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REPORT

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Substances to be Targeted in Laboratory and Technical Scale Experiments
Project OXIRED, Deliverable 1.1a

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Title
Substances to be Targeted in Laboratory and Technical Scale Experiments.
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Abstract

The combination of advanced oxidation (e.g. ozonation) and subsurface passage could overcome known limitations of MAR techniques with respect to dissolved organic carbon (DOC) and trace organics removal. The objective of the OXIRED project is to assess possibilities and limitations as well as practicability and technical feasibility of different combinations of advanced oxidation and subsurface passage with respect to this topic. As part of the first project phase, existing data on subsurface removal of organic trace substances was evaluated in order to identify substances that should be targeted in laboratory and technical scale experiments. This report summarizes the outcomes of this evaluation.

For the identification of substances to be targeted in laboratory and technical scale experiments, a literature survey was carried out on substances that are potentially persistent during subsurface passage. The basis for this survey was an extensive, publicly available data base on the behaviour of trace organics during natural drinking water treatment (bank filtration, aquifer recharge, slow sand filtration) compiled by the Schmidt (2005) at the German Technology Center for Water (TZW). This data was supplemented by results published by Stuyvzand et al. (2007) and a comprehensive analysis of NASRI data carried out at the KWB (Wiese et al. 2009).

For the 45 potentially persistent substances (for which only little removal had been stated in at least one of the mentioned sources) a comprehensive evaluation on potential for breakthrough in subsurface treatment systems was carried out. In addition, experts from BWB and Veolia were asked to classify the substances with respect to relevance (occurrence, persistence) in their respective water supply systems. The result was a list of 20 possible target substances, of which 4 were rated as 1st priority, due to the fact that they i) showed a high potential for breakthrough in subsurface treatment systems, ii) were classified as highly relevant by either BWB or Veolia (or both), iii) are not efficiently removed by advanced post-treatment techniques (e.g. GAC) and iv) for which an analytical method is available at BWB. These 1st priority substances for further investigations are: MTBE, sulfamethoxazole, EDTA and ETBE.

Possible target substances of 2nd priority are: carbamezipine, *primidone*, *1,5-NDSA*, *iopamidole*, bentazone, *1,7-NDSA*, *2,7-NDSA*, atrazine, desethylatrazine, linuron, diuron, diclofenac, *amidotrizoic acid* (italics indicate substances, for which there is currently no analytical method available at BWB).

In addition, it is recommended to investigate the behavior of the sum parameter AOI in the experiments, encompassing all iodinated contrast media which in total can not be determined as individual substances.

Zusammenfassung

Naturnahe Wasseraufbereitungsverfahren mit Untergrundpassage wie z.B. Uferfiltration oder künstliche Grundwasseranreicherung können eine ausreichende Elimination von organischen Spurenstoffen und gelöstem organischen Kohlenstoff (DOC) nicht in jedem Falle gewährleisten. Eine mögliche Lösung wäre die Kombination mit Oxidationsverfahren, wie z.B. Ozonierung. Das Ziel des Projektes OXIRED ist es, die Vor- und Nachteile wie auch die Praktikabilität und technische Machbarkeit verschiedener dieser Verfahrenskombinationen im Hinblick auf die Entfernung von DOC und organischen Spurenstoffen abzuschätzen. Innerhalb der ersten Phase des Projektes werden existierende Daten zur Spurenstoffelimination ausgewertet, um Einzelstoffe zu identifizieren, die in den Experimenten im Labor sowie im technischen Maßstab näher untersucht werden sollen. Der vorliegende Bericht dokumentiert die Ergebnisse dieser Einschätzung.

