 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-scake 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.

3.3 Water footprinting methods

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 2014)) aligned on the ISO 14040/14044, 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 ((Berger and Finkbeiner 2010); (Kounina et al. 2013)), 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 assessment WFP 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 as the volumetric approach of the Water Footprint Network ((Hoekstra et al. 2011)).

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 reuse, it is useful to include WFP into the list of indicators to reveal the potential impact of reusing water on the local water balance both in terms of quantity and quality. From the many available WFP methods in the scientific community, two approaches are explained in detail in this guideline to enable the LCA practitioner to include them in the LCA study.

Water scarcity footprint

Effects of water reuse on water quantity can be addressed using a water scarcity footprint. 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 WFP method, 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 [m³]
- Indirect water consumption of the background processes (e.g. for electricity production). This information can be extracted from latest LCA databases ((Ecoinvent 2014)) in [m³]
- Water scarcity indices (0.1-1) from literature ((Pfister et al. 2009)) which are also publicly available as a layer in Google Earth (http://www.ifu.ethz.ch/ESD/downloads/EI99plus) (Figure 12). National average WSI are available as excel-file.

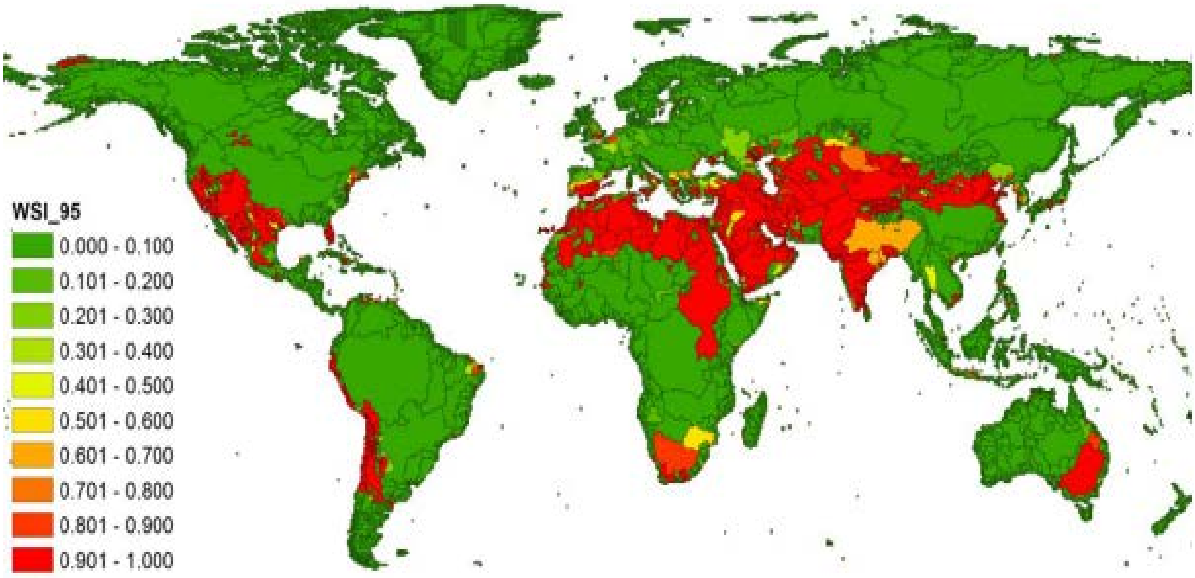


Figure 12 Water scarcity index ((Pfister et al. 2009))

Multiplying the water consumption data with the respective WSI gives a weighted water scarcity footprint. 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.

