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Decision support for water quality management of contaminants of emerging concern

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Abstract

Water authorities and drinking water companies are challenged with the question if, where and how to abate contaminants of emerging concern in the urban water cycle. The most effective strategy under given conditions is often unclear to these stakeholders as it requires insight into several aspects of the contaminants such as sources, properties, and mitigation options. Furthermore the various parties in the urban water cycle are not always aware of each other's requirements and priorities. Processes to set priorities and come to agreements are lacking hampering the articulation and implementation of possible solutions.

To support decision makers with this task, a decision support system was developed to serve as a point of departure for getting the relevant stakeholders together and finding common ground. The decision support system was iteratively developed in stages. Stakeholders were interviewed and a decision support system prototype developed. Subsequently, this prototype was evaluated by the stakeholders and adjusted accordingly. The iterative process led to a final system focused on the management of contaminants of emerging concern within the urban water cycle, from wastewater, surface water and groundwater to drinking water, that suggests mitigation methods beyond technical solutions. Possible wastewater and drinking water treatment techniques in combination with decentralised and non-technical methods were taken into account in an integrated way. The system contains background information on contaminants of emerging concern such as physical/chemical characteristics, toxicity and legislative frameworks, water cycle entrance pathways and a database with associated possible mitigation methods. Monitoring data can be uploaded to assess environmental and human health risks in a specific water system. The developed system was received with great interest by potential users, and implemented in an international water cycle network.

Keywords: contaminants of emerging concern, water quality management, urban water cycle, drinking water treatment, wastewater treatment, abatement methods.

1 Introduction

Chemicals are continuously produced for various beneficial purposes, such as protecting crops, conserving food or treatment of diseases. Over 3470.000 chemicals are registered and regulated via national and international authorities (CHEMLIST), new chemicals enter the market continuously and the global volume of production of chemicals is growing (CEFIC, 2013). Many of these chemicals and their transformation products enter the aqueous environment during their life cycle (Schwarzenbach et al., 2006).

Preliminary risk assessments consistently show that these environmental concentrations are lower than required for adverse human health effects, hence for individual compounds risks are not expected (Bruce et al., 2010; de Jongh et al., 2012; Debroux et al., 2012; Houtman et al., 2014; Schriks et al., 2010). However the toxicological risk of summed concentrations in complex environmental mixtures is heavily debated, especially related to potential endocrine disruption (Bergman et al., 2013; Dietrich et al., 2013; Nohynek et al., 2013; Vandenberg et al., 2012). This causes increasing concern for the public, regulators and users of surface water (Diamond et al., 2015; Schwarzenbach et al., 2006).

There are many definitions of these contaminants of emerging concern (CECs), but in this article the following definition is used: "manufactured or manmade chemicals or materials which have now been discovered or are suspected to be present in various environmental compartments and whose toxicity or persistence are likely to significantly alter the metabolism of a living being" (Sauvé and Desrosiers, 2014). CECs include, but are not limited to, drugs of abuse, artificial sweeteners, pesticides and biocides, musks and fragrances, perfluorinated compounds, industrial substances, nanoparticles,

1 plasticisers, pharmaceuticals and transformation products of these chemicals (Richardson, 2012;
2 Richardson and Ternes, 2011).

3 Information on CECs multiplies with rapid speed. Several legal frameworks, e.g. the Water Framework
4 Directive (WFD) and the EU chemicals regulation (REACH), are dealing with the issue both from a
5 water quality and authorisation perspective (EU, 2000, 2006). However water quality legislation, both
6 on a national and international level, are not meant to cover all individual substances authorised on
7 the market (Houtman, 2010). Furthermore there is often a time lag from the time a compound with
8 adverse effect is observed in the environment, to the time that the necessary legislation or policy is
9 implemented (Christensen et al., 2011; Halden, 2015). The time lag is due to complex decision
10 structures and the need for compromises (Halden, 2015; Houtman, 2010). This leaves water
11 authorities and drinking water companies with the question if, where and how to abate these
12 substances in the urban water cycle.
13

14
15 Many strategies are available to mitigate emissions. During the design and production stage of the
16 chemicals, legal regulations are in force. During the use stage, strategies such as drift reduction can
17 be used, especially for professional uses such as pesticides. Finally in the waste and removal stage,
18 strategies such as take-back schemes for pharmaceuticals or treatment of wastewater and drinking
19 water can be implemented (Schirmer and Schirmer, 2008). The most effective strategy under given
20 conditions are often not clear to stakeholders. It requires insight into several aspects of the
21 contaminants such as sources, properties, mitigation options, and their costs and benefits.
22 Furthermore, multiple stakeholders (such as water boards, drinking water companies and
23 municipalities) are often not aware of each other's requirements and priorities. Finally, processes to
24 set priorities and come to agreements are lacking and this hampers the finding and implementation of
25 possible solutions. The setup of river basin management plans required by the WFD address this
26 issue (EU, 2000).
27
28
29

30 In 2013 the European Interreg programme funded the TAPES programme (Transnational Action
31 Programme on Emerging Substances), with the aim to create a joint knowledge platform on CECs in
32 the urban water cycle. As part of this knowledge platform a Decision Support System (DSS) was
33 developed in strong cooperation with stakeholders within the whole water cycle. The objective of the
34 DSS was to facilitate decision makers with the complex task of deciding on effective and efficient
35 strategies to control CECs within their segment of the water cycle. To our best knowledge, no such
36 DSS exists at this moment. In this paper the development process of this DSS is described, starting
37 with the design criteria and finishing with the final DSS.
38
39
40

41 **2 Design criteria**

42 **2.1 DSSs and complex issues**

43
44 The definition of DSSs (Power and Sharda, 2009) is "an interactive computer-based system that helps
45 people use data, documents, knowledge, and models to solve problems and make decisions". DSSs
46 are built to *support* people in making decisions, not to *make* the decision itself (Angehrn and Jelassi,
47 1994; Power and Sharda, 2009). DSSs are regularly used by decision makers all over the world
48 (Delpla et al., 2014; Mysiak et al., 2005; Power and Sharda, 2009). There is no consensus on the
49 classification of various types of DSSs (Holsapple, 2003; Power and Sharda, 2009). The
50 categorisation by Power (2002) is the one that will be used here:
51
52
53

- 54 1. Communication-driven; DSS includes communication and collaboration supported by
55 technologies such as e-mails, bulletin boards, chat systems and interactive videos.
- 56 2. Data-driven; DSS gives access to tools to manipulate large sets of data.
- 57 3. Document-driven; DSS can be used to retrieve and analyse documents, such as product
58 specifications, minutes of meetings, policies and procedures.
- 59 4. Knowledge-driven; DSS suggests actions within a specific domain.
60
61
62
63
64
65

5. Model-driven; DSS gives access to a quantitative model.

Most DSSs are hybrids and consist of two or more of the above mentioned drivers (Power and Sharda, 2009).

DSSs shifted with time from solving semi-structured problems, to solving complex issues such as 'wicked' problems (Beynon et al., 2002; Courtney, 2001; McCown, 2002; Mysiak et al., 2005; Rauscher, 1999). The characteristics of a 'wicked' problem is that stakeholders cannot easily agree on the problem definition, and options for solutions are not clear beforehand (Rittel and Webber, 1973). To solve 'wicked' problems, a collectively accepted solution is required (Hocking et al., 2015). Therefore the main focus should be on the problem formulation, based on discussions with stakeholders, to incorporate their perspectives (Mitroff and Linstone, 1993; Shim et al., 2002) and to ensure that all relevant variables are included in the analysis (Shim et al., 2002; Wassen et al., 2011).

DSSs have several pitfalls that need to be accounted for in the design phase (McBride, 1997; Mysiak et al., 2005; Newman et al., 1999; Wassen et al., 2011). Common pitfalls are:

1. The process of decision making goes together with a learning process (Salewicz and Nakayama, 2004). It is difficult to know beforehand what information is needed to make decisions.
2. The acceptability of a DSS links to the stakeholders' possibilities to contribute and their abilities to communicate results, rather than the credibility of the underlying model (scientific soundness, high quality data etc.) (Wassen et al. 2011). Acceptability by the stakeholders is often known only at the last phase of the DSS development.
3. In order to meet new or more complex requirements of the decision makers, a DSS constantly needs to be kept up-to-date and further developed, otherwise it quickly becomes obsolete (Newman et al., 1999).