Für die Identifikation der zu untersuchenden Einzelstoffe wurde eine Literaturrecherche zu potentiell in Untergrund persistenten organischen Spurenstoffen durchgeführt. Die Basis für diese Recherche stellte eine umfangreiche, öffentlich zugängliche Datenbank des DVGW Technologiezentrums Wasser (TZW) in Karlsruhe dar. In dieser von Schmidt (2005) erstellten Datenbank sind Daten zum Verhalten von organischen Spurenstoffen während naturnaher Trinkwasseraufbereitung (Uferfiltration, künstliche Grundwasseranreicherung, Langsamsandfiltration) zusammengetragen. Ergänzt wurden diese Daten durch Ergebnisse von Stuyfzand et al. (2007) sowie durch eine umfangreiche Analyse von NASRI Daten des KWB (Wiese et al. 2009).

Für die 45 potentiell persistenten Substanzen (für die nur geringe oder keine Entfernung in mindestens einer der erwähnten Quellen dokumentiert war) wurde eine allgemeine Bewertung des Durchbruchspotentials bei der Untergrundpassage durchgeführt. Zusätzlich gaben Experten von BWB und Veolia ihre subjektive Bewertung zur Relevanz (Auftreten, Persistenz) der Einzelstoffe in ihren jeweiligen Wasserversorgungssystemen ab. Aus der resultierenden Liste von 20 möglichen Zielsubstanzen wurden vier mit höchster Priorität eingestuft, da sie i) ein hohes Durchbruchspotential aufwiesen, ii) mindestens von einem der beiden konsultierten Experten als höchst relevant eingestuft wurden, iii) nicht oder nur wenig durch weitergehende Aufbereitungstechniken wie z.B. Aktivkohle entfernt werden und iv) für die eine Analysenmethode bei BWB existiert. Diese Substanzen mit höchster Priorität für weitere Untersuchungen sind: MTBE, Sulfamethoxazol, EDTA und ETBE.

Mögliche Zielsubstanzen mit hoher (2.) Priorität sind: Carbamezipin, *Primidon*, *1,5-NDSA*, Iopamidol, Bentazon, *1,7-NDSA*, *2,7-NDSA*, Atrazin, Desethylatrazin, Linuron, Diuron, Diclofenac und *Amidotrizoesäure* (für kursiv gedruckte Substanzen ist zur Zeit keine Analysemöglichkeit bei BWB vorhanden).

Zusätzlich wird empfohlen, das Verhalten des Summenparameters AOI in den Experimenten zu erfassen, da er die Iod-haltigen Röntgenkontrastmittel beinhaltet, die in ihrer Gesamtheit nicht als individuelle Substanzen nachgewiesen werden können.

Résumé

La combinaison de l'oxydation avancée (par ex. l'ozonation) et de l'écoulement souterrain pourrait permettre de dépasser les limites connues des techniques intégrées de réalimentation des nappes MAR (Managed Aquifer Recharge) vis à vis du carbone organique dissous et de composés organiques traces. L'objectif du projet OXIRED est d'évaluer les possibilités et les limites, ainsi que la faisabilité technique et les conditions de mises en œuvre de diverses combinaisons d'oxydation avancée couplée à un écoulement souterrain pour ces paramètres. Lors de la première phase du projet, on a évalué les données existantes concernant l'épuration par percolation dans le sol de composés organiques traces afin d'identifier les substances à cibler lors d'expériences en laboratoire et à échelle pilote. Ce rapport fait la synthèse des résultats de cette évaluation.

Dans le but de sélectionner les substances à tester dans le cadre d'essais en laboratoire et à échelle pilote, une étude récapitulative des substances potentiellement persistantes lors de l'écoulement souterrain a été entreprise.

Cette étude se fonde sur un grand nombre de données publiques relatives au comportement de composés organiques traces pendant le traitement de l'eau potable naturelle (filtration sur berge, alimentation des nappes, filtration lente sur sable) compilées par Schmidt (2005) au Centre allemand de technologie de l'eau (TZW). Ces données sont complétées par les résultats de recherches publiés par Stuyvzand et al. (2007) et par une analyse exhaustive des données NASRI (Natural and Artificial Systems for Recharge and Infiltration) réalisée par Wiese et al. 2009 au Centre de compétences sur l'eau (KWB).

