Chemical Data collection summary

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Methodology for determining chemical contaminant removals

For potable reuse regulations/strategies are typically based on the removal and disinfection of pathogens (World Health Organization, 2017). The multiple-barrier design for the water treatment is widely accepted and should consider the entire system from collection of wastewater to production and supply of drinking-water to consumers. The use of a multiple-barrier approach ensures that performance failure at a single barrier should not lead to significant failure to remove microbial or chemical contaminants.

Figure 1. From WHO potable re-use

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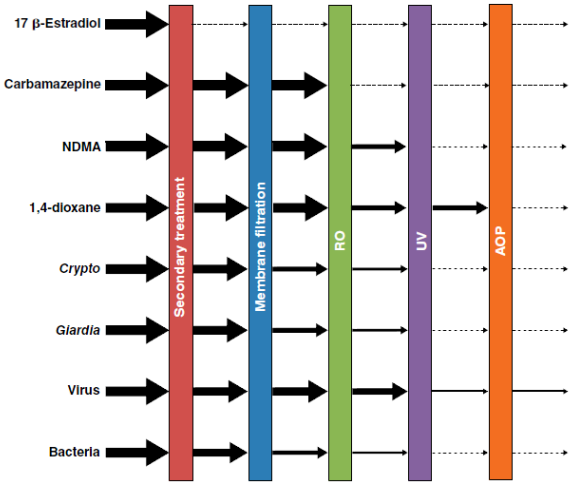
FIGURE 6 Effectiveness of a robust advanced treatment train (MF/RO/UV/AOP) in the control of chemical contaminants and pathogens*



AOP—advanced oxidation process, *Crypto*—*Cryptosporidium*, NDMA—*N*-nitrosodimethylamine, RO—reverse osmosis, UV—ultraviolet irradiation

*Dotted lines show concentrations below public health thresholds.

Approach: (Ruths working strategy)

1. Determine definitive list of chemicals of concern, based on the availability of health based (or aesthetic) guideline values (extracted from various guideline documents) (based on Freds database, added some more aesthetic and some new guideline recommendations)

A range of

2. Determine Log concentration ranges in source waters (secondary treated effluent). This can hopefully come primarily from Fred's database and we fill in the gaps. (See excel document)
3. Summarise what we know about LRV for each of the treatment barriers below (see text below)
4. For a particular specified treatment train, work through to determine when the log concentration is less than the log guideline value (after which process can we say this?) (Need to apply the total reductions, although this should be easily reached for most!)
5. Exclude each chemical from further consideration after the barrier at which the concentration is below the guideline. ("I'm applying groupings to make it more of a decision support tool" – The aim is to have a table like the one below – but with PDFs rather than % reduction ranges.)
6. See if any contaminants are remaining for relying on latter barriers such as environmental buffer. (Should be soon)

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Table 1. Indicative percent removals of organic chemicals during various stages of wastewater treatment

Chapter 6 | Treatment Technologies for Protecting Public and Environmental Health

Table 6-5 Indicative percent removals of organic chemicals during various stages of wastewater treatment

	Percent Removal										
			Pharmaceuticals					Hormones			
Treatment	B(a)p	Antibiotics[1]	DZP	CBZ	DCF	IBP	PCT	Steroid[2]	Anabolic[3]	Fragrance	NDMA
Secondary (activated sludge)	nd	10–50	nd	–	10–50	>90	nd	>90	nd	50–90	–
Soil aquifer treatment	nd	nd	nd	25–50	>90	>90	>90	>90	nd	>90	>90
Aquifer storage	nd	50–90	10–50	–	50–90	50–90	Nd	>90	nd	–	–
Microfiltration	nd	<20	<20	<20	<20	<20	<20	<20	nd	<20	
Ultrafiltration/ powdered activated carbon (PAC)	nd	>90	>90	>90	>90	>90	nd	>90	nd	>90	>90
Nanofiltration	>80	50–80	50–80	50–80	50–80	50–80	50–80	50–80	50–80	50–80	
Reverse osmosis	>80	>95	>95	>95	>95	>95	>95	>95	>95	>95	25–50
PAC	>80	20–>80	50–80	50–80	20–50	<20	50–80	50–80	50–80	50–80	
Granular activated carbon		>90	>90	>90	>90	>90		>90		>90	>90
Ozonation	>80	>95	50–80	50–80	>95	50–80	>95	>95	>80	50–90	50–90
Advanced oxidation		50–80	50–80	>80	>80	>80	>80	>80	>80	50–80	>90
High-level ultraviolet		20–>80	<20	20–50	>80	20–50	>80	>80	20–50	nd	>90
Chlorination	>80	>80	20–50	–<20	>80	<20	>80	>80	<20	20–>80	–
Chloramination	50–80	<20	<20	<20	50–80	<20	>80	>80	<20	<20	

(Sources: Ternes and Joss, 2006; Snyder et al., 2010)

B(a)p = benz(a)pyrene; CBZ = carbamazepine, DBP = disinfection by-product; DCF = diclofenac; DZP = diazepam; IBP = ibuprofen; NDMA=N-nitrosodimethylamine; nd = no data; PAC = powdered activated carbon; PCT = paracetamol.

[1] erythromycin, sulfamethoxazole, triclosan, trimethoprim

[2] ethynylestradiol; estrone, estradiol and estriol

[3] progesterone, testosterone

Collating Contaminants of Concern

Drinking water, and recycled water guidelines were collated in order to identify the range of risk based thresholds available for potential chemical contaminants in drinking water. Thresholds for aesthetic acceptability were also identified.

In total, 580 compounds were identified. Many of the compounds (148), were indirectly regulated, i.e having limits applied to groups of compounds. For example, the European Union (Council Directive 98/83/EC) set a 0.5 µg/L limit for total pesticides expected in drinking water.

Thirty three compounds had limits based on aesthetic acceptability; most of these also had health limits as only nine presented only aesthetic criteria.

Limitations: *What about emerging chemicals? which aren't currently regulated??*

Occurrence of contaminants

Data for concentrations of contaminants in wastewater effluent was compiled from a variety of sources from wastewater treatment plant effluent assuming the situation for potable reuse. Data sources were from around the world and considered effluents from a range of different catchments and wastewater treatment plant configurations.

Identification of priority contaminants

The identification of contaminants likely to be of concern was based on comparing concentrations of compounds in the wastewater effluent to the compiled drinking water thresholds.

The approach was conservative as the minimum thresholds for health and aesthetic acceptability were compared to the maximum reported concentrations in wastewater effluent.

In a large number of cases, chemical concentrations were below analytical detection limits. In such cases, the analytical detection limit was used for screening in place of the maximum possible value and used as a conservative surrogate.

Accordingly, care must be taken when interpreting the shortlisted compounds as assumptions were very conservative and does not necessarily imply that the chemical was ever measured at such a high concentration when LOQ's were assumed, or that the max values reported were likely to commonly occur or be part of normal operation

Of the 580 contaminants, there were 81 for which concentration data could not be found, while 133 were only reported once. Detection thresholds of the contaminants in the studies were also reported.

The maximum concentrations in wastewater effluent exceeded the minimum acceptance thresholds for health based standards for 94 compounds. In terms of aesthetic properties, there were 10 compounds found at concentrations exceeding the minimum recommended aesthetic acceptance thresholds.

Where compounds were not detected, the detection limits of the studies were also reported. It was noted that the method detection limits were higher than the lowest recommended guideline threshold for 133 compounds against health based limits and 11 for aesthetic based limits.

Therefore, a shortlist of 221 compounds were identified which were found at concentrations in wastewater exceeding the minimum reported guideline value; or had method detection limits which were higher than the minimum guideline values.

Limitations

- *This approach is rather conservative… method detection limits and limits for groups of compounds probably mean that many compounds are still being retained in the shortlist…*
- *We should probably also find some more data for the 81 compounds which concentrations could not be found ?*

Source water concentrations

Typically the initial treatment step in potable reuse schemes start in the wastewater treatment process. There is much variability introduced in the types of treatment, the treatment typically includes primary and secondary processes, however can also include advanced treatment processes which may also be used in water treatment plants.

Wastewater treatment set up and operation can affect the composition of the produced effluent. Typical variations include the use of conventional activated sludge, trickling filters or membrane bioreactors. These processes are likely to vary in their removals of degradable organic compounds.

Due to the large variability in removals, the risk assessment in this report is based on the chemical contaminant levels in treated effluent which have been reported in the literature or reports.

Chemical addition, coagulation, clarification

Description

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Coagulation and clarification have historically been used to reduce the TSS, nutrients and heavy metals in wastewater. The choice of coagulant depends on the effluent characteristics in particular heavy metal and ammonia levels (Khan, 2013). Typically metal coagulants are somewhat effective for the removal of inorganics (Bratby, 2016).

While coagulation is commonly used in wastewater treatment plants, its use in water purification depends on the effluent source. Apart from their effect on certain metals, coagulation and clarification are not expected to be the main barriers for other chemicals of concern. For example, in general clarification is only expected to account for about 15% of the reduction in average concentration during the treatment process (Stackelberg et al., 2007). Additives, which were monitored included alum, ferric chloride and softening processes. Lime was mainly reported for the removal of inorganics.