Water Impact Index

For calculating a water availability footprint, both water quantity and quality of water withdrawal and release have to be taken into account. A simple method for a water availability footprint is the Water Impact Index (WIIX) developed by Veolia ((Bayart et al. 2014)). This metrics is based on the weighting of all water flows withdrawn from the environment and released into the environment, weighted by the local scarcity index (e.g. WSI) and a quality indicator Q:

$$\text{Water Impact IndeX} = \left(W \times Q_w \times WSI_w\right) - \left(R \times Q_R \times WSI_R\right)$$

where W and R = withdrawn and released volumes of water [m³]
WSI = water scarcity index [0.1-1] (Pfister et al. 2009)
Q = Water Quality Index

The water quality index is calculated by comparing the actual concentration of selected pollutants against an environmental benchmark such as the environmental quality standards of the EU ((EU 2008)). The water quality parameter with the highest deviation from the quality standards determines the overall water quality index:

$$Q = \min_p\left(1; \frac{Cref_p}{C_p}\right)$$

with C_{refP} : Reference concentration of pollutant P
and C_p: Concentration of pollutant P in water flow

Hence, the data required for calculating the WIIX is more extensive:

- Direct water balance of the treatment process (water withdrawal, water release) [m^3/a]
- Local WSI [-] from Google Earth layer
- Concentration of major pollutants (COD, TP, TN, heavy metals…) in the water flows [mg/L]
- Reference concentrations of pollutants ((EU 2008))
- Indirect WIIX for background processes (e.g. electricity demand, chemicals production, transport), taken from specific databases (e.g. Quantis Water Database).

The calculation of the WIIX will allow the assessment of quantitative and qualitative effects of water use on the local water balance and availability. This WFP metrics can be used to demonstrate the benefits of water reuse for a specific case study: a decrease in water withdrawal of good quality will lower the WIIX if the use of primary water sources (e.g. groundwater, surface water) is substituted by water reuse. In addition, further treatment of water discharged into the environment (e.g. by tertiary treatment for reuse) will improve the quality of released water into the environment, also lowering the WIIX. Both effects will be even more pronounced in areas with high water stress, underlining the importance of water reuse in areas with high water scarcity.

Examples of water footprinting with Water Impact Index (WIIX) for water reuse systems

(data is not representative, for method demonstration only)

Input data:	WWTP discharge: 10,000 m^3/a, 100 mg/L COD, 1 mg/L P
	Electricity for tertiary treatment: 1 kWh/m^3
	Water demand for agriculture: 10,000 m^3/a taken normally from surface water (10 mg/L COD, 0.1 mg/L P)
	Environmental quality standards: 50 mg/L COD, 0.3 mg/L P
Indirect water use:	Electricity production uses 1 m^3/kWh (data from database ecoinvent)
Water Scarcity Index:	taken from Google Earth layer
	WSI = 0.8 (local at site, i.e. high water scarcity)
	WSI = 0.3 (country mix, for electricity production)
Water Quality Index:	WQI of discharged wastewater: WQI for COD = 50/100 = 0.5, WQI for P = 0.3/1 = 0.3, minimum WQI is 0.3
	WQI of surface water withdrawn for agriculture: WQI for COD 50/10 = 5, WQI for P = 0.3/0.1=3, minimum WQI is 1
	WQI for electricity = 1 (default, highest quality)
WIIX (status quo):	For WW discharge: WIIX = -(10,000*0.8*0.3) = -2400 m^3-eq/a
	For water withdrawal to agriculture: WIIX = 10,000*0.8*1 = 8,000 m^3-eq
	→ WIIX of existing system (no reuse) = 8000-2400 = 5600 m^3-eq/a
WIIX (reuse):	Scenario: tertiary treatment of WWTP effluent and reuse in agriculture
	No discharge of WW, WIIX = 0
	No withdrawal of water for agriculture, WIIX = 0
	Indirect WIIX for electricity in tertiary treatment (10,000 kWh/a):
	Indirect WIIX = 10,000*0.3*1 = 3,000 m^3-eq
	→ WIIX of reuse scenario = 0 - 0 + 3000 = 3000 m^3-eq
Result of WFP	Water reuse option can decrease WIIX by 46% or 2600 m^3-eq/a