Une évaluation détaillée de 45 substances potentiellement persistantes (pour lesquelles seule une élimination mineure a été mise en évidence dans au moins une des sources mentionnées) par rapport au potentiel de point de fuite dans les systèmes de traitement souterrains a été réalisée. Par ailleurs, les experts de la société des eaux berlinoise BWB et de Veolia ont eu à classer les substances selon leur pertinence (survenance, persistance) dans leurs ressources en eau utilisées en potabilisation. Il en résulte une liste de 20 substances cibles potentielles, dont 4 dans la catégorie de première priorité car i) elles présentent un fort potentiel de percement dans les dispositifs de traitement souterrains, ii) elles sont répertoriées comme étant très pertinentes soit par BWB ou Veolia (ou les deux), iii) elles ne sont pas suffisamment éliminées par les procédés d'affinage (par ex. le charbon actif en granulés et iv) pour lesquelles il existe une méthode d'analyse chez BWB. Ces substances de première priorité retenues pour des recherches ultérieures sont : le MTBE, le sulfaméthoxazole, le EDTA et l'ETBE.

Les substances cibles possibles de seconde priorité sont: la carbamazépine, la *primidone*, le *1,5-NDSA*, l'*iopamidole*, la bentazone, le *1,7-NDSA*, le *2,7-NDSA*, l'atrazine, la desethylatrazine, le linuron, le diuron, le diclofenac, l'acide *amidotrizoïque*

(les caractères en italique indiquent les substances pour lesquelles il n’existe pas encore de méthode d’analyse chez BWB).

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We greatly appreciate the input of P. Roche (Veolia, AR) and U. Dünnbier (BWB), who have shared their expertise with respect to relevance of the different organic trace compounds for their respective water supply systems. Finally, we thank U. Hübner (TUB), Iris Hülshoff (KWB) and Y. Moreau-Le Golvan (KWB) for their critical final review and P. Roche (Veolia, AR) for quality assurance.

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1. Introduction

Subsurface passage is a water treatment technique that is utilized e.g. during bank filtration (BF) and aquifer recharge (AR) and is recommended as pre-treatment of drinking water within a multi-barrier concept (WHO 2006). It also finds application as polishing step for treated waste water (referred to as soil aquifer treatment – SAT). Berlin has been relying on subsurface passage for both purposes since more than 150 years within an integrated water resource management. Many different research projects (e.g. NASRI, KWB 2002 – 2006) have lead to a sound understanding of the processes involved and the advantages and limitations of this technique.

During subsurface passage, especially particulate and particle-bound substances (e.g. algae and bacteria) are efficiently removed by physical straining. In addition, multiple bio- and geochemical reactions in the aquifer lead to a reduction of many dissolved substances like pharmaceuticals and industrial chemicals (for an overview see Hülshoff et al. 2009).

There are, however, limitations to this technique, as some trace organic substances have shown to be persistent in the subsurface. Also, efficient removal of bulk dissolved organic carbon (DOC) from surface waters with high concentrations or from treated wastewater can only be ensured for high shares of biodegradable DOC (BDOC), sufficient contact time and aerobic conditions.

In case of short retention times due to lack of aquifer volume (2 – 50 days) or in case of substantial pollution of the surface water, additional measures need to be taken to ensure sufficient drinking water quality or prevent long term degradation of ground water resources. Advanced oxidation (e.g. ozonation) as pre- or post-treatment may be a possible additional measure as it increases the share of biodegradable organic substances in water and has been shown to reduce concentrations of otherwise persistent trace organics in treated waste water (PILOTOX, KWB 2005). The aim of the project OXIRED1 is to assess the feasibility of combined advanced oxidation (e.g. ozonation) and subsurface passage for drinking water treatment or final waste water treatment step.

Work package 1.1 of the project aims at the identification of trace organic substances that shall be targeted in the experimental phase of the project. Criteria for this selection are:

i) high potential for breakthrough in subsurface infiltration systems (RBF / AR),

ii) high relevance for water suppliers (in this case Veolia and BWB),

iii) little or no removal by advanced drinking water treatment (e.g. granular activated carbon),

iv) analytical method established at BWB laboratories.

