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DOI
10.1039/C7EW00077D

Publication date
2017

Document Version
Final published version

Published in
Environmental Science: Water Research & Technology

Citation (APA)
Van Wezel, A. P., ter Laak, T., Fischer, A., Bäuerlein, P. S., Munthe, J., & Posthuma, L. (2017). Mitigation options for chemicals of emerging concern in surface waters; operationalising solutions-focused risk assessment. *Environmental Science: Water Research & Technology*, *2017*(3), 403-414. https://doi.org/10.1039/C7EW00077D

Environmental Science
Water Research & Technology

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Cite this: *Environ. Sci.: Water Res. Technol.*, 2017, **3**, 403

Mitigation options for chemicals of emerging concern in surface waters; operationalising solutions-focused risk assessment

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Received 8th March 2017, Accepted 7th April 2017

DOI: 10.1039/c7ew00077d

rsc.li/es-water

The water system provides many services to society; industries, municipalities and agriculture all withdraw, use and return water and demand a water quality fit for the intended purposes. Both global production of chemicals and global water withdrawal grow faster than human population. This implies increased chemical threats to water, and creates a strong driver for mitigation to protect human health, ecosystem integrity and ecosystem services. Here we connect the perspectives of the water cycle and the chemical life cycle and review possible mitigation options. We categorize mitigation options in various stages of the chemicals' life cycle, taking various sectors and environmental pathways into account. More technologically oriented *versus* other types of mitigation options are discerned, and their relevance on spatial and temporal scale is discussed. We review various water treatment techniques in relation to physical–chemical properties of chemicals. Finally we discuss how a mitigation database can be used to assess the effectiveness of interventions, by coupling them to regional or global hydrological models. A solution-focused and systems-oriented perspective combined with a mitigation database offers a common perspective amongst actors on the effects for water quality of possible mitigation options throughout the chemical's life cycle, in various sectors and at various places in the water system. This can stimulate coherent implementation of effective mitigation options, cross-sectoral learning and further innovations to improve water quality.

Water impact

Water quality research focuses on problem analysis, however for complex environmental mixtures prioritization of possible mitigation options might better drive effective and innovative approaches then prioritizing individual chemicals. Given the nexus of the water cycle and chemical life cycle, we propose how a mitigation database can be used to evaluate effective mitigation to improve water quality in a river basin.

1. Introduction

The water system provides many services to our society. Industries, municipalities and agriculture all withdraw, use and return water.[1] Depending on the world region, the withdrawal for industrial uses varies from 5 to 65%, for municipalities from 5 to 33% and for agriculture from 16 to 89% of the total withdrawal, respectively. Global water withdrawals increase 1.7 times faster than the global population growth. After it's use, water quality is changed with regard to chemicals, micro-organisms and renewable resources present in the water. This affects fit-for-purpose quality of the water for other users in the water cycle, and human and environmental risks related to the water quality. The water system integrates these various uses and requests, and upstream water use and return influence possible down-stream uses in a river basin (Fig. 1).

Chemicals are used for various beneficial purposes, such as crop protection, flame retardation, food conservation, disease recovery, *etc.* Over 347 000 chemicals are registered and regulated *via* national and international authorities (CHEMLIST), and new chemicals enter the market continuously. The global volume of production of chemicals grows faster than the global human population.[2] The chemicals and their transformation products enter the aqueous environment as a result of emissions that can occur during all stages

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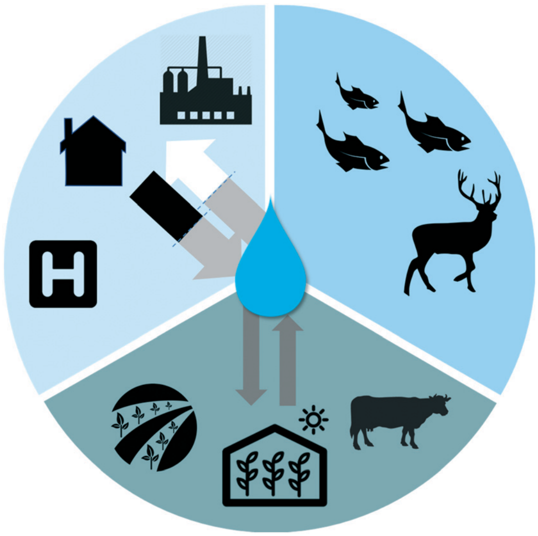

Fig. 1 The water system as integrator of urban and rural water withdrawals and returns, where sectors and nature demand sufficient water quality fit for purpose. Arrow widths summarize volumes abstracted in the EU context (FAO AQUASTAT data) for urban withdrawals (industry and municipalities) and rural withdrawals (agriculture), arrow darkness represents the presence and concentrations of chemicals.

