

Deliverable D4.4

Web based interactive tools for microbial risk and chemical water quality assessment

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COLOPHON

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	A web based QMRA application will be launched which allows the assessment of various treatment trains regarding the com- pliance with WHO health targets. Further this deliverable pro- vides a decision tree to select a treatment train based on chemi- cal water quality and application.
	This report is an accompanying document to the actual tools which are available at
	http://5.153.252.94:8080/QMRA/login.do http://5.153.252.91:8080/QCRA/welcome.do
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Executive Summary

The AquaNES project will catalyze innovations in water and wastewater treatment processes and management through improved combinations of natural and engineered components. Water quality assessment and associated risk assessment is essential for the evaluation of water treatment. It is not always possible to monitor water quality along treatment trains because of multiple reasons. For example: monitoring is too labor intensive, detection limits do not meet requirements, or dynamics in source water quality cannot be covered by occasional monitoring. Therefore, scenario studies are required to perform treatment assessment (and risk assessment) under different conditions. In that way the tools can assess whether the treatment of a particular type of water with an intended (re)use can meet defined quality criteria.

This report gives a description of two tools developed within the AquaNES project.

QMRA: Quantitative Microbial Risk Assessment is a preventive strategy for microbial safety of water The major components is determining the source water quality and the presence of microbial pathogens, assessment of the Pathogen Elimination Capacity of the treatment and exposure assessment and risk calculations.

QC(R)A: Quantitative Chemical (Risk) Assessment calculates the removal of a share of micro contaminants in treatment trains. The major components is determining the source water quality and the presence of micro contaminants, assessment of the chemical removal of the treatment and the estimation or residues of contaminants in the treated water.

These tools can assess treatment efficiency of customizable treatment trains for microbial and chemical contamination, respectively. The tools can be operated with literature data as well as data of a specific site to which the tool is applied. The tools are intended to assess the treatment efficiency, predict the concentrations of microbial and chemical contaminants in the treated water and evaluate whether the treated water meets quality criteria for safe use.

The tools are user friendly and target, operators and designers / planners of wastewater and drinking water treatment systems. It is also functional as an educative tool for employees of water utilities and authoroties. The tools were tested by AquaNES partners. Additionally, a workshop of the QMRA tool with potential users also illustrated its function as a dissemination tool for more generic audiences such as policy makers and students. Many tools developed within (EU) projects are not maintained after the project has ended. The life of the tools after the AquaNES project is guaranteed by incorporating the tools in the Watershare platform that is a cooperation of international research institutes and water companies (https://www.watershare.eu). Additionally, the adoption of the tools by this platform will support the dissemination and future projects and data of members will be used to improve the tools in future. Thereby they can provide a service to many potential users.

The Technology Readiness Level (TRL) of the QMRA tool is 6 it is a well-tested prototype that provides a risk assessment. The TRL of the QCRA tool is 4-5 as it is currently a demonstration of a prototype than needs testing as well as adjustments through additional data and usage.



1 About this document

1.1 Purpose and structure of this document

This document provides background information on two developed tools of Deliverable 4.4.

The QMRA tool is described and shortly evaluated in Chapter 2 and Chapter 3 describes and evaluates the QC(R)A tool. Chapter 4 discusses the future implementation of these tools in the water sector.

1.2 Relation to the project objectives

The AquaNES project demonstrates of the robustness and benefits of combined natural and engineered water treatment technologies. Water quality assessment in general, and especially treatment efficacy of natural treatment steps, that are generally less controllable and adaptable, requires tools to assess water quality already in the planning phase. The presented tools can help users to assess existing treatment schemes, adapt these schemes with additional natural or engineered treatment steps or build conceptual treatment schemes, and predict performance and perform a risk assessment.



