AquaNES

Demonstrating Synergies in Combined Natural and Engineered Processes for Water Treatment Systems

Deliverable 4.2

Blueprint for a water quality assessment framework for cNES

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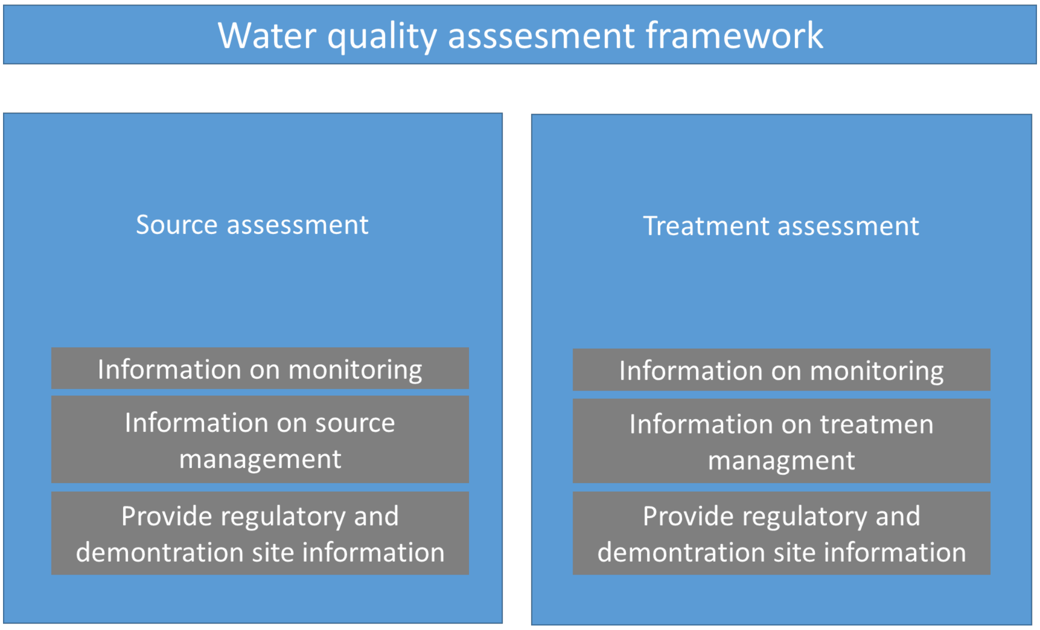
List of abbreviations

AC	Activated carbon
BF	Bankfiltration
BOD	Biological oxygen demand
CEC	Contaminant of emerging concern
cNES	Combined natural and engineered treatment system
COD	Chemical oxygen demand
CSO	Combined sewer overflow
CW	Constructed wetland
DOC	Dissolved organic carbon
DW	Drinking water
EC	Electrical conductivity
EDTA	Ethylenediaminetetraacetic acid (complexing agent)
MAR	Managed aquifer recharge
MS	Milestone
NDMA	N-Nitrosodimethylamine
NF	Nanofiltration
NTU	Nephelometric turbidity unit
QMRA	Quantitative microbial risk assessment
qPCR	quantitative polymerase chain reaction
RBF	Riverbank filtration
RO	Reverse Osmosis

RW	Rain water
SAT	Soil Aquifer Treatment
SW	Surface water
TOC	Total organic carbon
UV	Ultraviolet
UVA	Ultraviolet absorption
UVA_{254}	Ultraviolet absorption at 254 nm
UWWTD	Urban wastewater treatment directive
WP	Work package
WSP	Water safety plan
WW	Wastewater

Executive Summary

The AquaNES project will catalyze innovations in water and wastewater treatment processes and management through improved combinations of natural and engineered components. Among the demonstrated solutions are natural treatment processes such as bank filtration (BF), managed aquifer recharge (MAR) and constructed wetlands (CW). The project holds 13 demonstration sites that make use of BF, MAR or CW among other treatment techniques. Water quality assessment is essential for the evaluation of water treatment. This report presents a Water Quality Assessment Framework to support water quality assessment of combined natural and engineered treatments by evaluation source, treatment steps, monitoring and use of treated water. It also contains a preliminary assessment of all individual demonstration sites, providing suggestions for monitoring and other forms of water quality assessment for demonstration sites.



1 Introduction

1.1 Purpose of this document

The purpose of this document is to provide a framework for water quality assessment for drinking water and wastewater treatment. The provided information conduces to support the quality assessment of water treatment schemes with combined natural and engineered components.

1.2 Structure of the deliverable

The water quality assessment framework is presented (Chapter 2). Water quality assessment parameters and conventional and innovative tools are discussed (Chapter 3) and a preliminary water quality assessment is described for all demonstration sites (Chapter 4). Finally, the water quality assessment is evaluated (Chapter 5).

1.3 Relation to the project objectives

The AquaNES project demonstrates of the robustness and benefits of combined engineered and natural treatment technologies at 13 demonstration sites that make use of bank filtration (BF), managed aquifer recharge (MAR) and constructed wetlands (CW), among other treatment techniques. Proper assessment of chemical and biological water quality of sources, during treatment and after treatment is essential to control operation and safeguard water quality for its intended use (Figure 1).

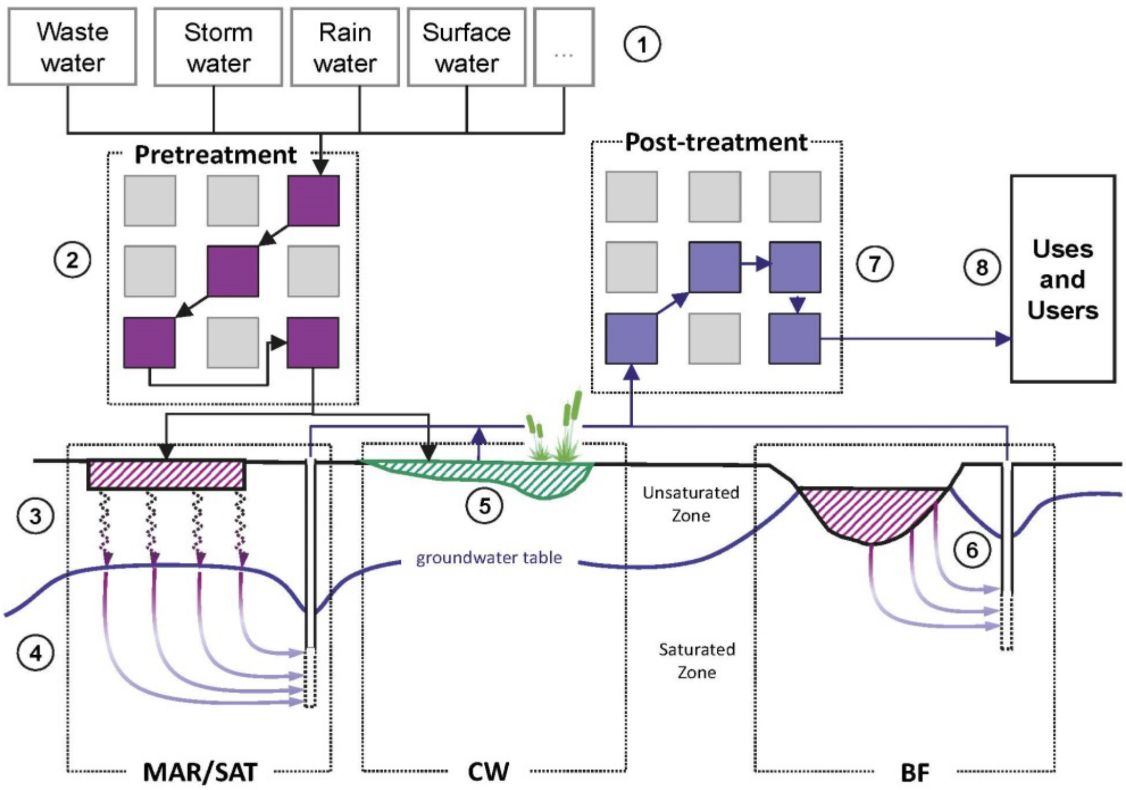


Figure 1 **Schematic overview of combined natural and engineered treatment technologies within AquaNES**
Legend: 1 Sources, 2 Engineered pre-treatment (Site 2, 6-13), 3/4; Managed Aquifer Recharge/Soil Aquifer Treatment (Site 6-9), 5 Constructed Wetland (Site 10-13), Engineered post-treatment (all sites)

2 Water quality assessment framework

2.1 Water quality assessment

Water quality assessment is a complex task since it requires assessment of (1) potential contamination of sources of the water, (2) assessment of treatment efficiency for this (potential) contamination, (3) the assessment of treated water and (4) knowledge on system hydrology and dynamics. This should all be related to (5) the intended transport and use of the water. The presented water quality assessment framework guides water quality assessment for water treatment schemes that hold combinations of natural and engineered components, as studied in the AquaNES project. Information gathered within this framework can be used for a water safety planning [1].

2.2 Source assessment

Water quality assessment starts with source characterization. The source of the treated water determines the potential pollution and undesired reactions with pipelines and other hardware and thereby the required monitoring to assess water quality. Below a flow scheme for source assessment is given (Figure 2). It provides generic information on potential contamination of different sources.

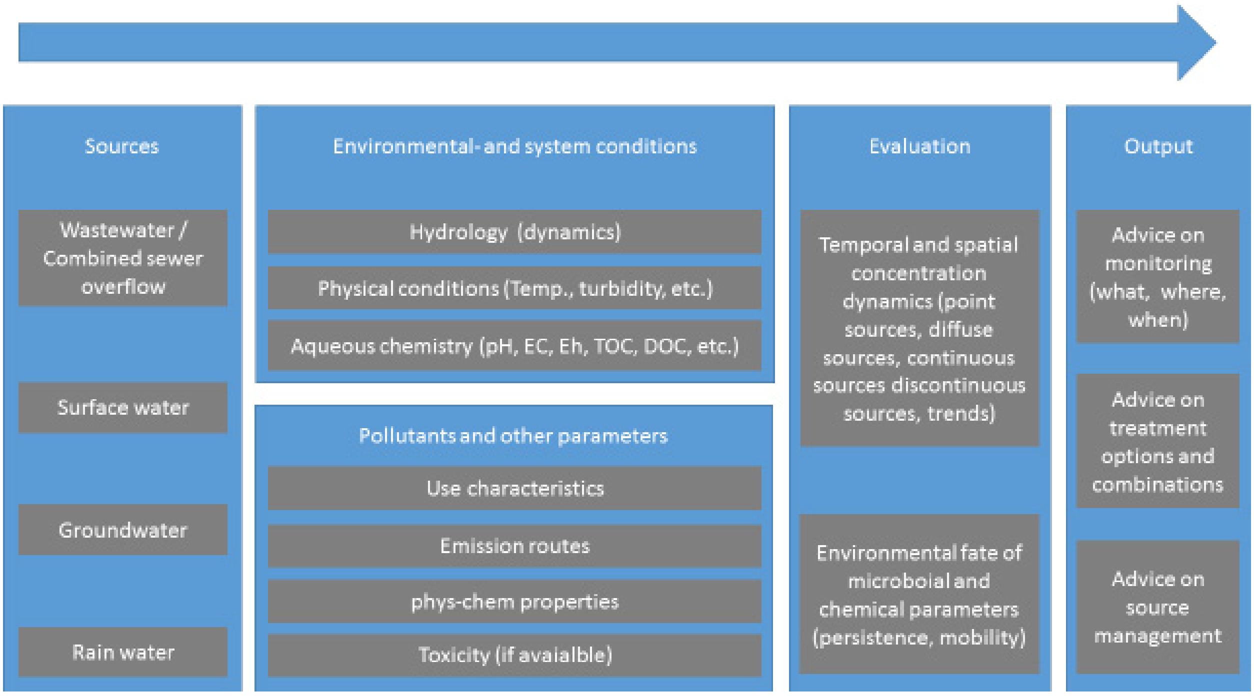


Figure 2 Water quality assessment framework for source assessment

The 13 demonstration sites studied within the AquaNES project use the following sources: 1) wastewater (site 7,8, 10-13) including combined sewer overflow (site 11), 2) surface water (site 1-6), and 3) collected rain water (site 9). The quality and characteristics of these sources differ, so therefore source quality monitoring will differ as well.

Raw wastewater generally contains the highest loads of organic material, nutrients, micro-pollutants and pathogens. Treated wastewater differs from raw wastewater since some components are better removed than other components.

Surface water quality is influenced by emissions to its catchment area. Surface water can receive treated (via sewage treatment plants) and untreated wastewater (via combined sewer overflow), industrial wastewater effluents, emissions from agricultural activities (e.g. pesticides, nutrients) and urban areas, polluted groundwater and deposition of pollutants and particles via air.

When water passes soil (groundwater and infiltrated water) many compounds and elements are removed to some extent by sorption or transformation/degradation. The removal efficiency depends on the hydraulic retention time, the composition of the soil material, and conditions such as the redox state, pH, temperature, salt content etc. In some cases the soil can also be a source of contaminants (e.g. arsenic, heavy metals, radon, historical contaminants).

Rainwater contains much less micro-pollutants and microorganisms, it can however contain compounds that are volatile and soluble or are bound to dust and particles from (for example) combustion processes that form aerosols in the air. Finally, surface run-off (when rain is collection from large surfaces) can lead to washing off of contaminants from these surfaces such as heavy metals, coating materials and paints, precipitated soot and dust bound contaminants, microbial contaminants and organic material from feces of animals, residues of plant materials etc. [2-5]. Since rain water at Site 8 is collected from rooftops, we defined water quality parameters relevant for rain collected from these surfaces in an urban of industrial environment. In Table 1 the generic relevance of parameter classes are given per type of source water.

Table 1 Relevant water quality parameters for source water quality assessment

Water source for treatment	Nutrients, Eutrophication indicator	Redox indicator	Metal	Organic carbon content indicator	Human Pharmaceuticals and personal care products	Veterinary pharmaceuticals	Combustion byproducts	Pesticide/biocide	Industrial chemicals (products) [4]	Industrial chemicals (intermediates)	Fecal indicators and pathogens	Biological stability indicators	Bioassay endocrine disruption [8]	Various organic chemicals Non-target chemical screening approaches [9]	Antibiotic resistance indicators
SW	+	-	+	+	+[1]	+[2]	+/-	+	+	+[5]	+[6]	-	+	+	+
GW	+/-	+	+	+	+/-	+[2]	-	+	+	-	-	-	+	+	+/-
RW (from rooftops)	-	-	+	-	-	-	+	-	+	+[5]	+/-[7]	-	+	+/-	-
WW	+	-	+	+	+	-[3]	+/-	+	+	-[5]	+	-	+	+	+
TWW	+	-	+	+	+	-[3]	+/-	+	+	-[5]	+	-	+	+	+
CSO	+	-	+	+	+	-[3]	+	+	+	-[5]	+	-	+	+	+

Legend: **Source water:** SW=surface water; GW=groundwater; WW= raw wastewater; TWW = treated wastewater; RW=rain water; CSO=combined sewer overflow

[1] analysis of human pharmaceuticals is relevant when water is directly or indirectly impacted by effluent from communal waste water; [2] analysis of veterinary pharmaceuticals is only relevant when water is directly or indirectly impacted by fields receiving manure; [3] veterinary pharmaceuticals with human applications are relevant [4] industrial products such as flame-retardants can end up in air (aerosols) or are released by coatings used on buildings and subsequently end up in harvested rain; [5] Industrial intermediates are used in chemical plants, they can unintentionally end up in effluent and the air, such parameters are relevant for rivers or wastewater treatment fed with industrial wastewater; [6] Fecal indicators are relevant in wastewater effluents and surface waters; [7] Harvested rainwater from rooftops can contain fecal contamination from surfaces contaminated with excrements of animals; [8] bioassays integrate effects of many contaminants and are therefore relevant in practically all water types; [9] non-target screening approaches cover chemicals of many classes and can therefore be relevant to all kinds of water types

2.3 Treatment assessment

Water treatment can lead to the removal or addition/formation of chemical and microbial contamination and the transformation of chemicals into other chemicals. The removal, addition or formation of pollutants during treatment depends on the presence of pollutants in source waters, environmental conditions, the used treatment technology, the conditions during treatment, the performance of the treatment steps. In Table 2 the generic relevance of monitoring parameters for treatment technologies are indicated.

Table 2 Relevant water quality parameters for different treatment steps / processes / technologies

Treatment technology (cluster)[1]	Nutrients, eutrophication indicator	REDOX indicator	Metal	Organic carbon content indicator	Human pharmaceuticals and personal care products	Veterinary pharmaceuticals	Combustion byproducts [2]	Pesticide/biocide	Industrial chemicals (products)	Industrial chemicals (intermediates)	Fecal indicators and pathogens [3]	Biological stability indicators [4]	Bioassay endocrine disruption [5]	Various organic chemicals Non-target chemical screening approaches [6]	Antibiotic resistance indicators [7]	Transformation product / Disinfection by-products [8]
Nitrification / denitrification	+	-	-	+	-	-	-	-	-	-	+/-	+	-	+	-	+/-
Coagulation & sedimentation	+	-	+	+	-	-	-	-	-	-	+	-	-	+	-	-
(UV) Disinfection	-	-	-	-	+	+	+	+	+	+	+	-	+	+	-	+
Advanced oxidation	-	-	-	+	+	+	-	+	+	+	+	-	+	+	+-	+
Soil/sediment passage	+	+	+	+	+	+	-	+	+	+	+	+	+	+	+	+
Sand filtration	+/-	-	+	+/-	-	-	-	-	-	-	+	+	+	+	+/-	+
Microfiltration	-	-	-	+/-	-	-	-	-	-	-	+	-	+	+	-	-
Nanofiltration & RO	+	-	+	+	+	+	-	+	+	+	+	-	+	+	-	-
AC filtration	+	-	+	+	+	+	-	+	+	+	+	+	+	+	+/-	+

Legend:

[1] treatment steps are clustered; [2] combustion byproducts such as PAHs are generally very hydrophobic, so they are easily removed by filtration techniques and soil or sediment passage, making monitoring of most of them less relevant for these treatment steps; [3] practically all treatment techniques affect the presence of microorganisms including pathogens; [4] biological stability indicators are mainly relevant in (filtration) techniques with biological activity; bioassays (for endocrine disruption) cover a wide array of bioactive chemicals, so this analysis is relevant for processes that potentially alter the chemical composition of the water through chemical and biological processes. Non-target approaches cover a wide array of chemicals, so this analysis is relevant for processes that potentially alter the chemical composition of the water through chemical and biological processes. [7] Antibiotic resistance indicators are of interest in treatment steps with high biological activity; [8] Transformation products can be formed in treatment techniques with high chemical reactivity (advanced oxidation) or biological activity (biological active filtration techniques and bioreactors).