of their life cycle.[3] Major environmental entry routes are household and industrial effluent treatment plants, agricultural run-off, infiltration into groundwater, combustion and evaporation and incidental spills. Since the analytical capabilities to detect the presence of chemicals in the water increase,[4] many stakeholders in the water cycle are more aware of the presence of many chemicals in waste water effluent, surface and ground water and drinking water.[5–7]

This triggers the question whether regulatory efforts are sufficient to understand and manage the problems arising at the water–chemical cycles' interface. A well-known approach is to derive environmental quality standards and judge environmental quality per chemical. For the majority of chemicals however, no official quality standards have been derived, neither for drinking water nor for environmental risks. When standards are available, environmental concentrations are normally lower than (preliminary) limits for adverse human health effects, so for individual compounds negligible human health risks are expected.[8] However, the toxicological relevance of complex environmental mixtures is debated, especially related to potential endocrine disruption.[9–11] Consumers express their concerns regarding chemical contamination of drinking water[12] and the topic of water pollution is increasingly mentioned in the media.[13] Impacts as a result from the presence of chemicals in aquatic ecosystems can be demonstrated,[14] as well as in the food chain[15] and there is evidence for adverse effects on human health and ecosystem threats at local to global scales.[16] As both water withdrawals and chemical emission grow, increasing deterioration of water quality can be a result. This may hamper sectors using the water, thus water quality deserves urgent attention as essential element of water security.[17] Moreover, in view of the circular economy a recently formulated policy goal is to strive towards a non-toxic environment by 2020.[18] For all these reasons, there is a strong drive to put additional efforts into measures that prevent chemicals from entering the water cycle, and to reduce exposures and effects.

Current research and policy attention is often mainly directed to prioritization of the most problematic chemicals,[19] in order to take measures to prevent and reduce specifically their particular emissions. As compared to other environmental problems such as climate change,[20] relatively little attention has been paid to mitigation possibilities for chemicals. This whilst smart solutions by tackling multi-chemical emissions may bring the non-toxic environment closer by. Mitigation strategies are defined in this context as 'interventions with the objective to reduce the chemical loads in water systems, thereby reducing the concentration, exposure and adverse effects for humans and the environment and increasing the possibilities to use the water safely for a variety of services'.

Here, we review possible mitigation options to improve water quality. We describe the nexus of the water cycle and the chemical life cycle, and the idea of a tailored multi-chemical mitigation strategy. We propose a mitigation database and discuss how such a mitigation database can be useful to generate tailored solutions to problematic chemical emissions, and to evaluate the effectiveness of packages of mitigation options for a river basin.

2. Existing chemicals' legislation

Existing regulations focus at various life stages of chemicals. In the European Union, legislation of chemicals for registration and authorization to gain access to the market is organized per chemical use type (Fig. 2). Examples for the a) industrial, b) agricultural, c) household and care sector are respectively a) the REACH legislation (EC 1907/2006) for industrial chemicals, b) the Plant Protection Product Regulation (1107/2009/EC) for pesticides and EU Directive 2001/82/EC for veterinary pharmaceuticals, and c) the Biocidal Product Regulation (528/2012/EC) for biocides, the EU Directive 2001/83/EC for pharmaceuticals and again the REACH legislation for chemicals used in cleaning products, paints and consumer articles, *etc.* Chemicals incorporated in products such as food additives, cosmetics or toys, are regulated under respectively EC 1331–1334/2008 for food additives including enzymes and flavourings, the EU Cosmetics Directive (76/768/EEC) and the EU Toys Directive 2009/48/EC. Information on authorizations and risk evaluations are typically operationalized for practical use *via* annexes to these regulations.

Second, regulations can focus on the end-of-life stage such as the EU Waste Framework Directive (2008/98/EC) and the Hazardous Waste Directive (91/689/EEC). There are also regulations concerning industrial effluents (2010/75/EU) and urban wastewater treatment (91/271/EEC).

