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Adaptive Decision Support System (ADSS) for the Integration of Stormwater Source Control into Sustainable Urban Water Management Strategies

D4.3 & D4.4

Selected stormwater priority pollutants (SSPP) – Introduction and database

Prepared by

**E. Eriksson, A. Baun, P.S. Mikkelsen and A. Ledin
Institute of Environment & Resources
Technical University of Denmark**



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Glossary/ Definitions / Acronyms: (new words used in the text)

Potential Stormwater Pollutant (PSP): A pollutant that can potentially be present in stormwater because (a) it has been identified in stormwater samples, or (b) it may be released to stormwater from materials, products, food, etc. or from activities conducted in the urban environment.

Potential Stormwater Priority Pollutant (PSPP): A potential stormwater pollutant (PSP) with hazardous or otherwise problematic inherent properties.

Stormwater Priority Pollutant (SPP): A stormwater pollutant with hazardous or otherwise problematic inherent properties, which is available at a critically high concentration, i.e. for which the environmental concentration exceeds the effect concentration. Thus, a SPP is a PSPP where the word “potential” is no longer needed.

Selected Stormwater Priority Pollutant (SSPP): A stormwater priority pollutant (SPP), which has been selected by a group of experts to be evaluated in the other work packages within the DayWater project. Thus, SSPP is a short list of a few selected SPP.

1 Introduction

DayWater is a direct translation of a Swedish word that means *water in daylight or surface runoff*. *DayWater* is also the acronym of a European research project aimed at developing an “adaptive decision support system (an ADSS) for the integration of stormwater source control into sustainable urban water management strategies”. The *DayWater* project, which runs from December 2002 to November 2005, is organised in seven work packages focused at different aspects of stormwater source control.

1.1 Objective

Work package 4 – Risk and Impact Assessment – deals with the potential negative effects of handling stormwater locally, i.e. it aims at developing principles, procedures and tools for managing risks that can be realistically foreseen when implementing stormwater source control on top of traditional, basic urban water management.

The report describes the output from the third task (T4.3) in work package 4: “Definition of potential stormwater priority pollutants (PSPP)”. The purpose is to propose a list of selected stormwater priority pollutants and to compile information on inherent properties and toxicity for these compounds into a database. This list will serve as input for various tools developed within *Daywater* used for assessing pollutant sources and fluxes (WP6), the behaviour, fate and toxicity of pollutants during passage of stormwater through BMPs (WP5) and the environmental risk associated with their subsequent dispersal in the environment (further tasks in WP4).

The list of selected stormwater priority pollutants is partly based on criteria identified in task 4.2 and agreements made during the first annual meeting of the *DayWater* project held in Athens during October 2003, although the major input derive from data found specifically in this task. The final selection of SSPP took place during the third annual meeting in Copenhagen in 2004. The report describes the content of two actual deliverables in the *DayWater* project: D4.3 “Selected Stormwater Priority Pollutants (SSPP)” and D4.4 “Database of SSPP”.

1.2 This deliverable

The final SSPP list is based on CHIAT – Chemical Hazard Identification and Assessment Tool, which is a procedure that has been developed as part of the second task of work package 4 (T4.2, “Development of methodology for evaluating and prioritising environmental risks). The CHIAT methodology is briefly outlined in chapter 2.

Chapter 3 presents the justified list of selected stormwater priority pollutants (SSPP), which presently contains 24 parameters. These are distributed between the following categories:

- *Basic parameters (5)*
- *Metals (7)*
- *PAH (3)*
- *Herbicides (4), and*
- *Miscellaneous organic compounds (5).*

This net list of selected stormwater priority pollutants is intended to be used in practice where it is not feasible to investigate many pollutants with similar or equal inherent properties. Behind this lies a *gross* list of compounds that have initially gone through the hazard and problem identification screening, see section 2.3. Furthermore, the output from this screening has been prioritised by a group of experts representing work packages 4, 5 and 6, who made the final selection of pollutants (section 2.5).