Treatment steps can have multiple purposes. We can distinguish storage of water, removal of (organic) solids, removal of nutrients, removal of (dissolved) organic material, removal of microbial contamination, changing pH, salt concentration, or ion composition or the removal of micro pollutants. Treatment performance can depend on selection, combination, dimensioning of applied treatment techniques, environmental conditions (e.g. temperature), properties of the raw or pre-treated water (e.g. TOC, DOC, pH, conductivity, BOD, COD) dynamics of the load of treated water, and the condition of the treatment techniques itself (e.g. treatment performance of especially filtration techniques change during use (with number of bed volumes) [6]).

A single treatment technique serves multiple purposes. Hence, the effect of a treatment technique is relevant for multiple classes of parameters. Especially "natural" treatment steps (e.g. bank filtration, constructed wetlands) or treatment techniques that involve natural processes such as biodegradation (e.g. sand filtration, active carbon filtration) cover many removal mechanisms and can therefore be relevant for many parameter classes.

Water is generally treated by a combination of treatment techniques in a specific order. This is done because (1) a combination of mechanisms can improve water quality in different ways, (2) treatment steps can improve treatment performance of successive steps [7] or (3) scavenge unwanted contamination from previous steps [8]. Furthermore, storage of water within treatment schemes can be very valuable in (1) balancing input and demands, (2) mute dynamics in water quality and (3) dodge contamination peaks in time. Storage of water is often not considered an active treatment step. However, a detailed analysis of micro-pollutants before 5 month storage in a reservoir, after storage and after full treatment illustrated that generic removal during storage was similar to removal during advanced treatment technologies [9]. This results illustrates the power of natural attenuation to remove (or transform) micro-pollutants. River bank filtration or managed aquifer recharge also improve water quality in many ways, but the quantification is often complex. It requires advanced knowledge on hydrology because of mixed residence times, and additional mixing with groundwater from other sources with different water quality than infiltrated water. Grischek et al. (2002) highlighted groundwater flow beneath the river towards RBF wells in the Elbe river valley at Meissen, Germany, where that groundwater portion was polluted with nitrate of >100 mg/L. At the RBF site in Mockritz, Germany, high sulfate concentration in landside groundwater affected the pumped water quality and had to be controlled by specific mixing ratios of groundwater and bank filtrate (Grischek et al. 2000).

The performance of a treatment scheme including natural and engineered components is defined by the combination, order and dimensions of treatment steps, in relation to quality and dynamics of the source water and environmental conditions.

The separation of engineered and natural treatment is rather arbitrary. Some "natural" treatment such as constructed wetlands have a natural appearance and an engineered design. Furthermore, similar processes such as sorption and (bio)degradation occur in both "engineered" and the "natural" systems. There is an overarching difference between most natural and engineered treatment steps. Most engineered steps focus on a single treatment process that is well defined, controllable and usually performed in a rather short treatment time. Most natural processes include multiple treatment processes that are more difficult to control and have (much) longer treatment times. The benefit of combining natural and engineered techniques lie in these differences. Combining a diverse set of treatment steps of different nature enables to cover a broader spectrum of contaminants. Furthermore, engineered techniques with short residence times are less suitable to treat water with highly variable quality and properties. Proper treatment of water with high variation in quality requires online monitoring to timely adjust operation or over-dimensioning treatment systems to fulfill treatment requirements under all water quality conditions. Since most natural treatment techniques have longer residence times, they are able to reduce water quality variation when they are applied as pre-treatment or primary treatment, thereby enabling further (engineered) treatment to be more stable, easier to control and more effective. Bank filtration and (sub)surface storage of water fulfills this requirement. This is done at demonstration sites 1-9. Furthermore, natural systems are also applied as post-treatment, as a polishing step. Examples of such approaches are shown at demonstration sites 10-13.

So theoretically, the combined techniques applied at the different demonstration sites enable more robust and effective treatment of water for its use. But how can the treatment performance and water quality be assessed? Figure 3 illustrates a water quality assessment framework for water treatment. It structures relevant information on treatment techniques, treatment conditions and associated water quality parameters in order to evaluate treatment efficiency, robustness and data processing for operation and performance assessment.

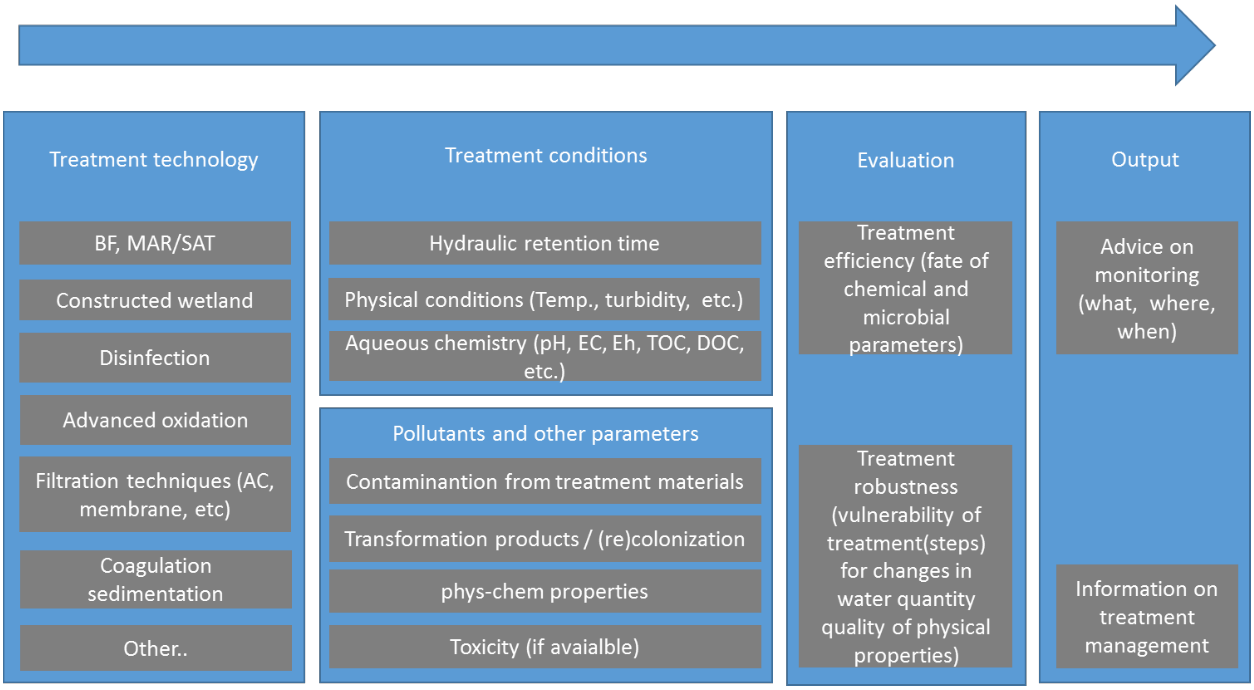


Figure 3 Water quality assessment framework for treatment assessment

2.4 Treated water assessment

Water treatment can lead to the removal or addition/formation of chemical and microbial contamination and the transformation of chemicals into other chemicals. The removal, addition or formation of contaminants during treatment depends on presence of contaminants in source water, environmental conditions, the design and operation of the treatment technologies. This requires the integration of the source assessment and the treatment assessment. The final goal of water treatment is its safe use.

The application of the treated water determines what parameters are of relevance since they can pose risks or affect receiving systems. The AquaNES project distinguishes (1) waste water treatment and combined sewer overflow for emission to surface water, (2) wastewater treatment for irrigation, (3) rain water treatment and storage for irrigation, (4) surface water for the production of drinking water, (5) bank filtrate (and groundwater) for drinking water. Table 3 indicates the relevant classes of parameters per use category.

Table 3 Relevance of water quality parameters per use category of treated water

Treatment technology (cluster)	Nutrients, eutrophication indicator	Redox indicator	Metal	Organic carbon content indicator	Human pharmaceuticals and personal care products	Veterinary pharmaceuticals	Combustion byproducts [2]	Pesticide/biocide	Industrial chemicals (products)	Industrial chemicals (intermediates)	Fecal indicators and pathogens [3]	Biological stability indicators [4]	Bioassay endocrine disruption [5]	Various organic chemicals Non-target chemical screening approaches [6]	Antibiotic resistance indicators [7]	Transformation product / Disinfection by-products [8]
WW and CSO effluent to SW	+	-	+	+	+	+/-	+/-	+	+	+	+	+/-	+	+	+	+
WW effluent for irrigation	+	-	+	+	+/-	+/-	+/-	+	+	+	+	+/-	-	+	+	+
RW for irrigation	-	-	+	+	-	-	+	+	+/-	-	+/-	-	-	+	-	-
SW for DW	-	-	+	+	+	+/-	-	+	+	+	+	+	+	+	+	+
BF & GW for DW	-	+	+	+	+	+	-	+	+	+	+/-	+/-	+	+	+	+

This overview is defined by the potential presence of certain parameters in water and the relevance for its use and not (necessarily) by regulatory frameworks. The table illustrates that practically all parameters are of relevance for wastewater since (municipal) wastewater contains many contaminants, and its emission to surface water or use for irrigation requires a certain water quality. The paragraph below discusses how all these water quality parameters before (Table 1) during (Table 2) and after treatment (Table 3) can be assessed and evaluated.

2.5 Information requirements for a water quality assessment

Proper water quality assessment and assessment of risks associated with the use of the water requires various activities that stretch further than monitoring only.

1. Selection of relevant parameters

Environmental waters can contain numerous pollutants, many of these chemicals. The large number of chemical pollutants challenges monitoring, water quality assessment and risk assessment [10]. Various approaches are available to track and prioritize emerging pollutants in certain compartments of the water cycle [9, 11-15]. Source assessment (paragraph >>) can provide relevant contamination sources and classes of contaminants associated with the type of source at a given location and under given conditions. Treatment assessment (paragraph>>) can indicate the suitability of a treatment to cope with pollutants that are expected in the used source of water.

2. Definition of relevant water quality criteria

The European Union has a defined set of water quality standards for various water types listed in the European Drinking Water Directive, the European Wastewater Directive, the Groundwater Directive etc (European Commission, 1991 #3144;European Commission, 1998 #1955;European Commission, 2000 #1312;European Commission, 2003 #2495;European Commission, 2003 #2608;European Commission, 2006 #2250;European Commission, 2006 #2607;Union, 2006 #3185;Union, 2006 #3186;European Commission, 2008 #2000;European Commission, 2010 #3143;Commision, 2015 #3193). Also outside the European Union governmental organizations set water quality standards (see for example https://www.epa.gov/wqc). Non-governmental organizations such as the WHO set (non-regulatory) water quality criteria [16-18]. These quality standards enable water quality assessment for drinking water, irrigation water or effluents emitted to surface water [19, 20]. However, many contaminants lack quality criteria, and not all criteria are health or risk based. For example, there are no regulatory criteria set for pharmaceuticals in the European drinking water Directive nor in the Water Framework Directive [16]. This means that not all parameters that are considered relevant for a specific site, treatment or intended use can be properly evaluated. For chemicals lacking criteria, a generic threshold of toxicological concern (TTC) is developed for human health risks. This threshold is based on a statistical approach where the distribution of effect based water quality criteria of a large training set is used to define the 5th percentile of distribution of safe exposure levels, assuming the same distribution for chemicals with and without a criteria [21-23]. The TTC can distinguish chemicals with endocrine effects and mutagenic or genotoxic effects (threshold 0.01 µg/L) from all "other" chemicals (0,1 µg/L) [23]. The exceedance of this TTC does mean that a human health effects cannot be excluded and additional information is required.

3. Methods to analyze or estimate these parameters / conditions

Not all relevant chemical and microbial parameters can be monitored at required frequencies for technical and practical reasons. Consequently, monitoring the treated water in order to assess water quality and potential risks is not always feasible.

Chemical water quality can be assessed by:

- Evaluation of sources, hydrology, properties and associated environmental fate of chemicals of interest in sources and treatment [5, 24 25], [26-30 31].
- prioritization of relevant / indicator parameters to optimize output of monitoring ([11, 32])
- Using reference data / literature data from demonstration sites [7, 33]
- Use innovative integrative monitoring approaches such as effect based monitoring and non-target screening [34-37]. (see section "innovative techniques for water quality assessment" for more detail)

Microbial water quality is often assessed by:

- evaluation of detectable concentrations in sources and estimations of removal rates
- estimation of concentrations or removal based on literature data on concentrations and or removal efficiencies [17, 38-44] (Quantitative Microbial Risk Assessment[17, 40, 43]).
- innovative monitoring approaches such as the analysis of specific DNA fragments or proteins to determine the presence of pathogens or indicate for their potential presence, or specific genes, for example, antibiotic resistance, that is considered to pose a human health threat [45].

The general concept of the "Water quality assessment framework" derived from the principles described above is shown in Figure 4.

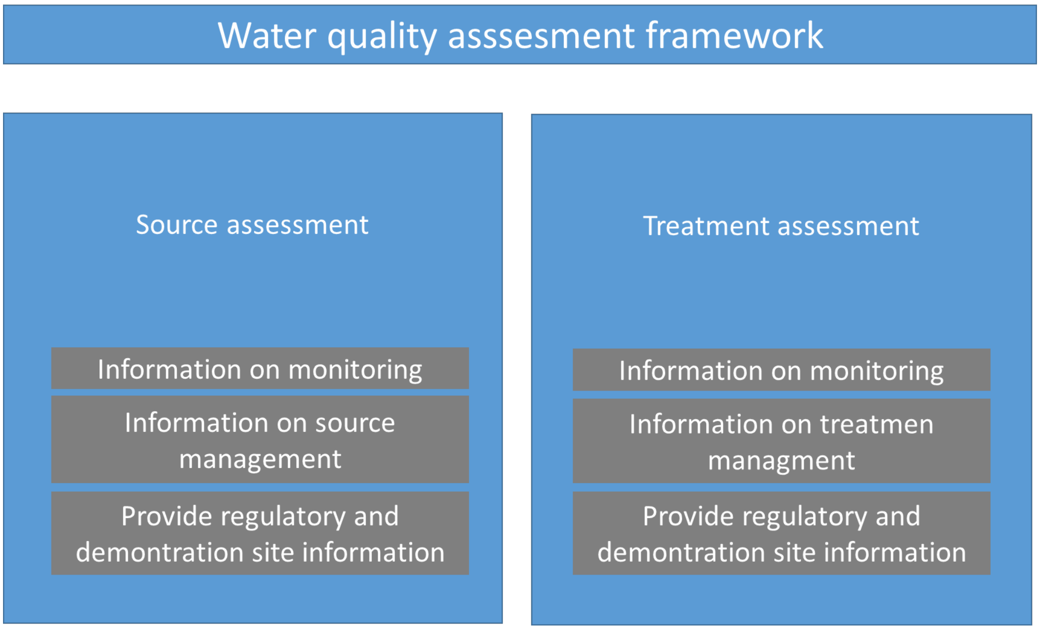


Figure 4 Water Quality Assessment Framework

2.6 Innovative techniques for water quality assessment

Chemical and microbial water quality assessment tools are developed at a high pace. While the advantages of innovative techniques are evident, water quality is generally assessed for a limited set of individual parameters using classic tools and methods. Innovative techniques can cover a wider array of contaminants, can be more sensitive, can enable faster detection and can integrate contamination and effects of complex mixtures. The limited set of individual regulated chemical water quality parameters might draw an incomplete picture of water quality and treatment performance. For example, most micro-pollutants under regulatory frameworks are parent compounds, when these parent compounds are transformed to other compounds, they are out of sight and control of regulatory frameworks, while persistent transformation products can be relevant in both in amount and potential effect [46]. Furthermore, persistent mobile (very polar) organic chemicals (PMOC) [47] are often ignored in monitoring and regulation, as these compounds are not well covered by current preparation and separation techniques, while their mobile and persistent nature makes them very hard to remove from water [48]. Additionally, environmental and human health effects and risks are not caused by individual chemicals but by the composition of the complex mixture. Bioassays allow to study toxic effects of complex mixtures for specific endpoints. Microorganism loads in water sources can have a very dynamic character, as some emissions are erratic and can be associated with rain events or local contamination. This requires frequent and event specific monitoring and fast detection. Classic plating techniques require days to obtain results and are labor intensive. They might not provide the speed and efficiency needed. Innovative microbial sensors can provide the required speed and efficiency and can be used as a first tier microbial water quality assessment tool.

Standard water quality parameters also might not sufficiently fulfill water quality monitoring with complex treatment systems and trains that hold combined natural and engineered treatment steps. For example, natural open systems risk microbial contamination, and therefore require robust microbial monitoring. Some examples of innovative water quality assessment tools, that might enable better water quality assessment in treatment with combined natural and engineered treatment steps are described below.

Integrated approaches – non target and suspect screening: Non-targeted chemical approaches analyze integrate responses of complex mixtures by scanning for all chemicals that can be isolated, separated and detected by available techniques. Such approach covers a far wider array of chemicals compared to targeted approaches. Starting from a suspect list of chemicals is also used more and more. Ongoing and future work on targeted databases and standardizations is expected to improve the use and implementation of these techniques [36, 49-51]. Non target approaches are most relevant for screening purposes in a research setting allowing substances to emerge, while suspect screening methods can be applied as a monitoring setting for water quality control.