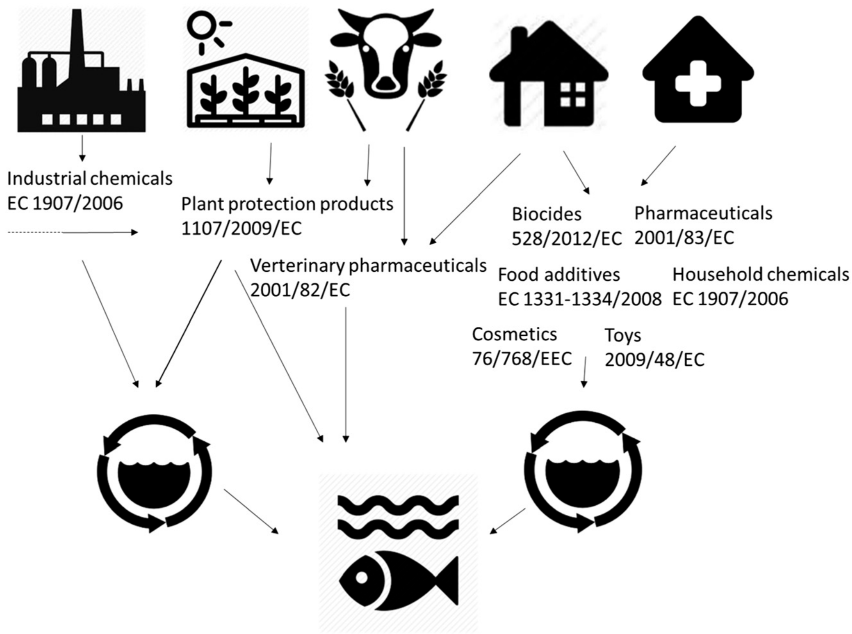

Fig. 2 Scheme of societal sectors, their chemical uses, the dedicated policy frameworks for registration and authorization, and pathways to the aqueous environment direct or *via* industrial- or household effluent treatment plants (circle symbols).

Third, there are dedicated regulations on various environmental compartments such as the water and air compartment *via* respectively the Water Framework Directive (2000/60/EC) and the Air Quality Directive (2008/50/EC). Specific susceptible functions of the water system have their own legislation. Examples are the Drinking Water Directive (98/83/EC) and the Bathing Water Directive (2006/7/EC). Also in other regions of the world, chemical legislation is focused on market authorization per individual chemical and per sector, chemical waste and environmental compartment. In addition several international conventions exist, where the focus is mainly on a small number of well-known chemical contaminants *i.e.* persistent organic pollutants (POPs), *e.g.* the Stockholm Convention on Persistent Organic Pollutants and the UN-ECE Convention on long range transboundary air pollution (CLRTAP). As cumulative nor dense uses are taken into account in the legislation for authorization, and illegal chemical uses or enforcement problems are found, problems with water quality do occur in spite of all current legislations.

3. Mitigation options for chemical water quality improvement

We collate and evaluate mitigation strategies, not starting from the individual chemical but from the systems perspective. We systematically collate and categorize possible mitigation options towards their possibilities in various stages of the chemicals' life cycle from *ex ante* interventions during design and authorization to *ex post* ones after emission.[16,21,22] These include mitigation options during the design, registration and authorization, production, use and waste phases, and ultimately technological interventions at the point of use, the point of environmental entry or at the point of a susceptible function of the water. Such a life cycle might span large spatial and time scales, as a result of trade, stocks, long-living products *etc.*, and influencing the time and space of effectiveness of mitigation options. We discern more technologically oriented mitigation options *versus* other types of mitigation, and discuss the relevance of mitigation options on spatial and temporal scales and identify which societal actors and stakeholders are or can be involved in the various steps.

3.1. Design of chemicals

'Green chemistry', 'sustainable chemistry' or 'green pharmacy' are often mentioned as a way to minimize environmental and health risks and increase the durability of resources. For a safe chemical economy, safe design is promoted as key principle.[23,24] A driver for increased use of safe design may be the Circular Economy, for which presence of hazardous chemicals in products is not a smart idea as those chemicals preclude re-use. The concept of green chemistry is based on twelve principles, amongst which the incorporation of health and safety issues and efficient use of materials already in the design phase.[25,26] In the practice of green chemistry however, issues of diminished toxicity and improved degradability of produced 'green' chemicals still receive relatively little attention.[27,28] Enhanced integration across disciplines – amongst which are toxicologists and chemists – is needed to better incorporate health and environment issues in green chemistry. A focus on developing chemicals that are more efficiently degraded in waste water treatment or in the environment seems promising.[29] An example is the design of better biodegradable pharmaceuticals, by small molecular changes in the drug molecule while the functional drug moiety remains intact.[30]

Currently, the share of green chemical products on the market is still low.[31] Full integration of all green chemistry principles appears to be a challenge for the chemical industry, regulatory bodies and society at large.

Major stakeholders in the development phase are the industry that develops and brings the chemicals to the market, educational institutions that train the developers of chemicals, and regulatory bodies that might influence market penetration of novel benign products through tailored regulations. A wide implementation of safely designed chemicals and products has the ability to improve water quality long-lasting, and can world-wide contribute to the sustainable development goals as defined by UN.