This report shall summarize the results of the literature study carried out and give a priority list of substances to target in the laboratory and technical scale experiments scheduled for 2009.

2. Methods

A literature study was carried out to compile data on the behavior of potentially persistent trace organics in the subsurface during bank filtration and aquifer recharge. A large number of relevant publications has already been subject to a similar literature study by the Water Technology Center, Karlsruhe (TZW). The results are available in a publicly accessible data base (http://hikwww1.fzk.de/ptwte/w/Export/Daten/Z_Materialien/Datenbank_Uferfiltration_Spurenstoffe.pdf). This information was supplemented with own results, obtained in an interpretational study with field data acquired during the NASRI project (Wiese et al. 2009). In addition, a recent study by Stuyfzand et al. (2007), covering a great number of trace organics, was included.

In a **first step**, substances were selected, that show the potential for high persistence in the subsurface, i.e. for which little or no removal is indicated in one of the three mentioned sources. These were compiled in an EXCEL-table (given in appendix 1) together with the classification obtained from the mentioned literature (columns 2 through 5).

For these 45 trace organic substances, a general assessment of the substances´ relevance with regard to potential breakthrough in BF / AR systems was carried out (column 7 in the EXCEL table, **step two**). This assessment was based on persistence in the subsurface documented in the different studies, with high priority given to substances that showed low removal (< 25 % removal according to Schmidt 2005 or category 3 for Wiese et al. 2009 and Stuyvzand 2007) in more than one study. Special consideration was given to substances that are not removed under aerobic conditions, as these are prone to be problematic at the sites aimed at in this study. Substances, that showed varying removal rates between the different studies or for which information was only found in one study, were rated to be of medium (2) to uncertain (1) relevance.

In a **third step**, experts at Veolia (P. Roche) and BWB (U. Dünnbier) were asked to assess the relevance of all 45 substances with regard to relevance (the term “relevance” referring to occurrence in source water – and possibly also drinking water – in their respective fields of experience). The results are given in columns 8 and 9 of the EXCEL table.

Subsequently (**step 4**), different categories of substances were defined:

1) Substances with high relevance for water suppliers and high potential for breakthrough in RBF / AR systems
2) Substances with high relevance for water suppliers and medium / uncertain potential for breakthrough in RBF / AR systems
3) Substances with unknown relevance for water suppliers and high potential for breakthrough in RBF/AR systems

4) Substances with medium, low or unknown relevance for water suppliers and medium / uncertain potential for breakthrough in RBF / AR systems

For the following steps, only substances from categories 1 to 3 were considered, plus substances of special interest, that had been subject to discussion during the project team meetings (isoproturone, iopromide, diclofenac, clofibric acid). The latter were added due to their high prevalence worldwide (isoproturone) or extensive data on their occurrence in Berlin (iopromide, diclofenac, clofibric acid). This gave a list of 20 substances that could be possible target substances for the laboratory and technical scale experiments within the OXIRED-1 project.

Finally (**step 5**), data on removal by GAC and ozone from Lenntech (2008), Ternes et al. (2003) and TZW (2006) as well as the analytical possibilities at the BWB laboratories were compiled into a priority list for target substances that was then subject to discussion with the technical committee.

3. Results

On the basis of the stepwise approach (chapter 2) 20 out of 45 potentially persistent substances were classified as possible target substances for the experiments in OXIRED. These substances are listed in table 1, together with information on removal by advanced drinking water treatment (GAC, ozone) and the availability of an analytical method at BWB.

Table 1: Twenty possible target substances for laboratory and technical scale experiments during OXIRED1.