2 QMRA tool

2.1 Introduction

The QMRA tool enables users to estimate the risk of effluents of a wide array of water treatment steps and combinations of these steps in treatment trains in regard to different purposes of water use. A calculation is performed according to the QMRA approach that involves the estimation of infection risk per person and year and the DALYs (disability-adjusted life years) per person and year for bacteria (*Campylopbacter jeuni*), virus (*Rotavirus*) and protozoae (*Cryptosporidium*). A more detailed description of the QMRA approach can be found in D3.1 of the European project DEMOWARE (D3.1 Appropriate and user friendly methodologies for Risk assessment, Life Cycle Assessment, and Water Footprinting).

The tool has an easy to use web interface and can be found here:

https://lnkd.in/gDHWYJW

http://5.153.252.94:8080/QMRA/login.do

It is integrated within the Watershare suite of tools <u>https://www.watershare.eu/</u> and can be accessed through the AquaNES DSS (<u>http://dss.aquanes.eu/Default.aspx?t=1743&ToolID=23</u>).

2.2 Description of steps

Steps for use of the tool are described below.

Step 1: Create new or open existing QMRA

QMRA	.6alpha				wate	ershare 🗦	AquaNES
	1 RISK ASSESSMENT	2 SOURCE	3 TREATMENT	4 USE	5 SUMMARY	6 EXPOSURE & RIS	ĸ
		Welcon	TREATMENT ne DanielW, Wha © Create new Risk As © Modify existing Risk SUBMIT	t do you want t		EXPOSURE & RIS	K

Step 2: Selection of source water with predefined water qualities

Several source water qualities can be selected, ranging from raw sewage over treated sewage, several types of surface water (e.g. contaminated, protected) to rain water. Ranges of microbiological concentrations associated with each source are shown.



1 RISK ASSES	SMENT	2 SOURCE	3 TREATMENT	4 USE	5 SUMMARY	6 EXPOSURE & RISK	
k Assessment: Test QMRA							
						« Back	Next >
under Pathogens.	This range will be	used in the risk assessm	ant to assess the risk. The range nent. The ranges are based on g nd the index pathogen for which Dath out	uidelines and references, the risk is calculated.			
under Pathogens.	This range will be n introduction for e	used in the risk assessme each pathogen group an	nent. The ranges are based on g nd the index pathogen for which	uidelines and references, v			
under Pathogens button displays a Test Source	This range will be n introduction for e	used in the risk assessm	nent. The ranges are based on g nd the index pathogen for which	uidelines and references, t the risk is calculated. gens (i		e Summary page. The 'i'	
under Pathogens. button displays a	This range will be n introduction for e	used in the risk assessme each pathogen group an	nent. The ranges are based on g nd the index pathogen for which Pathog	uidelines and references, t the risk is calculated. gens (i	which will be displayed on th	e Summary page. The 'i'	
under Pathogens. button displays a Test Source	This range will be n introduction for e	used in the risk assessme each pathogen group an	nent. The ranges are based on g nd the index pathogen for which Pathog	uidelīnes and references, the risk is calculated. GENS () ia → Min Value: 1.00	which will be displayed on th	e Summary page. The 'i' CFU/lter)	
under Pathogens. button displays a Test Source	This range will be n introduction for e	used in the risk assessme each pathogen group an	nent. The ranges are based on g nd the index pathogen for which Pathog Bacte	uidelīnes and references, the risk is calculated. GENS () ia → Min Value: 1.00	which will be displayed on th le-03, Max Value: 1.00e+03 (C	e Summary page. The 'i' CFU/lter)	

Step 3: Selection of Treatment Train

A wide range of predefined water treatment steps are available (>20) that can be selected to build customized treatment combinations:

- Adjust number of treatment steps as needed for the case study
- Insert treatment steps into blank boxes by drag and drop
- Default values for each treatment step are displayed, which can be adjusted later (in case site-specific monitoring data is available)