Performance

As coagulants aid in removing suspended solids, the removal of organic compounds which are associated with the suspended solids may also be removed (Snyder et al., 2007). Log Kow can provide a rough indicator of percent removal by coagulation. From studying a number of pharmaceuticals which exist as anions at ambient pH, only those with a log Kow greater than 5 achieved any notable removal by aluminium or iron salt coagulation (Snyder et al., 2007). The relationship between log Kow and coagulation/clarification for the chemicals of concern in this study is shown in Figure 2. While other factors may also contribute to contaminant removal, there is difficulty in isolating and predicting these effects.

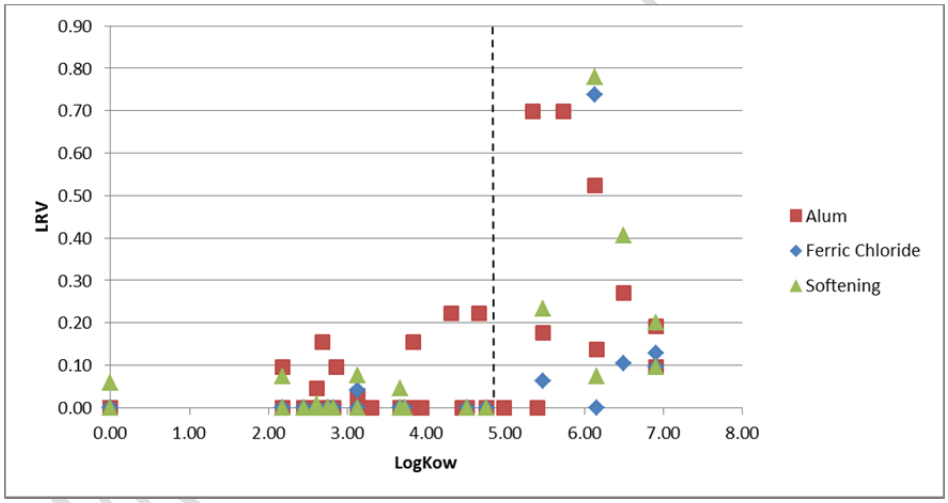

Figure 2. Relationship between LRV and Log Kow for organic chemicals of concern from the collated studies.

Based on the Log Kow values for the reported compounds expected PDFs for % reduction and LRVs were calcualted from the compiled dataset. Removals were minimal <20% for most compounds with lower Log Kow values, these will be assumed to be neglible. There didn't appear to be any signficant diffrence between the three main treatment methods (Figure 2).

Compounds with larger Log Kow values showed higher removals, however these were typically still only moderate with an average of 40% removal.

Sixteen compounds with Log Kow >5 were compiled, while there were 47 compounds with Log Kow < 5 . From the initial shortlist based on maximum influent composition compared to guideline values, of the compounds which should be monitored there were 11 and 24 of the Log Kow>5, and <5 respectively.

Table 2. Compounds with Log Kow > 5 with removals reported for different additives (showing the number of records). Compounds which should be monitored based on the initial shortlist are underlined.

Compound	Alum	Ferric chloride	Softening
4-tert-octylphenol	1		
a-chlordane	1	1	1
aldrin	1	1	1
Benzo(a)pyrene	1	1	1
benzo(b)fluoranthene	1	1	1
benzo(k)fluoanthene	1	1	1
DDD	1		
DDE	1	1	1
DDT	2	2	2
dieldrin	1		
fluoranthene	1		
Galaxolide	2	1	1
g-chlordane	1	1	1
heptachlor	1	1	1
Hexachlorobenzene	1		
Trifluralin	1		

Table 3. Compounds with Log Kow< 5 with removals reported for different additives (showing the number of records). Compounds which should be monitored based on the initial shortlist are underlined.

Compound	Alum	Ferric chloride	Softening
acenapthylene	1		
Acetaminophen	2	1	1
Ametryn	1		
Ametryn	1		
androsterone	1	1	1
anthracene	1		
Atrazine	3	2	2
BHC	1		
Caffeine	3	2	2
Carbamazepine	2	1	1
Chlorpyrifos	1		
Chlorpyrifos-methyl	1		
chrysene	1	1	1
DEET	3	2	2
Diazepam	1	1	1
Diclofenac	2	1	1
Diuron	1		
Erythromycin	2	2	2
estradiol	3	1	2
Estriol	2	1	1
Estrone	3	2	2
Ethynyl Estradiol	3	2	2
Fluorene	2	1	1
Fluorene	2	1	
Fluoxetine	2	2	2
Gemfibrozil	2	1	1

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Compound	Alum	Ferric chloride	Softening
heptachlor epoxide	1		
Ibuprofen	2	1	1
Iopromide	2	1	1
Lindane	1	1	1
Metolachlor	3	1	1
Musk Ketone	2	1	1
Musk Ketone	2	1	
Naproxen	2	1	1
napthalene	1		
napthalene	1		
Parathion	1		
Parathion-methyl	1		
phenanthrene	1		
Progesterone	3	2	2
pyrene	1		
Simazine	1		
Sulfamethoxazole	2	1	1
TCEP	3	2	2
Testosterone	2	1	1
Triclosan	2	1	1
Trimethoprim	2	1	1

While higher coagulant doses can aid the removal of chemicals, the dose is typically based on TSS removal inorder to protect upstream processes. There were minimial differences between the different processes.

For organics

- logKow < 5: assume LRV = 0
- logKow> 5: assume LRV = 0 (neglible/poor removal)
- logKow> 5: assume LRV = 0.32 ± 0.36 (poor/moderate removal based on total dataset)

Limitations:

- *Basis for estimating removal of inorganics is unclear*
- *Many organic compounds were only reported once*

Sand filters, Microfiltration and ultrafiltration

Sand filters also have minimal removal of organic compounds, with very poor removal of antibiotics (Le-Minh et al., 2010).

As there is expected to be minimal chemical removal through microfiltration processes, and the processes are typically proceeded by NF or RO systems. It is assumed that this stage will not contribute significantly compared to the later systems.

Limitations

- *May need to be included if in the GAC process.*
- *Some potential references are https://www.sciencedirect.com/science/article/pii/S0043135407002539#tbl5*

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Adsorptive Processes (GAC and PAC addition)

Description

Adsorption is commonly used to remove organic contaminants such as herbicides, pesticides, algal toxins and metabolites; it is also used to remove compounds that may have an adverse impact on the taste and odour of water.(NH&MRC, 2013). Activated carbon can be added to help adsorb organic chemicals, its removal performance can range from good to excellent (Le-Minh et al., 2010). However, its performance depends on pH, dose, contaminant concentration and contact time.

The most common forms of activated carbon for water treatment are known as granular activated carbon (GAC) and powdered activated carbon (PAC). These terms refer to the physical form, or particle size, in which the activated carbon is applied. Smaller particle sizes in PAC tend to have higher surface areas while large particle sizes in GAC tend to be more easily separated from the water subsequent to treatment. PAC is often used by direct addition to water with mixing and then separated by gravity and/or filtration. Alternatively, GAC is more commonly used as filtration media with the water being percolated through it.

The effectiveness of PAC and GAC to removal chemicals of concern has been related to the hydrophobicity of the compounds (Khan, 2013). For example, hydrophobic organics compounds as well as relatively hydrophobic inorganic compounds such as N, sulfides and heavy metals can be effectively removed. Hydrophilic compounds such as small carboxylic acids and alcohols are poorly removed. The use of PAC has been effective for the removal of pharmaceuticals, endocrine disruptors and pesticides from relatively clean water sources (Snyder et al., 2007; Westerhoff et al., 2005).

PAC removal

While amounts of PAC addition can vary, typical doses in water treatment plants range from 2 to 60 mg/L, but can be as high as 100 mg/L. Typical contact times of 10-30 minutes are noted in full scale plants, however longer may be needed for removal of taste and odour compounds. The percent removal of EDC/PPCPs were reported by Westerhoff et al. (2005) to be independent of the initial concentrations of contaminants.

The adsorption kinetics for PAC are better explained by the pseudo second order reaction model than the pseudo first order reaction (Park thesis 2016). While the initial adsorption rate can be correlated with the Log Kow and diffusion coefficient of the contaminants, the removals depend on contact time, adsorption equilibriums and bed characteristcs. In addition, the charge of the compound will also affected the relationship between initial adsorption rate and Log Kow (Figure 3). Where compounds with a pKa less than 7 will be negatively charged, and react slower, while those with high pKa will be positive and react faster.