3.2. Registration and authorization

Existing legislation for registration and authorization of chemicals to the market (Fig. 2) aims to prevent the production, trade and use of chemicals with unacceptable adverse effects to human and environmental health. Authorization is performed per individual chemical and per individual type of use. Industries that aim to bring chemicals to the market have to supply dossiers on emissions, exposures, hazards and risks, conforming to the requests by the specific sectoral legislation. Based on this information, public bodies (*e.g.* EFSA, ECHA, EMA) approve, adapt or reject their market introduction. Risk management modifications can be prescribed, such as limits to doses or use frequencies, technologies for application, or treatment after use. In view of enforcement, these risk management modifications are typically more used in the context of professional uses of chemicals, such as in the agricultural or the healthcare sector, compared to non-professional uses.

The registration and authorization follows well-defined and detailed frameworks and guidance, so industry works at an international 'level playing field' and knows what to expect.[32,33] Generally, both human and environmental risks are taken into account, pharmaceuticals are an exemption for which environmental risks do not influence authorization in the current EU framework. A certain level of risk is accepted in view of the benefits of using the chemical, but exceedance of pre-set thresholds is prohibitive. High risk chemicals can be selected as 'candidates for substitution'. These can over time be phased out, in case less harmful alternatives are available with similar use properties that can fulfill the intended service at comparable cost.[34–36]

The authorization mechanisms have an important effect on environmental quality, by reducing hazardous emissions. Although valuable, authorization cannot prevent all adverse effects. A major reason for this is that individual chemicals originating from different uses cumulate in mixtures in the environment. Authorization is based on generalized use scenarios, that do not consider very intensive and aggregated uses in areas with dense population, industries and/or agriculture. Finally, illegal use of chemicals may also contribute to the occurrence of adverse effects. Involved stakeholders during registration and authorization are industrial parties and the government that develops legislation and guidance and decides on the authorization. The legislation is organized on a national or continental level. However, when large markets are concerned, the influence of the legislation is global and spans long timeframes.

3.3. Industrial production

During industrial production emission of chemicals is prevented or mitigated using closed production processes and applying the best available techniques (BAT).[37] In Europe this is laid down in Directive 2010/75/EU on industrial emissions (IED). The prescribed BATs generally focus on 'classic' environmental pollutants such as heavy metals, organic halogens and nutrients and on standard parameters such as total oxygen demand, but not on the actually produced chemicals.[38] The enforcement of the IED by water managers also makes use of these general parameters. The total capacity of industrial waste water plants in industrialized countries is comparable to the capacity of sewage treatment plants. Industrial waste water plant effluents may seriously affect surface water quality.[39] Sector-specific information can be available and used for treatment of industrial effluents, for example in pharmaceutical industry.[40]

Industry is the stakeholder that invests in preventing emissions at the production site, which is a technologically oriented mitigation option especially relevant at local scale. Local or national governmental water quality managers provide licenses for industrial emissions to the surface water. Governments on a higher scale level are the relevant stakeholder drawing the legislative framework for industrial emissions.

3.4. Use and consumption

Chemicals are used non-professionally in households (*e.g.* biocides, pharmaceuticals, food additives, cosmetics, personal hygiene and cleaning products, stocked chemicals in various products), or professionally in agricultural practices (*e.g.* pesticides, veterinary pharmaceuticals) and in hospitals and healthcare facilities (*e.g.* pharmaceuticals and biocides). Emissions are relatively high during the use phase.[41]

Especially for professional use of chemicals, mitigation options can be taken to prevent emission and exposure. For pesticides, integrated pest management (IPM) measures can be prescribed by authorities or voluntarily taken by agrarians, such as pest prevention, use of non-chemical alternatives, low-dose spraying or use of drift-reducing spray devices and buffer zones. The compliance to mandatory measures is high and significantly reduces deterioration of water quality.[42] In closed agricultural systems such as greenhouses, effluents can be treated to prevent residual pesticides to enter surface waters.[43]

Pharmaceuticals are mainly used after prescription, in interplay between professionals and consumers. Prescription rates vary largely between states, which is reflected in surface water concentrations.[44,45] Reticence by doctors in prescription may improve water quality, as does a choice for less hazardous alternative pharmaceuticals if possible. A voluntary system for communicating environmental risks of pharmaceuticals is adopted in Sweden[46] to facilitate selection of pharmaceuticals with lower environmental risk, however adverse environmental effects are not a dominant consideration during prescription and use.[47] There are worldwide many (pilot) projects for advanced treatment of hospital effluents to remove pharmaceutical residues.[48] For the majority of pharmaceuticals less than 15% of the total load used is excreted in the hospital,[49,50] so decentralised treatment of hospital effluents only partly decreases pharmaceutical loads to surface waters. Other mitigation options for pharmaceuticals are related to the users of pharmaceuticals, *e.g.* programs to collect unused residual pharmaceuticals.[51]

For the high number and volumes of chemicals used non-professionally, a mandatory prescription of mitigation measures cannot be easily enforced. A non-mandatory mitigation option that might influence emissions on large spatial and time scales is to increase the consciousness of consumers on their contribution to diminished water quality connected to the use of chemicals. A life-cycle based environmental footprint for products, including an assessment of chemical risks is being developed in this context.[52]

The use and consumption is characterized by a plethora of stakeholders in many different sectors. In conclusion, for chemicals used professionally many mandatory and non-mandatory mitigation options are possible. For non-professional uses mitigation during the use phase is more difficult, though the evolution of foot printing approaches can develop into valuable approaches. Most of the described mitigation options have a strong technological component, and are relevant primarily on local scale.