2.2 DSSs in the water sector

DSSs are widely used in the water sector, mostly related to river management (Salewicz and Nakayama, 2004; Xu et al., 2007). DSSs are developed to help implementing aspects of the EU Water Framework Directive (WFD), such as MULti-sectoral INtegrated and Operational decision support system (MULINO), SOurce COntrol of Priority Substances in Europe (SOCOPSE), and the WFD Explorer (Baartmans et al., 2009; Giupponi, 2007; Junier and Mostert, 2014).

Many of the river management DSSs implicitly take CECs into consideration, for instance in combination with nutrients, but without attention for their specific behaviour, toxicity or mitigation options (Delpla et al., 2014). In most fresh water-related DSSs the whole urban water cycle from wastewater, surface water and groundwater to drinking water, is not taken into account. The systems usually focus on only one part, either drinking water, wastewater and/or surface water (Delpla et al., 2014; EPA, 2007; Junier and Mostert, 2014; WHO/IWA, 2009).

Table 1 gives an overview of the existing fresh water-related decision support systems that includes CECs. SOCOPSE and WFD-Explorer are the only two DSSs (not under development), which specifically can address CECs and possible mitigation strategies, and will therefore be discussed further. In general, the usefulness and success of a DSS can be difficult to assess. For the WFD-Explorer, a paper on the development and use of the system, concluded that the tool was generally not used as hoped for. This was due to issues concerning the definition of the user group, the appropriate level of analysis and the expertise to be included (Junier and Mostert, 2014). A new and improved version was released in 2013, which has not been evaluated yet, but was used to study mitigation measures for pharmaceuticals (Coppens et al., 2015). With regards to the SOCOPSE DSS, no evaluation of the success was found, however it has been used within the project for five case studies (www.socopse.se). One of the learning points was that not all stakeholders necessarily had

the same level of knowledge. This is when a DSS can help to level out this difference, and serve the relevant stakeholders to find common ground (personal communication R. Baartmans). The usefulness of SOCOPSE was reviewed in a master thesis from Uppsala University, and was found valuable, but points of improvements were also given (Andersson, 2009). None of both DSSs provides an information basis directed towards management of CECs in general, within the whole urban water cycle. Also none of the two DSSs address mitigation methods in an integrated way, such as wastewater and drinking water treatment techniques, in combination with decentralised and non-technical methods. With non-technical methods we think of mitigation methods that fall within managerial, legal or societal actions such as temporarily stop the intake of drinking water, lobby for restrictions/bans of certain compounds, or increase awareness of the consequences of using certain compounds/products.

The objective of the DSS developed within the TAPES project framework, is to fill these gaps, as this is seen as a valuable addition to the existing fresh water-related CEC DSSs. Such a DSS will facilitate decision makers with the complex task of deciding on effective and efficient strategies to control CECs within their segment of the water cycle. The aim is to do this by providing CEC specific information on mitigation options relevant to the whole urban water cycle, including both centralised (wastewater and drinking water treatment techniques) and decentralised (such as direct water treatment at hospitals for example) technical mitigation options, as well as non-technical options. The developed DSS will be referred to as the TAPES DSS (tDSS) in the remainder of this paper.

Table 1. *Table of existing fresh water-related decision support systems that include CECs*

Name	Organisation/Project	Type	Applicable for	Description	Year	References
MULINO	The MULINO consortium/ EU FP5	Computer system CD-ROM	Competent water authorities	Enables sustainable use of water resources at a catchment scale.	2004	(Giupponi, 2007)
HACCP	EPA (USA)	Guidance document	Drinking water suppliers	Enables identification and control of microbiological contamination in the distribution system.	2007	(EPA, 2007)
SOCOPSE	The SOCOPSE consortium/ EU FP6	Guidance document	Water authorities	Enables management of EU priority substances at European, national or river basin level.	2009	(Baartmans et al., 2009)
Water Safety Plan Manual	WHO/IWA	Guidance document	Drinking water suppliers	Enables development and implementation of Water Safety Plans to systematically assess and manage risks.	2009	(WHO/IWA, 2009)
ARTEM-WQ	LERES (France)	Computer system	Small water supply systems	Calculates a health assessment based on water quality (with regards to micro pollutants), catchment type, treatment in place and DOC removal.	2013	(Delpla et al., 2014)
WFDE	Deltares	Computer system	Water management authorities	Calculates effect of restoration and mitigation on ecological and chemical quality of surface waters.	2013	(Junier and Mostert, 2014)
RiBaTox (under development)	SOLUTIONS consortium/ EU FP7	Web based system	Water authorities	Enables prioritisation, risk assessment and abatement of emerging pollutants and their mixtures.	2015	(Brack et al., 2015)

Name	Organisation/ Project	Type	Applicable for	Description	Year	References
tDSS	TAPES consortium/ EU Interreg IV B	Web based system	Decision makers within the urban water cycle	Enables management of CECs in the urban water cycle.	2015	This paper

2.3 tDSS design criteria

The objective of the tDSS, as outlined above, is the management of CECs in the whole urban water cycle, including an integrated assessment of possible mitigation methods beyond technical solutions. In general the management of CECs can be considered a 'wicked' problem, as legislation lacks to assess CECs in specific water bodies. A 'one-size-fits-all' solution does not exist, as this depends on the specific compounds and catchments. Finally, stakeholders differ in their problem perception, urgency and possibilities to take additional measures. Due to this 'wicked' nature, CEC DSSs should be designed to provide the various stakeholders with a common ground, from where discussions on the approach towards CECs can start, as was also experienced in the development of the SOCOPSE DSS. This requires close collaboration with stakeholders and end users, to make sure that the DSS considers all the perspectives of the stakeholders, and to ensure that all relevant variables are included in the DSS (Mitroff and Linstone, 1993; Shim et al., 2002; Wassen et al., 2011).

Furthermore, a strategy to avoid the DSS pitfalls should be part of the design criteria. Therefore flexibility of the DSS should be in focus, together with the stakeholders' possibilities to contribute to the development. It is also important to communicate the results of this approach, to cater for the learning process of the stakeholders and end users during the development, and to heighten the acceptability of the final DSS (Salewicz and Nakayama, 2004; Wassen et al., 2011). Finally, it is crucial to design a DSS that can be further developed (Newman et al., 1999), as the subject of CECs is continuously developing (Diamond et al., 2015) and a CEC DSS will quickly become outdated or obsolete. Table 2 summarises the design criteria for the tDSS.

Table 2. *Design criteria for tDSS.*

Criteria	
1	Solve 'wicked' problem: provide stakeholders with common ground for starting discussions of CECs, ensure close communication with stakeholders to include all relevant aspects.
2	Avoid pitfall 1: account for learning process of stakeholders throughout the DSS development.
3	Avoid pitfall 2: heighten acceptability of DSS by giving stakeholders continuous possibility of contributing throughout the DSS development.
4	Avoid pitfall 3: keep developing and updating DSS to avoid it becoming obsolete.

3 Methodology

3.1 Iterative process for the DSS design

3.1.1 Problem identification

Given the tDSS design criteria, the following methodology was used. To make the idea of the tDSS more tangible, a preliminary framework for such a DSS was developed in close collaboration with a key stakeholder (a water research institute), shown in Figure 1. The preliminary framework consisted of three levels:

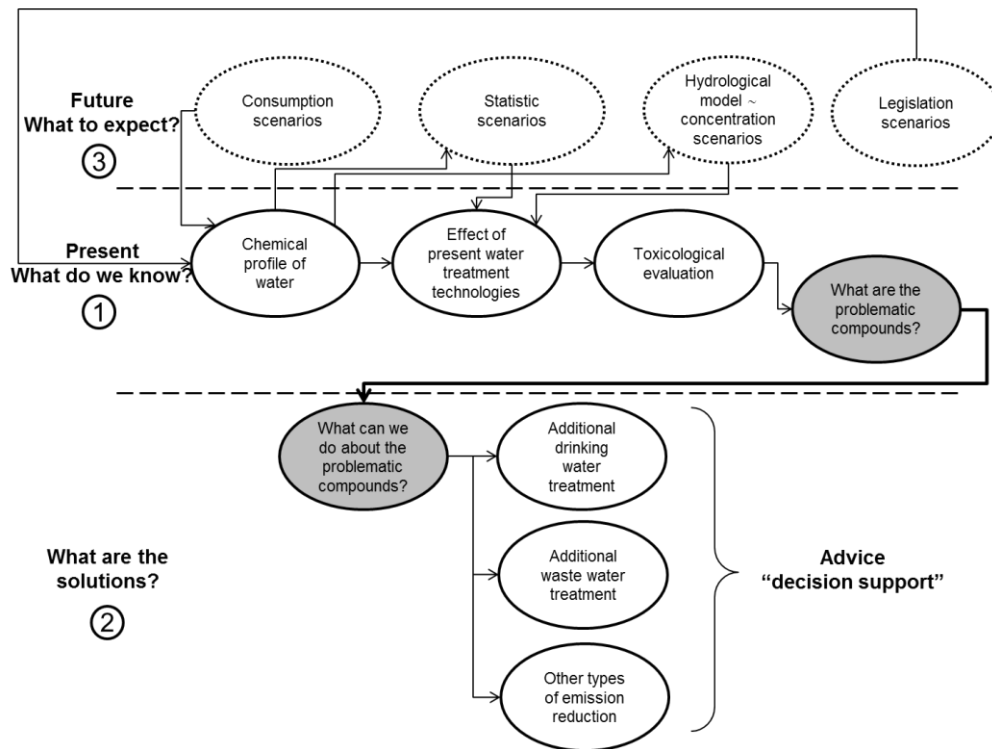


Figure 1. Schematic diagram of preliminary tDSS.

Level 1 – Present is mapping the present situation. This is done based on concentration levels of emerging substances in the surface waters of the catchment investigated. If needed, a post-treatment profile will be made, based on the water treatment technologies currently in place. Using this information a toxicological assessment will be made (Mons et al., 2013; Schriks et al., 2010).

Level 2 - Solutions is assessing which possible measures are available and applicable to the stakeholder, based on the outcomes of Level 1. This is evaluated within the categories additional drinking water treatment, additional wastewater treatment and possibly other types of mitigation methods such as legislation, decentralised removal techniques, awareness raising etc.

Level 3 - Future will simulate various future developments based on consumption, hydrological and/or legislative scenarios and statistics (van der Aa et al., 2011). In this way, the current situation mapped in Level 1 can be adjusted to future scenarios for decisions related to long term effects.

It is important to stress that this is the sketch of the *ideal* tDSS and an actual tDSS might not be able to fulfil all the desired functions due to cost, time or modelling issues.

With this preliminary framework as a basis, six potential users representing different actors within the water sector, were interviewed to understand the challenges they face when dealing with CECs (in this case a drinking water utility, a wastewater utility, a water board, two water research institutes, and a water management organisation). The interviewed parties were selected to cover the most relevant part of the urban water cycle. This was done to ensure that relevant stakeholder perspectives were heard and incorporated in the DSS. The stakeholders were contacted by e-mail and asked to participate in the interview. Employees relevant for the interviews, were identified by the companies and the interviews were scheduled. During a period of half a year, 21 people were interviewed mostly in groups of two, a few times one to one, and once a group of eight. All interviews were carried out as semi-structured interviews, and done face to face based on six open questions related to the preliminary tDSS framework (see supplementary materials 1). The open questions were deliberately very broad in scope in order to give the interviewed parties the possibility of addressing all the perspectives they felt were important to have included in the DSS. They were used as a starting point

for a discussion around that specific topic rather than a rigid structure that had to be confined to. The questions and the preliminary framework were emailed to the participants ahead of the interview to encourage the participants to prepare for the interview and ensure that all relevant aspects were touched upon. The interviews were recorded with a digital recorder, and notes were taken. When all interviews were carried out, the recorded interviews were analysed. In this case the interviews were used to obtain an overall idea of the stakeholders struggles with CECs. To analyse the interviews for this purpose, as efficient as possible, the interviews were not transcribed. The audio files were analysed by sampling and clustering (coding) the points raised in the interviews. The clusters were each related to a theme, and these main themes were then confirmed with a selected group of stakeholders, see section 3.1.2.

Based on the themes from the interviews, an initial framework for the *t*DSS was outlined detailing the information that should be available, see section 3.1.3. The *t*DSS was developed in iterative rounds in which three settings were used:

1. A larger group of stakeholders, water treatment experts and end users, focussing on the initial framework and first prototype
2. A smaller expert group (with people from the involved research institutes), focussing on the second prototype
3. Two DSS experts, focussing on the third prototype

This iterative development ensured continuous confirmation of the requirements for the DSS with the stakeholders, experts and end users. In this way the learning process of the stakeholders, experts and end users on what they need to make a good decision, could be followed and the content of the *t*DSS adjusted to the outcome of the learning (Salewicz and Nakayama, 2004). The close communication with all involved parties was also intended to improve the acceptability of the *t*DSS and avoid the second pitfall of many DSSs. The stakeholders could see an actual system develop and influence the process.

Finally, the iterative and ongoing development should prevent the DSS from becoming obsolete. The *t*DSS must continuously be developed further, in order to meet the expectations of the involved parties.

3.1.2 Problem formulation

The problem formulation for the *t*DSS was done based on the information obtained via the interviews. The overall conclusion from the interviews was that the stakeholders had sufficient information on CECs, but that the relevance of the information often was unknown. Main themes as identified from the analysis of the interviews are highlighted in table 3, for details on how the themes were derived see supplementary materials 2.

Table 3. *Main themes of tDSS derived from interviews*

Topic	Theme
CECs	Pathways
	Influence on environment
	Toxicity
	Monitoring/research
	Mitigation measures
	Cost of mitigation methods
	Policy
DSS	Integrated approach
	Issues
	Needs

Based on the themes and the points raised in the interviews, questions that the tDSS should answer to fulfil the wishes of the stakeholders were formulated:

1. What are the sources of CECs to water?
 - a. What is known on adverse effects on human health, the ecosystem or susceptible functions of the water system?
2. What are possible mitigation measures?
 - i. Which measures are available
 - ii. How to choose the location of these measures
 - iii. What are the future robustness of these measures, long term vs. short term
3. Possible future scenarios. The effects of climate change, changes in EU legislation, introduction of new chemicals on the market were mentioned amongst others in the interviews.
4. What are further research needs?

Other important points emerging from the interviews were the wish for a factsheet in the DSS, for easy access to information. Also transparency on the origin of all information included in the system, and the need for more than one answer to an issue was seen as important. An indication whether action on a short term basis should be taken (as response to a (eco)toxicological threat, or a breach of legislation), was an equally important point. Finally the system should be easy-to-use for both experts and non-experts.

The findings of the interviews and the formulated DSS questions were presented to a select group of stakeholders. The relevance of the questions was confirmed and it was decided to focus on the first two themes for the tDSS. This information was seen as most crucial, to enable better management of CECs in the urban water cycle.

3.1.3 Initial framework

Based on the problem formulation from the interviews, an initial framework for the content of the tDSS was constructed. This framework detailed the information that should be available in the tDSS in order to address the main questions deduced from the interviews. Figure 2 shows this framework.