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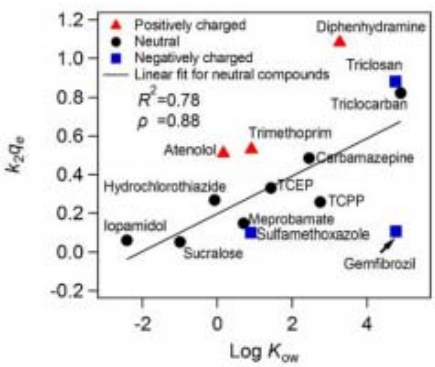

Figure 3. Correlation of the initial adsorption rate (k2qe) with hydrophobicity of contaminants (Park thesis 2016 – need to find corresponding articles)

Options for polyanski estimation method: and other methods as reported by Snyder et al 2007

However, relationships between the physiochemical parameters and percent removals are difficult to calculated without experimental data relating to equilibrium concentrations. Snyder et al. (2007) noted this difficulty and suggested that compounds be grouped according to the removal performance in AC studies reported in the literature. Data for PAC removal was gathered from a variety of literature sources.

Some of the compounds showed large variability in removal performance in the compiled records Figure 4. These are likely due to changes in PAC dose, for example diclofenac and iopromide showed a correlations between LRV and PAC dose with R2 = 0.47, 0.56 however even at high PAC doses (>50) removals only slightly exceeded 1 LRV. Testosterone LRVs on the other hand also showed a good correlation with PAC dose (R2 = 0.71), however showed much better performance with dose of 20mg/L giving ~ 2 LRV removal.

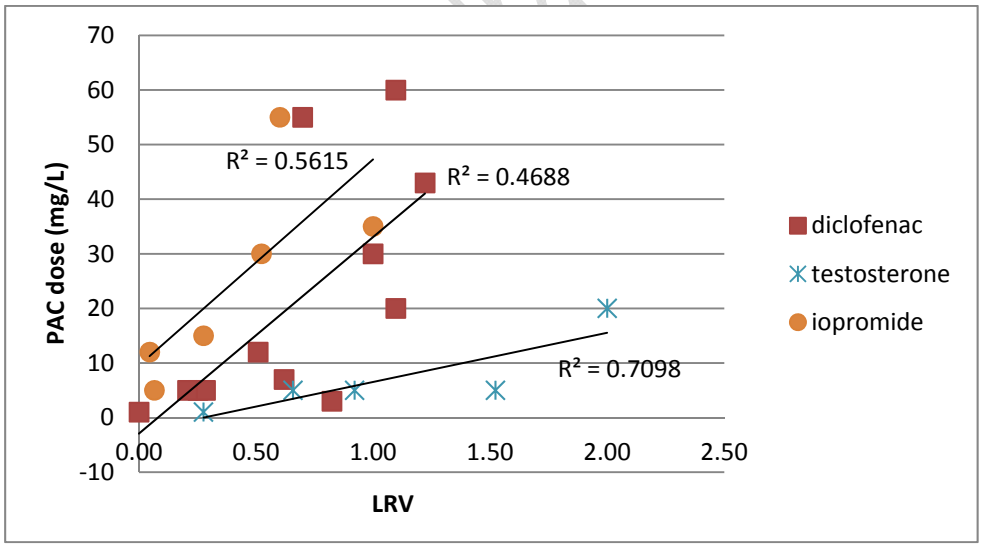

Figure 4.Effect of PAC dose on LRV for certain chemicals

The majority of the records were lab or pilot scale studies, using doses ≤20mg/L. Based on the collated references the removal performance of about 40 regulated compounds were reported. Depending on their median reported removals, the regulated compounds were grouped into either poor, moderate and good removals for low (≤15 mg/L) and high (>15 mg/L) PAC doses as shown in Table 1.

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PDFs for individual compound removals as well as total compounds and removal groups were calculated based on aggregated data. These groupings can be assigned as surrogates for removals for compounds where there is not data.

Limitations exist in that:

- Studies report % removals to a limited number of decimal points due to limits of detection, this means that higher range LRVs are not present
- Reporting of PAC doses were not always reported, and may not represent full range at operating WWTPs
- Based on the dataset, a maximum of 2 log reduction should be assigned.

Table 4.Removals of regulated compounds during PAC treatment, * shows where data was limited n=1, those underlined where identified as compounds which should be monitored during water treatment. Good removals (≥90%), Moderate removals (50-90%), Poor removals (<50%)

Compound	Removal groupings at different PAC doses	
	≤15 mg/L dose	>15 mg/L dose
4-Methylphenol	Good	no data
acenapththylene	Good	
anthracene	Good	
Endosulfan sulfate	Good *	
fluoranthene	Good	
fluorene	Good	
fluoxetine	Good	Good *
Methylbenzotriazole	Good *	Good *
Metoprolol	Good	Good
phenanthrene	Good	
pyrene	Good *	
17-Beta estradiol, E2	Moderate	Good
a-BHC	Moderate	
acetaminophen	Moderate	
a-chlordane	Moderate	
Ametryn	Moderate	
atrazine	Moderate	Good
b-BHC	Moderate	
benzo(b)fluroanthene	Moderate	
benzo(g,h,I)perylene	Moderate	
benzo[k]fluoranthene	Moderate	
Bezafribate	Moderate	Good
Bisphenol A	Moderate	Moderate*
caffeine	Moderate	
carbamazepine	Moderate	Good
Chlorpyrifos	Moderate*	
Chlorpyrifos-methyl	Moderate*	
Clarithromycin	Moderate	Good *
d-bhc	Moderate	
DDD	Moderate	
DDE	Moderate	
DDT	Moderate	
DEET	Moderate	Good *
diazepam	Moderate	
dieldrin	Moderate	
Diuron	Moderate*	
endrin	Moderate	
Erythromycin	Moderate	

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estiol	Moderate	
estrone	Moderate	
Ethynyl Estradiol	Moderate	Good
Galaxolide	Moderate	
g-BHC	Moderate	
g-chlordane	Moderate	
heptachlor epoxide	Moderate	
heptachlor	Moderate*	
indeno(1,2,3-cd]pyrene	Moderate	
Mecoprop	Moderate	
Metformin	Moderate*	
methoxychlor	Moderate	
Metolachlor	Moderate	
Microcystin	Moderate*	
musk ketone	Moderate	
napthalene	Moderate	
Parathion	Moderate*	
Parathion-methyl	Moderate*	
progesterone	Moderate	Good*
Simazine	Moderate*	
Sulfamethoxazole	Moderate	Moderate
TCEP	Moderate	Moderate*
testosterone	Moderate	Good *
Triclosan	Moderate	
Trimethoprim	Moderate	
diclofenac	Poor	Good
gemfibrozil	Poor	
Ibuprofen	Poor	Moderate*
iopromide	Poor	Moderate
naproxen	Poor	
Perfluorooctanesulfonic acid, PFOS	Poor*	

GAC removal

A study reported by Ternes et al. (2002) revealed GAC filtration to be an effective method for removing a variety of pharmaceuticals during drinking water treatment in Europe. GAC is typically used as an inert media filter, its performance is determined by the empty bed contact time, design flowrate and expected concentrations. Its performance can degrade overtime and need media replacement. Removals are due to both adsorption and biodegradation in the beds. The biodegradation rate is typically related to the DOC content.

Zearley and Summers (2012) proposed pseudo first order kinetics for operation at steady state.

$$\frac{C_e}{C_0} = \exp(-k' \cdot EBCT) \qquad (1)$$

where C_0 and C_e are the influent and effluent micropollutant concentrations, and k' is the pseudo-first-order rate constant.

Where k was the pseudo-first-order rate constant, which can be grouped as recalcitrant ($k' < 0.022$ min^{-1}), slow (0.022 $min^{-1} < k' < 0.093$ min^{-1}), fast (0.093 $min^{-1} < k' < 0.248$ min^{-1}), and very fast ($k > 0.248$ min^{-1}).

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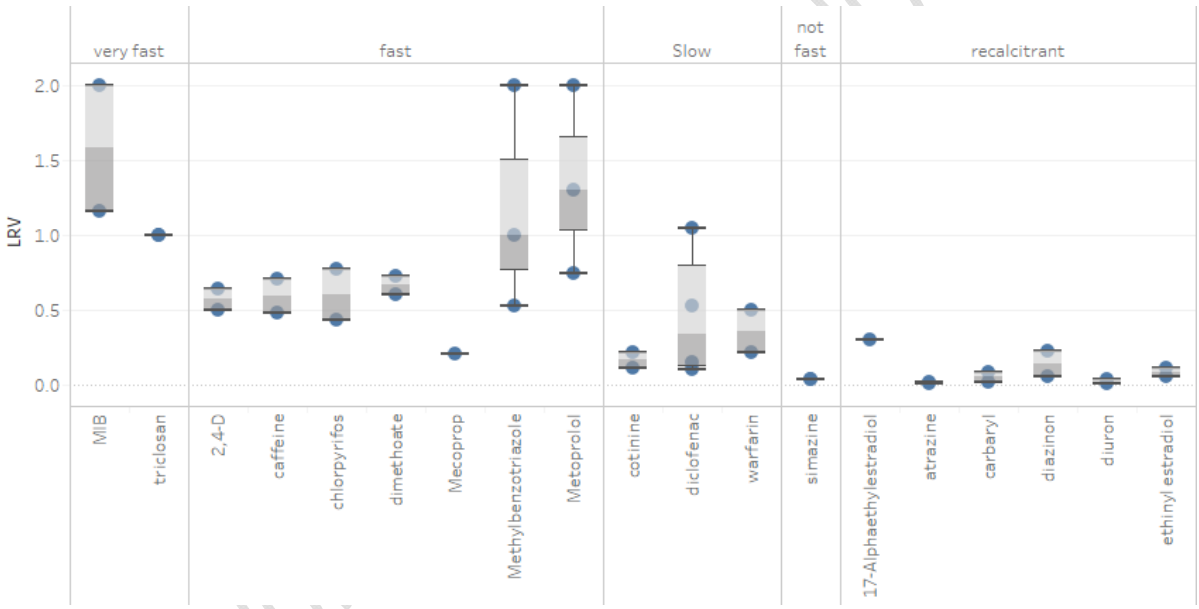
These categories of degradation potential can help group compounds and will be used to determine the expected likelihood for removal in GAC for compounds where no data is available. For an EBCT of 7 minutes the average LRVs from experimental data (Zearley and Summers, 2012) is shown below:

- Very fast, LRV= 1.2 ±.36
- Fast degradation, LRV = 0.65 ±0.21
- Slow, LRV = 0.23 ±0.15
- Recalcitrant, LRV = 0.04 ± 0.04 (assume no removal)

The Biowin degradation calculation was used for those compounds which were shortlisted and where no data was available. The Biowin1 and Biowin 2 models allocate readily biodegradable (fast or very fast degradation), or not readily biodegradable (slow or recalcitrant) for the other compounds based on their structure. Therefore:

- Readily degradable, (same as fast degradation), LRV = 0.65 ±0.21
- not readily degradable, (same as recalcitrant), LRV = 0



Calculating the average LRVs for the dataset of compiled values show large variability between some sources, for example the LRV PDFs reported by Walker et al. (2016) showed much higher removals compared to Zearley and Summers (2012).

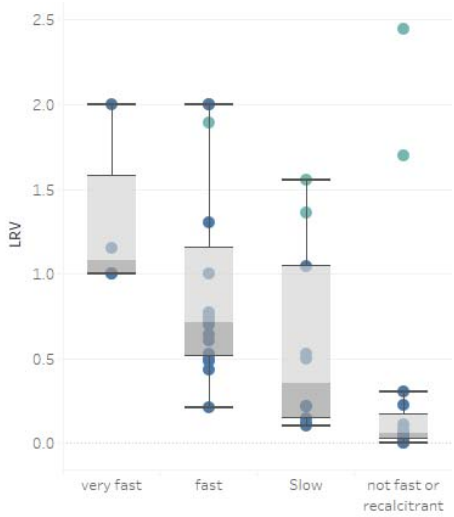


Figure 5.Compilation of LRVs from the compiled literature organised into groups based on biodegradability (EBCTs > 30 minutes were excluded). Point is the lighter blue are from Walker et al. (2016)

Limitations:

- *For compounds which are not adsorbable, or for GAC beds which are exhausted, the effectiveness of removal can be equated with inert media filters (Brown et al., 2017). The rate constants give similar ranges and performances for those from the GAC reported by Zearley and Summers (2012), however compounds with low biodegradability will not be removed at all.*
- *EBCT showed some variations, however still gave an acceptable range, due to the small amount of data low (<10 mins) and high (> 10 mins) groupings were not applied. A maximum EBCT of 30 mins was set to remove outliers.*

Ozone treatment may also be coupled with GAC which can promote the degradation of compounds.

Reverse osmosis and Nano filtration

Performance

Rejection of chemical contaminants using high pressure membrane systems are influenced by properties of the membrane (size exclusion, electrostatic interactions, hydrophobic interactions) and the contaminant (molecular size, polarity, hydrophobicity) (Le-Minh et al., 2010).

Organic chemicals

Bellona et al. (2004) proposed a model based on compound MW compared to membrane MWCO; pKa vs pH and log Kow can be used to allocate surrogates based on similar properties. The same model can be used to RO and NF, as the input parameters can be varied.

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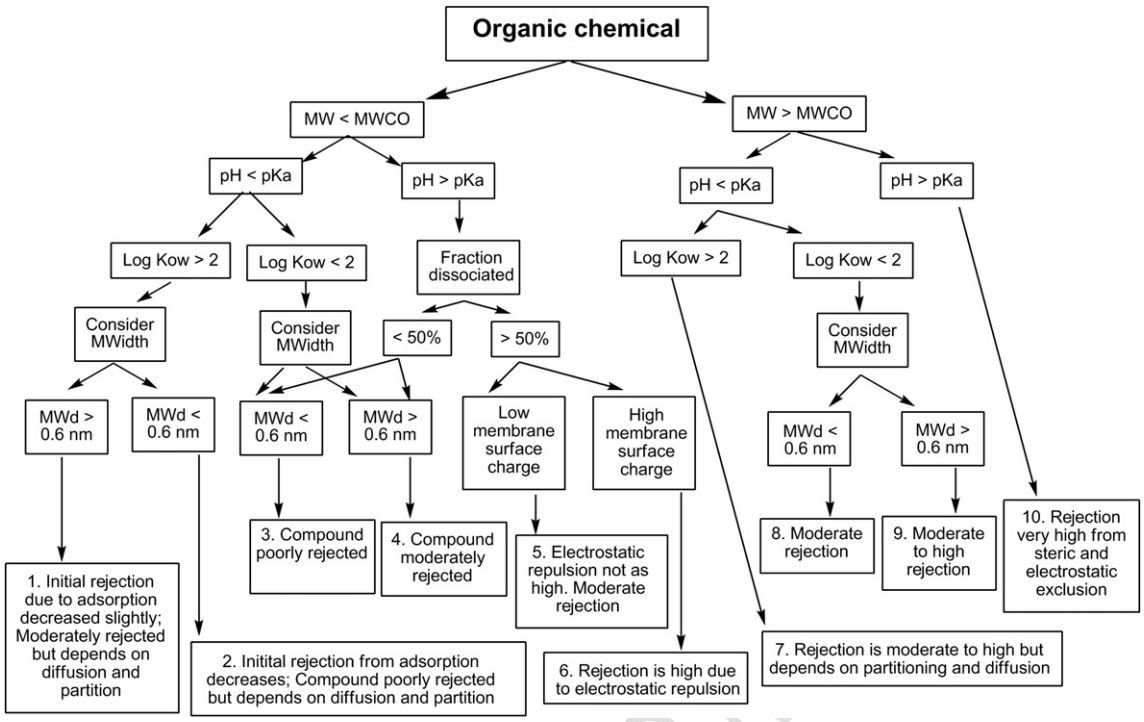

Figure 6.Rejection diagram for organic contaminants during membrane treatment, MW = molecular weight, pKa = acid (Bellona et al., 2004)

There are various approaches for determining the expected removals of organic compounds based on these groupings:

- Van der Bruggen et al. (2006) aimed to provide quantitative ranges to the qualitative removals of the groups 1-10 using nanofiltration. (see Spreadsheet)
- The report by Walker et al. (2016) uses the classifications for RO systems in full-scale water treatment plants. The data for each category has been collated for each of the categories. (see Figure 8)
- Assumptions based on poor and good removals for each group (based on 2012 report) (Figure 8)
- Another option for estimating removals is aggregating all the reported removal performance data for the different groups from the compiled data as shown in Figure 7 and Figure 8.

The variability between the approaches for estimating removals for each category is shown in Figure 8, the use of these methods provides the user options for evaluating compound removals.

Limitations:

- *Variability in removals and between methods for estimating potential group removals exist.*

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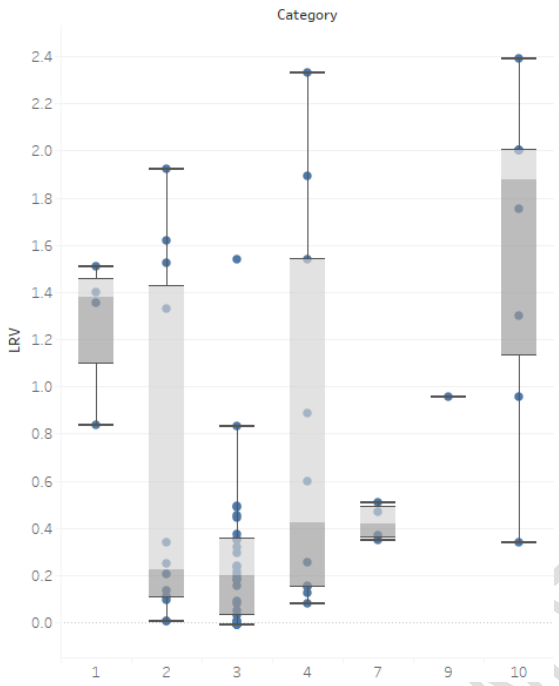