2 Methodology

The methodology used in this task (T4.3) is developed in T4.2 (Development of methodology for evaluating and prioritising environmental risks) and is reported in a separate deliverable (D4.2) as well as a scientific paper (Eriksson et al., 2005a). It is based on approaches used in environmental risk assessment of chemicals by governments, chemical industry, environmental organisations, and institutions responsible for issuing eco-labels as well as the scientific community (see e.g. European Commission, 2003). The present method is restricted to a problem-oriented hazard and problem identification and assessment, which includes on both environmental and/or health hazards and technical problems as well as an expert judgement. In general, hazard identification serves to map the inherent properties of chemicals by collecting and comparing relevant data on e.g. physical state, volatility, mobility, potential for degradation, bioaccumulation, and toxicity. Hazard assessment aims to find and evaluate the exposure and the effects. To perform a risk characterisation, which includes an evaluation of the probability for an effect to occur is beyond the scope of WP4.

The 5-step tool CHIAT for problem-oriented hazard identification and assessment is illustrated in Figure 1.

2.1 Source characterisation

In the first step, source characterisation, literature surveys are carried out in order to compile data concerning the potential content of chemical constituents in stormwater. One literature survey focuses on published studies regarding measured constituents, and the revealed information is divided into different categories depending on the type of surface the stormwater samples have been derived from (different types of source water). Another literature survey aiming at identifying compounds that may potentially be present in stormwater due to releases from materials, products, traffic etc. or from activities in the urban environment. The first survey thus aim to map what can be deduced from historical monitoring programs, while the other targets “new” pollutants which, no-one has yet included in their monitoring programs. These “new” potentially present pollutants were identified by studying use of chemicals (e.g. weed control and de-icing), release from materials (buildings, roads as well as brakes and tyres on cars), accidental spills and atmospheric deposition (Eriksson et al., 2005a). The compounds identified in the source characterisation is transferred to the potential pollutants list which consist of compounds that potentially can be present in stormwater; the so-called Potential Stormwater Pollutants (PSP).

2.2 Recipient, receptor and criteria identification

In the second step, the recipient, receptor and criteria identification, the use/reuse scenario is defined and the recipient (e.g. water, soil) is determined. The exposure objects, for example humans, aquatic organisms and crops, have to be established for each individual scenario. Other local information such as catchment’s size, annual average precipitation, local and regional legislation and BPM characteristics e.g. deriving from WP5 BMP-database are collected for use later on in the assessment. This step aims to compile site-specific information that will be used in the fourth step, the hazard assessment, as well as legislation that will be used in the fifth step, the expert judgement.

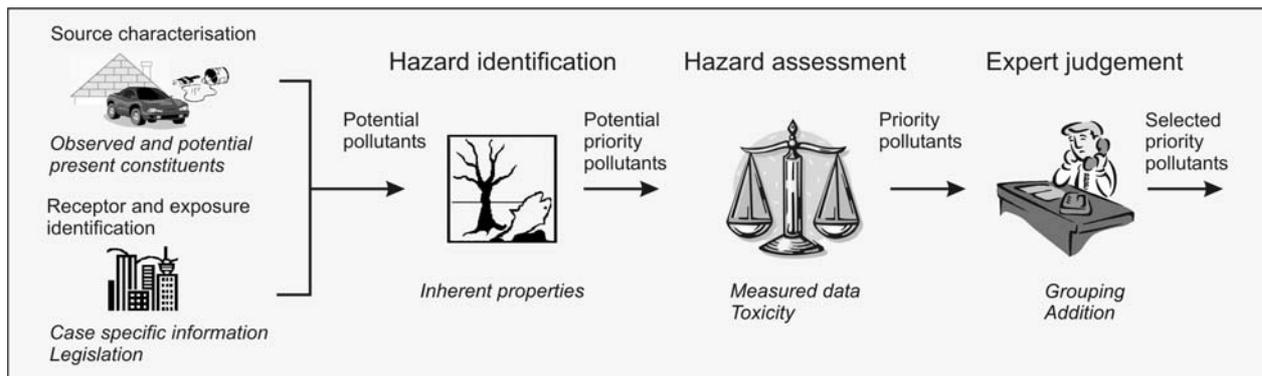


Figure 1: Outline of the methodology.

2.3 Hazard and problem identification

In the subsequent hazard and problem identification, inherent data needed to perform the hazard identification is compiled, criteria and cut-off levels are selected, and all chemicals identified as potential stormwater pollutants (PSP) are evaluated. The output of this step is a list of potential priority pollutants, which contains those chemical constituents that potentially constitute a hazard or problem based on their inherent properties.