Integrated approaches - Effect based monitoring: Biological effects of environmental complex mixtures can be monitored by a suite of bioassays such as isolated receptors, cells, biological tissues, whole organisms or ecosystems for very specific to very generic effect endpoints. The advantage is that such approaches cover a wider array of chemicals and outputs can be linked to biological effects [52]. However, the selection of (various) bioassays is crucial to cover relevant endpoints, and trigger values of such bioassays are still often lacking [14, 53, 54].

Microbial sensors – Microbial contamination can be detected by several sensors based on the detection of unique DNA fragments or proteins of for example fecal bacteria such as *E. coli (http://www.microlan.nl/)*. This enables continuous online or at line detection of microbial contamination and can function as an early warning system.

qPCR techniques – qPCR techniques enable to copy and identify specific DNA or RNA fragments of interest. This can be the presence of certain species for ecological profiling or the presence of antimicrobial resistance genes within and (environmental) microbial community. Such indicators enable to assess the ecological water quality and the effects of antimicrobial pressure on the water system, respectively. Antimicrobial resistance is a human health threat, and risks are clear in medical and veterinary settings [55]. However, the health risk of anti-microbial resistance in the water cycle is still unclear, as transfer of these genes from environmental microorganisms to pathogens and the exposure of humans via this route is largely unknown. Therefore the WHO advices to keep the number of ARGs in the environment as low as reasonably achievable. A further increase of resistance genes in the urban water cycle is therefore unwanted [56] [57, 58] [55].

Room is now given in the European Drinking Water Directive to develop a risk based monitoring program [59]. Customizing monitoring gives the freedom to exclude irrelevant parameters and apply alternative tools, but requires an evaluation of the output of these tools [60].

Requirements for acceptance and application are (1) the definition of health/risk based trigger values in order to evaluate samples and (2) collection of reference data on water types. Furthermore, and removal efficiencies of treatment systems enable comparison and prediction of treatment efficiencies [61].

3 Preliminary implementation of the WQAF

3.1 Water quality assessment framework

Technical and financial limitations normally prevent monitoring all (relevant) parameters with sufficient sensitivity at relevant frequencies. The current monitoring activities at the 13 demonstration sites are described in the AquaNES milestone report MS10. In short, this report and related data-file the treatment systems are summarized and the parameters that are monitored are given. The monitoring programs for the sites are rather diverse.

Efficient water quality assessment requires optimization of monitoring and application of other forms of information such as characterization of potential contamination in source water and evaluation of treatment robustness. The water quality assessment framework presented provides the ingredients to optimize and customize water quality assessment of treatment schemes. The paragraphs below describe some of the challenges of monitoring (data collection) and prerequisites to use this information for water quality assessment.

Selection of relevant emerging (chemical) contaminants. Both the number and volumes of synthetic chemicals that are globally produced and in use increase quickly, which during the production, use and waste phase can find their way to the aqueous environment [62]. Worldwide over 348.000 organic chemicals are produced [63], approximately 70.000 are registered for commercial application in Europe [64] and around 11.000 are produced or used in volumes over 100 tons per annum (TPA) in the European Union [65]. Most of these chemicals are not (regularly) monitored while they can potentially enter the water cycle during their production use and waste stage. Furthermore many of these chemicals can be transformed during use or after emission [46, 66]. Chemicals legislation such as REACH (Registration, Evaluation, Authorization and restriction of Chemicals) [67], the Authorization of Plant Protection Products Regulation (1107/2009/EC), the Cosmetics Regulation (1223/2009/EC), the Chemicals Agents Directive (98/24/EC), the Biocidal Product Regulation (528/2012/EC), and the Pharmaceutical Directive (2001/83/EC) are instrumental in safeguarding, production, formulation, use, service life and disposal of chemicals in the European Union. Information on production, use and properties of chemicals registered under various regulations can guide selection of relevant chemical contaminants for monitoring in specific sources and for specific uses.

3.2 Regulatory water quality criteria

Table 4 to Table 9 list water quality criteria and monitoring requirements for wastewater effluent, water for reuse as irrigation and groundwater recharge and drinking water. Since the different regulatory frameworks are define criteria for its use, this does not enable the evaluation of the treatment efficiency of and robustness of the applied treatment techniques. For further water quality assessment and assessment of treatment efficiency or risk assessment, other parameter classes are proposed along the treatment train in section 4.4.

The application of the treated water determines what parameters are of relevance since they can pose risks or affect receiving systems. The AquaNES project distinguishes:

- wastewater treatment and combined sewer overflow for emission to surface water
- wastewater treatment for irrigation
- rain water treatment and storage for irrigation
- surface water for the production of drinking water
- bank filtrate (and groundwater) for the production of drinking water

In order to determine relevant parameters for assessment of water quality, an overview was made on European guidelines and/or regulations that are available and may apply. In the following, information available from guidelines and regulations are organized according to the following themes:

- Wastewater treatment for emission to surface water
- Wastewater treatment (including run-off rain water) for irrigation
- Surface water and bank filtrate (and groundwater) for the production of drinking water

3.2.1 Wastewater treatment for emission to surface water

For wastewater treatment the source of wastewater considered here is the wastewater covered by the Urban Waste Water Treatment Directive (UWWTD; 91/271/EEC). Urban wastewater is defined as domestic wastewater or the mixture of domestic wastewater with industrial wastewater and/or run-off rain water.

Requirements for discharges from urban waste water treatment plants to surface water have been defined for Biochemical Oxygen Demand (BOD_5), Chemical Oxygen Demand (COD) and total suspended solids. For discharges to sensitive areas which are subject to eutrophication requirements for discharges have been defined for phosphorus and nitrogen. These requirements are presented in Table 4. The UWWTD does not include requirements for microbiological parameters and other chemical parameters.

Table 4 Requirements for discharges from urban waste water treatment plants as described in UWWTD. Tables modified from Table 1 and Table 2 as presented in Annex I of the UWWTD. Requirements regarding total phosphorus and total nitrogen only apply to discharges to sensitive areas which are subject to eutrophication. For more details, see UWWTD (91/271/EEC)

Parameter	Concentration	Minimum percentage of reduction
Biochemical Oxygen Demand (BOD_5 at 20 °C) without nitrification	≤ 25 mg O_2/L	70-90
Chemical Oxygen Demand (COD)	≤ 125 mg O_2/L	75
Total suspended solids	≤ 35 mg/L	90
Total phosphorus	≤ 1 mg/L	80
Total nitrogen	≤ 10 mg/L	70-80

3.2.2 Wastewater treatment (including run-off rain water) for irrigation

For wastewater treatment the only source of wastewater considered here is the wastewater covered by the UWWTD (91/271/EEC). Urban wastewater is defined as domestic wastewater or the mixture of domestic wastewater with industrial wastewater and/or run-off rain water.

There are no guidelines or regulations at the European Union (EU) level regarding (waste)water reuse, such as for irrigation. Recently, the Joint Research Centre (JRC) has published a report with proposed minimum quality requirements for water reuse in agricultural irrigation. This includes parameter values for microbiological parameters and parameters for Biochemical Oxygen Demand (BOD_5), Chemical Oxygen Demand (COD) and total suspended solids, but lacks chemical parameters for single compounds.

Four quality water classes (A, B, C and D) have been defined for which criteria for reclaimed water for agricultural irrigation were proposed. For different crop categories the JRC proposed which water classes can be used in combination with which irrigation methods (JRC, 2017). This information is summarized in Table 5.

Table 5 **Classes of reclaimed water quality with the associated agricultural use and irrigation methods applied. Table modified from JRC (2017)**

Crop category	Minimum reclaimed water quality class	Irrigation method
All food crops, including root crops consumed raw and food crops where the edible portion is in direct contact with reclaimed water.	Class A	All irrigation methods allowed
Food crops consumed raw where the edible portion is produced above ground and is not in direct contact with reclaimed water.	Class B	All irrigation methods allowed
Processed food crops. Non-food crops including crops to feed milk-or meat-producing animals.	Class C	Drip irrigation only
Industrial, energy, and seeded crops.	Class D	All irrigation methods allowed

The proposed quality criteria for these 4 reclaimed water classes for agricultural irrigation are presented in Table 6 (JRC, 2017).

Table 6 **Reclaimed water quality criteria for agricultural monitoring as proposed by JRC (2017).** Table modified from JRC (2017). Table A mentions refer to Table 5 of this document

Reclaimed water quality class	*E. coli* (cfu/100 mL)	BOD_5 (mg/L)	TSS (mg/L)	Turbidity (NTU)	Additional criteria
Class A	≤ 10 or below detection limit	≤ 10	≤ 10	≤ 5	*Legionella* spp.: ≤ 1 000 cfu/L when there is risk to aerosolization. Intestinal nematodes (helminth eggs): ≤ 1 egg/L when irrigation of pastures or fodder for livestock.
Class B	≤ 100	According to UWWTD (see Table A)	According to UWWTD (see Table A)	-	
Class C	≤ 1 000	According to UWWTD (see Table A)	According to UWWTD (see Table A)	-	
Class D	≤ 10 000	According to UWWTD (see Table A)	According to UWWTD (see Table A)	-	

Regarding chemical parameters, the JRC suggests that maximum concentrations in soils for a set of organic and inorganic chemicals as set by the WHO for soils (WHO, 2006) may be taken as a guidance if no updated scientific data are available. The JRC report indicates that the use of reclaimed water for irrigation may introduce toxic chemical compounds into soils, and pollutants accumulated in the soils may subsequently be taken up by crops and pose health risks to humans and animals. It indicates that especially heavy metals may require specific attention, but also that comtaminats of emerging concern (CECs) should get attention.

3.2.3 Surface water and bank filtrate (and groundwater) for the production of drinking water

The Drinking Water Directive (98/83/EC) concerns the quality of water intended for human consumption. Requirements for a series of microbiological, chemical and indicator parameters have been defined (Table 7, Table 8, Table 9). Member States of the European Union can include additional substances, or set higher standards, when translating the Drinking Water Directive into own national legislation.

Table 7 Microbiological parameters as defined in the European Drink Water Directive (98/83/EC)

Parameter	Parametric value
*Escherichia coli (*E. coli)	0/100 mL
Enterococci	0/100 mL
For water for sale in bottles or containers	
Parameter	Parametric value
Escherichia coli (E. coli)	0/250 mL
Enterococci	0/250 mL
Pseudomonas aeruginosa	0/250 mL
Colony count 22 °C	≤ 100/mL
Colony count 37 °C	≤ 20/mL

Table 8 Chemical parameters as defined in the European Drink Water Directive (98/83/EC)

Parameter	Parametric value
Acrylamide	≤ 0.10 µg/L
Antomony	≤ 5.0 µg/L
Arsenic	≤ 10 µg/L
Benzene	≤ 1.0 µg/L
Benzo(a)pyrene	≤ 0.010 µg/L
Boron	≤ 1.0 mg/L
Bromate	≤ 10 µg/L
Cadmium	≤ 5.0 µg/L
Chromium	≤ 50 µg/L
Copper	≤ 2.0 mg/L
Cyanide	≤ 50 µg/L
1,2-dichloroethane	≤ 3.0 µg/L
Epichlorohydrin	≤ 0.10 µg/L
Fluoride	≤ 1.5 mg/L
Lead	≤ 10 µg/L
Mercury	≤ 1.0 µg/L
Nickel	≤ 20 µg/L
Nitrate	≤ 50 mg/L

Nitrite	≤ 0.50 mg/L
Pesticides	≤0.10 µg/L
Pecticides - Total	≤ 0.50 µg/L
Polycyclic aromatic hydrocarbons	≤ 0.10 µg/L
Selenium	≤ 10 µg/L
Tetrachloroethene and trichlororethene	≤ 10 µg/L
Trihalomethanes - Total	≤ 100 µg/L
Vinyl chloride	≤ 0.50 µg/L

Table 9 **Indicator parameters as defined in the European Drink Water Directive (98/83/EC)**

Parameter	Parametric value
Aluminium	≤ 200 µg/L
Ammonium	≤ 0.50 mg/L
Chloride	≤ 250 mg/L
Clostridium perfringens (including spores)	0/100 mL
Colour	Acceptable to consumers and no abnormal change
Conductivity	≤ 2500 µS/cm at 20 °C
Hydrogen ion concentration	pH between 6.5 and 9.5
Iron	≤ 200 µg/L
Manganese	≤ 50 µg/L
Odour	Acceptable to consumers and no abnormal change
Oxidisability	≤ 5.0 mg/L O2
Sulphate	≤ 250 mg/L
Sodium	≤ 200 mg/L
Taste	Acceptable to consumers and no abnormal change
Colony count 22 °C	No abnormal change
Coliform bacteria	≤ 0/100 mL
Total organic carbon (TOC)	No abnormal change
Turbidity	Acceptable to consumers and no abnormal change

3.2.4 Evaluation of regulatory water quality criteria

It is obvious that the requirements for wastewater treatment for emission to surface water and the requirements that have been proposed for wastewater treatment for irrigation largely differ from the requirements that have been defined for drinking water. Further, it is interesting to note that the requirements for wastewater treatment for emission to surface water and the proposed requirements for wastewater treatment for irrigation, include values for a minimum percentage of reduction of the BOD_5, COD and total suspended solids (and total phosphorus and total nitrogen for discharges to sensitive areas which are subject to eutrophication). This indicates that besides measurements of the effluent of the waste water treatment plant, time-matched measurements of the influent are needed in order to determine this percentage of reduction. For drinking water, the European Drink Water

Directive's drinking water quality requirements only apply to the final product (drinking water). However, individual member states may have their own legislation with specific requirements for the water source that is used for the production of drinking water.

3.3 Optimizing quality of monitoring and data interpretation

3.3.1 Optimization of monitoring

Parameters can be selected based on known emissions, hydrology (origin of water, volumes, dilution, dynamics), system characteristics, parameter characteristics (mobility, persistence, volatility), available water quality data of system or similar systems from literature [11, 15, 47, 68] and legal requirements. The advantage of such parameters is their known source and emission and expected relevance. However, this approach is likely biased towards parameters that already have a large knowledge base, while other relevant but hardly studied or regulated parameters are omitted [69]. Information on production use and properties, as described above, can support the emergence of relevant contaminants. Furthermore, innovative techniques described in section 3.2 enable new chemicals and microbial contamination to emerge. Health/risk based guideline values or trigger values are required to evaluate whether these emerging chemicals and microbes pose a risk.

One should be aware of difficulties in monitoring specific parameters. For example, volatile or light sensitive parameters require specific sampling and storage procedures. While the use of specific materials and solvents should be avoided specific parameters as they might lead to losses or contaminations (e.g. metal equipment, plastic equipment and tubing, detergents used for cleaning equipment, extraction materials, solvents and salts added for storage and analysis, etc.). One should always be aware of materials and procedures that can compromise samples and sampling.

3.3.2 Evaluation of treatment robustness

One can *experimentally* determine water quality of raw and treated water by monitoring parameters of interest, experimentally determine operational parameters that indicate treatment performance, and/or *theoretically* assess the robustness of a treatment train by using removal rates of treatment steps from literature (see https://www.watershare.eu/tool/abates/ [40]). In all cases, the treated water quality or values of (indicative) parameters are compared to regulatory water quality criteria [17, 19, 20, 70-74] or provisional guideline values [16, 23, 75-78]. A recent inventory illustrated that removal rates lack standardization in experimental conditions resulting in a large variation of experimental removal rates and thereby lack large margins of uncertainty [61]. Furthermore, parameters derived in batch lab experiments are not always representative of long-term continuous operation of wastewater and drinking water treatment plants, and treatment assessment often focuses on the reduction of (chemical) pollutants without distinguishing between removal and transformation. Transformation products of substances that occur in sources are of special relevance when disinfection and oxidative techniques such as ozone treatment UV, UV-H_2O_2 and chlorination are applied in the treatment train. Also treatment techniques with high biological activity such as conventional activated sludge treatment and natural treatment steps such as constructed wetlands and passage of soil can lead to the formation of transformation products. The assessment of transformation product is challenging, since the transformation products formed are diverse and information is scarce. However, examples can be found in literature. Appendix 1 gives an overview of relevant transformation products of various classes of organic substances from literature.

3.3.3 Data quality and representativeness

Analysis of water quality parameters can be compromised by sampling, sample treatment and analysis. Variable concentrations of parameters due to dynamic concentrations in sources or treatment performance (e.g. microorganism blooms, seasonal or event specific emissions) require frequent or time integrated sampling, and knowledge on emission patterns and hydrology [79, 80]. Sample treatment and analysis should also be sufficiently sensitive to determine the parameters of interest at relevant levels. Sample treatment and analysis should not introduce contamination (by contaminated solvents, equipment, or accidental contamination) or lead to the loss of parameters of interest (by evaporation, poor extraction recovery of analytical issues). Blanks, correct sample handling and multiple analysis prevent misinterpretation of results of analysis.

3.3.4 Components of water quality assessment

Water quality assessment at a specific site consists of system analysis, determining potential pollutants, evaluating reference sites and data, design monitoring program (what to monitor when and where), and evaluating results. In the following paragraphs, a preliminary assessment of a selection of demonstration sites is presented. Whether the required data can be obtained, will in the end be a matter of available resources.

3.4 Water quality assessment framework applied to selected demonstration sites

Demonstration sites have a suite of sources, treatment technologies and uses (see MS 10). Three sites were selected for a preliminary assessment. The sites represent treatment schemes from work package 1, 2 and 3, being riverbank filtration (Site 1), managed aquifer recharge for drinking water production (Site 6) and a constructed wetland concept for raw wastewater (Site 10a) treatment.

3.4.1 Preliminary assessment of AquaNES Demonstration Site 1

At Site 1 (Berlin) drinking water is produced from bank filtrate and (recharged) groundwater. The treatment scheme for the demonstration site is depicted Figure 5.