QMRA v 0.9.6alpha					watershare 🗦 AquaN
1 RISK ASSESSMENT		2 SOURCE	3 TREATMENT	4 USE	5 6 SUMMARY EXPOSURE & RISK
isk Assessment: Test QMRA te Created : 2019-04-02 te Modified : 2019-04-02		Description: Test for Final User: DanielW	l Event		« Back Next
the selected process to display a brief intr	oductio	n. The range of log r	removal of each pathogen group by	y this process is sl	a box click '+' or drag and drop boxes to change the order. Point a nown. These log removals are used in the risk calculation. The add the process here and then adapt the log removal values on t Scheme
Bank filtration		No.	Process Orde		Log Removal
Chlorination, drinking water Chlorination, wastewater		1.	Primary treatment	×	Bacteria Minimum: 0.0 , Maximum: 0.5 Viruses Minimum: 0.0 , Maximum: 0.1 Protozoa Minimum: 0.0 , Maximum: 1.0
Chlorine dioxide Conventional clarification Dissolved air flotation		2.	Wetlands, subsurface flow	v ×	Bacteria Minimum: 0.5 , Maximum: 3.0 Protozoa Minimum: 0.5 , Maximum: 2.0
Dual media filtration Granular high-rate filtration		3.	Chlorination, wastewate	r ×	Bacteria Minimum: 2.0 , Maximum: 2.0 Viruses Minimum: 2.0 , Maximum: 2.0
High-rate clarification					Protozoa Minimum: 2.0 , Maximum: 2.0



Step 4: Select foreseen type of water usage

Water use can be selected from several predefined usages (e.g. different types of irrigation, drinking water, car washing), each associated with an ingestion volume and a number of events per year. A description and respective values for number of events and ingestion volumes are displayed for information, which will be used as input parameters for the risk calculation.

QMRA v 0.9.6ªpha				water	share 🗦 AquaNES
1 RISK ASSESSMENT	r SOURCE	3 TREATMENT	4 USE	5 SUMMARY	6 EXPOSURE & RISK
	User: DanielW use. If multiple uses are cons	it for Final Event idered, select the one with the hij gested each time. Literature refe			« Back Next »
Water L			elected Water U		арч.
Irrigation, Public		unlikely to be directly ex via contact with lawns, e	posed to large amounts of etc. Likely to be higher whe ek) grounds and golf cours I to 50 events	pal areas sparingly (estimate f spray and therefore exposur n used to irrigate facilities su es (estimate 1/week)	e is from indirect ingestion

Step 5: Summary page with all assumptions made for the QMRA

The summary page includes the following functionalities:

- Overview of all input parameters is shown in fold-out tables
- Log-removal of treatment steps can be adapted (e.g. if local monitoring data is available) by selecting "Entry Treatment Data" opening the summary table "Treatment Process"
- Min/Max removal can be adjusted and distribution type can be modified (e.g. set to "norm" = normal distribution), which automatically changes the reference to "user data"
- Clicking on the button "User Treatment Data" opens an excel file which can be used to calculate the appropriate log-removal credits for each treatment step from available monitoring data
- Input data for QMRA can be exported as pdf (button "Export PDF")
- Start calculation by selecting the "Calculate"-button



	2	3	4	5	6
RISK ASSESSMENT	SOURCE	TREATMENT	USE	SUMMARY	EXPOSURE & RISK
ssessment: Test QMRA					
ated : 2019-04-02 dified : 2019-04-02					« Back Calculate
nmary of Data					
				User Treatment Data	rt PDF Entry Treatment Dat
nber of Monte Carlo Simulatior	: 1000				
on a heading below to display a full over					
ment performance. lick on 'User Treatm pers and distribution in the treatment ta					
		Water Sou	rce: Test Source		
		Treatm	nent Process		
Treatment Process	Order	Data	Bacteria	Viruses	Protozoa
Treatment Process Primary treatment	Order 1			Viruses	Protozoa
		Data	Bacteria		
		Data Minimum Log Removal	Bacteria	0.0	0.0
		Data Minimum Log Removal Maximum Log Removal	Bacteria 0.0 0.5 uniform	0.0 0.1 uniform	0.0 1.0 uniform
		Data Minimum Log Removal Maximum Log Removal	Bacteria 0.0 0.5	0.0	0.0
		Data Minimum Log Removal Maximum Log Removal Distribution	Bacteria 0.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	0.0 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1	0.0 1.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0
		Data Minimum Log Removal Maximum Log Removal Distribution	Bacteria 0.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	0.0 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1	0.0 1.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0
		Data Minimum Log Removal Maximum Log Removal Distribution Reference	Bacteria 0.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	0.0 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1	0.0 1.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0
		Data Minimum Log Removal Maximum Log Removal Distribution Reference	Bacteria 0.0 0.5 uniform DEMEAUWARE Deliverable 3.1 Io18-197: NRMMO-EPHC-AHMQ (2006). WHO 2008)	0.0 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1	0.0 1.0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0