Figure 7. Group removals for shortlisted reported compounds based on MWCO = 210 and pH = 7. Compounds in Group 1= Tetrachloroethylene; Group 2 = 1,1-Dichloroethylene, 1,4-Dichlorobenzene, Benzene; Group 3 = 1,1,2-Trichloroethane, 1,2-Dichloroethane, 1,2-Dichloropropane, N-Nitrosomorpholine, NDMA, trans-1,2-Dichloroethene; Group 4= Bromodichloromethane, Caffeine, Cotinine, Simazine; Group 7 = Bromoform; Group 9 = Diatrizoate sodium; Group 10 = Amoxycillin, Atrazine, Diatrizoic acid, Diclofenac, PFOA, PFOS

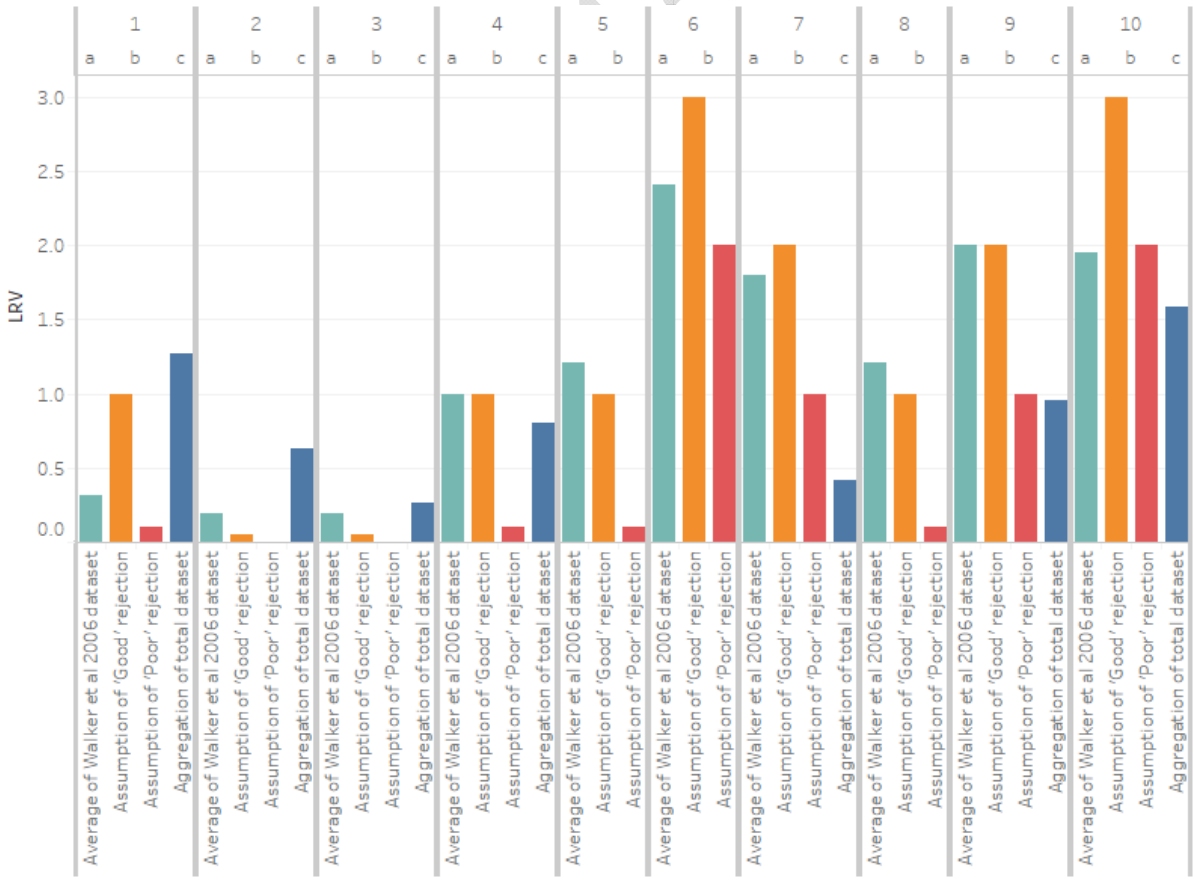

Figure 8. Comparison of average LRVs for the different categories according to different approaches. a = Walker et al 2006, b = Replacement flows 2012 paper, c = Aggregated dataset results

Inorganic compounds

The presence of inorganic compounds or ions in the RO permeate depends on the particle size and charge. Charged particles are more likely to be rejected. The probability distributions of a range of inorganic removals were reported in Walker et al. (2016).

Rejection categories for inorganic compounds were based on the expected valance of each ionic substance at a near neutral pH in conventionally treated wastewater.

Smaller compounds such as boron are expected to have very poor removal. Boron removal can provide an assessment of RO performance in removing low molecular weight chemicals as it is normally present in reasonable concentrations in wastewater and is partly removed by RO (Drewes et al, 2008). Correlations between the removal of poorly rejected small compounds such as boron and NDMA were noted by Fujioka et al. (2014)

Limitations:

- *groupings for inorganics isn't completed yet, need to aggregate existing data for inorganic compounds.*

Oxidation and Advanced Oxidation Processes (AOP)

Description

The removal of organic compounds which are biologically recalcitrant and/or poorly retained by membranes or activated carbon can be aided by oxidative processes (Khan, 2013).
Oxidative degradation can occur directly with the applied oxidant such as ozone, or via the production of highly reactive secondary species such as hydroxyl radicals (-OH). Ultraviolet (UV) light can also be used to degrade organic chemicals in water and it too can promote the formation of hydroxyl radicals. Ozone and UV light can be used to degrade contaminants, however molecular ozone or UV light alone are relatively specific in the chemical groups that they attack. There are a range of processes which promote the formation of hydroxyl radicals for the degradation or organics, these are generally referred to as advanced oxidation processes (AOP). The addition of hydrogen peroxide to ozone or in UV treatment is a commonly used method.

The coupling of these methods with hydroxyl radicals leads to non-specific degradation where all organics are ultimately susceptible if a sufficient dose is applied (Shemer et al., 2006). Thus AOPs widen the range of organic chemicals that may be oxidised as well as significantly increase reaction rates (von Gunten, 2003). For example, the addition of small amounts of H2O2 prior to ozonation generally improved by 5-15% the extent of EDC/PPCP oxidation as compared to ozone alone. (Westerhoff et al., 2005).

Innovative processes are currently being developed electrochemical or photocatalytic oxidation processes, or sonolysis (Rizzo et al., 2019). However, these are mostly lab or pilot scale studies and therefore are not included in the model due to lack of full scale studies.

The efficiency of AOPs depends on the contact time as well as the concentration of scavengers in the water (i.e. non-target oxidisable species). Due to the impacts of high concentrations of DOC and carbon/bicarbonate on the effectiveness of AOP, it is assumed that advanced oxidation is only

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applied following either GAC or RO which are effective reducing the levels of these hydroxyl scavengers. Indeed, AOP is commonly used to degrade chemicals which are not well removed by RO such as NDMA and 1,4-dioxane.

Performance

Ozonation

Due to its high reactivity, ozone decays quickly and does not maintain a residual for downstream processes. The faster compounds react with ozone, the quicker they degrade, those which decay slower will likely not be effectively removed as the ozone will be quickly depleted. Compounds with higher molecular ozone second-order rate constants in the literature were noted to have higher percentage removals (Westerhoff et al., 2005).

There have been various approaches made to group and predict removals during ozonation.

- Dickenson et al. (2009) grouped compounds into 5 different categories based on percentage reductions, and indicated relationships with ozone rate constants.
- Lee et al. (2013) acknowledged the contributions of hydroxyl radicals formed from the ozone dose. As –OH is less selective than ozone, this can lead to the reduction of other compounds. Lee et al. (2013) proposed the grouping of compounds into 5 groups according to both the ozone and the hydroxyl rate constants, showing the expected removals for surrogate compounds in each group
- While recently Rizzo et al. (2019) grouped a number of compounds into 3 groups according to the ozone rate constants and showed the relationship with ozone dose for a number of compounds. This is a simpler model, resulting in a wider expected PDF range

Based on the groupings and findings of Lee et al. (2013) a decision tree (Figure 9) was constructed in order to estimate the removal of unknowns during the ozonation process.

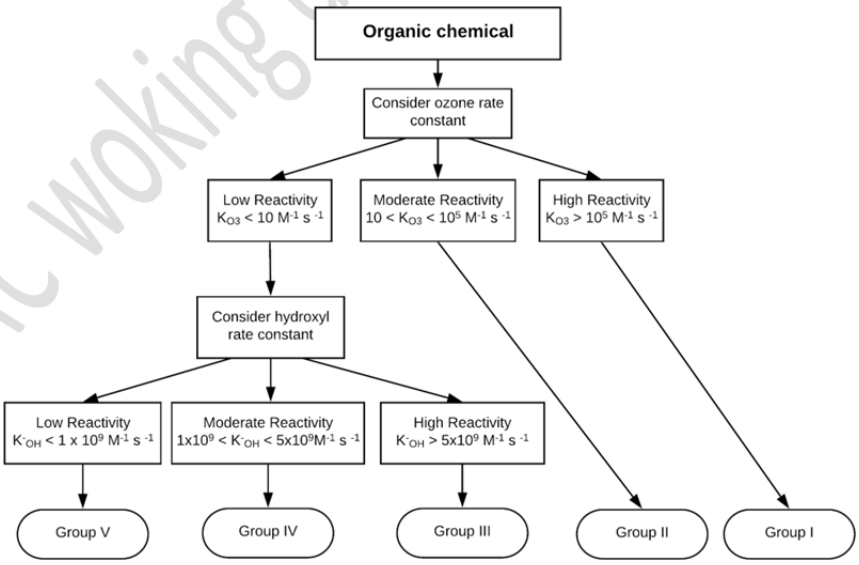

Figure 9. Decision tree for grouping organic contaminants during ozonation. Based on (Lee et al., 2013).