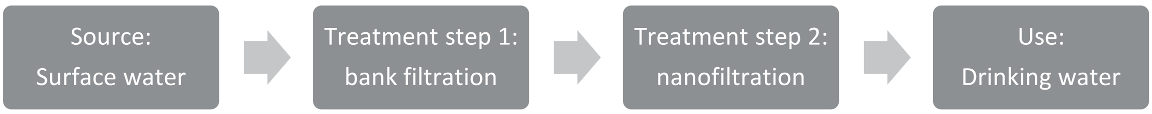


Figure 5 Simplified treatment scheme of site 1 - Water quality can be assessed after each step

3.4.1.1 Source assessment

Site 1 is a low land area that consist of rivers and lakes. The catchment of the Havel river catchment, with the Spree as a main contributory, holds a population of 4-5 million people and contains agricultural land and industrial activities and many lakes. The average discharge of the river is rather low for the size of its catchment (average 38 m^3 from the Havel and 15 m^2 from the Spree at the point in Berlin where the two rivers merge) because of the rather low annual precipitation in this region (500-600 mm/y). The contribution of the Spree is reduced during the last decades. This is a result of the abandoning of lignite mining upstream of Berlin leading to a reduction of so-called “sump water” extracted from the mining areas. The low discharge provides limited dilution for wastewater streams from the population of Berlin and surroundings. The water collected for drinking water production mainly consist of bank filtrate. The residence time of the bank filtrate varies from a month to years. The bank filtrate that is extracted is generally a mixture of water with different residence times in the underground.

Water quality parameters for surface water and bank filtrate are separated since the first can provide relevant information on pollutants that might reach latter in due time, and enable to determine treatment efficiency of bank filtration.

3.4.1.2 Treatment assessment

At demonstration site 1 pilot plant, drinking water is produced from bank filtrate that is further purified by nanofiltration. The treatment efficiency of bank filtration for microorganisms and micro pollutants is dependent on the soil material, the conditions and the residence time of the water in the riverbank. Characterization of the hydrology is relevant for the assessment of relevant parameters. Extracted bank filtrate from a single site is composed of water with different ages (i.e. residence times in the bank). The water with the shortest retention time largely determines the load of microorganisms. Micro pollutants can be retarded by sorption to the soil, or transformed into other substances [81, 82]. As a consequence the composition of the micro pollutants in extracted river bank filtrate are a mixture of substances that were emitted recently and substances that were emitted years or decades ago. Typically, polar persistent neutral and negatively charged molecules (e.g. carbamazepine, sulfamethoxazole, diatrizoic acid, EDTA), pass a riverbank while more hydrophobic substances and positively charged substances (the latter depending on cation exchange capacity, pH and presence of other cations) are retained (e.g. PAHs, metformin, (heavy) metals [83]). Hydrology and retardation can lead to the observation of obsolete substances that are hardly found in surface waters any more (e.g. phenazone and its transformation products [84] [85]). Banning or changing use of substances will therefore have a delayed effect on the composition of river bank filtrate. Nanofiltration separates water from larger molecules and charged molecules. Consequently, substances that are small and polar and are not electrostatically rejected by the membrane are most likely to pass nanofiltration membranes [86].

3.4.1.3 Monitoring parameters

Water quality standards for drinking water are listed in Paragraph 4.2. However, monitoring microorganisms is most relevant in sources, as limits of quantification are generally insufficient for analysis meeting water quality standards in produced drinking water.

Considering treatment and source characteristics, chemical monitoring should be directed towards polar neutral and negative substances that are rather persistent, and able to pass the treatment barriers [47, 48]. This can be both substances that are commonly found in wastewater effluents such as pharmaceuticals, personal care products that are used in households as well as a selection of industrial chemicals and pesticides that are related to industrial activities and agriculture in the region, respectively. For example, parameters associated with lignite mining including indirect effects such as metal mobilization due to acidification as a result of pyrite oxidation might be relevant. Monitoring efforts can be reduced by finding indicator parameters for specific sources and emission routes (e.g. an indicator pharmaceutical or artificial sweetener for municipal wastewater, a pesticide for agricultural activities, and a microbial indicator for fecal contamination). Indicator parameters need to be validated from time to time since emission patterns and routes can change with time. When parameters are specifically selected to study treatment performance, one should design the sampling scheme in such a way that samples before and after treatment can be related. Furthermore, relevant (environmental) conditions should be covered in order to assess the robustness of the treatment performance.

The water quality of river surface water is dynamic, however the long residence in the riverbank allows mixing. Monitoring frequency of bank filtrate can be adapted to the hydraulic retention time of the bank filtration system.

Table 10 Relevant water quality parameters for monitoring besides legal monitoring requirements

	Generic monitoring											*Innovative techniques*		
Treatment step	Nutrients, eutrophication indicators	Redox conditions	Metal	Organic carbon content indicator	Substances from communal wastewater sources	Substances from agricultural sources	Substances from (specific) industrial sources	Transformation product / Disinfection by-products	Biological activity/stability indicators	Fecal indicators and pathogens		Results from innovative integrative techniques	Online and at-line sensors for operational purposes	(Antibiotic) resistance indicators
Source (SW)	+	-	+ [4]	+	+	+	+	-	- [7]	+ [4]		+ [4]	-	- [7]
Source (RBF)	+	+ [2]	+ [4]	+	+ [4]	+ [4]	+ [4]	+ [4,5]	-	+ [4]		+ [4]	+ [8]	- [7]
Treatment (NF)	-	-	+ [4]	+	+ [4]	+ [4]	+ [4]	-	-	+ [4]		+ [4]	+ [9]	- [7]
Product (DW)	+ [1]	-	+ [4]	+ [1]	+ [4]	+ [4]	+ [4]	+ [6]	-	+ [4]		+ [4]	+ [10]	- [7]
Examples of parameters	N, P	Chemical and microbial Redox indicators (e.g. SO_4, sulfur bacteria)	e.g. Pb, C, Cd Cr, As	DOC, BOD, COD, suspended solids	Pharmaceuticals, personal car, products	Pesticides, veterinary pharmaceuticals	Benzene, PAHs, chlorinated hydro0carbons	Phenazone transformation products, chloride disinfection byproducts	ATP, algae	Colony count, Coliforms, E coli, Enterococci		Bioassays (CALUX), non-target screening approaches	Sensors for microbial activity, coliforms, specific pathogens	DNA fragments of antibiotic resistance genes

Legend: [1] for regrowth potential, [2] for relevant transformation and speciation processes in the underground, [4] for assessing treatment efficiency, [5] bank filtrate is known to hold environmental transformation products of (sometimes obsolete) substances, [6] chlorination can lead to disinfection byproducts, [7] not a specific interest for this demonstration site. [8] macro parameters indication age and source of bank filtrate can affect extraction and mixing of water from different wells in well fields (temperature, macro chemical composition), [9] parameters indication membrane integrity and performance (e.g. Pressure), [10] parameters indication flow and demand.

3.4.2 Preliminary assessment of AquaNES Demonstration Site 6

At Site 6 (Basel) drinking water is produced from surface water that is pretreated with UV &H_2O_2 and subsequently filtered by the ground (MAR/SAT). The treatment scheme for the demonstration site is depicted in Figure 6.

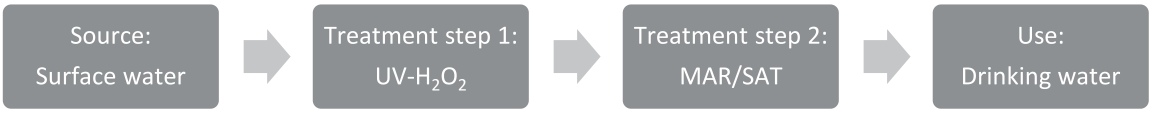


Figure 6 Simplified treatment scheme of site 6 - water quality can be assessed after each step

3.4.2.1 *Source assessment*

Site 6 is situated at the foothills of the Alps in the catchment of the Rhine river. This catchment upstream of Basel holds over 5 million people, mostly from Switzerland. The average discharge of the river Rhine at Basel is around 900 m³/s. therefore the percentage of treated wastewater from industries and municipal wastewater effluent is lower than in the lower stretches of the river Rhine [87] and many low land rain fed rivers in Europe. The relatively high discharge provides dilution for wastewater upstream from Basel. However, the mountain landscape can lead to surface run off that can lead to high turbidity, organics during heavy rain events or snow melt.

Table 11 shows relevant water quality parameters for the surface water that provides can provide relevant information on pollutants and materials that can affect treatment performance.

Table 11 Relevant water quality parameters for monitoring besides legal requirements

	Generic monitoring											*Innovative techniques*		
Treatment step	Nutrients, eutrophication indicators	Redox conditions	Metal	Organic carbon content indicator	Substances from communal wastewater sources	Substances from agricultural sources	Substances from (specific) industrial sources	Transformation product / Disinfection by-products	Biological activity/stability indicators	Fecal indicators and pathogens		Results from innovative integrative techniques	Online and at-line sensors for operational purposes	(Antibiotic) resistance indicators
Source (SW)	+	-	+[3, 4]	+	+	+	+	-	-[7]	+[4]		+[4]	-	-[7]
(pre) treatment (UV-	+	-	+[4]	+	+[4]	+[4]	+[4]	+[3]	-	+[4]		+[4]	+[8]	-[7]
MAR/SAT	-	+ [2]	+[4]	+	+[4]	+[4]	+[4]	+[5]	-	+[4]		+[4]	+[9]	-[7]
Product (DW)	+[1]	-	+[4]	+[1]	+[4]	+[4]	+[4]	+[6]	-	+[4]		+[4]	+[10]	-[7]
Examples of parameters	N, P	Chemical and microbial Redox indicators (e.g. SO_4, sulfur	e.g. Pb, C, Cd Cr, As	DOC, BOD, COD, suspended solids	Pharmaceuticals, personal car, products	Pesticides, veterinary pharmaceuticals	Benzene, PAHs, chlorinated hydro0carbons	NDMA, chloride disinfection byproducts (trihalomethanes)	ATP, algae	Colony count, Coliforms, E coli, Enterococci		Bioassays (CALUX), non-target screening approaches	Sensors for microbial activity, coliforms, specific pathogens	DNA fragments of antibiotic resistance genes

Legend: [1] for regrowth potential, [2] for relevant transformation and speciation processes in the underground, [3] UV-H_2O_2 can lead to transformation products, [4] for assessing treatment efficiency, [5] soil passage is known to hold environmental transformation products of (sometimes obsolete) substances, [6] chlorination can lead to disinfection byproducts, [7] not a specific interest for this demonstration site. [8] parameters indicating performance (oxidation potential, free radicals, turbidity) [9] parameters indication soil condition (pH, conductivity, temperature), [10] parameters indication flow and demand.

3.4.2.2 Treatment assessment

At demonstration site 6, drinking water is produced from surface water that is pre-treated sand filtration and then with UV-H_2O_2 for disinfection and break down of micro-contaminants. The formation of transformation products is largely dependent by the dosage of light and H_2O_2 in relation to the properties of the source water. When turbidity and suspended solids and dissolved organic materials rise, more light and H_2O_2 is needed to obtain the same performance.

The treated water is subsequently infiltrated in the soil and extracted after an average residence time of several months (in the full scale system, residence time in the pilot set-up is shorter). The UV- H_2O_2 leads to microorganism removal and transformation of micro contaminants and organic matter. The MAR/SAT enables to dilute peak emissions (due to accidents, spills or heavy rain events), remove microorganisms and either sorb or transform micro-contaminants. Substances that are difficult to oxidize and insensitive to UV light pass UV-H2O2 treatment [88], furthermore this treatment step generates transformation products from micro contaminants as well as organic matter present in the source water [89]. Polar persistent neutral and negatively charged molecules potentially pass the soil while positively charged substances (the latter depending on cation exchange capacity, pH and presence of other cations) can be retained.

3.4.2.3 Monitoring parameters

Water quality standards for drinking water are listed in Paragraph 4.2. Monitoring microorganisms is most relevant in sources, as limits of quantification are generally insufficient for analysis of water quality standards in produced drinking water, there are however legal requirements to monitor (indicator) microorganisms in drinking water.

Considering treatment and source characteristics, chemical monitoring should be directed towards transformation products of UV-H_2O_2 treatment and polar neutral and negative substances that are rather persistent, and able to pass soil [47, 48]. This can be substances that are commonly found in wastewater effluents such as pharmaceuticals, personal care products that are used in households as well as a selection of industrial chemicals and pesticides that are related to industrial activities and agriculture in the region. Since the site is situated at the foothills of the Alps, one should perform event specific monitoring on source quality and treatment performance associated with heavy rain event (surface run off, and snow melt, as this can both lead to large emissions of certain pollutants (pesticides, and fecal microbes and can compromise the UV-H_2O_2 treatment by light and radical scavenging of DOC/turbidity.

3.4.3 Preliminary assessment of AquaNES Demonstration Site 10a

At Site 10a (Thirasia) raw wastewater is treated by photocatalytic treatment using natural light, a constructed wetland and chlorination for disinfection. The treated water is intended to be used for irrigation of public space/ groundwater recharge. The treatment scheme for the demonstration site is depicted in Figure 7.

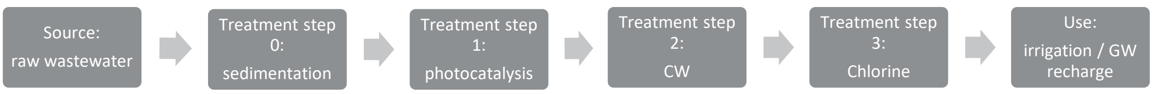


Figure 7 Simplified treatment scheme of site 10A - Water quality can be assessed after each step

3.4.3.1 Source assessment

Site 10a is situated at Thirasia Island (Greece) in the Aegean Sea. The treatment is fed with raw wastewater from inhabitants and tourists. The population on the island is very small ~200, but in tourist season the number of inhabitants increase almost tenfold. Currently, only a small part of the island population and tourist venues bring their wastewater to the treatment plant, but it is intended that these numbers increase. The transport by trucks and the seasonal differences in volumes of wastewater is a challenge for the treatment system and require specific wastewater and treatment management.

Table 12 shows relevant water quality parameters for the surface water and relevant information on pollutants and materials that can affect treatment performance.

Table 12 Relevant water quality parameters for monitoring besides legal requirements

	Generic monitoring											*Innovative techniques*		
Treatment step	Nutrients, eutrophication indicators	Redox conditions	Metal	Organic carbon content indicator	Substances from communal wastewater	Substances from agricultural sources	Substances from (specific) industrial sources	Transformation product / Disinfection by-products	Biological activity/stability indicators	Fecal indicators and pathogens		Results from innovative integrative techniques	Online and at-line sensors for operational purposes	(Antibiotic) resistance indicators
Source (WW)	+	-	-	+	+	-	-	-	-[7]	+[4]		-[7]	-	-[7]
(pre) treatment (Photocatalysis	-	-	-	-	+[4]	-	-	+[3]	-[7]	+[4]		-[7]	+[8]	-[7]
CW	+	+	-	+	+[4]	-	-	+[5]	-[7]	+[4]		-[7]	+[9]	-[7]
Cl	-	-	-	-	-	-	-	+[6]	-[7]			-[7]	+[10]	-[7]
Product	+[1]	-	+[4]	+[1]	+[4]	-	-	+	-[7]	+[4]		-[7]	+[11]	-[7]
Examples of parameters	N, P	Chemical and microbial Redox indicators (e.g. SO_4,	e.g. Pb, C, Cd Cr, As	DOC, BOD, COD, suspended solids	Pharmaceuticals, personal car, products	Pesticides, veterinary pharmaceuticals	Benzene, PAHs, chlorinated hydro0carbons	chloride disinfection byproducts (trihalomethanes)	ATP, algae	Colony count, Coliforms, E coli, Enterococci		Bioassays (CALUX), non-target screening approaches	Sensors for microbial activity, coliforms, specific pathogens	DNA fragments of antibiotic resistance genes

Legend: [1] for regrowth potential, [2] for relevant transformation and speciation processes in the underground, [3] Photocatalysis can lead to transformation products, [4] for assessing treatment efficiency, [5] Constructed wetlands can lead to environmental transformation products, [6] chlorination can lead to disinfection byproducts, [7] not a specific interest for this demonstration site. [8] parameters indicating performance (oxidation potential, natural illumination, temperature) [9] parameters indication CW condition (pH, conductivity, temperature), [10] chlorine levels, [11] parameters indication flow and demand. [12] dynamic flows and conditions make continuous monitoring valuable.

3.4.3.2 Treatment assessment

At demonstration site 10a, wastewater is collected, and after sedimentation, photocatalytic reactors with natural sunlight and TiO_2 surfaces provide oxidation of organic material micro contaminants and removal of microbes. Subsequently, the water is lead over an horizontal constructed wetland in order to remove nutrients before it is collected and chlorinated for further disinfection. Since fresh water is scarce on these islands, the intended use of the water is irrigation and groundwater recharge. The main purpose of the treatment is to remove microbial contamination for reuse.

The catalytic oxidation leads to disinfection and can also lead to transformation of micro contaminants and organic matter. Further treatment in constructed wetlands enable to remove nutrients and transform or assimilate organic matter. Finally, chlorination disinfects the water further and can also lead to disinfection by-products.

3.4.3.3 Monitoring parameters

Suggested European minimum water quality standards for irrigation and groundwater recharge water are listed in Table 5 and Table 6. The actual Greek limit values are summarized in a paper by Paranychianakis et al.[1]. Monitoring microorganisms (or its indicators) is very relevant as reuse for irrigation or groundwater recharge indirectly can lead to exposure of humans.

Considering treatment and source characteristics and intended use, monitoring should be directed towards microbial water quality parameters, besides legal requirements set for the treated water, it is relevant to monitor treatment efficiencies in order to provide valuable information on treatment efficiency of the different components and the total treatment scheme of this demonstration site. Specific attention should be drawn towards dynamics in flow over the seasons and the batch wise loading (by trucks), as well as the seasonal and diurnal treatment efficiencies of especially the photo catalysis driven by natural light and seasonal effects on the constructed wetland. Chemicals such as pharmaceuticals and household products are of special interest since the wastewater is largely from domestic origin. The treatment steps can lead to the transformation of organic micro pollutants, so evaluation of transformation products might also be of interest.