Substances with high relevance to water suppliers and high potential for breakthrough in RBF/AR systems	Removal by advanced post-treatment GAC	Ozone	Analytical Method established at BWB
MTBE	-	+/-	yes
Sulfamethoxazole	+/-	+	yes
EDTA	-	+/-	yes
ETBE	-	+/-	yes
Carbamazepine	+	+	yes
Primidone	-	+/-	no (under development)
Naphthalene-1,5-disulfonate (1,5-NDSA)	+		no
Substances with high relevance to water suppliers and medium / uncertain potential for breakthrough in RBF/AR systems			
Iopamidol	-	+/-	no
Bentazone	+/-	+	yes
Naphthalene-1,7-disulfonate (1,7-NDSA)	+		no
Naphthalene-2,7-disulfonate (2,7-NSSA)	+		no
Atrazine	+	+/-	yes
Desethylatrazin	+	-	yes
Linuron	+	+/-	yes
Diuron	+	+	yes
Diclofenac	+	+	yes
Substances with unknown relevance to water suppliers and high potential for breakthrough in RBF/AR systems			
Amidotrizoic acid	-	+/-	no
Other substances / parameters of interest			
Isoproturone	+	+	yes
Iopromide	-	+/-	no
Clofibric acid	-	+/-	yes

+: good removal, +/-: medium / partial removal, - low removal, no symbol: no information

On this basis, the following substances were classified “highest” (1^{st}) or “high” (2^{nd}) priority for further investigations (in order of descending priority). If not stated otherwise, the analytical method for the mentioned substance is available at BWB.

Substances with highest relevance for laboratory and technical scale experiments in OXIRED-1 (1^{st} priority) are:

1) **MTBE**

   The fuel additive MTBE has been shown to be only poorly removed by bank filtration (Schmidt 2005). This is in line with frequent occurrence in MAR systems (Stuyvzand 2007) and in Berlin bank filtrate (Wiese et al. 2009). MTBE is not removed well by GAC and only partially by ozone. The consulted experts from BWB and Veolia have classified MTBE as highly relevant. In combination with frequent detection in surface water at comparatively high concentrations (0.4 µg/L in average) this leads to an overall classification as highly relevant for the ongoing investigations.

2) **Sulfamethoxazole**

The removal of this antibiotic has been shown to be redox dependent with high removal under anaerobic and low removal under aerobic conditions (Wiese et al. 2009, Schmidt 2005 and 2007). It is therefore relevant especially for short subsurface passage. The consulted experts from BWB and Veolia have classified it as highly relevant. Therefore and due to relatively high mean concentrations in source waters (0.8 µg/L, Schmidt 2005), this substance is classified as highly relevant for the ongoing study.

3) **EDTA**

This chelating agent has been subject to various investigations in the past. It occurs at relatively high concentrations in surface waters (average: 10 µg/L) and is frequently observed at BF sites (Wiese et al. 2009, Schmidt 2005). Removal is consequently regarded as low (0-50 % in aerobic and anaerobic systems). Although its toxicity is low, it has been widely acknowledged as a problematic substance, hardly removable by natural treatment (BF, AR or slow sand filtration). Advanced treatment methods also show only poor to partial removal. The EDTA producing industry has therefore committed itsself to a 50 % reduction within 10 years. However, this has not been achieved and surface water concentrations remain comparatively high. Therefore it is classified as highly relevant for experiments (the consulted expert from BWB declared the relevance to be high and for Veolia no information was available).

4) **ETBE**

As ETBE has only recently been brought into use as substitute for MTBE there is little information on its removal during subsurface passage. Schmidt (2007) mentions no removal at aerobic bank filtration sites. Therefore – and because conventional activated carbon treatment does not show any removal – ETBE is classified as highly relevant for the ongoing investigations (the consulted expert from BWB declared the relevance to be high and for Veolia no information was available).

Substances with high relevance for laboratory and technical scale experiments in OXIRED-1 (2^{nd} priority) are:

5) **Carbamazipine**

Different studies have shown that this pharmaceutical (antiepileptic / antidepressant) is frequently detectable in aquifers influenced by RBF / AR (Stuyfzand 2007, Wiese et al. 2009). Under aerobic conditions usually only little removal can be observed (while under anaerobic conditions up to 100 % removal is possible). The experts from BWB and Veolia have classified it as highly relevant in their systems. On the other hand, carbamazipine is well removed by advanced drinking water treatment. In combination with relatively high average surface water concentrations, carbamazipine is classified as highly relevant for further investigations (2^{nd} priority).