3.5. Sewage effluent and drinking water treatment

Many chemicals used in households enter the water *via* sewage effluent. Sewage treatment plants (STPs) are in general not equipped with technologies that remove especially the more polar and persistent chemicals.[53] Additional technologies are needed for efficient removal, and in various states currently programs are running to upgrade STPs.[54,55] Hydrological models that relate STP emissions to susceptible parts of the water system showed that only a small part of all STPs explain the majority of impact on susceptible functions,[56] so advanced treatment techniques at STPs can be efficiently placed on those major contributors to the impact. Another use of this type of models is the evaluation of various mitigation scenarios, *e.g.* a general upgrade of all large STPs in a region *versus* a more targeted upgrade.[57]

Advanced water treatment technologies for removal of contaminants are generally used at drinking water production plants, especially when surface water is used as source. Large investments are currently being made at drinking water production sites throughout Europe. Drinking water production plants where groundwater is used as source generally have lower production volumes, and less advanced technology in place.

The water sector is primarily the relevant stakeholder for advanced treatment at STP and drinking water utilities. The implementation of technological mitigation options is relevant at a regional scale.

3.6. Integrated mitigation strategy

An overview of the aforementioned mitigation options in the various stages of a chemicals' life cycle is summarized in Table 1, with a qualification on the technological character of the mitigation option, the scale at which effects are expected, the efficiency to improve water quality and the probability of implementation.

It is concluded that early in the chemical life cycle non-technological mitigation options that are relevant on large spatial scales dominate, while at the end of the life cycle technological options relevant at regional scale dominate. While the options early in the cycle are comparable for various use types, they are more differentiated towards specific uses later in the cycle. In some stages of the life cycle, especially the use and consumption phase, many different stakeholders have possibilities for mitigation.

An efficient mitigation strategy will combine options in various stages of the life cycle, and use both preventive and curative options. A focus on preventive options early in a chemical's life cycle, may deliver the most long-term and large-scale benefits. Many transformation products might be formed when relying on technical treatment only.[58] In view of the current growing chemical demand by society, it is inevitable to also use emission-reduction and curative mitigation options later in the chemical's life cycle. Here, we focus on emission-reduction and curative mitigation options for the aqueous environment, but this could be elaborated for other environmental compartments too. The implementation of technological options later in the life cycle may provide a cost-price related stimulus, that enhances consideration for implementing lower-net-cost mitigation options earlier in the chemical life cycle.

4. Qualitative and quantitative detailing mitigation options: water treatment processes

In the water treatment technologies as used for treatment of industrial, greenhouse, hospital or household waste waters or for drinking water treatment, three basic processes can be discriminated being a) sorption and biodegradation, b) oxidative processes and c) size exclusion processes. Several reviews describe removal efficiencies of water treatment processes in combination with physico-chemical properties of the

Table 1 Chemical life-stages based overview of mitigation options, including a characterization of expected applicability and efficacy (+: applicable and/or important, − not applicable and/or unlikely, ± applicability depends on circumstances or uncertain)

Phase in chemical life cycle	Mitigation option	Relevant stakeholder	Technological character	Large spatial scale	Efficiency to reduce chemical load to water system	Probability of implementation	Remarks
Development							
	Green chemistry	Industry Education	+	+	+	−	Toxicity and degradability still receive little attention
Registration and authorization							
	Legislation and guidance	Government Industry	−	+	±	+	Environmental risks not included for pharmaceuticals. Cumulative effects and dense use not included
Production							
	Implement best available techniques	Industry Government	+	−	±	+	Treatment evaluated on generic parameters only
Use and consumption							
Professional	Emission prevention during professional use	Agriculture Health sector Government	±	−	+	±	Per sector and use type
Non-professional	Increase consciousness consumers	Education Industry Consumers	−	+	+	−	
Water treatment							
	Upgrade sewage treatment plants with advanced technologies	Water manager	+	−	See Table 2		Efficient allocation in relation to susceptible functions water system
	Advanced drinking water treatment	Drinking water utility	+	−			Treatment dependent on source quality associated risks