Depending on the site and the water characteristics, particularly the nitrite concentration, the ozone dose will have different effects. The expected removals for categories allocated by Lee et al. (2013)

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were calculated using data for removals of representative compounds from lab scale trials from 10 different plants for a range of ozone doses. The probability distributions for each group were based on the Lee et al. (2013) labscale trials (Table 5), as well as distribution from broader literature data (Figure 10).

Ozone and hydroxyl rate constants were gathered for a range of compounds from a variety of sources, e.g . (Mandal, 2018; Sudhakaran and Amy, 2013; Westerhoff et al., 2005; Wols and Hofman-Caris, 2012). For compounds where data was not available, will be indicated and assigned as minimal expected removal.

Table 5 Grouping compounds according to ozone and hydroxyl rate constants, based on Lee et al. (2013)

Group	*Representative compound*	*<Need to calculate removals PDFs*	
I	***Triclosan***, diclofenac, carbamazepine, bisphenol A, sulfamethoxazole, trimethoprim, and naproxen		
II	Atenolol, Gemfibrozil		
III	DEET, ibuprofen, phenytoin, and primidone		
IV	*Meprobomate* *Atrazine*		
V	*TCEP*		
?			

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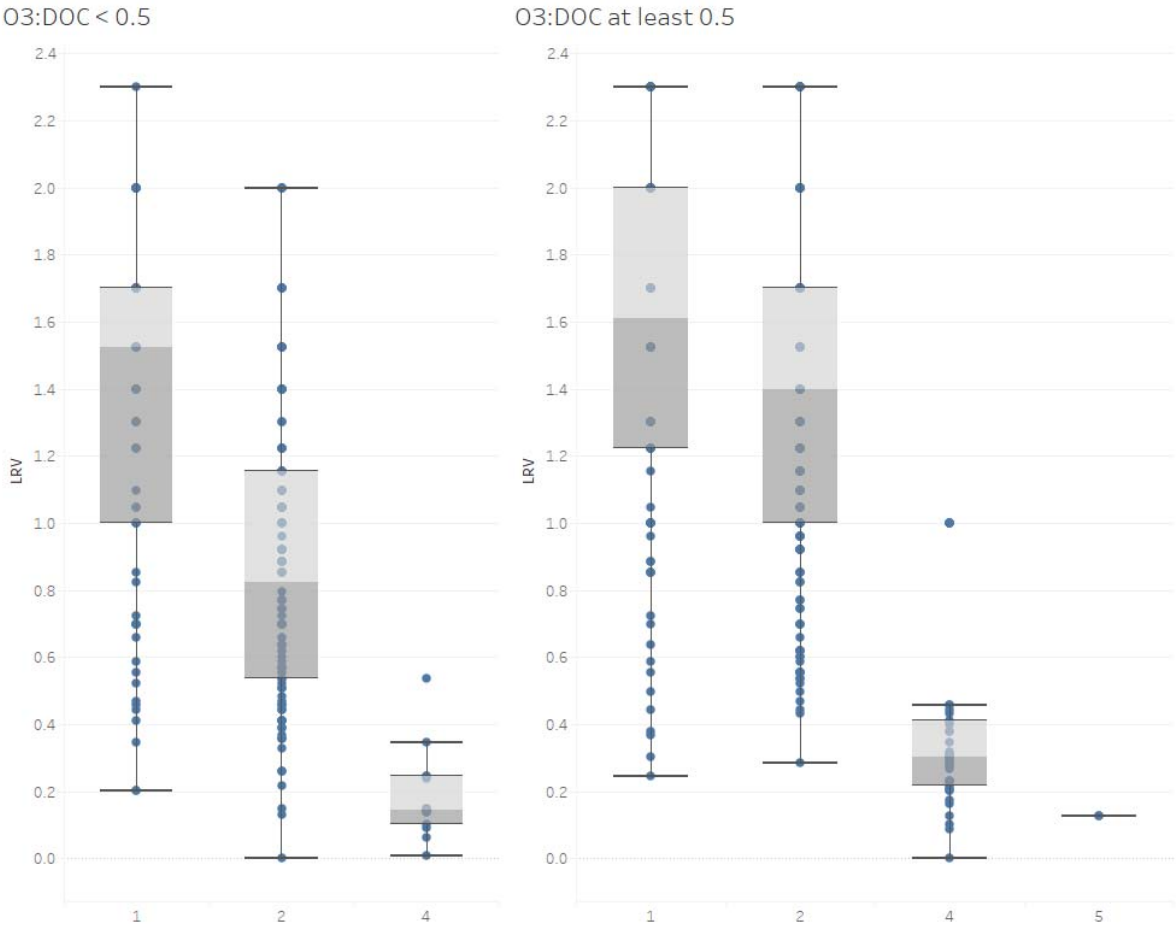

Figure 10. LRV distributions for Ozone treatment for each of the compound groupings (Figure 9) at different O3 dose rates based on compiled data from the literature

Acknowledged limitations of these approaches are:

- *While temperature will also influence the degradation rates, for the grouping of compounds it is assumed the range is minimal and close to 20˚C.*
- *Nitrite can also react fast with ozone in a molar ratio of 1:1, consuming 3.43 g O_3 per g NO_2-N. The fast reaction results in a competition with CECs abatement (Rizzo et al., 2019).*
- *Similarly, components such as EfOM, bicarbonate/carbonate, bromide and ammonia can contribute to the overall –OH consumption (Lee et al., 2013)*
- *The rate constants of compounds with pKa close to the water pH can vary dramatically and affect their removal. Such compounds include:*
- *Filtration prior to ozonation can increase the removal efficiency (Lee et al., 2013)*
- *Rate constant data was not available for all compounds. Where not available another decision matrix needs to be added detailing how it was assigned to a group or a null category.*

Ozonation + H2O2

The addition of H2O2 during ozone causes ozone to react with the peroxide anion (HO2−) to form ˙OH precursors. This process is known as the Peroxone process. Lee et al. (2013) also investigated the effect of H2O2 addition for each of the allocated groups (I to V). Concentrations of 0.5 to 1 H2O2 to O3 were tested, there did appear to be a slight increase in the removal rate for higher H2O2 doses. However, the optimal ratio is 0.5 = H_2O_2 : O_3 (Miklos et al., 2018). H2O2 addition only appeared to

improve the reduction rates slightly for compounds in groups Table 6. The use of H2O2 does however reduce the formation rates of bromate during ozonation (Miklos et al., 2018). Ozone also does not lead to the formation of chlorinated DBPs when applied.

Table 6 Effect of H_2O_2 addition during ozonation on contaminant removals. Lee et al. (2013) Table S2 – S5

Group I:	little effect, may in fact reduce removal efficiency due to faster decay of ozone
Group II:	
Group III:	<to be calculated>
Group IV:	<10% enhancement
Group V:	<10% enhancement

UV Disinfection (UV dose 40-180 mJ/cm²)

The energy carried by UV-C radiation (200-280 nm) is sufficient to break chemical bonds in organic chemicals capable of adsorbing those wavelengths, however a typical doses (~40 mJ/cm^2) used for disinfection it is expected that oxidation of contaminants is extremely small (Snyder et al., 2007).

Certain compounds have been documented to be affected at the typical disinfection doses. For example some micropollutants, such as boldenone, diclofenac, ketoprofen, sulfamethoxazole, can be effectively degraded at reasonably low dosages (>90% degradation at dose of around 230 mJ/cm^2) (Yang et al., 2014).

However, due to the low removals and uncertainty for many compounds it is assumed that UV treatment at levels used for disinfection will not significantly remove any contaminants.

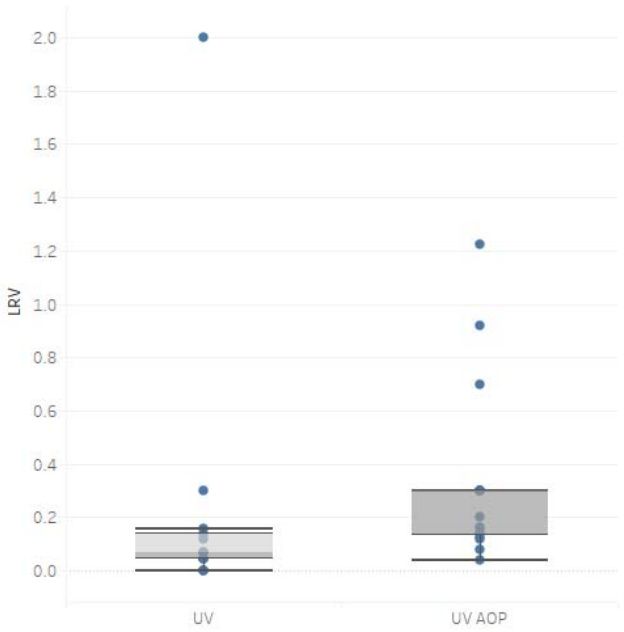

Figure 11. LRVs for the UV and UV AOP (H2O2) for UV dosage less than 500 mJ/cm^2 from the compiled datasets.