6) **Primidone**

This pharmaceutical (anticonvulsant) has been observed frequently in bank filtrate in Berlin with only very little removal (Wiese et al. 2009). Also, Schmidt 2005 and 2007 documented removal neither under aerobic nor under anaerobic conditions. The experts from BWB and Veolia have classified it as highly relevant in their systems. In addition, primidone is not well removed by activated carbon and only partially by ozone. It is therefore classified as highly relevant for this study. However, there is currently no analytical method available at BWB (to be developed within 2009), so it is proposed to carry out experiments with primidone in the next project phase.

7) **Naphthalene-1,5-disulfonate (1,5-NDSA)**

This substance is an industrial chemical used for various applications (e.g. as intermediate in the manufacturing of paper chemicals or as plasticizer for concrete). It is usually associated with naphtalene-1,7-disulfonate and naphtalene-2,7-disulfonate (which are, however, better biodegradable). NASRI (Wiese et al. 2009) and other investigations (Schmidt 2005) have shown 1,5 NDSA to be quite persistent at bank filtration sites (the consulted expert from BWB declared the relevance to be high and for Veolia no information was available). On the other hand, it is well removed by advanced drinking water treatment. Although it has been classified as relevant for further investigations, there is currently no analytical method available at BWB.

8) **Iopamidole**

This x-ray contrast media has been shown to occur frequently in MAR influenced aquifers (Stuyvzand 2007). Further investigations are, however, lacking. It shows medium to poor removal during advanced drinking water treatment and was classified as highly relevant by the Veolia expert (for BWB there is no information available). Iopamidol is therefore recommended for further investigations with 2^{nd} priority.

9) **Bentazone**

This herbicide is sporadically found in surface waters (TZW 2006) and is hardly reduced during aerobic subsurface passage (Schmidt 2005). The interviewed expert from Veolia classified it as highly relevant, however, for BWB only low relevance was identified. Bentazone is removed well by advanced drinking water treatment and is therefore classified as relevant for the experiments at 2nd priority.

10) **Naphthalene-1,7-disulfonate and Naphtalene-2,7-disulfonate (1,7-NDSA and 2,7-NDSA)**

Both substances occur similar to 1,5-NDSA, however, they are better removed by subsurface passage (Wiese et al. 2009 and Schmidt 2005). Currently, there is no analytical method available at BWB. Therefore, they are classified as relevant for the experiments at 2nd priority.

11) **Atrazine, Desethylatrazine, Linuron, Diuron**

All these substances are pesticides and are not removed well by subsurface passage (< 30 % under aerobic conditions according to Schmidt 2005). All four are classfied as highly relevant by the Veolia experts. However, due to their prevalence in rural areas there is little relevance seen for BWB (although measured regularly). With exception of desethylatrazine this group of substances is well removed by advanced drinking water treatment. Therefore, they are classified as relevant for the experiments at 2nd priority.

12) **Diclofenac**

Although the NASRI investigations have shown a good removal of diclofenac under aerobic conditions, it is classified as highly relevant BWB, due to widespread detections in raw water. It is removed well by advanced drinking water treatment and therefore classified as relevant for the experiments at 2nd priority.

13) **Amidotrizoic Acid**

This iodinated X-ray contrast media has been shown to occur frequently in MAR influenced aquifers (Stuyvzand 2007) and shows no removal by RBF under aerobic conditions (Schmidt 2007). In addition, it is not removed well by advanced drinking water treatment. There is no information on relevance for BWB or Veolia and an analytical method is currently not available at KWB. Amidotrizoic Acid is therefore classified with 2nd priority relevance for further investigations.

In addition, in the experiments it is recommended to investigate the behavior of the sum parameter **AOI**, encompassing all iodinated contrast media which in total can not be determined as individual substances.