Raw wastewater influent collected from a small touristic island by trucks is very variable in composition and its load. Monitoring should take into account these dynamics. This strongly advocates for (near) continuous monitoring of the most relevant microbial parameters. Alternatively, or for other parameters event specific monitoring can be applied to define various influent quality and quantity conditions under various environmental (temperature, sun light intensity) conditions to define the treatment efficiency under all relevant conditions.

3.5 The water quality assessment framework and its use for Water Safety Planning

The water quality assessment framework guides the user towards the collection of relevant information to assess the water quality. This stretches further than water quality criteria set by legal frameworks. It consist of data from monitoring, but also relevant reference data from other (similar systems) and non-regulatory water quality criteria or guidelines. It covers information on sources, treatment and produced water as well as relevant quality criteria to interpret these data. This information enables to perform a risk assessment of the treatment system and product that is produced for its intended use. Furthermore, the reference data on treatment systems and system dynamics can be used to manage risks and define relevant measures to monitor and control these risks. The system evaluation, risk assessment and risk management is the knowledge base on a system level to perform water safety

[1] N. V. Paranychianakis, M. Salgot, S. A. Snyder & A. N. Angelakis (2015) Water Reuse in EU States: Necessity for Uniform Criteria to Mitigate Human and Environmental Risks, Critical Reviews in Environmental Science and Technology, 45:13, 1409-1468, DOI: 10.1080/10643389.2014.955629

planning (WSP) for effluent [90], reuse and irrigation water and drinking water [1]. It can help to evaluate essential water treatment steps. Additionally these data and their relationship with sources hydrology as well as the robustness of treatment (steps) also can be applied for scenario studies and evaluating the resilience of existing treatments and (conceptual) alternative treatment schemes. This enables tools for planning investments.

4 Discussion and concluding remarks

There is no one size fits all solution for water quality assessment since source quality and quantity, treatment technology as well as intended use of water differs and available resources for water quality assessment differ. Regulatory frameworks provide a basic set of water quality parameters and criteria to monitor or assess the treated water. Water quality assessment within the AquaNES project has also other purposes such as the illustration and evaluation of pilot treatment plants and evaluation of the treatment robustness and safety. Furthermore, the most relevant and critical steps in water treatment train that can be obtained with water safety planning, differ per (combination of) source water treatment train and intended use of the water. Similarly, the most relevant steps within the demonstration sites for the AquaNES project differ per site. Therefore, a customized water quality assessment approach, consisting of evaluation of contamination sources, monitoring, treatment and evaluation of results with reference data or risk based water quality criteria is necessary. Multiple forms and sources of information can (and need to be) used to enable efficient effective and robust water quality assessment, in order to perform risk assessment and management provide water quality that fits its intended use under all circumstances.

The following issues and activities are relevant:

- Evaluate systems / contamination sources and potential threats and customize monitoring and other forms of water quality assessment accordingly
- look beyond regulatory frameworks and its water quality criteria, as risks are not solely determined by regulated parameters, and emerging issues of today might be regulated tomorrow and various non-governmental water quality criteria are available [17, 21]
- Use reference data of similar systems and situations (e.g. demonstration sites, data on treatment techniques or source contamination). Build a community with parties using similar techniques to enable first hand data and knowledge transfer (https://www.watershare.eu/)
- Define key treatment processes and evaluate its robustness under various conditions with information from previous activities
- Use innovative tools if they provide additional and relevant information or have advantages in efficiency or speed
- Use tiered approaches and event specific monitoring in order to use funds and capacity more efficiently for water quality assessment
- Develop and use data processing tools that enable better monitoring and interpretation of changing (environmental) conditions and treatment performance and the relation of those aspects to product quality
- Apply gathered information for Water Safety Planning or scenario studies to test system resilience

5 Literature

Please note, references from no. 91 on only appear in the Appendix.

1. World Health Organization Water Safety Plans: Managing drinking-water quality from catchment to consumer; WHO: Geneva, Switzerland, 2005; p 244.
2. Majumdar, D.; Rajaram, B.; Meshram, S.; Suryawanshi, P.; Chalapati Rao, C. V., Worldwide distribution of polyclyclic aromatic hydrocarbons in urban road dust. International Journal of Environmental Science and Technology **2017,** 14, (2), 397-420.
3. Young, I.; Smith, B. A.; Fazil, A., A systematic review and meta-analysis of the effects of extreme weather events and other weather-related variables on Cryptosporidium and Giardia in fresh surface waters. Journal of water and health **2015,** 13, (1), 1-17.
4. Huber, M.; Welker, A.; Helmreich, B., Critical review of heavy metal pollution of traffic area runoff: Occurrence, influencing factors, and partitioning. *Science of the Total Environment* **2016,** *541*, 895-919.
5. Tran, N. H.; Gin, K. Y. H.; Ngo, H. H., Fecal pollution source tracking toolbox for identification, evaluation and characterization of fecal contamination in receiving urban surface waters and groundwater. *Science of the Total Environment* **2015,** *538*, 38-57.
6. Oen, A. M. P.; Beckingham, B.; Ghosh, U.; Kruså, M. E.; Luthy, R. G.; Hartnik, T.; Henriksen, T.; Cornelissen, G., Sorption of organic compounds to fresh and field-aged activated carbons in soils and sediments. *Environmental Science and Technology* **2012,** *46*, (2), 810-817.
7. Bartak, R.; Grischek, T.; Ghodeif, K.; Ray, C., Beach Sand Filtration as pre-treatment for RO desalination. *Int J Water Sciences* **2012,** *1*, (2), 1-10.
8. Heringa, M. B.; Harmsen, D. J. H.; Beerendonk, E. F.; Reus, A. A.; Krul, C. A. M.; Metz, D. H.; Ijpelaar, G. F., Formation and removal of genotoxic activity during UV/H2O2-GAC treatment of drinking water. *Water Research* **2011,** *45*, (1), 366-374.
9. Sjerps, R.; Nugteren, S.; Maessen, M.; Ter Laak, T. L. *Evaluatie meetgegevens organische microverontreinigingen Evides (2012-2014)*; KWR watercycle research institute: Nieuwegein, the Netheralnds, 2016; p 48.
10. Altenburger, R.; Ait-Aissa, S.; Antczak, P.; Backhaus, T.; Barceló, D.; Seiler, T. B.; Brion, F.; Busch, W.; Chipman, K.; de Alda, M. L.; de Aragão Umbuzeiro, G.; Escher, B. I.; Falciani, F.; Faust, M.; Focks, A.; Hilscherova, K.; Hollender, J.; Hollert, H.; Jäger, F.; Jahnke, A.; Kortenkamp, A.; Krauss, M.; Lemkine, G. F.; Munthe, J.; Neumann, S.; Schymanski, E. L.; Scrimshaw, M.; Segner, H.; Slobodnik, J.; Smedes, F.; Kughathas, S.; Teodorovic, I.; Tindall, A. J.; Tollefsen, K. E.; Walz, K. H.; Williams, T. D.; Van den Brink, P. J.; van Gils, J.; Vrana, B.; Zhang, X.; Brack, W., Future water quality monitoring - Adapting tools to deal with mixtures of pollutants in water resource management. *Science of the Total Environment* **2015,** *512-513*, 540-551.
11. Sjerps, R. M. A.; Vughs, D.; van Leerdam, J. A.; ter Laak, T. L.; van Wezel, A. P., Data-driven prioritization of chemicals in various water types using suspect screening LC-HRMS. *Water Reseach* **2016**, 254-264.
12. Ji, K.; Han, E. J.; Back, S.; Park, J.; Ryu, J.; Choi, K., Prioritizing human pharmaceuticals for ecological risks in the freshwater environment of Korea. *Environmental Toxicology and Chemistry* **2016,** *35*, (4), 1028-1036.
13. Helwig, K.; Hunter, C.; McNaughtan, M.; Roberts, J.; Pahl, O., Ranking prescribed pharmaceuticals in terms of environmental risk: Inclusion of hospital data and the importance of regular review. *Environmental Toxicology and Chemistry* **2016,** *35*, (4), 1043-1050.
14. Brack, W.; Ait-Aissa, S.; Burgess, R. M.; Busch, W.; Creusot, N.; Di Paolo, C.; Escher, B. I.; Mark Hewitt, L.; Hilscherova, K.; Hollender, J.; Hollert, H.; Jonker, W.; Kool, J.; Lamoree, M.; Muschket, M.; Neumann, S.; Rostkowski, P.; Ruttkies, C.; Schollee, J.; Schymanski, E. L.; Schulze, T.; Seiler, T. B.; Tindall, A. J.; De Aragão Umbuzeiro, G.; Vrana, B.; Krauss, M., Effect-directed analysis supporting monitoring of aquatic environments - An in-depth overview. *Science of the Total Environment* **2016,** *544*, 1073-1118.
15. Schollée, J. E.; Schymanski, E. L.; Avak, S. E.; Loos, M.; Hollender, J., Prioritizing Unknown Transformation Products from Biologically-Treated Wastewater Using High-Resolution Mass Spectrometry, Multivariate Statistics, and Metabolic Logic. *Analytical Chemistry* **2015,** *87*, (24), 12121-12129.
16. Moermond, C. T. A.; Smit, C. E., Derivation of water quality standards for carbamazepine, metoprolol, and metformin and comparison with monitoring data. *Environmental Toxicology and Chemistry* **2016,** *35*, (4), 882-888.

17. WHO *Guidelines for drinking-water quality - 4th ed.*; World Health Organisation: Geneva, Switzerland, 2011; p 568.
18. Wirtz, F., Danube, Meuse and Rhine MEMORANDUM 2008. *Environmental science and pollution research international* **2009,** *16 Suppl 1*, S112-115.
19. European Commission, EU Water Framework Directive In Brussels, Belgium, 2000.
20. European Commission, The Drinking Water Directive, 98/83/EC. In Brussels, Belgium, 1998.
21. Baken, K.; Sjerps, R. The Threshold of Toxicological Concern (TTC): refinement of the concept and application to drinking water; BTO 2016.069; KWR Watercycle Reserach Institute: Nieuwegein, The Netherlands, 2016; p 50.
22. Kroes, R.; Galli, C.; Munro, I.; Schilter, B.; Tran, L. A.; Walker, R.; Wurtzen, G., Threshold of toxicological concern for chemical substances present in the diet: A practical tool for assessing the need for toxicity testing. Food and Chemical Toxicology **2000,** 38, (2-3), 255-312.
23. Mons, M. N.; Heringa, M. B.; van Genderen, J.; Puijker, L. M.; Brand, W.; Van Leeuwen, C. J.; Stoks, P.; van der Hoek, J. P.; van der Kooij, D., Use of the Threshold of Toxicological Concern (TTC) approach for deriving target values for drinking water contaminants. Water Research **2013,** 47, (4), 1666-1678.
24. Lapworth, D. J.; Baran, N.; Stuart, M. E.; Ward, R. S., Emerging organic contaminants in groundwater: A review of sources, fate and occurrence. Environmental Pollution **2012,** 163, (0), 287-303.
25. Coppens, L. J. C.; Gils, J. A. G.; ter Laak, T. L.; Raterman, B. W.; van Wezel, A. P., Towards spatially smart abatement of human pharmaceuticals in surfacewaters: Defining impact of sewage treatment plants in susceptible functions. *Water Research* **2015,** *81*, 356-365.
26. Hamann, E.; Stuyfzand, P. J.; Greskowiak, J.; Timmer, H.; Massmann, G., The fate of organic micropollutants during long-term/long-distance river bank filtration. *Science of the Total Environment* **2016,** *545-546*, 629-640.
27. Snip, L. J. P.; Flores-Alsina, X.; Plo´sz, B. G.; Jeppsson, U.; Gernaey, K. V., Modelling the occurrence, transport and fate of pharmaceuticals in wastewater systems. *Environmental Modelling and Software* **2014,** *62*, 112-127.
28. Henzler, A. F.; Greskowiak, J.; Massmann, G., Modeling the fate of organic micropollutants during river bank filtration (Berlin, Germany). *Journal of Contaminant Hydrology* **2014,** *156*, 78-92.
29. Scheurer, M.; Michel, A.; Brauch, H. J.; Ruck, W.; Sacher, F., Occurrence and fate of the antidiabetic drug metformin and its metabolite guanylurea in the environment and during drinking water treatment. *Water Research* **2012,** *46*, (15), 4790-4802.
30. Monteiro, S. C.; Boxall, A. B. A., Occurence and fate of human pharmaceuticals in the environment. *Rev Environmental Contamination Toxicology* **2010,** *202*, 53-154.
31. Manzetti, S.; Van Der Spoel, E. R.; Van Der Spoel, D., Chemical properties, environmental fate, and degradation of seven classes of pollutants. *Chemical Research in Toxicology* **2014,** *27*, (5), 713-737.
32. Brack, W.; Dulio, V.; Slobodnik, J., The NORMAN Network and its activities on emerging environmental substances with a focus on effect-directed analysis of complex environmental contamination. *Environmental Sciences Europe* **2012,** *24*, (1).
33. Bertelkamp, C.; Puijker, L.; Baken, K.; Schriks, M.; Cornelissen, E.; Hofman-Caris, R. *Robuustheid zuiveringen DPWE bedrijven - Inventarisatie nieuwe stoffen en selectie voor experimenteel onderzoek*; KWR 2016.005; KWR: Nieuwegein, 2016.
34. Hernandez, F.; Portoles, T.; Pitarch, E.; Lopez, F. J., Target and nontarget screening of organic micropollutants in water by solid-phase microextraction combined with gas chromatography/high-resolution time-of-flight mass spectrometry. *Analytical Chemistry* **2007,** *79*, (24), 9494-9504.
35. Escher, B. I.; Fenner, K., Recent advances in environmental risk assessment of transformation products. *Environmental Science and Technology* **2011,** *45*, (9), 3835-3847.
36. Hogenboom, A. C.; Van Leerdam, J. A.; De Voogt, P., Accurate mass screening and identification of emerging contaminants in environmental samples by liquid chromatography-LTQ FT Orbitrap mass spectrometry. *J. Chromatogr. A* **2009,** *1216*, 510–519.
37. ter Laak, T. L.; Puijker, L. M.; van Leerdam, J. A.; Raat, K. J.; Kolkman, A.; de Voogt, P.; van Wezel, A. P., Broad target chemical screening approach used as tool for rapid assessment of groundwater quality. *Science of the Total Environment* **2012,** *427-428*, 308-313.
38. Schoen, M. E.; Garland, J., Review of pathogen treatment reductions for onsite non-potable reuse of alternative source waters. *Microbial Risk Analysis* **2017,** *5*, 25-31.

39. Hamilton, K. A.; Weir, M. H.; Haas, C. N., Dose response models and a quantitative microbial risk assessment framework for the Mycobacterium avium complex that account for recent developments in molecular biology, taxonomy, and epidemiology. *Water Research* **2017,** *109*, 310-326.
40. Petterson, S. R.; Ashbolt, N. J., QMRA and water safety management: Review of application in drinking water systems. *Journal of water and health* **2016,** *14*, (4), 571-589.
41. Benami, M.; Gillor, O.; Gross, A., Potential health and environmental risks associated with onsite greywater reuse: A review. *Built Environment* **2016,** *42*, (2), 212-229.
42. Ashbolt, N. J., Microbial Contamination of Drinking Water and Human Health from Community Water Systems. *Current environmental health reports* **2015,** *2*, (1), 95-106.
43. Smeets, P. W. M. H.; Rietveld, L. C.; Van Dijk, J. C.; Medema, G. J., Practical applications of quantitative microbial risk assessment (QMRA) for water safety plans. *Water Science and Technology* **2010,** *61*, (6), 1561-1568.
44. Smeets, P. W. M. H.; Medema, G. J., Combined use of microbiological and non-microbiological data to assess treatment efficacy. In *Water Science and Technology*, 2006; Vol. 54, pp 35-40.
45. Knapp, C. W.; Dolfing, J.; Ehlert, P. A. I.; Graham, D. W., Evidence of Increasing Antibiotic Resistance Gene Abundances in Archived Soils since 1940. *Environmental Science & Technology* **2010,** *44*, (2), 580-587.
46. Lambropoulou, D. A.; Nollet, L. M. L., *Transformation Products of Emerging Contaminants in the Environment*. Wiley: Chichester, UK, 2014; Vol. 1, p 1-383
47. ter Laak, T. L.; Sjerps, R. M. A.; Kools, S. *Classifying persistent mobile organic compounds*; KWR Watercycle Research Institute: 2015; p 40.
48. Reemtsma, T.; Berger, U.; Arp, H. P. H.; Gallard, H.; Knepper, T. P.; Neumann, M.; Benito Quintana, J.; Voogt, P., Mind the gap: persistent and mobile organic compounds - water contaminants that slip though. *Environmental Science & Technology* **2016,** *asap*, asap.
49. Zedda, M.; Zwiener, C., Is nontarget screening of emerging contaminants by LC-HRMS successful? A plea for compound libraries and computer tools. *Analytical and Bioanalytical Chemistry* **2012,** *403*, (9), 2493-2502.
50. Krauss, M.; Singer, H.; Hollender, J., LC-high resolution MS in environmental analysis: From target screening to the identification of unknowns. *Analytical and Bioanalytical Chemistry* **2010,** *397*, (3), 943-951.
51. Lebedev, A. T.; Polyakova, O. V.; Mazur, D. M.; Artaev, V. B., The benefits of high resolution mass spectrometry in environmental analysis. *Analyst* **2013,** *138*, (22), 6946-6953.
52. Oulton, R. L.; Kohn, T.; Cwiertny, D. M., Pharmaceuticals and personal care products in effluent matrices: A survey of transformation and removal during wastewater treatment and implications for wastewater management. *Journal of Environmental Monitoring* **2010,** *12*, (11), 1956-1978.
53. Wieczerzak, M.; Namieśnik, J.; Kudłak, B., Bioassays as one of the Green Chemistry tools for assessing environmental quality: A review. *Environment International* **2016,** *94*, 341-361.
54. Di Paolo, C.; Ottermanns, R.; Keiter, S.; Ait-Aissa, S.; Bluhm, K.; Brack, W.; Breitholtz, M.; Buchinger, S.; Carere, M.; Chalon, C.; Cousin, X.; Dulio, V.; Escher, B. I.; Hamers, T.; Hilscherová, K.; Jarque, S.; Jonas, A.; Maillot-Marechal, E.; Marneffe, Y.; Nguyen, M. T.; Pandard, P.; Schifferli, A.; Schulze, T.; Seidensticker, S.; Seiler, T. B.; Tang, J.; van der Oost, R.; Vermeirssen, E.; Zounková, R.; Zwart, N.; Hollert, H., Bioassay battery interlaboratory investigation of emerging contaminants in spiked water extracts – Towards the implementation of bioanalytical monitoring tools in water quality assessment and monitoring. *Water Research* **2016,** *104*, 473-484.
55. WHO *Antimicrobial resistance: global report on surveillance* WHO: 2014.
56. Berendonk, T. U., Manaia, C.M., Merlin, C., (...), Baquero, F., Martinez, J.L., Tackling antibiotic resistance: The environmental framework. *Nature Reviews Microbiology* **2015,** *13*, (5), 310-317.
57. Huijbers, P. M. C.; Blaak, H.; De Jong, M. C. M.; Graat, E. A. M.; Vandenbroucke-Grauls, C. M. J. E.; De Roda Husman, A. M., Role of the Environment in the Transmission of Antimicrobial Resistance to Humans: A Review. *Environmental Science and Technology* **2015,** *49*, (20), 11993-12004.
58. Larsson, D. G. J., Antibiotics in the environment. *Upsala Journal of Medical Sciences* **2014,** *119*, (2), 108-112.
59. Commision, E., Commision Directive (EU) 2015/1787 Amending annexes II and III to Councel Directive 98/83/EC on the quaity of water intended for human consumption. In Union, E., Ed. Brussels, belgium, 2015.
60. Guillén, D.; Ginebreda, A.; Farré, M.; Darbra, R. M.; Petrovic, M.; Gros, M.; Barceló, D., Prioritization of chemicals in the aquatic environment based on risk assessment: Analytical, modeling and regulatory perspective. *Science of the Total Environment* **2012,** *440*, (0), 236-252.
61. Fischer, A.; Bertelkamp, C.; Wezel, A. v.; Verliefde, A. R. D.; Hoek, J. P. v. d., Toxicity Assessment of Organic Micropollutant Removal During River Bank Filtration. In Delft University: in prep.; p 1.