chemicals to be removed.[48,59,60] Physico-chemical properties of these chemicals vary widely. Hydrophobicity, volatility, biodegradability and reactivity drive the fate and exposure and thus chemical risk assessment,[32] and may also explain removal efficiencies for water treatment technologies.[61,62] In general the more polar, low molecular weight persistent chemicals are difficult to remove,[53] and typically can be retrieved at low concentrations in drinking waters.[63] In the context of risk assessment, the use of quantitative structure activity relationships (QSARs) is well-established to describe the relation between chemical properties and fate processes.[64] Well-used and freely available toolboxes and databases for QSAR application for environmental fate ease the use of QSARs for risk assessors, such as the OECD toolbox or EPI-suite. For water treatment however, such QSARs are less well established.[65]

4.1. Treatment processes based on sorption processes combined with biodegradation

Use of granulated, biological or powder activated carbon (AC), sand filtration, river bank and dune filtration, and soil passage are all broadly applied in water treatment, especially for drinking water treatment. Sorption and biodegradation are the dominant removal processes for these technologies.

Sorption of molecules to activated carbon depends on solvability, hydrophobicity and electrostatic interactions. Adsorption can be nonlinear due to saturation and competition, reason why bed volumes are of importance. Furthermore the conditions of the environmental matrix, *e.g.* pH and salinity, directly influence sorption.

QSARs for removal by AC are available, using a variety of descriptors.[61,66–69] Some authors mention that QSARs should be developed for each type of AC separately, and how much water it has treated should be taken into account.[67,68,70] Compared to the approach taken for QSARs for environmental fate, where simple QSARs based on the octanol–water partition coefficient (K_{ow}) are applied to a variety of soils after normalization for organic carbon content,[71,72] this seems a rather detailed approach. For soil sorption QSAR models including multiple descriptors such as quantum-chemical descriptors, topological descriptors *etc.*, do not perform better than simple QSARs based upon K_{ow} solely.[73] Indeed, a simple QSAR based on K_{ow} predicts removal by AC treatment quite well above $\log K_{ow}$ of 4[74–76] when hydrophobic interactions dominate. For more hydrophilic and especially charged chemicals electrostatic interactions can dominate, resulting in underestimation of sorption based on hydrophobic interactions. Additionally, sequestration or slow diffusion in poorly accessible parts of the AC can cause non-linearity, so some authors combine QSARs for removal with a so-called pore surface diffusion model to account for specificities of the AC and changes in sorption capacity in time.[77] The majority of chemicals except relatively polar chemicals can be removed cost-efficiently with AC, QSARs derived by several authors are consistent in this prediction.[78] The application of QSARs for water treatment using activated carbon predicts removal rates between 10 to >95 percent.

For river bank filtration, it was shown that biodegradation processes generally dominate over sorption processes, although relatively few compounds show high persistence.[79,80] It takes over 6 months before bacterial communities are well developed for sufficient effective biodegradation in newly developed sand bank filtration sites. Especially negatively charged and more hydrophobic chemicals were shown to have high biodegradation rates, as well as chemicals with ethers and carbonyl groups. Slow sand filters are effective in biodegradation of compounds that are difficult to remove by other treatment processes, such as iodinated X-ray contrast media, at low hydraulic loading rates and thus long contact times.[81] Under abiotic conditions, removal during soil passage was much lower.[82] Depending on the physico-chemical properties of the chemical, river bank filtration and slow sand filters give a high variation in removal rates (<20 to >90%).

4.2. Treatment processes based on (advanced) oxidation processes

Oxidative processes are widely applied in drinking water treatment, especially UV or UV/H_2O_2 oxidation and ozonation. A relevant physico-chemical parameter is the reactivity of the chemical, often expressed by the parameter E_{homo}, the sigma constant expressing the electron-donating or -withdrawing properties, the double bond equivalence, the ionisation potential, the electron-affinity or the bond strength of carbon–halogen.[83–86]

For ozonation, compounds with activated aromatic rings are highly reactive, whereas substances with deactivated aromatic rings such as phthalate, halogen substituted compounds and saturated aliphatic show low reactivity.[87] In a review on QSARs for environmental fate processes[64] E_{homo} appeared a useful and most often used descriptor for oxidative processes.