Step 6: Exposure and Risk: Summary of results

After running of the Monte-Carlo simulation (takes 2-30 s, depending on use scheme) the results are displayed as boxplots. The red line indicates the maximum acceptable risk level according to WHO guidelines. The following results are given as figures:

- Infection risk per person per year
- DALYs per person per year (DALY: disability-adjusted life years)

Below the graph the more detailed results are given as fold-out tables (values exceeding the guideline risk level are shown in red). Results can be exported as pdf by clicking on the "Export PDF" button.



1	2	3	4	5	6
RISK ASSESSMENT	SOURCE	TREATMENT	USE	SUMMARY	EXPOSURE & RISK
Assessment: Test QMRA					
rested : 2019-04-02 lodified : 2019-04-02					« Back Export PD
immary of Result					
risk of this scenario can be compar	red to two commonly ann	lied health hased targets (WHO	GDWO 2011)-		
1 in 10,000 Annual risk of infection o			0011220113.		
0.000001 Disability Adjusted Life Yea					
estimated risk of infection exceeds	the health target of 1 infe	ection per 10,000 people per yea	r for Protozoa		
estimated health risk exceeds the h	health target of 1 microDA	LY per person per year for Proto			
	In	fection risk per p	erson per vea		
			h based target)		
	1			Bacteria	
	1		T	Virus	
	0.01		T		
1	1			Virus	
	1 (80) 0.01			Virus	
	1 (80) Juga (10-4 ug			Virus	
	1 (80) 0.01 1e-4			Virus	
	1 (80) Juga (100) 1e-4 1e-6 1e-6			Virus	
	1 001 1001			Virus	
	(i) 1e-4 -e-1			Virus	
	1 (00) 100 100 100 100 100 100 100			Virus	
	(60) 0.01 1e-4 1e-4 1e-6 1e-6 1e-10			Virus	

Virus Risk Assessment							
Protozoa Risk Assessment							
Data	Number/log10	Mean	5%	50%	95%		
Source Concentration	N/L	5009.31	3918.86	5004.80	6168.37		
Primary treatment	log10	0.499	0.0496	0.5	0.946		
Secondary treatment	log10	1.0	0.551	1.0	1.45		
Ozonation, wastewater	log10						
Slow sand filtration	log10	2.65	0.557	2.64	4.78		
Conventional clarification	log10	15	1.05	15	1.95		
Total Treatment	log10	5.64	5.09	5.64	6.22		
DALY per Year	/person/year	1.525-6	3.9E-7	1.145-6	2.67E-8		
Exposure per Year	number/person/year	0.022	0.00849	0.0189	0.0476		
Infection Risk per Year	/person/year	0.00128	3.715-4	0.00106	0.00275		
Ingestion per Event	liter/event	0.001	0.001	0.001	0.001		
Events per year	number/jear	50	50	50	50		



2.3 Data sources, adding pown measured data

The tool is based on data (e.g. regarding source concentrations and log removals achieved in selected treatment steps) from guidelines such as the WHO drinking water guideline. The references of all data are displayed on the summary page (Step 5, see above). If monitoring data for log removals of individual treatment steps is available, data can be used as described above (step 5).

The database qmra.db (v.0.10.0) included in the tool is publically available on the EU funded repository Zenodo (<u>https://doi.org/10.5281/zenodo.3339322</u>) under the permissive MIT license and its content is documented under the following link:

https://kwb-r.github.io/qmra.db/

Under the menu item "Database content", an overview of the current database content is given.