62. Vasquez, M. I.; Lambrianides, A.; Schneider, M.; Kümmerer, K.; Fatta-Kassinos, D., Environmental side effects of pharmaceutical cocktails: What we know and what we should know. *Journal of Hazardous Materials* **2014,** *279*, 169-189.
63. Chemical Abstract Service Regulated Chemicals - CHEMLIST http://www.cas.org/content/regulated-chemicals (June 17),
64. Schwarzenbach, R. P.; Escher, B. I.; Fenner, K.; Hofstetter, T. B.; Johnson, C. A.; von Gunten, U.; Wehrli, B., The challenge of micropollutants in aquatic systems. *Science* **2006,** *313*, (5790), 1072-1077.
65. European Chemicals Agency (ECHA) Information on Chemicals http://echa.europa.eu/web/guest/regulations/reach/substance-registration/publishing-information-from-dossiers (June 17),
66. Lambropoulou, D. A.; Nollet, L. M. L., *Transformation Products of Emerging Contaminants in the Environment*. Wiley: Chichester, UK, 2014; Vol. 2, p 384-935
67. European Chemicals Agency (ECHA) REACH - Registration, Evaluation, Authorisation and Restriction of Chemicals. http://echa.europa.eu/information-on-chemicals/registered-substances (July 15),
68. de Voogt, P.; Janex-Habibi, M.-L.; Sacher, F.; Puijker, L. M.; Mons, M., Development of a common priority list of pharmaceuticals relevant for the water cycle. *Water Sci Technol* **2009,** *59*, 39-46.
69. Brack, W.; Altenburger, R.; Schüürmann, G.; Krauss, M.; López Herráez, D.; van Gils, J.; Slobodnik, J.; Munthe, J.; Gawlik, B. M.; van Wezel, A.; Schriks, M.; Hollender, J.; Tollefsen, K. E.; Mekenyan, O.; Dimitrov, S.; Bunke, D.; Cousins, I.; Posthuma, L.; van den Brink, P. J.; López de Alda, M.; Barceló, D.; Faust, M.; Kortenkamp, A.; Scrimshaw, M.; Ignatova, S.; Engelen, G.; Massmann, G.; Lemkine, G.; Teodorovic, I.; Walz, K. H.; Dulio, V.; Jonker, M. T. O.; Jäger, F.; Chipman, K.; Falciani, F.; Liska, I.; Rooke, D.; Zhang, X.; Hollert, H.; Vrana, B.; Hilscherova, K.; Kramer, K.; Neumann, S.; Hammerbacher, R.; Backhaus, T.; Mack, J.; Segner, H.; Escher, B.; de Aragão Umbuzeiro, G., The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. *Science of the Total Environment* **2014**.
70. European Commission, Urban Waste Water Directive In Commision, E., Ed. Brussels, Belgium, 1991.
71. European Commission, Restriction of Hazardous Substances Directive 2002/95/EC & 2003/11/EC. In European Union: Brussels, Belgium, 2003; p L42/45.
72. European Commission, Directive on the restriction of the environmentally harmfull PFOS, 2006/122/EC. In European Union: Strassbough, France, 2006; Vol. 2006/122/EC, p 3.
73. European Commission, Priority Substances Directive, 2008/105/EC. In European Union, Ed. Brussels, Belgium, 2008.
74. European Commission, The Industrial Emissions Directive. In European Commision, Ed. Brussels, Belgium, 2010.
75. Moermond, C. T. A. Environmental risk limits for pharmaceuticals - Derivation of WFD water quality standards for carbamazepine, metoprolol, metformin and amidotrizoic acid; 270006002/2014; RIVM, Dutch national Institute of Public Health and the Environemnt: Bilthoven, the Netherlands, 2014; p 56.
76. Montforts, M. H. M. M. The trigger values in the environmental risk assessment for (veterinary) medicines in the European Union: a critical appraisal; 601500002/2005; RIVM: Bilthoven, 2005.
77. Schriks, M.; Heringa, M. B.; Kooi, V. D.; De Voogt, P.; Van Wezel, A. P., Toxicological relevance of emerging contaminants for drinking water quality. *Water Research* **2010,** *44*, 461-476.
78. Brand, W.; de Jongh, C. M.; van der Linden, S. C.; Mennes, W.; Puijker, L. M.; van Leeuwen, C. J.; van Wezel, A. P.; Schriks, M.; Heringa, M. B., Trigger values for investigation of hormonal activity in drinking water and its sources using CALUX bioassays. *Environment International* **2013,** *55*, 109-118.
79. Ort, C.; Gujer, W., Sampling for representative micropollutant loads in sewer systems. In *Water Science and Technology*, 2006; Vol. 54, pp 169-176.
80. Ort, C.; Lawrence, M. G.; Rieckermann, J. r.; Joss, A., Sampling for Pharmaceuticals and Personal Care Products (PPCPs) and Illicit Drugs in Wastewater Systems: Are Your Conclusions Valid? A Critical Review. *Environmental Science & Technology* **2010,** *44*, (16), 6024-6035
81. Bertelkamp, C.; Reungoat, J.; Botton, S.; Cornelissen, E.; Ghadiri, E.; de Jonge, M.; Singhal, N.; van der Hoek, J. P.; Verliefde, A. R. D., Transformation of organic micropollutants during river bank filtration: Laboratory versus field data. *Water Practice and Technology* **2012,** *7*, (4).
82. Bertelkamp, C.; Reungoat, J.; Cornelissen, E. R.; Singhal, N.; Reynisson, J.; Cabo, A. J.; van der Hoek, J. P.; Verliefde, A. R. D., Sorption and biodegradation of organic micropollutants during river bank filtration: A laboratory column study. *Water Research* **2014,** *52*, 231-241.

83. Semple, K. T.; Morriss, W. J.; Paton, G. I., Bioavailability of hydrophobic organic contaminants in soils: fundamental concepts and techniques for analysis. *European Journal of Soil Science* **2003,** *54*, 809-818.
84. Reddersen, K.; Heberer, T.; Dunnbier, U., Identification and significance of phenazone drugs and their metabolites in ground- and drinking water. *Chemosphere* **2002,** *49*, (6), 539-544.
85. de Jongh, C. M.; Kooij, P. J. F.; de Voogt, P.; ter Laak, T. L., Screening and human health risk assessment of pharmaceuticals and their transformation products in Dutch surface waters and drinking water. *Science of the Total Environment* **2012,** *427-428*, 70-77.
86. Verliefde, A. R. D.; Cornelissen, E. R.; Heijman, S. G. J.; Verberk, J. Q. J. C.; Amy, G. L.; Van der Bruggen, B.; van Dijk, J. C., Construction and validation of a full-scale model for rejection of organic micropollutants by NF membranes. *Journal of Membrane Science* **2009,** *339*, (1-2), 10-20.
87. ter Laak, T. L.; van der Aa, M.; Houtman, C.; Stoks, P.; van Wezel, A. *Temporal and spatial trends of pharmaceuticals in the Rhine*; Association of River Waterworks, RIWA: Nieuwegein, the Netherlands, 2010; p 44.
88. Hofs, B. In *DPW(E) Robuustheid: samenvatting en bioassays*, DPWE miniworkshop HWL, 2014; 2014.
89. Kolkman, A.; Martijn, B.; Vughs, D.; Baken, K. A.; van Wezel, A. P., Tracing nitrogenous disinfection byproducts after medium pressure UV water treatment by stable isotope labeling and high resolution Mass Spectrometry. *Environmental Science & Technology* **2015,** *49*, 4458-4465.
90. World Health Organisation Sanitaion safety planning, manual for safe use and disposal of wastewater, grey water and excreta; WHO: France, 2016; p 156.
91. ter Laak, T.; Baken, K.; van Leerdam, T.; Sjerps, R.; Bäuerlein, P. *Literature survey of transformation products in the water cycle*; BTO 2015.060; KWR: Nieuwegein, 2015.
92. Fenner, K.; Canonica, S.; Wackett, L. P.; Elsner, M., Evaluating pesticide degradation in the environment: Blind spots and emerging opportunities. *Science* **2013,** *341*, (6147), 752-758.
93. Boxall, A. B. A.; Sinclair, C. J.; Fenner, K.; Kolpin, D.; Maund, S. J., When synthetic chemicals degrade in the environment. *Environmental Science and Technology* **2004,** *38*, (19), 368A-375A.
94. Hladik, M. L.; Roberts, A. L.; Bouwer, E. J., Removal of neutral chloroacetamide herbicide degradates during simulated unit processes for drinking water treatment. *Water Res.* **2005,** *39*, 5033-5044.
95. Taylor, J. P.; Mills, M. S.; Burns, R. G., Dissipation of acetochlor and its distribution in surface and sub-surface soil fractions during laboratory incubations. *Pest Management Science* **2005,** *61*, (6), 539-548.
96. Stewart, M.; Olsen, G.; Hickey, C. W.; Ferreira, B.; Jelić, A.; Petrović, M.; Barcelo, D., A survey of emerging contaminants in the estuarine receiving environment around Auckland, New Zealand. *Sci. Total Environ.* **2014,** *468–469*, (0), 202-210.
97. Mercurio, P.; Flores, F.; Mueller, J. F.; Carter, S.; Negri, A. P., Glyphosate persistence in seawater. *Marine Pollution Bulletin*, (0).
98. Osano, O.; Admiraal, W.; Klamer, H. J. C.; Pastor, D.; Bleeker, E. A. J., Comparative toxic and genotoxic effects of chloroacetanilides, formamidines and their degradation products on Vibrio fischeri and Chironomus riparius. *Environmental Pollution* **2002,** *119*, (2), 195-202.
99. Heberer, T.; Dünnbier, U., DDT Metabolite Bis(Chlorophenyl)acetic Acid: The Neglected Environmental Contaminant. *Environmental Science & Technology* **1999,** *33*, (14), 2346-2351.
100. Fang, H.; Cai, L.; Yang, Y.; Ju, F.; Li, X.; Yu, Y.; Zhang, T., Metagenomic analysis reveals potential biodegradation pathways of persistent pesticides in freshwater and marine sediments. *Sci. Total Environ.* **2014,** *470–471*, (0), 983-992.
101. Shayeghi, M.; Khoobdel, M.; Bagheri, F.; Abtahi, M.; Zeraati, H., Organophosphorous residue in Liza aurata and Cyprinus carpio. *Asian Pacific Journal of Tropical Biomedicine* **2012,** *2*, (7), 564-569.
102. Bavcon, M.; Trebše, P.; Zupančič-Kralj, L., Investigations of the determination and transformations of diazinon and malathion under environmental conditions using gas chromatography coupled with a flame ionisation detector. *Chemosphere* **2003,** *50*, (5), 595-601.
103. Morgan, M. K.; Sheldon, L. S.; Jones, P. A.; Croghan, C. W.; Chuang, J. C.; Wilson, N. K., The reliability of using urinary biomarkers to estimate children's exposures to chlorpyrifos and diazinon. *Journal of Exposure Science and Environmental Epidemiology* **2011,** *21*, (3), 280-290.
104. Kolpin, D. W.; Thurman, E. M.; Linhart, S. M., Occurrence of Cyanazine Compounds in Groundwater: Degradates More Prevalent Than the Parent Compound. *Environmental Science & Technology* **2001,** *35*, (6), 1217-1222.

105. Dixit, V.; Tewari, J. C.; Obendorf, S. K., Identification of degraded products of aldicarb due to the catalytic behavior of titanium dioxide/polyacrylonitrile nanofiber. *Journal of Chromatography A* **2009,** *1216*, (36), 6394-6399.
106. Brown, C. D.; van Beinum, W., Pesticide transport via sub-surface drains in Europe. *Environmental Pollution* **2009,** *157*, (12), 3314-3324.
107. Tiwari, M. K.; Guha, S., Kinetics of biotransformation of chlorpyrifos in aqueous and soil slurry environments. *Water Res.* **2014,** *51*, 73-85.
108. Nam, S.-W.; Choi, D.-J.; Kim, S.-K.; Her, N.; Zoh, K.-D., Adsorption characteristics of selected hydrophilic and hydrophobic micropollutants in water using activated carbon. *J. Hazard. Mat.* **2014,** *270*, (0), 144-152.
109. Furman, O. S.; Yu, M.; Teel, A. L.; Watts, R. J., Water quality parameters controlling the photodegradation of two herbicides in surface waters of the Columbia Basin, Washington. *Chemosphere* **2013,** *93*, (9), 1734-1741.
110. Lurker, P. A.; Berman, F.; Clapp, R. W.; Stellman, J. M., Post-Vietnam military herbicide exposures in UC-123 Agent Orange spray aircraft. *Environmental Research* **2014,** *130*, 34-42.
111. Kern, S.; Singer, H.; Hollender, J.; Schwarzenbach, R. P.; Fenner, K., Assessing Exposure to Transformation Products of Soil-Applied Organic Contaminants in Surface Water: Comparison of Model Predictions and Field Data. *Environmental Science & Technology* **2011,** *45*, (7), 2833-2841.
112. Buttiglieri, G.; Peschka, M.; Frömel, T.; Müller, J.; Malpei, F.; Seel, P.; Knepper, T. P., Environmental occurrence and degradation of the herbicide n-chloridazon. *Water Res.* **2009,** *43*, (11), 2865-2873.
113. Devers-Lamrani, M.; Pesce, S.; Rouard, N.; Martin-Laurent, F., Evidence for cooperative mineralization of diuron by Arthrobacter sp. BS2 and Achromobacter sp. SP1 isolated from a mixed culture enriched from diuron exposed environments. *Chemosphere* **2014,** *117*, (1), 208-215.
114. Amine-Khodja, A.; Boulkamh, A.; Boule, P., Photochemical behaviour of phenylurea herbicides. *Photochemical and Photobiological Sciences* **2004,** *3*, (2), 145-156.
115. Laganà, A.; Bacaloni, A.; De Leva, I.; Faberi, A.; Fago, G.; Marino, A., Occurrence and determination of herbicides and their major transformation products in environmental waters. *Analytica Chimica Acta* **2002,** *462*, (2), 187-198.
116. Knauber, W. R.; Krotzky, A. J.; Schink, B., Microbial metabolism and further fate of bentazon in soil. *Environmental Science and Technology* **2000,** *34*, (4), 598-603.
117. Chiron, S.; Abian, J.; Ferrer, M.; Sanchez-Baeza, F.; Messeguer, A.; Barcelo, D., Comparative photodegradation rates of alachlor and bentazone in natural water and determination of breakdown products. *Environmental Toxicology and Chemistry* **1995,** *14*, (8), 1287-1298.
118. Yan, S.; Song, W., Photo-transformation of pharmaceutically active compounds in the aqueous environment: A review. *Environmental Sciences: Processes and Impacts* **2014,** *16*, (4), 697-720.
119. Celiz, M. D.; Tso, J.; Aga, D. S., Pharmaceutical metabolites in the environment: Analytical challenges and ecological risks. *Environmental Toxicology and Chemistry* **2009,** *28*, (12), 2473-2484.
120. Escher, B. I.; Fenner, K., Recent Advances in Environmental Risk Assessment of Transformation Products. *Environ. Sci. Technol.* **2011,** *45*, (9), 3835-3847.
121. ter Laak, T.; Kooij, P.; Hofman, J.; Tolkamp, H., Different compositions of pharmaceuticals in Dutch and Belgian surface waters explained by consumption patterns and treatment efficiency. *Environmental Science and Pollution Research* **2014,** *21 (22)*, 12843-12855.
122. ter Laak, T.; Baken, K. *The occurrence, fate and ecological and human health risks of metformin and guanylurea in the water cycle - A literature review*; KWR 2014.001; KWR Watercycle Research Institute & Rijkswaterstaat: Nieuwegein, The Netherlands, 2014; p 26.
123. Ternes, T. A., Occurrence of drugs in German sewage treatment plants and rivers. *Water Research* **1998,** *32*, (11), 3245-3260.
124. Poiger, T.; Buser, H. R.; Müller, M. D., Photodegradation of the pharmaceutical drug diclofenac in a lake: Pathway, field measurements, and mathematical modeling. *Environmental Toxicology and Chemistry* **2001,** *20*, (2), 256-263.
125. Hofs, B. *Overzicht DPW robuustheid 2010-2013 – de verwijdering van een selectie van organische microverontreinigingen in zomer en winter*; KWR: Nieuwegein, the Netherlands, 2014; p 23.
126. Michael, I.; Achilleos, A.; Lambropoulou, D.; Torrens, V. O.; Pérez, S.; Petrović, M.; Barceló, D.; Fatta-Kassinos, D., Proposed transformation pathway and evolution profile of diclofenac and ibuprofen transformation products during (sono)photocatalysis. *Applied Catalysis B: Environmental* **2014,** *147*, 1015-1027.