The aim of the source characterisation (step 1) is to ensure that no pollutants are forgotten from the start. The “hazard and problem identification” step, the “I” in CHIAT, is where “Ranking and Identification of Chemical Hazards” (RICH) occurs, and for this part of the CHIAT methodology a special tool (called RICH) has been developed for hazard identification of Potential Stormwater Priority Pollutants (PSPP’s) based on their inherent properties. The details of the RICH methodology are reported in a journal paper (Baun et al., 2006) and are elaborated on the DayWater ADSS (see <http://www.daywater.cz>). The RICH tool is furthermore presented as a web-tool where users can obtain information about the many PSPP’s that have been screened in the DayWater project in a user friendly manner (physically located at a server at DTU, <http://chiat.er.dtu.dk>, but with direct links from the ADSS). The RICH tool is one of the operational risk screening tools developed as an outcome of WP4 in the DayWater project.

In the current version of RICH only screening procedures for organic chemicals are included, but “filters” for e.g. heavy metals, nutrients or other water quality parameters may also be constructed and fitted with filters developed for screening of problems and hazards related to these specific compound groups. In the DayWater project the heavy metals and basic water quality parameters has been selected in the expert judgement step. The obtained list with PSPP is a *gross* list of potential stormwater priority pollutants that have all gone through the hazard and problem identification *screening*.

2.4 The hazard assessment

Hazard assessment is carried out as the fourth step in CHIAT. Measured or estimated environmental concentrations for the site in question are compared with predicted no-effect concentrations derived according to the technical guidance document for risk assessment of chemicals in EU (European Commission, 2003). The sources and flux models (SEWSYS and STORM) used and developed in WP6 could potentially be applied in this step to estimate environmental concentrations. The output from this step is a list containing those chemical constituents that will constitute a hazard or problem in the specific recipient if the stormwater is handled according to the selected principle.

Possible oversaturation, i.e. potential for precipitation can be estimated by geochemical modelling (e.g. PHREEQC, Parkhurst and Appelo, 2000) and pollutants that are oversaturated (receiving a saturation index above one) are classified as stormwater priority pollutants (SPP).

This list of SPP may contain more compounds than what is feasible from a practical point of view; lack of data or financial constraints may simply limit the number of compounds that can be realistically included in the subsequent monitoring programme or investigation of environmental problems related to source control measure etc. Thus, it may be relevant to group the compounds based on chemical similarities and only select a *net* subset for use as *indicator compounds* in further investigations.

2.5 Expert judgement

The “expert” is not necessarily a single person (for example an environmental chemist) but can be a group of decision-makers with different scientific backgrounds. The expert/experts select priority pollutants for which some actions need to be taken according to the following;

- Grouping – compounds may be grouped based on chemical structure (e.g. PAH) or based on same specific sources (e.g. car catalysts) or similar fate in the environment.
- Adding – compounds present in national and European legislation on limit values e.g. drinking water standards, environmental quality standards and emission limit values for watercourses, lakes or the sea can be used to identify pollutants that may need to be added to the list. Compounds originating from specific urban sources may be relevant to add for further investigation.
- Removing – may take place based on use patterns in the catchments, due to ban of use or production

Additionally high levels of easily degradable organic material can cause oxygen depletion and fish death and can be monitored by organic summation parameters such as BOD and COD.

The output is a list containing individual pollutants and summa parameters that constitute a hazard after evaluation by the expert: the selected stormwater priority pollutants.

3 Selected Stormwater Priority Pollutants

About 600 compounds were identified as potential stormwater pollutants in the first step Source characterisation and inherent data have been found for 233 of these (Baun et al., 2006). Focus has been of herbicides (pesticides) and PAHs. The datasheet (appendix 1) contains a template on how the data is structured in the database and inherent data for the organic compounds found on the SSPP-list. However, the hazard identification (step 3) was hampered by the lack of data on the inherent properties, and all SSPP could not be fully evaluated due to the lack of data, see appendix 2.

Step 4, the hazard assessment was excluded since the major purpose was to identify compounds that should be used for further evaluation in the other work packages, i.e. site-specific information regarding environmental concentrations would not be feasible to apply in this selection. Step 2 was excluded since the information compiled in this step was going to be used in step 4.