Interested users can also provide suggestions for further improving the database by using GitHub`s issue tracking system as described under the menu item "Update Database":

https://kwb-r.github.io/qmra.db/articles/update_database.html#suggest-your-changes-on-github

2.4 Description of calculations

The calculation engine (R package kwb.qmra v0.1.1) was initially developed within EU-project DEMOWARE and adapted to the needs of a web-based front end developed by KWR. Functions were programmed in *R* and integrated in the open-source *R*-package kwb.qmra (v0.2.0) accessible through GitHub (https://github.com/kwb-r/kwb.qmra) under the permissive MIT license, made citable via Zenodo (https://doi.org/ 10.5281/zenodo.3341401) and documented under the following link:

https://kwb-r.github.io/kwb.qmra/

Following this link, the installation procedure, functions and examples are described. These considerations sum up to TRL of 6, as it is a well-tested prototype that provides a risk assessment.

2.5 Implementation of QMRA

The tool presents a user friendly and simple interface to assess treatments and to perform a risk assessment either on generic data or by including user defined data of a specific treatment. Monte Carlo simulations enable to assess the concentrations potential concentrations of bacteria, viruses and protozoa during treatment. These concentrations can be related to risk based water quality criteria in order to perform a risk assessment of existing and conceptual treatment trains. Site specific data can be included in the assessment to obtain more site specific risk assessment.

The tool has a user-friendly front end, and is therefore very useful to 1) make employees in utilities and water authorities, which are no experts in QMRA, familiar with the concept of QMRA, as well as a support in evaluating and designing treatments. As of yet, the tool is intended as a first evaluation and aid in discussing treatment options in existing and newly designed treatment trains. Discussions with AquaNES partners and a public workshop revealed that there is a lot of interest for this particular tool (see appendix 1). These considerations sums up to TRL of 6, as it is a well-tested prototype that provides a risk assessment.

AquaNES

3 QC(R)A tool

3.1 Introduction

The QC(R)A tool enables users to estimate the removal efficiency of organic micro pollutants in a wide array of water treatment steps and combinations of these steps in treatment trains. The tool has an easy to use web interface. The data for the calculation of removal is extracted from a database holding data on micro pollutants in sources and removal for a wide array of treatment steps. It includes both literature data and data from selected AquaNES demonstration sites. The 'R' in QCRA is given between brackets, as the risk assessment of micro pollutants in treated water is not easily deducted from concentrations due to the finding that risks are not determined by individual chemicals (van Loon, Verwoerd et al. 1997, Parkerton, Stone et al. 2000, Chèvre, Maillard et al. 2008, Backhaus and Faust 2012, Houtman, Kroesbergen et al. 2014, Altenburger, Ait-Aissa et al. 2015, Schoenfuss, Furlong et al. 2016) and risk based thresholds are not always available for individual chemicals and for all use categories. Therefore, the outcome of the assessment can be related either to regulatory quality criteria. These criteria are not necessarily related to human health or ecological risks (e.g. Water Framework Directive, Drinking water directive or criteria set for water intended for irrigation (European Commission 1998, European Commission 2000, European Commission 2008)). Additionally or alternatively, guideline values given by non-governmental organizations, or to thresholds of toxicological concern (TTC) can be applied. The TTC is a safe level below which there would be no appreciable risk to human health assuming lifetime exposure (Mons, Heringa et al. 2013). For many chemicals, no specific quality standards are available and if they do exist, they are often not directly linked to effects or risks.

Relating risks associated with the presence of individual chemicals in water sources is very complex. Therefore, the 'R' is between brackets. Hence, the risk aspect is not tackled by this tool as of yet. Because of the similarity to the QMRA tool, and the intention to include the aspect in future, we decided to use this abbreviation nevertheless.

The web tool can be found here: http://5.153.252.91:8080/QCRA/welcome.do

It is integrated within the Watershare suite of tools <u>https://www.watershare.eu/</u> and can be accessed through the AquaNES DSS (<u>http://dss.aquanes.eu/Default.aspx?t=1743&ToolID=21</u>).