127. Schulze, T.; Weiss, S.; Schymanski, E.; von der Ohe, P. C.; Schmitt-Jansen, M.; Altenburger, R.; Streck, G.; Brack, W., Identification of a phytotoxic photo-transformation product of diclofenac using effect-directed analysis. *Environ. Pol.* **2010,** *158*, (5), 1461-1466.
128. Scheurer, M.; Sacher, F.; Brauch, H. J., Occurrence of antidiabetic drug metformin in sewage and surface waters in Germany. *J. Environ. Monit.* **2009,** *11*, 1608-1613.
129. Oosterhuis, M.; Sacher, F.; ter Laak, T. L., Prediction of concentration levels of metformin and other high consumption pharmaceuticals in wastewater and regional surface water based on sales data. *Science of the Total Environment* **2013,** *442*, 380-388.
130. Scheurer, M.; Sacher, F.; Brauch, H.-J., Occurence of the antidiabetic drug metformin in sewage and surface waters in Germany. *Journal of Environmental Monitoring* **2009,** *11*, 1608-1613.
131. Vulliet, E.; Cren-Olivé, C., Screening of pharmaceuticals and hormones at the regional scale, in surface and groundwaters intended to human consumption. *Environmental Pollution* **2011,** *159*, (10), 2929-2934.
132. De Laurentiis, E.; Prasse, C.; Ternes, T. A.; Minella, M.; Maurino, V.; Minero, C.; Sarakha, M.; Brigante, M.; Vione, D., Assessing the photochemical transformation pathways of acetaminophen relevant to surface waters: Transformation kinetics, intermediates, and modelling. *Water Res.* **2014,** *53*, 235-248.
133. Kolpin, D. W.; Skopec, M.; Meyer, M. T.; Furlong, E. T.; Zaugg, S. D., Urban contribution of pharmaceuticals and other organic wastewater contaminants to streams during differing flow conditions. *Science of the Total Environment* **2004,** *328*, (1-3), 119-130.
134. Jelic, A.; Michael, I.; Achilleos, A.; Hapeshi, E.; Lambropoulou, D.; Perez, S.; Petrovic, M.; Fatta-Kassinos, D.; Barcelo, D., Transformation products and reaction pathways of carbamazepine during photocatalytic and sonophotocatalytic treatment. *Journal of Hazardous Materials* **2013,** *263, Part 1*, (0), 177-186.
135. Wetzstein, H. G.; Stadler, M.; Tichy, H. V.; Dalhoff, A.; Karl, W., Degradation of ciprofloxacin by basidiomycetes and identification of metabolites generated by the brown rot fungus Gloeophyllum striatum. *Applied and Environmental Microbiology* **1999,** *65*, (4), 1556-1563.
136. Miege, C.; Choubert, J. M.; Ribeiro, L.; Coquery, M., Fate of pharmaceuticals and personal care products in wastewater treatment plants - conception of a database and first results. *Environmental Pollution* **2009,** *157*, 1721-1726.
137. Hirsch, R.; Ternes, T. A.; Haberer, K.; Kratz, K. L., Occurrence of antibiotics in the aquatic environment. *Science of the Total Environment* **1999,** *225*, (1-2), 109-118.
138. García-Galán, M. J.; Silvia Díaz-Cruz, M.; Barceló, D., Identification and determination of metabolites and degradation products of sulfonamide antibiotics. *TrAC - Trends in Analytical Chemistry* **2008,** *27*, (11), 1008-1022.
139. Arikan, O. A.; Rice, C.; Codling, E., Occurrence of antibiotics and hormones in a major agricultural watershed. *Desalination* **2008,** *226*, (1-3), 121-133.
140. Otagiri, M.; Nakamura, H.; Imamura, Y.; Matsumoto, U., Circular dichroic investigations into binding of sulfonamides to serum albumin. *Pharmaceutisch Weekblad Scientific Edition* **1989,** *11*, (6), 207-212.
141. Kühne, M.; Ihnen, D.; Möller, G.; Agthe, O., Stability of tetracycline in water and liquid manure. *School of Veterinary Medicine* **2000**.
142. Halling-Sorensen, B.; Sengelov, G.; Tjornelund, J., Toxicity of tetracyclines and tetracycline degradation products to environmentally relevant bacteria, including selected tetracycline-resistant bacteria. *Archives of Environmental Contamination Toxicology* **2002,** *42*, 263-271.
143. Díaz-Cruz, M. S.; Barceló, D., Determination of antimicrobial residues and metabolites in the aquatic environment by liquid chromatography tandem mass spectrometry. *Analytical and Bioanalytical Chemistry* **2006,** *386*, (4), 973-985.
144. Giger, W.; Alder, A. C.; Golet, E. M.; Kohler, H.-P. E.; McArdell, C. S.; Molnar, E.; Siegrist, H.; Suter, M. J.-F., Occurence and fate of antibiotics as trace contaminants in wastewaters, sewage sludges, and surface waters. *Chimica* **2003,** *57*, 485-491.
145. Winker, M.; Faika, D.; Gulyas, H.; Otterpohl, R., A comparison of human pharmaceutical concentrations in raw municipal wastewater and yellowwater. *Science of the Total Environment* **2008,** *399*, (1-3), 96-104.
146. Jarukamjorn, K.; Thalhammer, T.; Gollackner, B.; Pittenauer, E.; Jäger, W., Metabolism of roxithromycin in the isolated perfused rat liver. *Journal of Pharmacy and Pharmacology* **1998,** *50*, (5), 515-519.
147. Liu, Z. Y.; Wu, Y.; Sun, Z. L.; Wan, L., Characterization of in vitro metabolites of trimethoprim and diaveridine in pig liver microsomes by liquid chromatography combined with hybrid ion trap/time-of-flight mass spectrometry. *Biomedical Chromatography* **2012,** *26*, (9), 1101-1108.

148. Donoho, A. L., Biochemical studies on the fate of monensin in animals and in the environment. *Journal of animal science* **1984,** *58*, (6), 1528-1539.
149. McGregor, E. B.; Solomon, K. R.; Hanson, M. L., Monensin is not toxic to aquatic macrophytes at environmentally relevant concentrations. *Archives of Environmental Contamination and Toxicology* **2007,** *53*, (4), 541-551.
150. Pospíšil, S.; Sedmera, P.; Halada, P.; Spížek, J., Oxidation of lincomycin by hydrogen peroxide restricts its potential Biotransformation with haloperoxidases. *Folia Microbiologica* **2001,** *46*, (5), 376-378.
151. Barnes, K. K.; Christenson, S. C.; Kolpin, D. W.; Focazio, M. J.; Furlong, E. T.; Zaugg, S. D.; Meyer, M. T.; Barber, L. B., Pharmaceuticals and other organic waste water contaminants within a leachate plume downgradient of a municipal landfill. *Ground Water Monitoring and Remediation* **2004,** *24*, (2), 119-126.
152. Kolpin, D. W.; Furlong, E. T.; Meyer, M. T.; Thurman, E. M.; Zaugg, S. D.; Barber, L. B.; Buxton, H. T., Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999-2000: a national reconnaissance. *Environmental Science and Technology* **2002,** *36*, 1202-1211.
153. American Medical Association *Council on Drugs AMA Drug Evaluations Annual*; American Medical Association,: Chicago, IL, USA, 1994; p 902.
154. Zuccato, E.; Castiglioni, S.; Fanelli, R.; Reitano, G.; Bagnati, R.; Chiabrando, C.; Pomati, F.; Rossetti, C.; Calamari, D., Pharmaceuticals in the environment in Italy: Causes, occurrence, effects and control. *Environmental Science and Pollution Research* **2006,** *13*, (1), 15-21.
155. MacLeod, S. L.; Sudhir, P.; Wong, C. S., Stereoisomer analysis of wastewater-derived β-blockers, selective serotonin re-uptake inhibitors, and salbutamol by high-performance liquid chromatography-tandem mass spectrometry. *Journal of Chromatography A* **2007,** *1170*, (1-2), 23-33.
156. Fraile, L. J.; Bregante, M. A.; Garcia, M. A.; Solans, C., Altered diltiazem metabolism in the neonatal rabbit following intra-uterine chronic exposure to diltiazem. *Xenobiotica* **2001,** *31*, (4), 177-185.
157. Daughton, C. G.; Ternes, T. A., Pharmaceuticals and personal care products in the environment: Agents of subtle change? *Environmental Health Perspectives* **1999,** *107*, (SUPPL. 6), 907-938.
158. Krkošek, W. H.; Payne, S. J.; Gagnon, G. A., Removal of acidic pharmaceuticals within a nitrifying recirculating biofilter. *Journal of Hazardous Materials* **2014,** *273*, 85-93.
159. van Nuijs, A. L. N.; Pecceu, B.; Theunis, L.; Dubois, N.; Charlier, C.; Jorens, P. G.; Bervoets, L.; Blust, R.; Meulemans, H.; Neels, H.; Covaci, A., Can cocaine use be evaluated through analysis of wastewater? A nation-wide approach conducted in Belgium. *Addiction* **2009,** *104*, (5), 734-741.
160. Benotti, M. J.; Trenholm, R. A.; Vanderford, B. J.; Holady, J. C.; Stanford, B. D.; Snyder, S. A., Pharmaceuticals and endocrine disrupting compounds in U.S. drinking water. *Environmental Science and Technology* **2009,** *43*, (3), 597-603.
161. Kolodziej, E. P.; Sedlak, D. L., Rangeland grazing as a source of steroid hormones to surface waters. *Environmental Science and Technology* **2007,** *41*, (10), 3514-3520.
162. Klečka, G.; Persoon, C.; Currie, R., Chemicals of emerging concern in the Great Lakes Basin: An analysis of environmental exposures. In *Reviews of Environmental Contamination and Toxicology*, 2010; Vol. 207, pp 1-93.
163. Kools, S. *Microplastics in de waterketen (een verkenning)*; BTO 2013.060; KWR: Nieuwegein, 2013; p 24.
164. Guerra, P.; Kim, M.; Kinsman, L.; Ng, T.; Alaee, M.; Smyth, S. A., Parameters affecting the formation of perfluoroalkyl acids during wastewater treatment. *Journal of Hazardous Materials* **2014,** *272*, (0), 148-154.
165. Loganathan, B. G.; Sajwan, K. S.; Sinclair, E.; Senthil Kumar, K.; Kannan, K., Perfluoroalkyl sulfonates and perfluorocarboxylates in two wastewater treatment facilities in Kentucky and Georgia. *Water Res.* **2007,** *41*, (20), 4611-4620.
166. Eschauzier, C.; Haftka, J.; Stuyfzand, P. J.; De Voogt, P., Perfluorinated compounds in infiltrated river rhine water and infiltrated rainwater in coastal dunes. *Environ. Sci. Technol.* **2010,** *44*, (19), 7450-7455.
167. Kim, M. H.; Wang, N.; McDonald, T.; Chu, K. H., Biodefluorination and biotransformation of fluorotelomer alcohols by two alkane-degrading Pseudomonas strains. *Biotechnology and Bioengineering* **2012,** *109*, (12), 3041-3048.
168. Burka, L. T.; Sanders, J. M.; Herr, D. W.; Matthews, H. B., Metabolism of tris(2-chloroethyl) phosphate in rats and mice. *Drug Metabolism and Disposition* **1991,** *19*, (2), 443-447.
169. Stackelberg, P. E.; Gibs, J.; Furlong, E. T.; Meyer, M. T.; Zaugg, S. D.; Lippincott, R. L., Efficiency of conventional drinking-water-treatment processes in removal of pharmaceuticals and other organic compounds. *Science of the Total Environment* **2007,** *377*, (2-3), 255-272.

170. Williams, D. T.; Nestmann, E. R.; LeBel, G. L.; Benoit, F. M.; Otson, R.; Lee, E. G. H., Determination of mutagenic potential and organic contaminants of Great Lakes drinking water. *Chemosphere* **1982,** *11*, (3), 263-276.
171. Paxéus, N., Organic pollutants in the effluents of large wastewater treatment plants in Sweden. *Water Research* **1996,** *30*, (5), 1115-1122.
172. Andresen, J. A.; Grundmann, A.; Bester, K., Organophosphorus flame retardants and plasticisers in surface waters. *Science of the Total Environment* **2004,** *332*, (1-3), 155-166.
173. Bollmann, U. E.; Möller, A.; Xie, Z.; Ebinghaus, R.; Einax, J. W., Occurrence and fate of organophosphorus flame retardants and plasticizers in coastal and marine surface waters. *Water Research* **2012,** *46*, (2), 531-538.
174. Bacaloni, A.; Cavaliere, C.; Foglia, P.; Nazzari, M.; Samperi, R.; Laganà, A., Liquid chromatography/tandem mass spectrometry determination of organophosphorus flame retardants and plasticizers in drinking and surface waters. *Rapid Communications in Mass Spectrometry* **2007,** *21*, (7), 1123-1130.
175. Asimakopoulos, A. G.; Wang, L.; Thomaidis, N. S.; Kannan, K., Benzotriazoles and benzothiazoles in human urine from several countries: A perspective on occurrence, biotransformation, and human exposure. *Environment International* **2013,** *59*, 274-281.
176. Huntscha, S.; Hofstetter, T. B.; Schymanski, E. L.; Spahr, S.; Hollender, J., Biotransformation of benzotriazoles: Insights from transformation product identification and compound-specific isotope analysis. *Environmental Science and Technology* **2014,** *48*, (8), 4435-4443.
177. Ruan, T.; Liu, R.; Fu, Q.; Wang, T.; Wang, Y.; Song, S.; Wang, P.; Teng, M.; Jiang, G., Concentrations and composition profiles of benzotriazole UV stabilizers in municipal sewage sludge in China. *Environmental Science and Technology* **2012,** *46*, (4), 2071-2079.
178. Dubroca, J.; Brault, A.; Kollmann, A.; Touton, I.; Jolivalt, C.; Kerhoas, L.; Mougin, C., Biotransformation of nonylphenol surfactants in soils amended with contaminated sewage sludges. In *Environmental Chemistry: Green Chemistry and Pollutants in Ecosystems*, 2005; pp 305-315.
179. Sun, Q.; Li, Y.; Chou, P. H.; Peng, P. Y.; Yu, C. P., Transformation of bisphenol A and alkylphenols by ammonia-oxidizing bacteria through nitration. *Environmental Science and Technology* **2012,** *46*, (8), 4442-4448.
180. Trautwein, C.; Berset, J. D.; Wolschke, H.; Kümmerer, K., Occurrence of the antidiabetic drug Metformin and its ultimate transformation product Guanylurea in several compartments of the aquatic cycle. *Environment International* **2014,** *70*, 203-212.
181. Scheurer, M.; Schmutz, B.; Happel, O.; Brauch, H. J.; Wülser, R.; Storck, F. R., Transformation of the artificial sweetener acesulfame by UV light. *Science of the Total Environment* **2014,** *481*, (1), 425-432.
182. Liang, L.; Zhang, J.; Feng, P.; Li, C.; Huang, Y.; Dong, B.; Li, L.; Guan, X., Occurrence of bisphenol A in surface and drinking waters and its physicochemical removal technologies. *Frontiers of Environmental Science & Engineering* **2014**.
183. Kormos, J. L.; Schulz, M.; Kohler, H.-P. E.; Ternes, T. A., Biotransformation of selected Iodinatede X-ray contrast media and characterization of microbial transformation pathways. *Environmental Science & Technology* **2010**.
184. Zuehlke, S.; Duennbier, U.; Heberer, T., Investigation of the behavior and metabolism of pharmaceutical residues during purification of contaminated ground water used for drinking water supply. *Chemosphere* **2007,** *69*, (11), 1673-1680.
185. ter Laak, T. L.; Tolkamp, H.; Hofman, J. *Geneesmiddelen in de Watercyclus in Limburg - Fase 1: Voorkomen, herkomst en ernst van geneesmiddelen in het watersysteem*; KWR Watercycle Research Institute: Nieuwegein, The Netherlands, 2013; p 86.
186. Baken, K. A. *Toxicological properties of disinfection by-products* BTO 2013.230(s); KWR: Nieuwegein, 2013; p 33.
187. Nawrocki, J.; Andrzejewski, P., Nitrosamines and water. *Journal of Hazardous Materials* **2011,** *189*, (1-2), 1-18.
188. Qian, Y.; Wang, W.; Boyd, J. M.; Wu, M.; Hrudey, S. E.; Li, X. F., UV-induced transformation of four halobenzoquinones in drinking water. *Environmental Science and Technology* **2013,** *47*, (9), 4426-4433.
189. Huerta-Fontela, M.; Pineda, O.; Ventura, F.; Galceran, M. T., New chlorinated amphetamine-type-stimulants disinfection-by-products formed during drinking water treatment. *Water Research* **2012,** *46*, (10), 3304-3314.
190. Rodil, R.; Quintana, J. B.; Cela, R., Transformation of phenazone-type drugs during chlorination. *Water Research* **2012,** *46*, (7), 2457-2468.