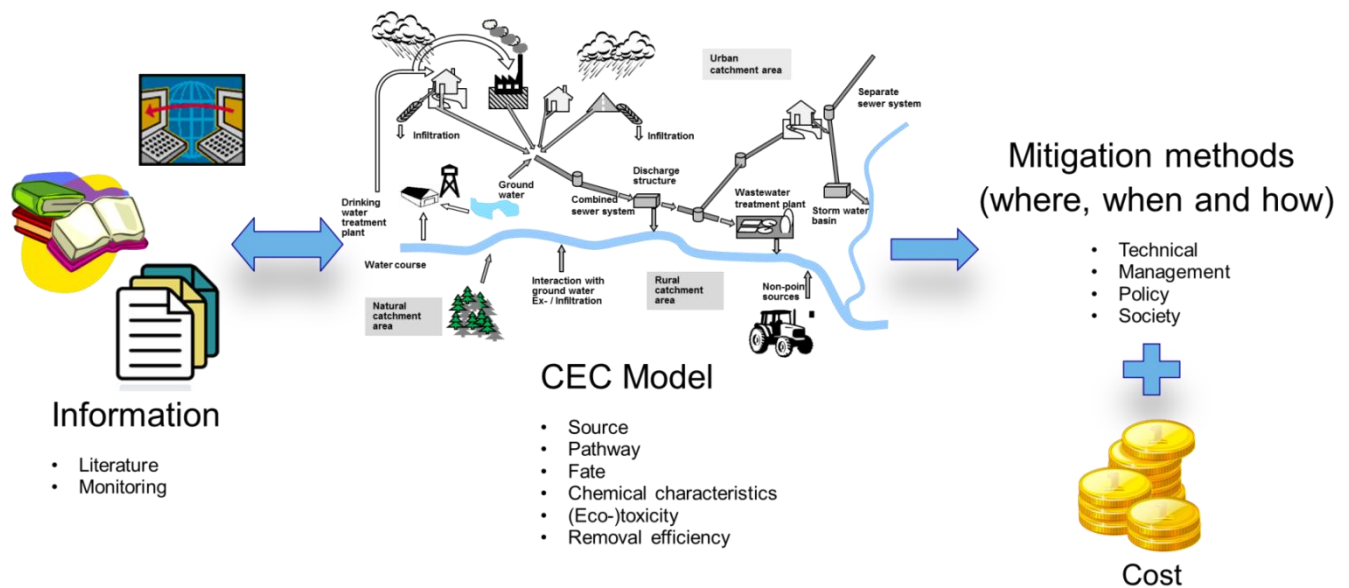


Figure 2. Initial framework of tDSS (water cycle diagram used by courtesy of Dr. E. Christoffels, Ertverband).

It was agreed with the stakeholders (setting 1) that the tDSS should provide the user with general substance information, such as physical/chemical characteristics and legislative framework, hazard (toxicity), water cycle entrance pathways and associated possible mitigation methods, and the ability to include monitoring results in order to assess environmental and human health risks. Data on water treatment efficiencies should be compiled for various drinking water and wastewater treatment technologies, as well as including decentral technical and non-technical mitigation methods, and where possible, the costs of these methods. The information in the tDSS should be relevant for many types of CECs. This because a variety of CECs from different uses, with different environmental entrances, different environmental fate and different toxicological properties all can be important to various stakeholders.

The stakeholders also agreed, that from the DSS typologies discerned (Power et al. 2002), a data and knowledge driven DSS would fit the requests best.

3.1.4 tDSS prototypes

Based on the previously described framework a first tDSS prototype was developed. This prototype was not well received by the involved parties (setting 1), even though the content was as previously agreed upon. There were discussions on the usefulness of the system and the presentation of the content. It was clear that the stakeholders and end-users were not sufficiently involved in the actual development of the prototype.

Based on this experience, an expert group consisting of a smaller group of the parties interviewed was created (setting 2). This group developed a more extensive and detailed framework for the tDSS (Figure 3), where it was ensured that the requests from the stakeholders were met. More elaborate illustrations of the way the content will be presented were also included. This framework was distributed in a wider group and agreed upon by all the involved parties.

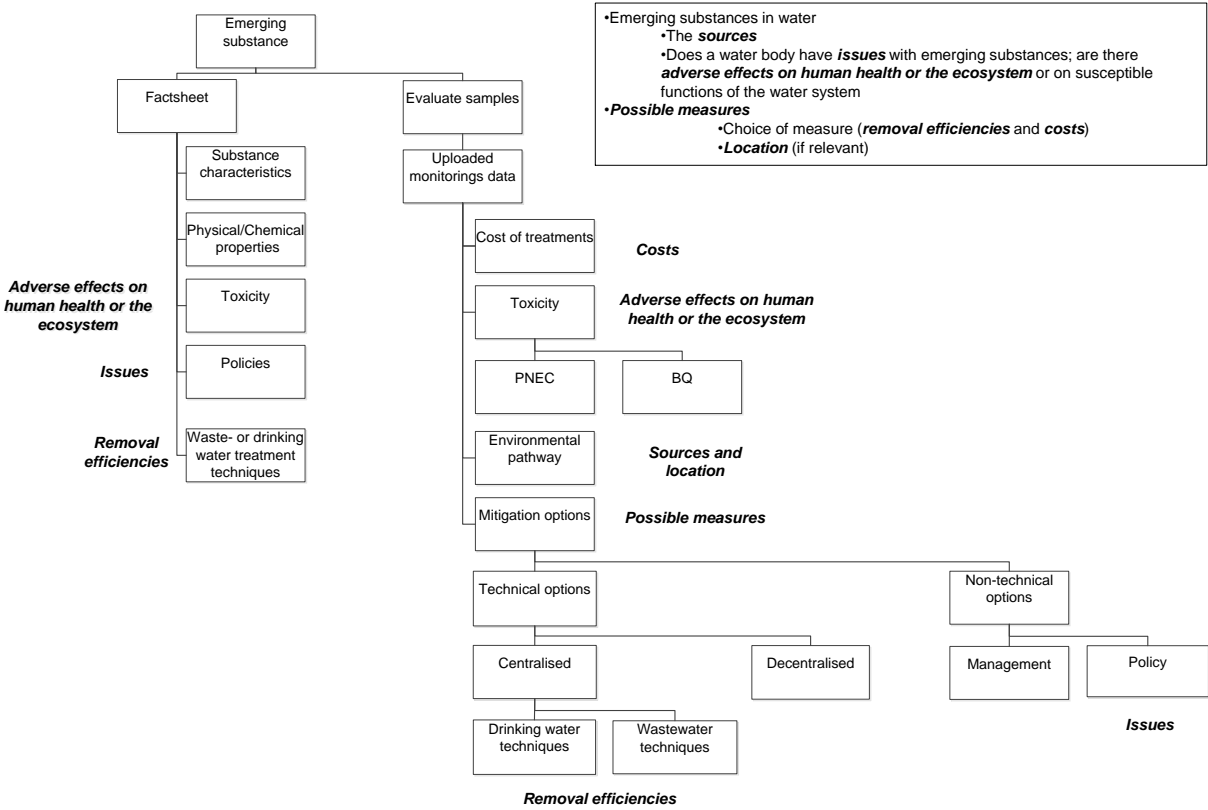


Figure 3. Diagram of information included in the DSS as per stakeholders requests.

1 Also a group of water treatment experts were approached to decide which physical/chemical
2 characteristics should be included in the system and which information on the treatment techniques
3 was relevant (see section 4.1, for details). The second prototype was well received, and development
4 of a third and final version was agreed upon. During this final phase (setting 3), the prototype was
5 tested on technical aspects (by a drinking water research company, experienced in developing
6 decision support systems), such as bugs, understanding of screen texts, ease of use of the DSS etc.
7 At the same time, the content of the system was tested, e.g. on the relevance of the diagrams and the
8 information given.

9
10 The main lesson from the development phase of the *t*DSS was that the presentation of the data was
11 crucial, especially since the *t*DSS was also meant to be used by non-experts. The output should be
12 unambiguous. It is important that this is thoroughly discussed at length and that agreements are well
13 documented.

14 **3.2 DSS Data sources**

15
16 A literature study was used to gather a database of removal efficiencies for the central mitigation
17 options, wastewater and drinking water treatment technologies. Currently the CEC groups industrial
18 by-products, solvents, flame retardants, pharmaceuticals, pesticides and the group other (for
19 compounds from road traffic or surface water usage) are in the *t*DSS. The focus was on the reduction
20 of concentrations of these chemicals by various commonly used treatment techniques for drinking
21 water and wastewater, such as flotation/coagulation, powdered activated carbon dosage, granular
22 activated carbon filtration, advanced oxidation and membrane filtration. These techniques were
23 chosen as there is a vast amount of data available on their efficiency in removing CECs, that could be
24 fed into the *t*DSS. Negative efficiencies were not included in the collected data as they can be a result
25 of; lower recovery and detection of substances in influent matrixes; random differences due to high
26 fluctuations of concentrations in influents and effluents; or transformation processes during treatment
27 leading to increasing concentrations of certain substances. Including such data would increase
28 uncertainty and were therefore not included in the current *t*DSS. The scale of the test (lab, pilot or full
29 scale), the initial concentration, the contact time, the range and average of removal efficiencies
30 measured, and cost per m³ water treated were included to differentiate between seemingly similar
31 treatments. In total, approximately 1000 entries for more than 80 chemicals were collected. So far nine
32 of these compounds are included in the *t*DSS, namely AMPA, bentazon, carbamazepine, chloridazon,
33 diclofenac, glyphosate, MCPA, metamitron and sulfamethoxazole. These compounds were seen as
34 relevant to the project partners and represented two of the CEC groups the *t*DSS was built to
35 accommodate namely pharmaceuticals and pesticides.