Please do not use Explorer as not all functionalities are supported by that browser, rather use Chrome or Firefox.



3.2 Description of steps

Water quality assessment is a complex task with many aspects. It includes assessment of (1) potential contamination of sources of the water, (2) evaluation of treatment efficiency for this (potential) contamination, (3) and the evaluation of treated water.

Step 1: Create new or open existing QCRA

The tool stars with the selection of the source water. On the entry page a project can be defined.

QCRA v 0.9.2alpha			watershare	AquaNES
	1 PROJECT	2 TREATMENT	3 WATER SOURCE	4 RESULT
	Welcom	e User, What do y	ou want to do?	
		 Create new Project Modify existing Project 		
New Project Project Name				
Project Description	×			
		SUBMIT		

Step 2: Selection of Treatment Train

A wide range of predefined water treatment steps are available (>20) that can be selected to build customized treatment combinations:

- Adjust number of treatment steps as needed for the case study
- Insert treatment steps into blank boxes by drag and drop

QCRA v 0.9 28649		2	3	watershare 🗦 Aqua
PROJECT		TREATMENT	WATER SOURCE	RESULT
				e Back Ne
Drag one Type of Treatment into the Process Orc To add new Process press + button				
Type of Treatment			Process Scheme	
Activated Carbon		No.	Process Order	
Conventional WWTP		0.	Water Intake	
Conventional WWTP, Full Conventional WWTP, Primary			*	
Conventional WWTP, Secondary		1.		
Membrane			Conventional WWTP, Full	
Oxidation	1000	2.	Oxidation, O3	
Oxidation, O3				
Oxidation, O3 + H2O2 Oxidation, UV		3.	Constructed Wetland ×	
Oxidation, UV + H2O2				
Natural Treatment			=	
Bank filtration				
Constructed Wetland				
MAR/SAT				
٢	» ×			



Step 3: Selection of Water Source

Subsequently, the source water can be selected, and water quality data for various micro-contaminants typically found in this particular source are presented. The micro-contaminants of interest can be selected. These data are based on literature data. The database holds data for many combinations of chemicals and water types, but not for all, this is work in progress.

QCRA v 0.9.24pm				watershare 🗦 AquaN
	1 PROJECT	2 TREATMENT	3 WATER SOURCE	4 RESULT
ject: example 1 Creased : 2019-07-02 Modified : 2019-07-02	Description:	uampia 1		e Back Next
		on combination of Treatments and Water Source that are nts available for those combination. To add another Sul		
Water Source	2		Selected Micropollutants Information	
		Micropollutants	Initial Concentration	
Waste Water	•	Diclofenac	1.0 µg/L	
		Carbamazepine	€.0 µg/L	
		Sulfamethoxazole	➡ 281.5 µg/L	
		•		

Step 4: Exposure, summary of results

After source selection concentration estimates along the treatment train are presented, using generic literature data. Water quality strongly varies between sources, locations and in time. Collected data on concentrations and removal also vary. The presented removal and expected concentrations can therefore deviate from the real life situations. Furthermore, if there are no data available, a default value (0% removal) is presented. In the example below this percentage is given for the constructed wetland treatment, as this treatment is at the moment of compiling this report not included in the database (Figure 4). The use of a default value can be recognized by the absence of references from which this factor is obtained (o references).