191. Chusaksri, S.; Sutthivaiyakit, S.; Sedlak, D. L.; Sutthivaiyakit, P., Reactions of phenylurea compounds with aqueous chlorine: Implications for herbicide transformation during drinking water disinfection. *Journal of Hazardous Materials* **2012,** *209-210*, 484-491.

6 Appendix 1

Overview of transformation products, based on report [91]:

6.1 TPs of pesticides in the environment

Around 10 to 20% of pesticides detected in the environment are transformed[92] according to currently available analytical techniques. Transformation of pesticides is affected by physicochemical (hydrolyis, oxidation, reduction), biological, and to a lesser extent photochemical processes. Microbial transformation is the most important process in soil and groundwater, due to the long residence times that enable microbial degradation.

Transformation of (chloro)acetanilide herbicides (e.g. acetochlor, metolachlor, alachlor and propachlor) produce numerous TPs. Microbially transformed ethanesulfonic acids are the most important products. Triazine herbicides transformation is studied intensively (atrazine, simazine, cyanazine, terbutylazine, propazine, sebuthylazine, terbutryn). They hydrolyze rapidly under acidic conditions. Besides hydroxylation, dealkylation, dehalogenation and deamination occur by biotransformation. Phenylurea herbicides (monuron, chlorotoluron, fluometuron, diuron, monolinuron, linuron, neburon) are dealylated at the amide group or the amide group, leaving an aniline. Amide insecticides (amitraz and chlordimeform) are transformed to anilines (see reference [46, 92] and references therein).

Table 13 gives an overview of TPs of pesticides.

Table 13 Examples of pesticides and their TPs

Parent compound	Class	Transformation product(s)	Transformation process	Occurence
Acetochlor [93-95]	Herbicide	Acetochlor ethane sulfonic acid Acetochlor oxanilic acid Acetochlor sulfinylacetic acid	Biotransformation (microbial)	Surface water, Groundwater
Glyphosate [93, 96, 97]	Herbicide	Aminomethylphophonic acid (AMPA)	Biotransformation (microbial)	Surface water, Sediment
Metolachlor [93, 94, 98]	Herbicide	2-ethyl-6-methylanliline 2-ethyl-6-methyl chloroacetanilide Metholachlor ethane sulfonic acid Metholachlor oxalinic acid	Biotransformation (microbial)	Groundwater Surface water
DDT [99, 100]	Insecticide	DCB DDD DCB DDE	Photolysis and Biotransformation (microbial)	Surface water
Diazinon [101-103]	Insecticide	3,5,6-trichloro-2-pyridinol 2-isopropyl-6methyl-4-pyrimidinol	Biotransformation (human)	Surface water
Atrazine [104]	Herbicide	Desethylatrzine Deisopropylatrazine Hydroxyatrazine Didealkylatrazine Hydroxydeethylatrazine Hydroxydeisopropylatrazine Ammeline Cyanuric acid	Biotransformation (microbial)	Groundwater
Cyanazine	Herbicide	Cyanazine acid	Biotransformation (microbial)	Groundwater

Parent compound	Class	Transformation product(s)	Transformation process	Occurence
[104]		Cyanazine amide Deethylcyanazine Deethylcyanazine acid Deethylcyanazine amide		
Aldicarb [93, 105, 106]	Insecticide	Aldicarb sulfone Aldicarb sulfoxide	(chemical) oxidation	drainflow
Chlorpyrifos [107]	Insecticide	Chloropyrisfos oxam Diethyl thiophosphate Trichloro pyridinol Diethyl phosphate Trichloro methoxypyridine	Biotransformation (microbial) in sludge and water	Water, sediment
2,4-Dichlorophenoxyacetic acid (2,4-D) [108-110]	Herbicide	4-chlorophenol	Photolysis (direct / indirect)	Surface water
Chloridazon [111, 112]	Herbicide	Desphenyl chloridazon Methyl-desphenyl chloridazon	Biotransformation (microbial)	Groundwater Surface water
Linuron [113, 114]	Herbicide	1-(3,4 dichlorophenyl) urea 1-(3,4 dichlorophenyl 3-methylurea 3,4 dichloroaniline	Photolysis and Biotransformation (microbial)	
Bentazone [115-117]	Herbicide	Bentazone methyl 8-hydroxybentazone	Photolysis Biotransformation (microbial)	Surface water Soil Groundwater

6.2 TPs of pharmaceuticals in the environment

Pharmaceuticals can be transformed after consumption by the user (human or animal), as well as in the environment. There is a large knowledge base on transformation in users from pharmacological and medical research, while relatively little is known on further transformation of pharmaceuticals (and TPs) in the environment. Some pharmaceutically active compounds are biodegradable, while others are more persistent in the aquatic environment [118]. Conjugated drug metabolites formed by phase II metabolism (see paragraph 3.3.3), especially glucoronide and sulphate conjugates, have the potential to deconjugate back to the parent compound in the environment or during water treatment [119, 120]. Phase I metabolites can be detected widely in the environment. Examples are hydroxyl-ibuprofen that exceeds its parent pharmaceutical, various hydroxilated forms of carbamazepine [121] or demethylated TPs such as desmethyl tramadol and desmethyl venlafaxine [85]. Conjugated substances can also produce reactive metabolites [119].

Furthermore, guanyl urea (a TP of metformine) [29, 122], salisylic acid (formed from acetylsalicylic acid [123]), and some pharmaceuticals (diclofenac, amoxicillin, cephalexin FQs, and cimetidine) are photoreactive [118, 124]. Many environmental TPs of pharmaceuticals are known, as they are considered during the authorization process. Most TPs mentioned in Table 6-2 are transformed within the (human or animal) user. The transformation processes during (drinking)water treatment such as advanced oxidation processes (ozonation, UV/H_2O_2 treatment) often focus on the dissipation of parent compounds [125], while TPs that are potentially formed are only studied sparsely [89].

Table 14 lists some pharmaceuticals and environmentally relevant TPs.

Table 14 Examples of pharmaceutics, their TPs (TPs) and their occurrence

Parent compound	Class	TP	Transformation process	Occurrence
Phenazone [84]	Analgesic	AMDOPH AMPH DMOAS	Biotransformation (human)	Ground-water River bank filtration [84, 85]
Methamizole [84]	Analgesic	AMPH AAA FAA	Biotransformation (human)	Ground-water River bank filtration [84, 85]
Diclofenac [126, 127]	Analgesic	numerous	Photolysis (catalytic oxidation)	Surface water Wastewater effluent
Ibuprofen [126]	Analgesic	numerous, most common: hydroxy ibuprofen	Biotransformation Photolysis (catalytic oxidation)	Ground-water Surface water
Metformine [128]	Anti-diabetic	Guanylurea	Biotransformation (Microbial, in wastewater treatment)	Wastewater effluent Surface water [29, 121, 129, 130] Ground-water [131]
Paracetamol [132]	Analgesic	4-acetaminophen sulfate 1,4 benzoquinone	Photolysis	Surface water [121, 133]
Carbamazepine [134]	Anti-epileptic	10, most common: 10-11 trans diol carbamazepine Hydroxy carbamazepine Epoxy carbamazepine [121]	Biotransformation (human) Photolysis (catalytic oxidation)	Surface water [121]
Tramadol	Analgesic	*O*-desmethyl tramadol	Biotransformation (human)	Surface water [121]
Ciprofloxacin	Antibiotic	Piperazine [135]	Biotransformation (human)	Wastewater influents and effluents [136]
Sulfamethoxazole [136, 137]	Antibiotic	*N*-4 acetyl-sulfamethoxazole	Biotransformation (human)	Wastewater influent and effluent Surface water Groundwater [136]
Sulfamethazine	Antibiotic	*N*-4 acetyl-sulfamethazine *N*-4 acetyl-sulfonamide Desaminosulfamethazine *N*-4 glucose conjugate of sulfamethazine	Biotransformation (human)	Wastewater influent and effluent Groundwater Surface water, Bottled water [136-139]
Sulfadimethoxine	Antibiotic	*N*-4 acetyl-sulfadimethoxine [140]	Biotransformation (human)	Surface water [139]
Sulfamerazine	Antibiotic	4 acetyl-sulfadimerazine 4-methyl-2-aminopyrimidine	Biotransformation (human)	Surface water [139]
Tetracycline	Antibiotic	5 among which: Iso-teracyclines 4-epi-tetracyclines [141, 142]	Biotransformation (human/ veterinary) Photolysis	Wastewater influent and effluent Surface water [139]
Chlorotetracycline	Antibiotic	Iso-chloroteracyclines 4-epi-chlorotetracyclines Etc. [142]	Biotransformation (human/ veterinary) Photolysis	Surface water [139]
Oxytetracycline	Antibiotic	Iso oxyteracyclines 4-epi-oxytetracyclines Etc. [142, 143]	Biotransformation (human/ veterinary) Photolysis	Surface water [139]
Erythromycine	Antibiotic	Dehydro erytromycine	Oxidation in wastewater treatment	Wastewater influent and effluent [136]

Parent compound	Class	TP	Transformation process	Occurrence
		n-desmethyl erythromycin [144, 145]	Biotransformation (human)	Surface water [137]
Roxithromycin	Antibiotic	N-monodemethyl-roxithromycin [146]	Biotransformation (human)	Surface water [139]
Trimethoprim	Antibiotic	TMP oxides and hydroxy TMP [147]	Biotransformation (human)	Wastewater influent and effluent [136]
Monesin	Antibiotic	Various among which O-desmethyl monesin [148]	Biotransformation (human)	Surface water [149]
Lincomycin	Antibiotic	Lincomycin sulfoxide, N-oxide sulfones, N-desmethy-lincomycin sulfoxide [150]	Biotransformation (human)	Ground-water, surface water, Wastewater effluent [151, 152]
Ranitidine	Antacid	desmethylranitidine, ranitidine-oxides [153]	Biotransformation (human)	Wastewater effluent, Surface water [154]
Fluoxetine	Anti-depressant	Norfluoxetine	Biotransformation (human)	Wastewater influent and effluent, surface water [155]
Diltiazem	Anti-hypertensive	Deacetyldiltiazem N-demethyldiltiazem [156]	Biotransformation (human)	Surface water [152]
Salbutamol	Anti-asthmatic	4'-- sulfate ester	Biotransformation (human)	Wastewater influent and effluent, surface water [157]
Gemfibrozil	Anti-hyper-lipidemic	various	Biotransformation (human / wastewater treatment)	Wastewater influent and effluent, surface water [123, 158]
Cannabinoids	Illicit drug	11-OH-THC and THC-COOH	Biotransformation (human)	Wastewater influent and effluents
Cocaine	Illicit drug	Benzoylecgonine	Biotransformation (human)	Wastewater influent and effluents [159]
Estradiol	hormone	Estrone, Estirol	Biotransformation	Surface water Drinking water [160-162]

TPs of other pharmaceuticals appear in relevant fractions compared to their parents [85, 121]. These examples stress the importance to monitor TPs and not merely parent compounds.

6.3 TPs of industrial chemicals in the environment

Industrial chemicals are a large and diverse group of chemicals with numerous applications that determine their potential emission routes into the environment and sources of drinking water. These routes influence the transformation processes that can occur. To organize this group, we distinguish (1) consumer chemicals that are emitted via wastewater (personal care products, household chemicals, food additives) for which many transformation processes take place in the wastewater treatment plant. (2) Industrial products applied in consumer goods (*e.g.* flame retardants, dirt repellants) are likely emitted via solid waste or by wear and tear and (3) chemicals used in industrial processes, examples are intermediates such as monomers used to produce polymers, reagents, solvents and catalysts [64]. These chemicals are potentially emitted via industrial effluent, fume or industrial solid waste. Some chemicals have multiple applications and emission routes [67].

Table 15 lists some industrial chemicals and their TPs.

Table 15 Examples of industrial products/chemicals and their TPs (TPs).

Parent compound	Class	TP	Transformation process	Occurrence
Plastic mm scale	Packaging material	microplastics and nanoplastics	Abrasion during use and in the environment [163]	surface water wastewater sea water
Fluorotelomer alcohols [164-166]	PFC precursor	Ketones and perflorinated carboxylic acids	Biotransformation [167]	waste water influent and effluent surface water rainwater
Tris(2-chloroethyl) (TCEP)	Flame retardant	Bis(2-chloroethyl) hydrohen Phosphate [168]	Biotransformation (human)	surface water [169]
Tris(1,3-dichloroisopropyl)phosphate (TDCPP)	Flame retardant	1,3 dichloropropene 1,2,3-trichloropropane acrolein	Biotransformation	wastewater influent and effluent, surface water, drinking water [170-172]
Ethanol-2-buthoxyphosphate (TBEP)	plasticizer	Hydrolysis products	Probably biotransformation	surface water [173]
Triphenylphosphate (TPP)	Plasticizer	Diphenylphosphoric acid		surface water drinking water [174]
Benzotriazoles	Corrosion inhibitor	Phthalic acid, 1-methyl benzotriazole, dimethylbenzylamine, 1H-benzotriazole 4 and 5 methoxy, dimethyl benzylamine, carbazole	Biotransformation (microbial, human) [175-177]	surface water, wastewater effluent
Alkylphenols (e.g. Bisphenol A)	Plasticizer /surfactant	Shortening of the alkyl chain [178, 179]	Biotransformation (microbial)	groundwater surface water
Aminopolycarboxylic acids (APCAs) (e.g. EDTA)	Chelating agent		Photolysis Biotransformation (microbial)	surface waters
Brominated flame retardant	Flame retardant	Very resistant against transformation, but can lose bromine atoms	photolysis	soil, sediment (due to their hydrophobicity) [66]

6.4 Environmental TPs in drinking water

TPs may end up in drinking water either if they are not removed during drinking water treatment or when they are introduced as, for example disinfection byproducts during drinking water treatment. Examples of both are addressed below.

TPs which are not removed from source water during drinking water treatment are listed inTable 16 .

Table 16 Examples of TPs that (can) end up in drinking water including concentration ranges.

Parent compound	Compound class	Transformation product(s)	Measured concentration range in drinking water (ng/L)	reference
Metformin	Pharmaceutical (antidiabetic)	guanylurea	2-61	180
Acesulfame	Artificial sweetener	hydroxylated acesulfame and iso-acesulfame	*Not reported*	181
various	Industrial contaminant	Bisphenol-A (BPA)	*Up to 10,000*	182
Iomeprol	iodinated X-ray contrast media (persistent class of compounds)		*Up to 500*	183
Phenazone	Pharmaceuticals	1,5-dimethyl-1,2-dehydro-3-pyrazolone (DP)	*1500 (95 percentile)*	184
propyphenazone	Pharmaceuticals	4-(2-methylethyl)-1,5-dimethyl-1,2-dehydro-3-pyrazolone (PDP)	*280 (95 percentile)*	184
dimethylaminophenazone (DMAA)	Pharmaceuticals	1-acetyl-1-methyl-2-phenylhydrazide (AMPH), acetoaminoantipyrine (AAA), formylaminoantipyrine (FAA), and 1-acetyl-1-methyl-2-dimethyloxamoyl-2-phenylhydrazide (AMDOPH)	*AMPH: 190 (95 percentile)* *AAA, and FAA: <loq* *AMDOPH: 990 (95 percentile)*	184
carbamazepine	Pharmaceuticals	10,11- trans diol carbamazepine; 3-hydroxy carbamazepine 2 hydroxy carbamazepine carbamazepine 10,11-epoxide	*TDC-CBZ 160-1110 (averages)* *3H-CBZ 10-90 (averages)* *2H-CBZ 10-70 (averages)* *CBZ 10,1- E 10-50 (averages)*	185

6.5 TPs formed by drinking water treatment

TPs which are introduced by drinking water treatment are listed in Table 17. More information on disinfection byproducts formed by drinking water treatment techniques applied in the Netherlands can be found in Baken, 2013 [186].

Table 17 Examples of TPs formed during drinking water treatment (MDA : 3,4-methylenedioxyamphetamine; MDEA: 3,4-methylenedioxyethylamphetamine; MDMA: 3,4-methylenedioxymethamphetamine.)

Parent compound	Compound Class	Treatment process	Transformation product(s)	Measured concentration range in drinking water (ng/L)	reference
dichloramine & dimethylamine diclofluanide tolylfluanide	Industrial compounds / biocide	chloramination & Ozonation	NDMA	1-66 ng/L	187
halobenzoquinones (HBQs)	Industrial compounds	UV	3-hydroxyl-2,6-dichloro-1,4-benzoquinone;	Not reported	188

Parent compound	Compound Class	Treatment process	Transformation product(s)	Measured concentration range in drinking water (ng/L)	reference
			5-hydroxyl-2,6-dichloro-3-methyl-1,4-benzoquinone; 5-hydroxyl-2,3,6-trichloro-1,4-benzoquinone; 3-hydroxyl-2,6-dibromo-1,4-benzoquinone		
Amphetamine and analogs	Illicit drugs	chlorination	(3-chlorobenzo)-1,3-dioxole from MDA and MDEA; 3-chlorocatechol from MDMA*	0,5-5.8	189
Phenazone and propyphenazone	analgesics and antipyretics	chlorination	chloro-hydroxy-phenazone; and N-demethyl-chloro-hydroxy-phenazone; N-demethyl-hydroxy-propyphenazone and N-demethyl-chloro-hydroxy-propyphenazone	n.r.	190
Phenylurea herbicides		chlorination	different	n.r.	191
diclofluanide			NDMa	n.r.	191