4 Comparison and critical discussion of LCA, WFP, and risk assessment

This report has shown the major features of RA, LCA and WFP as assessment methods for quantification of the environmental and human health-related implications of water reuse systems. While all three assessment methods may substantially support the decision making towards implementing water reuse, the shortcomings of the individual assessment methods have to be critically reflected. Moreover, the different assessment methods show their strengths at different points of the decision making processes:

- LCA and WFP methods are the most effective when they are conducted as early as possible in the decision making process to understand the environmental consequences of a water reuse system. If the environmental impact of different alternatives for achieving the pre-defined goals of reuse (functional unit) is known before taking large and long-term investments into a specific technical system, a more informed decision can be taken towards a balanced perspective for environmental benefits and additional impacts.
- In contrast, risk assessment in general is a more continuous and “living” assessment method. As part of a larger risk management system, periodic revision and continuous improvement of the system assessment is a key characteristic of RA.

Moreover, the three assessment methods differ in their spatial and temporal boundaries. While LCA in general takes a broad and global perspective of environmental impact assessment where the exact location and time of the emission is (in most cases) not explicitly addressed, WFP and RA for water supply and reuse systems are specific tools for taking into account local and regional conditions. The precise location or time of an emission may significantly impact the actual effects because e.g. if there is no human exposure to pathogens there is no risk for human health.

LCA aggregates emissions over space and time and may not reflect the actual impacts of a specific water reuse site on its environment. However, the life-cycle view can reveal existing trade-offs between local and global impacts (e.g. local water quality vs. greenhouse gas emissions) and quantifies all effects with a comparable impact assessment model, thus enabling a comparison between local, regional and global interventions. WFP has a more regional connection by taking into account regional water balances and water scarcity, but the time-dependent assessment (e.g. difference between dry and wet season) has yet to be improved. Again, WFP as described in this report with the WIIX methodology indicates the shift in water inputs and outputs on a local or regional basis and evaluates it on the basis of water quantity and quality.

Shortcomings of QMRA can be attributed to the limited amount of available and reliable dose-response relations. Due to ethical concerns of human feeding studies it does not seem to be likely that this shortcoming will be overcome soon. Moreover, the large variability und uncertainty regarding the occurrence and distribution of microbial parameters but also regarding the reliability of analytical methods often leads to results ranging over multiple orders of magnitude. The separation of uncertainty and variability is still a major challenge in QMRA.

In QCRA, risk can be formulated in several ways, which can be adapted to the situation which has to be assessed. Usually the assessment of single substances is based on the result of exposure assessment and a limited amount of toxicological test. Limitations can be seen in the fact that even if the RQ exceeds the value of 1 it is not at all clear what the risk is. The real risk stays in the areas of unknowns (van Leeuwen and van Vermeire 2007).

5 Summary and conclusion

This report provides an overview and method guideline for the three assessment tools LCA, WFP, and risk assessment in the field of water reuse:

- LCA shows the environmental impacts of water reuse systems in a global life-cycle perspective, i.e. taking into account direct effects (e.g. water discharge) and indirect effects (e.g. production of electricity and chemicals). With LCA, existing trade-offs can be identified between different environmental targets to enable an informed decision on potential system alternatives for water reuse.
- WFP is a tool for assessing qualitative and quantitative effects of water reuse on the local or regional water balance, thus showing potential benefits of water reuse by mitigating additional water stress on locally scarce water resources.
- For risk assessment, QMRA is a suitable tool to calculate potential health risks from water reuse through pathogenic microorganisms and define minimum treatment targets or minimum water quality to minimize human health risks of water reuse to an acceptable level.
- Several simplified exposure models are available for QCRA, which allow for a quantitative expression of the present chemical risk and related uncertainties due to chemical substances in the the treated water. Thereby related risk can be communicated transparently and treated in a systemized and reproducible manner.

With this report, the reader can understand the principles and methodological steps behind LCA, WFP and risk assessment and receive guidance in their application for assessing water reuse systems. This guideline should help to promote adequately safe and environmentally beneficial systems for water reuse and support decision making towards a wider implementation of water reuse in the European water sector.

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