	1 PROJEC	т		2 TREATMENT		y	3 WATER SOURCE			4 IESULT	
										« Ba	ack Si
Source: Waste	Water									Edit Data	Refresh
n Number of Refere	ence cell to see the Refere	Emclency, click Edit Data bu inces	itton. Click kerresh Calcula	ation to recalculate the E	nd Concentration.						Reliesi
on Number of Refere	ance cell to see the Refere	Emiciency, click Loit Data bu inces	tton. Click kerresh Calcula		nd Concentration. Treatmer	nt Order 2	Treatmen	it Order 3			Renesi
Micro Pollutants	Initial Concentration	Eniciency, click Loit Data bu		t Order 1	Treatmer	it Order 2	Treatmen Constructe		End Concentration	Lon Data	remesh
	ence cell to see the Refere	inces	Treatmen	t Order 1	Treatmer				End Concentration	Edit Uata	Renesi
	ence cell to see the Refere	inces	Treatmen	t Order 1 I WWTP, Full	Treatmer Oxidati	ion, O3	Constructe	d Wetland	End Concentration	EditUata	Renesi
n Number of Refere	ence cell to see the Refere	initial Concentration Unit	Treatmen Conventiona Removal Efficiency (%)	t Order 1 I WWTP, Full	Treatmer Oxidat Removal Efficiency (%)	ion, O3 Number of Reference	Constructe Removal Efficiency (%)	ed Wetland Number of Reference			rten esi

The tool gives the opportunity to include own measured, site specific data, to customize the assessment for a location. The tool calculates concentrations, but all treatment technologies and especially natural



treatment technologies will have variable treatment efficiency both between different systems as well as within systems, due to changing conditions.

A tool as presented here can never cover all aspects. The intention of this tool is therefore to build scenarios, discuss treatment systems and evaluate which treatment steps are key in removing micro contaminants. It is not intended to replace monitoring activities.

For many chemicals, no specific quality standards are available and if they do exist, they are often not directly linked to effects or risks. Therefore the 'R' in QCRA (Quantitative Chemical (Risk) Assessment) is between brackets. Relating risks associated with the presence of individual chemicals in water sources is very complex. This cannot be tackled by the current version of this tool. But because of the similarity to the QMRA tool that was developed, we decided to use this abbreviation nevertheless.

3.3 Implementation of QC(R)A

The tool presents a user friendly and simple interface to assess treatments. However, the tool holds data for 228 chemicals, and not all treatment steps are covered for these chemicals. There is an option to include own measured data, but this needs to be aggregated data presented as (average) removal rates.

Currently the variation in removal rates within and between different studies is not incorporated in the assessment, as is the case for the QMRA tool where this variation is included by using Monte Carlo simulations. Such an assessment would not only result in an average variation but also a distribution around this average.

The tool has a user-friendly front end, but considering the available data, the evaluation of the uncertainty and the evaluation in relation to thresholds are aspects which can be further improved. As of yet, the tool is intended as a first evaluation and aid in discussing treatment options in existing and newly designed treatment trains. For more detailed assessments, the tool needs additional data and features. Furthermore, it is recommended to further test and evaluate the functionalities of the tool by (potential) users, in order to layout feature requests in order to improve and widen its applicability. These considerations sums up to TRL of 4 to 5, as it is currently a demonstration of a prototype than needs testing as well as adjustments through additional data and usage.



4 Appendix 1: Workshop QMRA @ IWA Berlin 2019

Conference: 12th IWA International Conference on Water Reclamation and Reuse, Berlin Germany (<u>iwareuse2019.org</u>)

Date: June 16 2019 Agenda: 9:00 Welcome and round of table 9:15 Introduction QMRA methods (P. Smeets) 9:45 Overview Aquanes (U. Miehe) 10:00 Introduction Workflow of QMRA Tool (U. Miehe) 10:15 Usage of QMRA tool by participants 10:45 Coffee Break 11:00 Discussion on tool output and options to refine results (U Miehe) 11:30 Feedback on QMRA Tool

QMRA workshop summary & user feedback:

The workshop aim was to promote the QMRA tool developed in AquaNES within Europe and beyond. 15 Participant from Europe and USA, China, Singapore and Saudi-Arabia received training on the tool and tested it in small groups for different water reuse scenarios. Feedback from the participants regarding the tool setup and usability was very positive. One participant (Hultquist, Robert, California SWB, United States) gave the following feedback: "The tool is exactly what we need to make employees in utilities and water authorities, which are no experts in QMRA, familiar with the concept of QMRA and also the impacts of the different treatment stages". Several participants have continued to try out the tool after the workshop and have contacted us about implementation and further development of the tool.



5 Literature

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