The expert judgement (Step 5) was carried out in two rounds as it was decided by the Daywater partners at the PSPP work meeting in Athens (MoM work meeting, 2003) that some basic physical-chemical parameters should be included (organic material, suspended material and nutrients). Round two was held during the PP work meeting in Copenhagen (MoM work meeting, 2004) where experts representing DayWater WP4, 5 and 6 made the final agreement was made on metals and organic compounds.

The output in this deliverable is a *net* list of selected stormwater priority pollutants (SSPP) that are intended to be used in practice as representative *indicator parameters* where it is not feasible to investigate many pollutants with similar or equal inherent properties. Behind this lies a *gross* list of compounds (potential stormwater priority pollutants, PSPP, see <http://chiat.er.dtu.dk>) that have initially been pointed out as potential priority pollutants in the hazard and problem identification as well as an expert judgement.

3.1 The SSPP list

The list of selected stormwater priority pollutants proposed in this report (Table 1) consists of 24 parameters divided into the following categories

- *Basic parameters* (5)
- *Metals* (7)
- *PAH* (3)
- *Herbicides* (4)
- *Miscellaneous organic compounds* (5)

All metals are persistent to degradation but the seven metals on the list also have other properties, which imply that they should be given high priority. Some of them cause chronic effects (carcinogenic, mutagenic, reproduction hazardous and/or endocrine disrupting effects), high acute toxicity, and are suspected to have hazardous effects and/or derive from specific human sources (platinum-palladium exhaust catalysts). Additionally, the metal speciation has been taken into account, including an assessment of dissolved and particulate/colloidal bound metals, and among the dissolved cationic and anionic metal species, Table 1.

The PAH group identified as potentially present in runoff was found to consist of more than 50 compounds of which seven were found to be hazardous in the water phase and 36 in the solid phase. It has been possible to group the compounds and select a few representative compounds due the structural similarities of the chemical compounds; 1) naphthalene (2 rings) was found to constitute a hazard in both the water and solid phases. Two compounds were found to constitute a hazard in the solid phase 2) pyrene (4 rings) and 3) benzo[a]pyrene (5 rings and known to be carcinogenic). These have different inherent properties and are therefore expected to have different fates.

Out of the large number of herbicides defined as potential stormwater pollutants, 23 herbicides that are used in large quantities in Europe, as well as those herbicides that have been detected in food produced from plants, were selected for hazard identification. Fourteen of these were identified as stormwater priority pollutants. Three herbicides were selected since they are classified as hazards in both water and solid phase and one due its toxicity and vast use in urban areas and along motorways in e.g. Sweden, Denmark, England and France (glyphosate).

Five representative compounds have been selected from the group of miscellaneous compounds. One chlorinated phenol (pentachlorophenol), one PCB representing old persistent chloro-organo-compounds (polychlorinated biphenyl 28), one phthalate (di(2-ethylhexyl) phthalate), one petrol additive with known aesthetical problems (methyl tert-butyl ether) as well as an non-ionic detergents and its short chain degradation products (nonylphenol ethoxylates and nonylphenol) (Table 1).

Table 1: List of Selected Stormwater Priority Pollutants (indicator parameters).

Type	Constituents			Justification
Basic parameter	BOD/ COD	-	Biological/chemical oxygen demand	Basic parameter
	SS	-	Suspended solids	Basic parameter
	N	-	Nitrogen	Basic parameter
	P	-	Phosphorus	Basic parameter
	pH		pH	Basic parameter
Metals	Cd	7440-43-9	Cadmium	P, CMR
	Cr	7440-47-	Chromium	P, anionic in natural waters
		311104-59-9	Chromate	
	Cu	7440-50-8	Copper	P, T
	Ni	7440-02-0	Nickel	P, CMR
	Pb	7439-92-1	Lead	P, CMR
	Pt	7440-06-4	Platinum	P, CMR, specific human sources
	Zn	7440-66-6	Zinc	P, load
PAH		91-20-3	Naphthalene	Indicator of PAH, water and sediment phase, PB
		129-00-0	Pyrene	Indicator of PAH, sediment phase, PB
	BaP	50-32-8	Benzo [a] pyrene	Indicator of PAH, sediment phase, PB, CMR
		40487-42-1	Pendimethalin	PB, use statistics
Herbicides		13684-63-4	Phenmedipham	PB, use statistics
		1071-83-6	Glyphosate	BT, use statistics
		5915-41-3	Terbutylazine	Indicator of triazines, PB, use statistics
	Miscellaneous	NPEO	25154-52-3	Nonylphenol ethoxylates and nonylphenol
104-40-5				
27986-36-3				
1916-45-9 etc				
PCP		87-86-5	Pentachlorophenol	PB
DEHP	117-81-7	Di(2-ethylhexyl) phthalate	PB	
PCB 28	7012-37-5	Polychlorinated biphenyl 28	PB, water solubility	
MTBE	1634-04-4	Methyl <i>tert</i> -butyl ether	Technical problems (odour)	