UV AOP (UV dose >500 mJ/cm², no oxidation catalyst)

The higher doses of UV increases the formation of hydroxyl radical reactions while some compounds may be removed by direct photolysis (Wols and Hofman-Caris, 2012). Based on the structures of

compounds, higher removals are likely for those with aromatic rings or double C = C bonds, which absorb photons under UV irradiation. The variability between compounds is linked to their structure and susceptibility to photolysis.

Might be some useful data for NDMA. Also some others which are degraded by photolysis. Lots of papers by Karl Linden over last 20 years. I'll present the data better in this bit - link to compound properties to help classify unknowns.

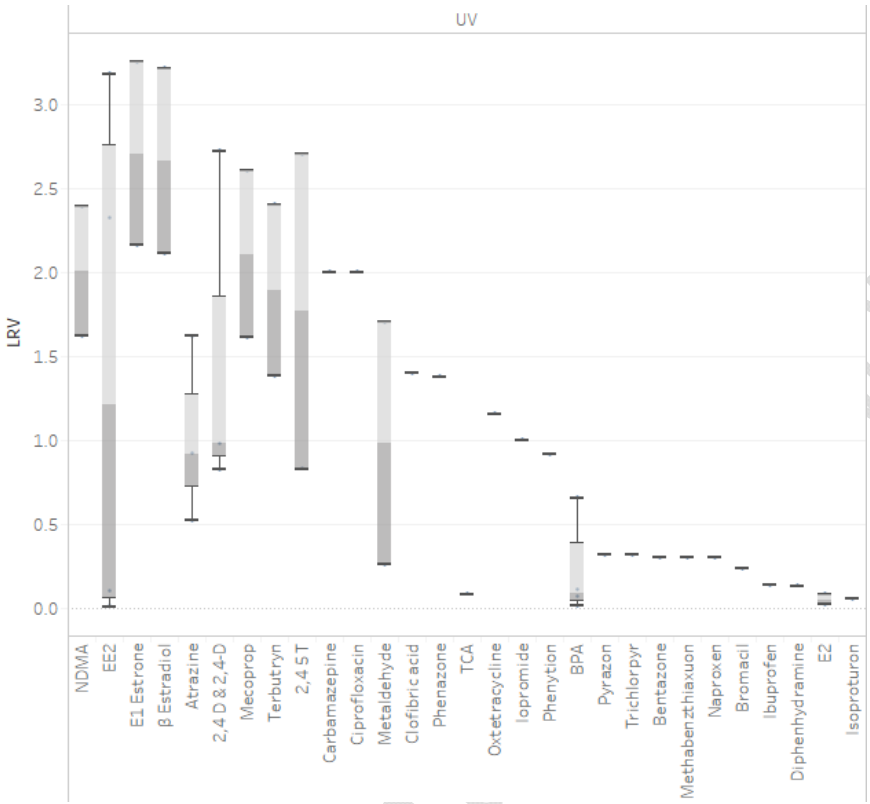

Figure 12. Box and Whisker diagram for the LRVs for UV where the dosage is greater than 500mJ/cm2. Note that large range of UV fluences are used.

UV AOP (UV dose >500 mJ/cm², H_2O_2)

Addition of UV energy in the presence of H_2O_2 is an advanced oxidation process (AOP), means much of the micropollutant oxidation occurs via a highly reactive intermediate, the hydroxyl radical ($^{\bullet}OH$). Similar to the ozonation, the UV AOP process is sensitive to water quality and the presence of hydroxyl scavengers.

UV/H2O2 processes are currently applied in full scale UV systems in order to remove recalcitrant contaminants such as 1,4 dioxane, methyl tert butyl ether (MTBE), trichloroethylene (TCE), N-nitrosodimethylamine (NDMA) and other organics (Snyder et al., 2007). Conditions which favour the removal of NDMA also result in the removal of taste of odour compounds such as geosmin, MIB as well as microcystin (Swaim et al., 2008).

Removals of 1,4-dioxane with UV AOP (5 mL/L H2O2) were dependant on UV dose with LRVs ranging from 0.08 to 0.4 for doses from 300 – 2200 mJ/cm^2 (Swaim et al., 2008).

Approaches to modelling the UV AOP process includes the steady-state $^{\bullet}OH$ radical method and the as well as the commercially available AdOx method. Both approaches rely on theoretical hydroxyl

rate constants (Rosenfeldt and Linden, 2007). However, other more precise methods proposed by Rosenfeldt and Linden (2007) require compound specific rate constants for direct photolysis and OH radical oxidation, the latter of which is not as commonly presented in the literature.

Might be some useful data for 1,4-dioxane. Also some others which are degraded by hydroxyl radicals. Lots of papers by Karl Linden over last 20 years.

Chlorine disinfection

Description

During chlorination processes, HOCl is generally the major reactive species for the reaction with micropollutants. Oxidation, addition and electrophilic substitution reactions of chlorine with organic compounds are reported in literature. Addition and oxidation reactions are typically slow. Only electrophilic attacks of chlorine on the organic compounds are usually fast enough to be significant. Therefore, chlorine is highly selective towards organic compounds and its reactivity is commonly limited to particular sites (such as amine and reduced sulfur functional groups or activated aromatic systems) (Deborde and von Gunten, 2008). For the reaction of chlorine with organic compounds, second-order rate constants can vary over more than 10 orders of magnitude.

While many inorganic and organic micropollutants can be transformed by chlorine however for certain compounds, the chlorine reactivity is low and only small modifications in the parent compound's structure are expected under water treatment conditions (Deborde and von Gunten, 2008).

Performance

Wil be some data from Southern Nevada Water Authority (Shane Snyder, Paul Westerhoff, Eric Dickenson). Should be able to get some Log (order of magnitude) removal values. Don't need much, just enough to get a sense of how useful this barrier might be.,

For inorganic and organic compounds, linear structure–activity relationships can be proposed based on the electron-donor/acceptor characteristics, structural analogy and from the expected chlorination mechanisms. Considering the known chlorine reactivity with the main functional groups, an estimation of the order of magnitude of chlorination reaction rate constants can be carried out. Such estimations were shown to be in agreement with literature data for numerous pharmaceuticals and endocrine disruptors. However, due to more complex chemical structures, such estimations are more difficult to be obtained in the case of certain heterocycles or cyanotoxins (Deborde and von Gunten, 2008). In addition, a pH dependence of organic and inorganic micropollutant transformation is commonly observed due to chlorine speciation in solution.

Interestingly, Deborde and von Gunten (2008) observed that for compounds with an electrophilic ozone and chlorine attack on the aromatic ring, a good linear correlation between chlorination and ozonation rate constants.

The effective removal of antibiotics by chlorination from drinking water requires sufficient free chlorine concentration and contact time (Le-Minh et al., 2010) With the use of free chlorine at 1.0 mgL_1 (as Cl2), 90% removal has been reported with contact times greater than 16 min for most

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sulfonamides and greater than 40 min for trimethoprim in river water (Adams et al., 2002). The longer term storage in reticulation systems can also result in the transformation of certain compounds (Gibs et al., 2007) , as this study deals with the drinking water treatment plant the focus is on the short term storage studies (e.g less than 1 day). Huerta-Fontela et al. (2011) noted that peroxidation with chlorine at breakpoint concentrations reduced the concentrations of certain compounds. For example, primary and secondary amines in amlodipine, tamoxifen, sertraline, oxazepam and furosemide were reduced at percentages higher than 99%. Some beta blockers were expected to have high reactivity (labetalol, betaxolol and doxazosin had high removals) – however others had poor removal, (Huerta-Fontela et al., 2011). Chlorination is suggested for the removal of microcystin LR (Sorlini and Collivignarelli, 2011), however the performance depends on the addition method. For example chlorine was more effective than chlorine dioxide.

In their study of pharmaceutical compounds, Glassmeyer and Shoemaker (2005) noted that compounds fell into three distinct groups; those that were unchanged, those that were chlorinated, those that were changed but not chlorinated .

Table 7. Effect of chlorination on pharmaceuticals, adapted from Glassmeyer and Shoemaker (2005)

No change	Signs of chlorination	Changes (but not strictly chlorinated)
continin aspartame caffeine 1,7 dimethylxantine aspirin 6a-methyl-17a-hydroxy progesterone acetate	gemfibrozil acetaminophen	Amxicillin cephalexin cimetidine trimethoprim diltiazem warfarin

< I'm still updating the table in excel - however there's large variability in the LRVs for certain compounds as to when chlorine is added – e.g pre or post chlorination. Typically LRVs wereb;t higher than 2 as the units were reported in % reductions and due to LOQ.