36
37 New data were created for a set of approximately 73 chemicals, which involved the drinking water
38 treatment techniques including; UV/H₂O₂, nanofiltration, granular activated carbon (GAC) filtration,
39 affinity adsorption (Bäuerlein et al., 2012), and the wastewater treatment techniques powdered
40 activated carbon (PAC), ozonation, retention soil filters (Christoffels et al., 2014), UV (+H₂O₂), the 1-
41 STEP filter (Hulsmann, 2016) and Dissolved Air Flotation (DAF). These new data on removal
42 efficiencies will also be included in the *t*DSS, except for; the affinity adsorption, as this is a new
43 technique and not yet commercially available; the 1-STEP filter which is currently not suitable for long
44 term treatment; and DAF which is not effective against CECs. An in-depth overview of the data
45 covered in this treatment database including the search criteria and experimental methods used, and
46 analysis of these results, will be published at a later stage.

47
48 In addition to central mitigation techniques, a desk study on possible decentralised technical and non-
49 technical abatement methods was carried out. As for many of these solutions the efficiency and costs
50 are currently difficult to quantify, qualitative information on these issues are provided in the *t*DSS when
51 relevant to the nine compounds in the system.

4 Results and discussion

4.1 tDSS content

In the following the information included in the tDSS to answer the problem formulation is discussed. It is detailed what information is available under the headings of figure 2, section 3.1.4.

4.1.1 Substance characteristics and physical/chemical properties

The CECs are characterized by name, CAS number, chemical structure (SMILES) and use(s). Based on the relevance for environmental fate and water treatment, the following chemical-physical properties are included; vapor pressure, melting point, polarizability, solubility, log K_{ow} and log D, flash point, pK_a , molecular mass, total biodegradation and estimated total wastewater treatment removal (de Ridder et al., 2010; Delgado et al., 2012; Schriks et al., 2010). The total biodegradation and total waste water treatment removal are based on the information given in EPI Suite™ Version 4.11 (EPA, 2012).

4.1.2 Environmental pathway

A common way to group substances is based on their type of use, such as pharmaceuticals, pesticides, industrial compounds, personal care products etc. (Schwarzenbach et al., 2006). The source is the place where the substances are originally used, such as household and healthcare sector, agriculture and greenhouses, trade and industry, road traffic and surface water usage such as shipping or recreation. The input routes (environmental pathways) are often comparable for a type of chemical use, as is the legislative framework for their market authorization. Major input routes are wastewater treatment plants (WWTP) effluents and sludge, sewer overflows, industrial discharges, and diffuse entrances such as soil erosion, surface runoff, interflow through the soil and deposition, or direct emission to the surface water through shipping or recreational use. When the environmental pathway of a specific (group) of CECs is known it is often easier to decide on which mitigation options are most suitable as these options are typically coupled to sources and/or input routes. The types, sources, input routes and mitigation categories used in the tDSS are outlined in Figure 4.

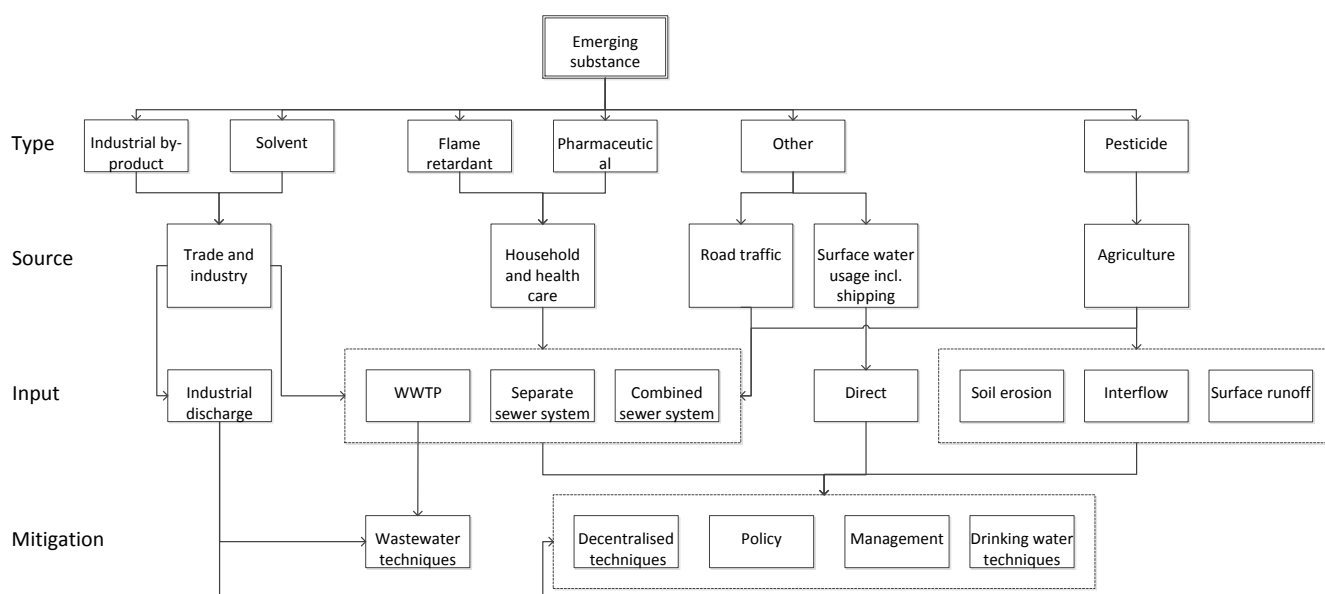


Figure 4. Types, sources, input routes and mitigation categories included in the tDSS.

4.1.3 Toxicity

Adverse effects of CECs to both humans and the ecosystem are of importance. To assess the effects and associated risk, information on both toxicity and exposure is necessary and can be used to assess if action is needed and to prioritize the CECs. Human toxicity of CECs and their mixtures, is relevant with regards to drinking water production, agriculture, fishing and recreation. The tDSS is

1 firstly focused on drinking water relevance by comparing a (provisional) drinking water limit to
 2 occurrence data (Bruce et al., 2010; Schriks et al., 2010). This method can be used for substances
 3 when a Tolerable Daily Intake (TDI), Advisable Daily Intake (ADI) or toxicity data, such as No
 4 Observed Adverse Effect Levels (NOAELs) from literature, is available. For substances where such
 5 information is lacking, as a first conservative approximation, the Threshold of Toxicological Concern
 6 (TTC) can be used (Kroes et al., 2000; Kroes et al., 2004; Mons et al., 2013; Schriks et al., 2010).

7 Predicted No Effect Levels (PNEC) which are relevant for the aquatic ecosystem were added to give
 8 an indication of the ecotoxicity of the compound.
 9

10 4.1.4 Policies

11 Various water quality limits for chemicals in surface waters are included in the rDSS to give water
 12 managers insight into whether they are in breach with any legislation. Limits currently included are the
 13 Water Framework Directive, the Dutch drinking water law, and the non-legally binding Danube, Meuse
 14 and Rhine Memorandum (Drinkwaterwet, 2015; EU, 2000; Wirtz, 2009). The information consists of
 15 the name of the compound (for which it is in force), limit value, name of the legislation and country
 16 (where it is in force).
 17
 18

19 4.1.5 Mitigation options

20 Within the rDSS the mitigation options are categorised based on their technical or non-technical nature
 21 as shown in Table 4. The technical measures are split into centralised options such as wastewater
 22 and drinking water treatment technologies, and decentralised options, such as technical measures at
 23 the source. The non-technical mitigation methods, such as, additional policy making, raising
 24 awareness of consumers, or agreements with farmers are divided in to the categories management,
 25 policy and society.
 26
 27
 28

29 Table 4. CEC DSS mitigation categories
 30

31 Main category	32 Sub category 1	33 Sub category 2	34 Examples of mitigation methods	35 Currently included in CEC DSS
36 Technical	37 Centralised	38 Drinking water treatment techniques	39 Flotation/coagulation, activated carbon, advanced oxidation, membranes and biological treatment.	40 All except biological treatment
		41 Wastewater treatment techniques	42 Flotation/coagulation, activated carbon, advanced oxidation, membranes and biological treatment.	43 All except biological treatment
	44 Decentralised	45 Agriculture - spray free zones, drip appliances. 46 Sewer overflow - retention soil filters. 47 Household and healthcare – on site treatment.	48 Yes	
49 Non-technical	50 Management	51 Change abstraction source. 52 Temporarily stop water intake.	53 Yes	
	54 Policy	55 Restrictions/bans of certain CECs.	56 Current restrictions in place included	
	57 Society	58 Increase awareness of the consequences of using certain CECs for both producers and consumers. 59 Change CEC production process.	60 Not included at the moment due to the complexity of quantifying the effect of such a measure	

In the *tDSS*, it is possible to choose between the mentioned mitigation subcategories to access information on the various mitigation methods in the selected sub category. The information available is based on the literature studies described in the methodology section. The removal efficiencies of the central water treatment techniques are presented using box plots (Figure 5).