CMR = has carcinogenic/mutagenic/reproduction hazardous and/ or endocrine disrupting effects

P = Persistent compound

PB = Persistent and bioaccumulating compound

T = Compound with high acute aquatic toxicity

3.2 Database

The "Database of SSPP" (D4.4) has been made available at a publicly available website, physically located at a server at DTU (<http://www.er.dtu.dk/daywater>) with direct links from the ADSS. The database interface is a list of all 23 parameters (25 actual entries because BOD and COD have been split and because pH has been added) along with their CAS-number and their type (basic parameter, metal, PAH, herbicide, misc. XOC). Fig 2. shows a screenshot from the database

Clicking a compound name gives access to the following information for that compound:

- Description: textual information about that compound as well as an image of its chemical structure when relevant.
- Inherent data used in the RICH procedure, i.e. information about: water solubility (mg/L), vapour (mmHg), Kh (atm m³/mole at 25°C), Kd, Koc, pka, Log Kow, BCF, biodegradability, aerobic degradability, anaerobic degradability, toxicity (algae) (mg/L), toxicity (crustacean) (mg/L), toxicity (fish) (mg/L), health classification, environmental classification, technical problems and long-term chronic effects based on human and non-human data (carcinogenicity, mutagenicity, reproduction hazards, and endocrine disrupting effects).
- Information about legislation addressing the compound: EU WFD, DEPA, EPER, ESR, UK and Ireland, SEPA, FR river quality, UN POP, LRTAP, Stockholm POP, WWF POP, OSPAR priority, OPSAR concern, HELCOM, and USEPA (for the significance of these acronyms, see <http://www.er.dtu.dk/daywater>).
- Other information.

A list of abbreviations and references are also provided from the database interface. The database makes all data used about SSPP's in the DayWater project available to external parties.

The screenshot shows a web browser window titled "Daywater - index - Microsoft Internet Explorer". The address bar shows the URL <http://www2.er.dtu.dk/daywater/comproresults.php?id=21>. The page header includes the "DayWater" logo and the text "Adaptive Decision Support System" and "BETA VERSION". A left-hand navigation menu contains links for "Home" and "Compound List", with sub-links for "Description", "Inherent data", "Legislation & Priority pollutants", and "Other information". The main content area is titled "Description:" and contains the following information:

- Compound:** Di-(2-ethylhexyl)-phthalate
- CAS nr.:** 117-81-7
- Description:** DEHP will, based on the very high adsorption to organic carbon (Koc) and low water solubility (Sw), almost exclusively adsorb to suspended solids, organic material and sediments. It is persistent to biodegradation and is bioaccumulating (BCF, Kow) which yield long-half life in the environment and high concentrations in organisms. High acute (ECLC50) and long-term chronic (teratogenic effects i.e. causes malformations of an embryo or foetus) makes DEHP a very toxic compound.
- Image:** A chemical structure diagram of Di(2-ethylhexyl)phthalate is displayed.