Oxidative processes can be highly efficient in their removal of chemicals, but again there is a high variation in removal efficiencies from 5 to 99% depending on the chemical structure.[88,89] Treatment efficiencies depend on process conditions, such as ozone dose or for UV treatment lamp types including UV spectra and intensities used, duration of the irradiation and addition of H_2O_2 or Fe.[90–92] Furthermore, treatment efficiencies are influenced by matrix effects such as the natural dissolved organic matter content of the water. Oxidative processes are well-known for their possible creation of disinfection by-products, their formation also depends on process conditions and matrix properties such as nitrate and DOC content.[93–95]

4.3. Treatment processes based on size exclusion processes

Water treatment by membranes such as reverse osmosis or nanofiltration, can be an effective way to remove chemicals. Removal efficiencies are influenced by characteristics of the treatment process – *i.e.* pore size, membrane material and charge, fouling – as well as the physico-chemical properties of the chemicals to be removed such as size and polarity, and the matrix composition.[96–98] Especially hydrophobic chemicals may sorb and accumulate in the membrane material.[96] This sorption depends on the type of polymer used for the membrane,[99] a phenomenon which is relatively well studied in the context of passive samplers for environmental monitoring purposes.[100–102] Several processes play a role in the removal efficiencies, being size exclusion, charge repulsion, ad/absorption, solute/solute interactions and interaction with the fouling layer.[99,103] A model including solute size, membrane pore size, and solute-membrane affinity was well able to predict removal efficiencies for a limited set of compounds.[104] Removal efficiencies generated *via* RO membranes are generally high (>85%), however especially small hydrophilic or negatively charged molecules remain difficult to remove by membranes.[105,106] The brine in which removed chemicals are concentrated might contaminate the environment again, if not disposed well.[107]

4.4. No 'one size fits all'

A database on quantitative efficacies on (technical) mitigation strategies is of high value for practical decisions regarding a smart and effective set of mitigation options for a problem case situation.[108] Currently such a database is being established for approximately 100 different CECs, sorptive, oxidative and size exclusion techniques,[108–110] including quality criteria for the original data and detailed analysis. Table 2 shows that removal efficiencies of the different treatment processes strongly vary across options and physico-chemical properties of the chemicals. In environmental aqueous samples complex mixtures of many different chemicals are found, optimal mitigation in this curative stage of a chemicals' life-cycle typically includes a combination of technologies to optimally cover the total chemical space. A combination of technologies is therefore mostly applied in pilot or full-scale situations, especially for drinking water production plants having surface water as a source. For waste water treatment plants and drinking water production plants with river bank or groundwater as a source, typically sorptive and biodegradation processes are used for treatment. Advanced oxidation or membrane processes are less often used in these situations, however also these sources are susceptible for contamination by chemicals.[111,112]

5. Integration of mitigation options into solutions-oriented strategy

As both water use and chemical emissions rise, increasing problems can be expected at the nexus of the chemical life

Table 2 Summary characterization of removal efficiency of various water treatment processes

Process	Mitigation option	Efficiency to reduce chemical load to water system	Remarks regarding physico-chemical properties
Sorption	AC	10 to >95%	High removal for hydrophobic chemicals
Biodegradation	Sand filtration	<20 to >90%	Higher removal for biodegradable chemicals, *e.g.* negatively charged and hydrophobic
Oxidation	UV (+H_2O_2), ozone	5 to >99%	Higher removal for reactive chemicals
Size exclusion	NF, RO membrane	Generally >85%	Lower removal for small hydrophilic compounds, or fouled membranes.

cycle and the water cycle. Intensification of current regulatory pathways presumably cannot yield a full solution to reach the policy goal of a non-toxic environment, so additional approaches seem warranted. We propose a solutions-focused risk assessment and management framework, which puts exploring mitigation strategies upfront in the assessment and management of chemicals of emerging concern and their risks for the water system.[109,110,113–115] Solution-focused research integrates analysis of the problem and the range of optional solutions in an early stage of the assessment, where scientists together with stakeholders coproduce and implement the knowledge.[116,117] An integration of the classical risk assessment and system analysis approach, based on mainly natural sciences, with engineering perspectives and social sciences is requested. A wide variety of disciplines may be involved including chemistry, (eco)toxicology, hydrology and geosciences to define *e.g.* geospatially smart and technically effective solutions and to implement those solutions *via* the application of expertise in the social and juridical disciplines. The use of a solution-focused approach can be supported by a mitigation database such as elaborated in section 3 and 4, to store and retrieve the wide variety of options including information of the efficacy of (technical) options to reduce chemical emissions to and concentrations in (drinking) water systems.

Currently the exploration of various mitigation possibilities is not well-integrated in risk assessment practices. Current practice is that risk assessments focus primarily on problem diagnosis: the 'risk management' step has developed to be a disparate step sequential to the risk assessors task. Various mitigation options, especially the ones already implemented at broad scale, can be integrated in models used for risk assessment. There is latitude to improve on regulatory and practical approaches here, as currently only some basic assumptions regarding sorption and biodegradation of the chemicals in sewage water treatment are integrated in the scenario's used for exposure and risk assessment.[118,119]

A solutions-focused approach helps to develop a coherent view amongst stakeholders regarding 'low-hanging fruit' and longer-term mitigation options, and identify areas where further innovations are needed. The goal of solutions-focused risk assessment is to generate a comprehensive insight in the effects of possible sets of mitigation options throughout the chemical's life cycle, in various sectors and at various places in the water system, appreciation there-off by the stakeholders involved and ultimately implementation of the chosen set of options.