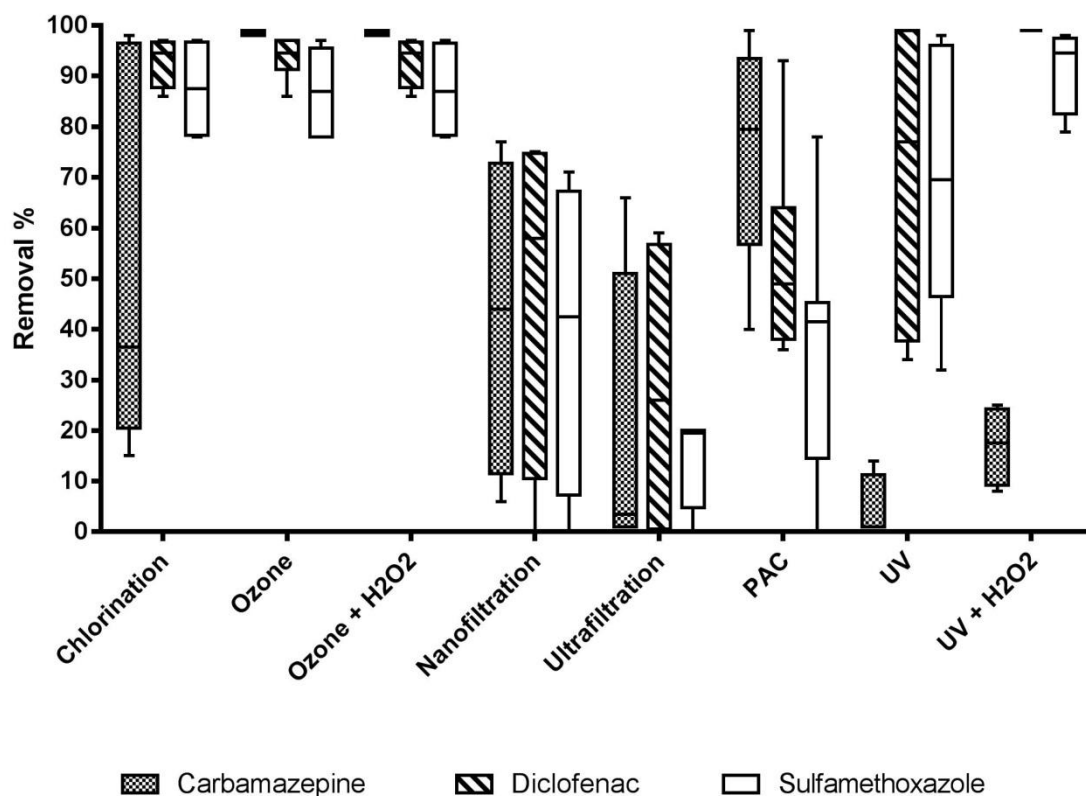


Figure 5. Boxplot of the removal efficiencies of a selection of drinking water treatment techniques for the compounds carbamazepine, diclofenac and sulfamethoxazole from the database. The whiskers of the box plot (25th and the 75th percentile) depicts the minimum and maximum of the removal efficiencies.

The information on possible decentralised technical and non-technical abatement methods are given in the form of a list detailing the compound for which; the option is valid, the option itself, possible location of the option, target groups of compounds, removal efficiency if known, costs if known, and references to the literature used.

This information informs the user on which mitigation options are possible for a given compound, their efficiency and where available, the costs of these.

All the above information detailed in sections 4.1.1 to 4.1.5, can only be filled in by individuals with an administrator password. Currently this is limited to the people who developed the system.

4.1.6 Monitoring measurements

To assess the situation for a specific water body or location, location-specific monitoring data can be uploaded in the *tDSS*. In this scenario, the following information is requested: compound(s) measured, location of sample, date, concentration of compounds measured, level of detection/level of quantification (LOD/LOQ) of the analytical technique, analytical-chemical technique used and unit of concentration. Each user can upload this information to the system. This is used to assess the potential drinking water relevance by comparing the monitored concentration to a (provisional) drinking water limit, as also mentioned in section 4.1.3 (Bruce et al., 2010; Schriks et al., 2010).

4.2 tDSS output

In summary, the tDSS provides the user with a factsheet containing information of a single substance (Figure 6), and the ability to upload monitoring results and get information relevant for a specific water matrix. The factsheet contains:

- Physico-chemical characteristics, relevant to the removal efficiency for different water treatment techniques.
- Human toxicological values relevant to assess safe exposure levels (ADI,TDI,NOAEL).
- Overview of relevant policies per compound (European Water Framework Directive, local drinking water policies etc.)
- Type, source and input route of the compound.
- Overview of drinking water and wastewater treatment removal efficiencies
- Overview on possible decentral technical and non-technical mitigation methods.

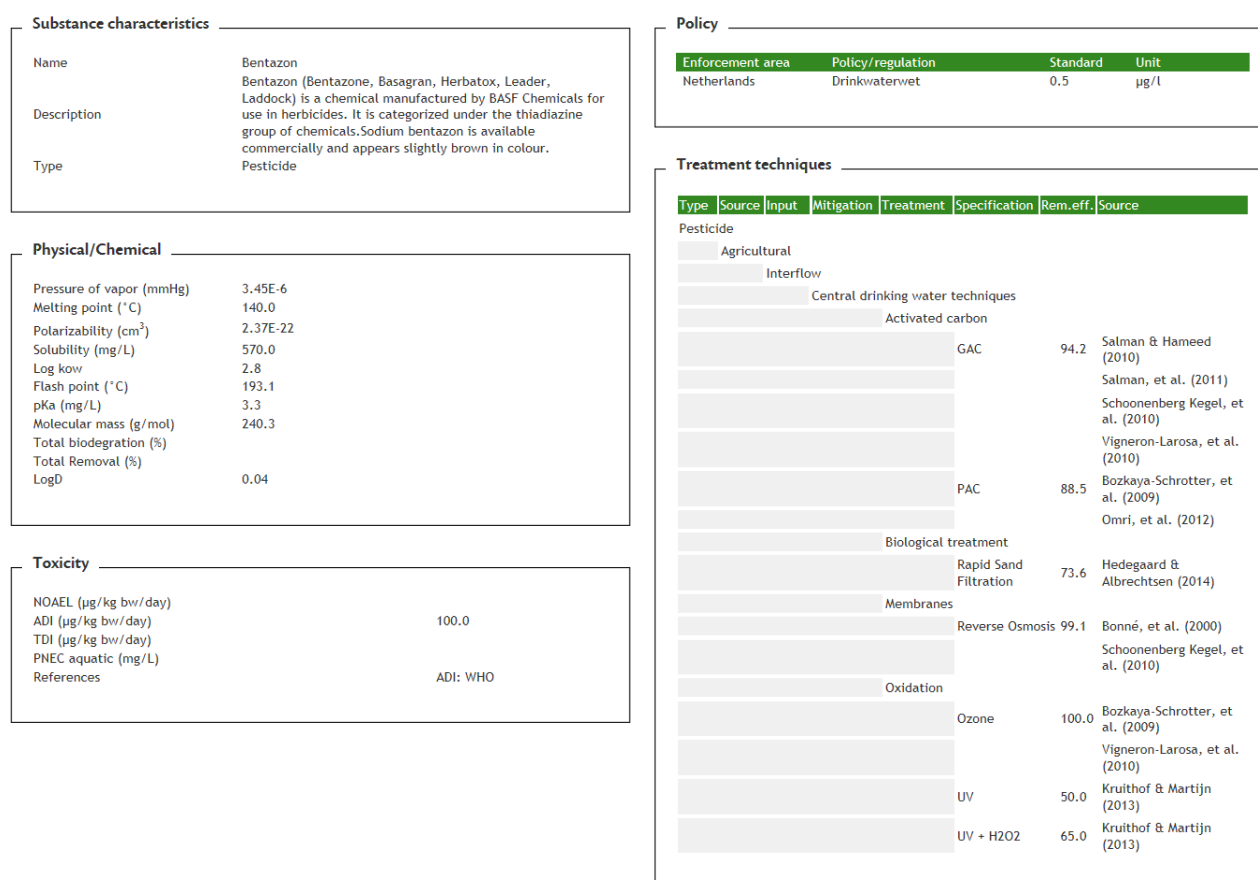


Figure 6. Screenshot of the factsheet for the compound bentazon.