4. Conclusions

The literature study and the interviews conducted with experts from BWB and Veolia resulted in the following list of possible target substances for further investigations (in descending priority; substances for which there is currently no analytical method available at BWB are given in italics):

1st priority:

1) MTBE
2) Sulfamethoxazole
3) EDTA
4) ETBE
5) AOI (sum parameter for iodinated x-ray contrast media)

2nd priority:

6) Carbamezipine
7) *Primidone*
8) *1,5-NDSA*
9) *Iopamidol*
10) Bentazone
11) *1,7-NDSA*
12) *2,7-NDSA*
13) Atrazine
14) Desethylatrazine
15) Linuron
16) Diuron
17) Diclofenac
18) *Amidotrizoic Acid*

This list was approved by the Technical Committee during the Technical Committee Meeting on 9th Febr. 2009 in Berlin.

Appendix A

1	2	3	4	5	6	7	8	9
	Removal (NASRI data, Wiese et al. 2008)	**Occurence in MAR (Stuyfzand, 2007)**	**Elimination bank filtration (%) Schmidt 2005**			**Resulting assessment of possible breakthrough in BF / AR systems (KWB)**	**Relevance assessment by P. Roche (Veolia)**	**Relevance assessment by U. Dünnbier (BWB)**
Substance	3: < 25 % removal under aerobic conditions 2: 25 - 75 % removal under aerobic conditions or < 25 % under anaerobic conditions 1: 25 - 75 % removal under anaerobic conditions 0: > 90 % removal	3: often and >0.1µg/L, 2: often or >0,1 µg/L, 1: sometimes and <0.1 µg/L	aerobic	anaerobic	Number of studies	3: high, 2: medium, 1: uncertain	3: high, 2: medium, 1: low, 0: don't know	3: high, 2: medium, 1: low, 0: don't know
Primidone	3	1	0	0	3	3	3	3
Carbamazepine	3	3	0	100	9	3	3	3
MTBE	3	3	0-50	0-50	3	3	3	3
EDTA	3		0-50	0-50	28	3	0	3
Naphthalene-1,5-	3		10	10	15	3	0	3
Sulfamethoxazole	2	2	0	100	5	3	3	3
Methylbenzene		3	0-100	0-100	2	3	0	1
Tris(chloroethyl)phosphate (TCEP / TCPP)		3	43-50	0-90	6	3	0	1
Amidotrizoic acid		3	0	100	2	3	0	0
ETBE			0			3	0	3
1,2-Dichlorpropane			0	100	3	3	0	1
2,4-Dichloraniline			0	0	4	3	0	1
2,5-Dichloraniline			0	0	6	3	0	1
PFOS / PFOA						3	0	1
Naphthalene-1,7-	2		0	50	4	2	0	3
Naphthalene-2,7-	2		0	50	5	2	0	3
AAA	2		77	90	2	2	0	2
Atrazine		1	25	50	34	2	3	1
Bentazone		2	0	25	11	2	3	1
Iopamidol		3				2	3	0
Chloroform		3	50	85	23	2	2	1
Iso-Nonylphenol		3	99	34-99	3	2	2	1
1,3 and 1,4		3	50	75	21	2	0	1
1,4 Dioxane		3				2	0	0
Chlortoluron			0-100	0	6	2	2	1
Diethylentriaminpentaacetic acid [DTPA]			0	25	4	2	0	2
2-Chlorophenol			0	0	2	2	0	1
Dikegulac			0	0	5	2	1	0
2-Hydroxy-4,6-bis(4-sulfanilo)-1,3,5-triazine			0		1	2	0	0
Phenazone	1	3	85	0	4	1	0	2
1,2,4 Trimethylbenzene		2	90		1	1	1	1
1,2-Dichloroethane		2	0-70	0-70	4	1	1	1
1,3,5 Trimethylbenzene		2	90	0	2	1	1	1
Bisphenol A		3	100		2	1	2	1
Diglyme		3	100		1	1	0	0
Desethylatrazin [Atrazine-Metabolite]			0-30	45-79	10	1	3	1
Linuron			0		1	1	3	1
Diuron			25	25	9	1	3	1
Diclofenac						1		3
Isoproturon			75	0	15	1	2	1
Tetrachloroethene [PER]			0	100	30	1	2	1

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