5.1. Coupling of mitigation options to hydrological models

By combining hydrological models, data on emission and fate of chemicals and possible mitigation options, proposed sets of mitigation options to improve water quality can be evaluated with currently predicted concentrations as background scenario. Space and time variable emissions, factors influencing environmental fate and behaviour, and hydrological processes determine environmental concentrations and their variability. Various approaches have been developed to model concentrations of contaminants of emerging concern,[39,56,57,120,121] mostly on a river basin scale and for specific down-the-drain consumer chemicals. The models are based on hydrological knowledge of the water system, the systems' climate variability, and the location and amount of sector specific inputs *via* point or diffuse sources. The impact of emissions by various sectors (industry, households, agriculture, care) can be combined.

There has been much development in global-scale hydrological models given available global data sets.[122,123] Such models have thus far hardly been applied in the context of exploring mitigation strategies for chemicals of emerging concern, but can be used to study the interaction of the water system and the various sectors demanding, using and returning water. In this way it is possible to reflect on the effects of possible mitigation options on a global scale as compared to a more traditional optimization on local scale. By coupling the mitigation options geospecifically to a river catchment water quality model that enables to model chemical emissions from various sectors in relation to the systems' hydrology, alternative sets of mitigation strategies can be evaluated.

5.2. Valuing effects of mitigation options

Improvement of environmental quality by implementing sets of mitigation options can be expressed in terms of a) decreased concentrations, b) diminished adverse effects on environmental and human health and c) better possibilities to obtain the demanded water system services (*e.g.* for drinking water production, food production, recreation). An option is to express improvement in terms of net chemical footprint, where emissions of a mixture of chemicals in a given river basin are compared to the available environmental water volume.[124] Given the common non-linearity of emissions-to-impact relationships, the efficiency of a mitigation strategy expressed in terms of concentration of a single chemical does not translate in equivalent reduction in expected impact on environmental or human health. Alternative packages of mitigation strategies may be evaluated whether, when and where they substantially contribute to improved water quality. This type of evaluation relates closely to the definition of safe boundaries, both at the local scale and at the scale of planetary boundaries.[16,125]

For the appreciation of mitigation options, next to improvement of environmental quality also other aspects are of key interest such as costs, energy, space, timeframe, and support by stakeholders and the public. The effects per mitigation option can be expressed for chemicals with typical environmental entrance pathways – coupled to specific sectoral uses and stakeholders – and for chemicals from various classes regarding their physical–chemical properties.

6. Conclusions

• Research on the topic of deterioration of water quality by chemicals is currently focused mainly on problem and risk analysis, while little attention is paid to mitigation options.

• As in the environment chemicals occur in complex mixtures, prioritization of possible (packages of) mitigation options might be a better way to derive effective and innovative approaches then prioritization of individual chemicals.

• The approach of solution-focused assessments can be supported by a mitigation database, including technical and non-technical options. Mitigation options can be defined along the whole pathway of a chemicals' life cycle, accounting for the characteristics of the water cycle.

• Early in the chemical life cycle, non-technological mitigation options relevant on large spatial scales dominate, while later in the life cycle technological options relevant at regional scale dominate. An efficient mitigation strategy combines preventive and curative options.

• In view of growing societal chemical demand it is inevitable to include curative mitigation options later in the chemical's life cycle, which may create a price stimulus for more preventive options earlier in the chemical life cycle.

• For water treatment of industrial, greenhouse, hospital or household waste waters or for drinking water treatment, similar techniques are applied. Techniques rely on sorption, biodegradation, oxidative processes and size exclusion processes. Removal efficiencies depend on the treatment process and physico-chemical properties of the chemicals. Optimal mitigation of complex mixtures in the curative stage typically uses of a combination of various technologies. Polar and low molecular weight persistent chemicals are difficult to remove.

• A database that lists mitigation options per sector and phase in the chemical's life cycles can be used to assess their effectiveness by coupling to hydrological models.

• Improvement of environmental quality after mitigation can be expressed in terms of decreased concentrations, diminished adverse effects on environmental and human health, or better possibilities to obtain water system services.

Acknowledgements

This work was funded by the European Commission, FP7 project SOLUTIONS, contract number 603437. LP was also funded by the Strategic Research Program of RIVM, project nr. S/121503, executed under the auspices of the RIVM Scientific Advisory Board.

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