Information on multiple compounds at the same time, can be presented based on the uploaded water quality monitoring results, and provides:

- Assessment of the safety of drinking water production, based on uploaded concentrations and (provisional) drinking water guidelines.
- Eco-toxicological values relevant to assess safe exposure levels (PNEC). At a later stage, a similar approach as for the drinking water safety assessment, can be incorporated to assess adverse effects on ecosystem using relevant eco-toxicological thresholds.
- Diagrams showing the water cycle entry routes for the selected compounds.
- Boxplots of drinking water and wastewater treatment removal efficiencies.
- Overview of relevant policies for the compounds (European Water Framework Directive, local drinking water policies etc.)

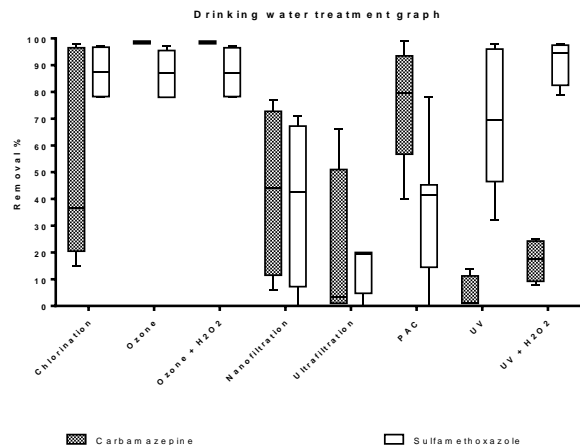
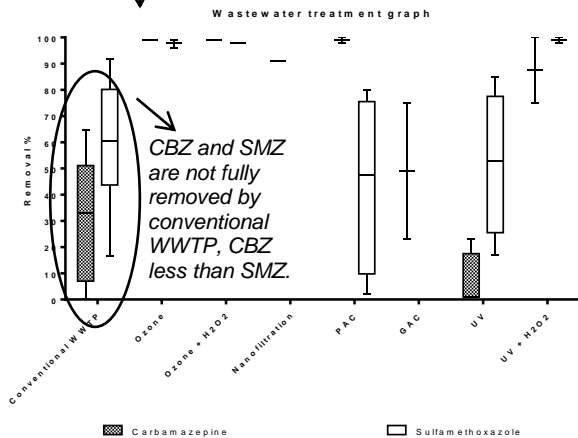
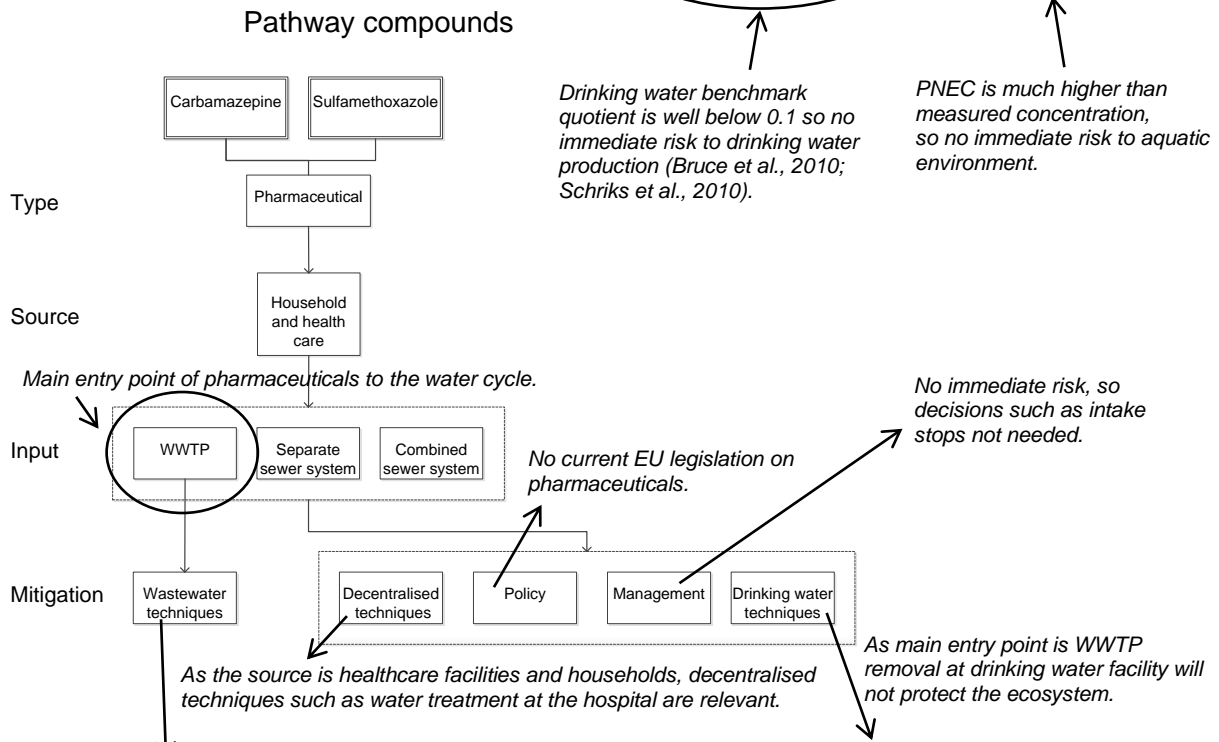
- Overview of decentral technical and non-technical mitigation options.

In Box 1 an example of the decision support the tDSS offers is highlighted for the two pharmaceuticals carbamazepine and sulfamethoxazole.

Box1: tDSS decision support in case of the two pharmaceuticals carbamazepine and sulfamethoxazole

General Information	Carbamazepine	Sulfamethoxazole
Description	Carbamazepine (CBZ) is an analgesic/antiepileptic drug. It was discovered in Switzerland in 1953.	Sulfamethoxazole (SMZ or SMX), is an antibiotic. It was used for bacterial and is effective against both gram negative and positive bacteria such as <i>Listeria monocytogenes</i> and <i>E. coli</i> .
Type	Pharmaceutical	Pharmaceutical

Concentration	Chemical of emerging concern	Drinking water benchmark quotient	PNEC
0.1 µg/L	Carbamazepine	0.002	0.0025 mg/L
0.01 µg/L	Sulfamethoxazole	0.00013	0.0021 mg/L



Most additional treatment steps will when optimised remove the pharmaceuticals in wastewater, except UV for CBZ.

Ozone (+H₂O₂) treatment seems the most promising technique to remove the substances from drinking water. PAC is also an option for CBZ, and UV (+H₂O₂) for SMZ.

4.3 Comparison of final *t*DSS to the original design criteria

4.3.1 *Addressing the design criteria*

Due to the 'wicked' nature of the problem formulation for the *t*DSS, the system is designed to provide the various stakeholders with a common ground, where discussions on the approach towards CECs can start. This is done by developing the *t*DSS in iterative rounds, in close collaboration with stakeholders and end users, to make sure that the *t*DSS considers all the perspectives of the stakeholders, and to ensure that all relevant variables are included in the *t*DSS. The *t*DSS is developed as a data and knowledge driven system. To fulfil the specific wishes of the stakeholders, a factsheet is available, together with clarity on the origin of all information included in the system. The *t*DSS does not dictate whether action should be taken, as mentioned in section 2.1, the role of DSSs are to *support* people in making decisions, not to *make* the decision itself. The *t*DSS supports the decision making by giving access to relevant CEC information, indicating whether current legislation is breached, if adverse effects may occur, and by providing the user with possible mitigation options (Halden, 2015). The request for information on the susceptible functions of the specific water systems and details on short term vs. long term solutions, has not (yet) been fulfilled. However, it is planned to incorporate these functions into the *t*DSS in the future. The system is considered simple and easy to use for both experts and non-experts. Effort has been made to make the system self-explanatory with informative screen texts and a few short instruction videos.