From the data compounds with the highest removals had aromatic rings (THC, THC-COOH, Setraline, Venlafaxine clofibric acid, parathion), or triazine

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Environmental buffer – Surface water reservoir

Dilution

Explain how Californian Title 22 regulations only recently produced "criteria for surface augmentation". In that regulation, they base LRV credits (for pathogens) on assumption of surface water dilution values, with benchmarks of (up to) 1% and 10% of reservoir volume during any 24 hour period. So we can adopt these benchmarks (1 LRV and 2 LRV) for our modelling.

Other removal mechanisms

Summary of how fugacity models can capture:

- *Biotic*
- *Abiotic (hydrolysis)*
- *Volatilisation*
- *Partitioning to sediment, etc*

Might make sense to only consider this for chemicals for which insufficient removal has already been demonstrated for previous treatment barriers.

But lets hold off on doing any work on this until the chemicals have been short-listed (probably to nothing). (Ok – holding off! July meeting?)

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References

Bellona, C., Drewes, J.E., Xu, P., Amy, G., 2004. Factors affecting the rejection of organic solutes during NF/RO treatment—a literature review. Water research 38(12), 2795-2809.

Bratby, J., 2016. Coagulation and Flocculation in Water and Wastewater Treatment. IWA Publishing.

Brown, J., Summers, R.S., Dickenson, E., Upadhyaya, G., 2017. Biological removal of hazardous pollutants in drinking water treatment, in: Çeçen, F., Tezel, U. (Eds.), Hazardous Pollutants in Biological Treatment Systems: Fundamentals and a Guide to Experimental Research. IWA Publishing, p. 0.

Deborde, M., von Gunten, U., 2008. Reactions of chlorine with inorganic and organic compounds during water treatment—Kinetics and mechanisms: A critical review. Water Research 42(1), 13-51.

Dickenson, E.R.V., Drewes, J.E., Sedlak, D.L., Wert, E.C., Snyder, S.A., 2009. Applying Surrogates and Indicators to Assess Removal Efficiency of Trace Organic Chemicals during Chemical Oxidation of Wastewaters. Environmental Science & Technology 43(16), 6242-6247.

Fujioka, T., Tu, K.L., Khan, S.J., McDonald, J.A., Roux, A., Poussade, Y., Drewes, J.E., Nghiem, L.D., 2014. Rejection of small solutes by reverse osmosis membranes for water reuse applications: A pilot-scale study. Desalination 350, 28-34.

Gibs, J., Stackelberg, P.E., Furlong, E.T., Meyer, M., Zaugg, S.D., Lippincott, R.L., 2007. Persistence of pharmaceuticals and other organic compounds in chlorinated drinking water as a function of time. Science of The Total Environment 373(1), 240-249.

Glassmeyer, S.T., Shoemaker, J.A., 2005. Effects of Chlorination on the Persistence of Pharmaceuticals in the Environment. Bulletin of Environmental Contamination and Toxicology 74(1), 24-31.

Huerta-Fontela, M., Galceran, M.T., Ventura, F., 2011. Occurrence and removal of pharmaceuticals and hormones through drinking water treatment. Water Research 45(3), 1432-1442.

Khan, S., 2013. Drinking water through recycling: The benefits and costs of supplying direct to the distribution system. Australian Academy of Technological Sciences and Engineering.

Le-Minh, N., Khan, S.J., Drewes, J.E., Stuetz, R.M., 2010. Fate of antibiotics during municipal water recycling treatment processes. Water Research 44(15), 4295-4323.

Lee, Y., Gerrity, D., Lee, M., Bogeat, A.E., Salhi, E., Gamage, S., Trenholm, R.A., Wert, E.C., Snyder, S.A., von Gunten, U., 2013. Prediction of Micropollutant Elimination during Ozonation of Municipal Wastewater Effluents: Use of Kinetic and Water Specific Information. Environmental Science & Technology 47(11), 5872-5881.

Mandal, S., 2018. Reaction Rate Constants of Hydroxyl Radicals with Micropollutants and Their Significance in Advanced Oxidation Processes. Journal of Advanced Oxidation Technologies 21(1).

Miklos, D.B., Remy, C., Jekel, M., Linden, K.G., Drewes, J.E., Hübner, U., 2018. Evaluation of advanced oxidation processes for water and wastewater treatment – A critical review. Water Research 139, 118-131.

NH&MRC, 2013. AUSTRALIAN DRINKING WATER GUIDELINES 6 2011 Version 2.0 updated December 2013. pp 1305.

Rizzo, L., Malato, S., Antakyali, D., Beretsou, V.G., Đolić, M.B., Gernjak, W., Heath, E., Ivancev-Tumbas, I., Karaolia, P., Lado Ribeiro, A.R., Mascolo, G., McArdell, C.S., Schaar, H., Silva, A.M.T., Fatta-Kassinos, D., 2019. Consolidated vs new advanced treatment methods for the removal of contaminants of emerging concern from urban wastewater. Science of The Total Environment 655, 986-1008.

Rosenfeldt, E.J., Linden, K.G., 2007. The ROH,UV Concept to Characterize and the Model UV/H2O2 Process in Natural Waters. Environmental Science & Technology 41(7), 2548-2553.

Snyder, S.A., Wert, E., Lei, H., Westerhoff, P., Yeomin, Y., 2007. Removal of EDCs and pharmaceuticals in drinking and reuse treatment processes. IWA publishing,

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Awwa Research Foundation,

AWWA,, Denver, USA.
Sorlini, S., Collivignarelli, C., 2011. Microcystin-LR removal from drinking water supplies by chemical oxidation and activated carbon adsorption. Journal of Water Supply: Research and Technology-Aqua 60(7), 403-411.
Stackelberg, P.E., Gibs, J., Furlong, E.T., Meyer, M.T., Zaugg, S.D., Lippincott, R.L., 2007. Efficiency of conventional drinking-water-treatment processes in removal of pharmaceuticals and other organic compounds. Science of The Total Environment 377(2), 255-272.
Sudhakaran, S., Amy, G.L., 2013. QSAR models for oxidation of organic micropollutants in water based on ozone and hydroxyl radical rate constants and their chemical classification. Water Research 47(3), 1111-1122.
Swaim, P., Royce, A., Smith, T., Maloney, T., Ehlen, D., Carter, B., 2008. Effectiveness of UV Advanced Oxidation for Destruction of Micro-Pollutants. Ozone: Science & Engineering 30(1), 34-42.
Ternes, T.A., Meisenheimer, M., McDowell, D., Sacher, F., Brauch, H.-J., Haist-Gulde, B., Preuss, G., Wilme, U., Zulei-Seibert, N., 2002. Removal of Pharmaceuticals during Drinking Water Treatment. Environmental Science & Technology 36(17), 3855-3863.
Van der Bruggen, B., Vandecasteele, C., 2002. Modelling of the retention of uncharged molecules with nanofiltration. Water Research 36(5), 1360-1368.
Van der Bruggen, B., Verliefde, A., Braeken, L., Cornelissen, E.R., Moons, K., Verberk, J.Q., van Dijk, H.J., Amy, G., 2006. Assessment of a semi-quantitative method for estimation of the rejection of organic compounds in aqueous solution in nanofiltration. Journal of Chemical Technology & Biotechnology 81(7), 1166-1176.
Walker, T., Stanford, B.D., Khan, S.J., Robillot, C., Snyder, S., Valerdi, R., Dwivedi, S., Vickers, J., 2016. Critical Control Point Assessment to Quantify Robustness and Reliability of Multiple Treatment Barriers of a DPR Scheme. Water Environment & Reuse Foundation, Alexandria, VA.
Westerhoff, P., Yoon, Y., Snyder, S., Wert, E., 2005. Fate of endocrine-disruptor, pharmaceutical, and personal care product chemicals during simulated drinking water treatment processes. Environmental science & technology 39(17), 6649-6663.
Wols, B.A., Hofman-Caris, C.H.M., 2012. Review of photochemical reaction constants of organic micropollutants required for UV advanced oxidation processes in water. Water Research 46(9), 2815-2827.
World Health Organization, 2017. Potable reuse: guidance for producing safe drinking-water. World Health Organization,, Geneva, Switzerland.
Yang, W., Zhou, H., Cicek, N., 2014. Treatment of Organic Micropollutants in Water and Wastewater by UV-Based Processes: A Literature Review. Critical Reviews in Environmental Science and Technology 44(13), 1443-1476.
Zearley, T.L., Summers, R.S., 2012. Removal of Trace Organic Micropollutants by Drinking Water Biological Filters. Environmental Science & Technology 46(17), 9412-9419.

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Technical notes:

In order to group chemicals of concern according to the Bellona et al. (2004) classifications, the molecular width (MWd) was estimated based on the logarithmic relationship with molecular weight proposed by Van der Bruggen and Vandecasteele (2002). The equation for estimating molecular width was MWd = A(MW)^B where A = 0.065 and B = 0.438, which is valid for the molecular weight range up to +_600Da.

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