The iterative process has helped to avoid typical aforementioned pitfalls for DSSs. It enabled insight to the learning process of the stakeholders and end users, and made clear what information was needed to support them in managing CECs in the urban water cycle. This approach also heightened the acceptability of the *t*DSS, as was seen in the positive response to the final prototype. To avoid the developed DSS becoming obsolete, it was decided that several stakeholders would continue to develop the *t*DSS.

In conclusion the design criteria highlighted in section 2.3 have been fulfilled.

4.3.2 *Stakeholder responses*

The stakeholders involved in the process of developing the *t*DSS were satisfied with the third and last *t*DSS prototype, the information it contained and the way this information was presented. A follow up of the *t*DSS named AbatES is now part of the international Watershare network, which contains expert tools for the water sector (www.watershare.eu). The Watershare network has 18 members from 15 countries. Furthermore a Community of Practice has formed for this tool to share their experiences with it, and possibly develop it further.

To assess the usefulness of the system for a new user group that had not been involved in the development, the final prototype was presented to an international group of potential new users to obtain their initial reactions to the system. Also in this setting, the system was well received and seen as useful and relevant. One of the participants, a water treatment manager, stated that the *t*DSS contained exactly the information he was interested in and it was therefore seen as a useful application.

4.3.3 *Future developments*

The following future developments are planned:

- Inclusion of all information required via literature research, beyond the nine test compounds,
- Inclusion of an ecotoxicology risk calculation, based on uploaded monitoring data or effect measurements;
- Inclusion of evaluation for the complete mixture of compounds, based on uploaded monitoring data;
- Inclusion of other water uses with relevance for human health, next to drinking water;
- Inclusion of more data on (non)-technical abatement options; and

- Expansion of the possibilities to upload monitoring data, and possibility of sharing monitoring data with others.

5 Conclusions

The objective of the *t*DSS was to facilitate decision makers with the complex task of deciding on effective and efficient strategies to control CECs within their segment of the water cycle. The *system* had to meet various design criteria such as to provide the various stakeholders with a common ground, where discussions on the approach towards CECs could start, while avoiding common DSS pitfalls. Also, specific stakeholder requests should be fulfilled in the system such as by the inclusion of a factsheet, transparency on the information in the system, an indication of the possible need for short term action, while it being easy-to-use for both experts and non-experts. Via an iterative development process in close communication with the stakeholders, these criteria were met. The final *t*DSS contains; CEC related information on physical/chemical characteristics, legislative framework, hazards, water cycle entrance pathways and associated possible mitigation methods, it includes the possibility of uploading monitoring data to assess risks in a specific water system. The novelty of the system is the integrated way of addressing mitigation options, such as wastewater and drinking water treatment techniques in combination with decentralised and non-technical methods. The iterative development process and the resulting *t*DSS was positively received by the involved stakeholders and with interest from potential new users. A follow up of the *t*DSS named AbatES is now part of the international Watershare network, which contains expert tools for the water sector (www.watershare.eu). Further development is planned to make sure that the system will continue to meet the requirements of current and new users.

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Decision support for water quality management of contaminants of emerging concern

Supplementary Material 1: Discussion points

1. What kind of decisions do you need to make with regards to the management of emerging substances within your organisation?
2. In general when making decisions regarding the management of emerging substances within your organisation what do you struggle with?
3. Do you feel that lack of knowledge in certain areas are preventing you from making informed decisions on how to manage emerging substances within your organisation? If yes in which areas are knowledge missing?
4. How should an ideal Decision Support System in your opinion help you make the right decisions?
5. What kind of output would you like/expect from a Decision Support System that should help you make informed decisions with regards to the management of emerging substances within your organisation?
6. What possible barriers could you think of that might prevent your organisation from implementing a solution given by the Decision Support System?

Decision support for water quality management of contaminants of emerging concern

Supplementary Material 2: Derived themes from interviews

	Theme	Points from interview	Stakeholder
CECs	Pathways of CECs	<ul style="list-style-type: none"> Total pathway (above and under catchment) Identify important players with regards to source, pathway and fate Insight into the source (linked to measures) Mass balance Total emissions Effluent emissions 	drinking water utility, wastewater utility, water board, and water management organisation
	CEC influence on environment	<ul style="list-style-type: none"> Effect of CECs on ecology Species related Target species Water Framework Directive limits Sensitive stretches Impact of WWTP at sensitive stretches of rivers 	wastewater utility, water board, water research institute
	Toxicity of CECs	<ul style="list-style-type: none"> Toxic effects <ul style="list-style-type: none"> Is there an issue? Mixture toxicology Toxicity of groups of compounds <ul style="list-style-type: none"> Long term Acute Metabolites and their toxicity <ul style="list-style-type: none"> Effect measurements before and after treatment More stable More toxic Cumulative effect of concentrations already in the water and legal discharge 	drinking water utility, wastewater utility, water board, water research institute, water management organisation
	Monitoring/research	<ul style="list-style-type: none"> Where should research money go Set-up of monitoring programme: <ul style="list-style-type: none"> Which compounds Best way of monitoring (bioassay-measurements-consumption) How much do we need to monitor (screening, relevance, ecology) Based on legal limits (to comply with legislation) 	wastewater utility, water board, water research institutes
	Mitigation measures	<ul style="list-style-type: none"> QSARS Predict behaviour <ul style="list-style-type: none"> WWTP drinking water treatment plant environment Removal efficiency of treatment technology <ul style="list-style-type: none"> Based on literature Own tests In treatment plants 	drinking water utility, wastewater utility, water board, water research institute, water management organisation
	Cost	<ul style="list-style-type: none"> Where can I use the EUR best? Cost of measures <ul style="list-style-type: none"> Cost of adaptation of WWTP Cost of monitoring 	drinking water utility, wastewater utility, water board, water management organisation
	Policy	<ul style="list-style-type: none"> Factsheets related to legislation (health 	drinking water utility,

		<p>based values)</p> <ul style="list-style-type: none"> • Legislation is too slow • EU legislation is too political • Lack of legislative limits (EU based on annual averages, issue for pesticides) • Lack of norms (threshold limits) • EU aim for simpler water treatment vs. need to deal with CECs 	wastewater utility, water board, water research institutes, water management organisation
DSS	DSS integrated approach	<ul style="list-style-type: none"> • Not only technical solutions • Social <ul style="list-style-type: none"> • Raising awareness (pharmaceutical) industry • Limit production • Intake management • Show examples of measures and techniques • Integrated effect of more aspects (cost & efficiency) • Transnational issue <ul style="list-style-type: none"> • International cooperation • Looking at the whole water cycle <ul style="list-style-type: none"> • Cooperation in whole water cycle (also NGO's) • Compound specific approach 	drinking water utility, wastewater utility, water board, water research institutes, water management organisation
	DSS issues	<ul style="list-style-type: none"> • Lack of monitoring data • Language (in DSS) • Sensitivity of information (where is the water not safe) • Will there be enough information on level (concentration, load, use) of ES for local use • Can the DSS consider all (important) aspects • The interest in CECs is variable • No harmonisation in the water cycle (different players have different approaches to established issues) • Validation (who, how) • Validity of possible toxicological evaluation • Complexity! • Needs to be maintained • Who controls the DSS • Does it already exist • Who will pay (for the mitigation measures) 	drinking water utility, wastewater utility, water board, water research institutes, water management organisation
	DSS needs	<ul style="list-style-type: none"> • Factsheet! • Regionally adaptable • Simple • Convincing • More than one answer • Easy to use • For policy makers • For management • Transparent • Tailored to user • Realistic • Give advice • Scientifically sound • Traffic light to indicate if action is needed 	drinking water utility, wastewater utility, water board, water research institute, water management organisation