Figure 2: Example of the DayWater SSPP datasheets for the Di(2-ethylhexyl)-phthalate

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5 Appendix 1 Inherent data for the organic SSPP

Compound	Cas-nr.	mmHg		atm m ³ /mole @ 25°C				Sorption Koc	Ref Koc	pKa	Ref pKa
		Vapour pressure	Ref VP	Henrys Kh	Ref Kh	Kd	Ref Kd				
Benzo(a)pyrene	50-32-8	1.99E-08	10	4.57E-07	3		8000-65000	3			
Di-(2-ethylhexyl)-phthalate	117-81-7	1.42E-07	8	0.00000013-0.0000103	1&3		510000-2000000000	1&3			
Glyphosate	1071-83-6	4.30E-10	12	4.08E-19	12		18.79	12	0.8	8	
MTBE	1634-04-4	250	8	5.87E-04	8		11	1	-3.7	8	
Naphtalene	91-20-3	7.50E-05	3	4.40E-04	8		1837	12			
Nonylphenol (NPE)	25154-52-3	0.0000236	8	1.10E-06	3		31000	3	10.25	3	
Nonylphenol di ethoxylate (NPEO2)	-										
Nonylphenol mono ethoxylate (NPEO1)	9016-45-9	0.000094	3	2.45E-09	3		6100	3			
4-Nonylphenol	104-40-5	0.000818	8	0.000034	3		32400	3			
PCB 28	7012-37-5	1.95E-04	8	2.00E-04	8						
Pendimethalin	40487-42-1	0.00003-0.000202	3&10	8.60E-07	3		2622	12			
Pentachlorophenol	87-86-5	0.0011-0.00011	8	0.000000245-0.00002345	8		1000-25000	3	4.5-4.7	8	
Phenmedipham	13684-63-4	1.00E-11	8	2.50E-08	8		3020	10	0.1	8	
Pyrene	129-00-0	0.000000345-0.0000045	8&10	1.19E-05	8		65300-1300000	1&3			
Terbutylazin	5915-41-3	1.12E-06	8	3.72E-08	8		516.1594188	7	2	8	

Compound	Cas-nr.	Log Kow	Ref Kow	Calc. BCF		Ref BCF	Biaccumulation	Biodegradability	Ref	Aerob degr.		Anaerob degr.	
				(fra log Kow)	BCF [L/kg]					[T½ d]	Ref P	[T½ 1/d]	Ref P
Benzo(a)pyrene	50-32-8	6.13	1	32396.6	134248	10	+	not easily	6	Persistent	1	Persistent	1
Di-(2-ethylhexyl)-phthalate	117-81-7	7.6	8		0.08-24500	4		Not inherently	10	Persistent	4	Persistent	4
Glyphosate	1071-83-6	-4.47	6		10	4	-	Ready	9				
MTBE	1634-04-4	0.94	8										
Naphtalene	91-20-3	3.3	3		69.34	12		Persistent	12				
Nonylphenol (NPE)	25154-52-3	5.71	3		350	3				Persistent	4	Persistent	3
Nonylphenol di ethoxylate (NPEO2)	-												
Nonylphenol mono ethoxylate (NPEO1)	9016-45-9												
4-Nonylphenol	104-40-5	5.76	8		4120	10		Inherent	10				
PCB 28	7012-37-5	5.62	8		17783	10		Not inherently	10				
Pendimethalin	40487-42-1	5.18	3		1400-1950	6&10				Inherent	3		
					2-45000						3		3
Pentachlorophenol	87-86-5	5.12	8			3		Persistent	10&12	Persistent		Inherent	
Phenmedipham	13684-63-4	3.49	6					Persistent	12				
Pyrene	129-00-0	4.88-5.1	1&8	4315.2	12000-16000	1&3	+	not easily	10	Inherent	1	Persistent	1
Terbutylazin	5915-41-3	3.1	6	86.1			+	Persistent	12				

Compound	Cas-nr.	Algae		Crust.		Fish			Environmental classification	Ref. cl.
		EC/LC50 [mg/L]	Ref Alg.	EC/LC50 [mg/L]	Ref Cru.	EC/LC50 [mg/L]	Ref Fish	Classification		
Benzo(a)pyrene	50-32-8 117-81-7	0.005	6	0.005	6	0.0056	6	R45-46,60-61	R50/53	10
Di-(2-ethylhexyl)-phthalate		0.1-130	4	0.133-300	4	0.16-10000	4	R60-61	10	
Glyphosate	1071-83-6	13	6	0.01	6	10	6	Xi;R41	N;R51/53	13
MTBE	1634-04-4									
Naphtalene	91-20-3	0.05	5	0.0008	5	0.01	5	Xn;R22	N;R50/53	13
Nonylphenol (NPE)	25154-52-3	0.027-1.3	4	0.043-140	4	0.00635-0.9	5	Xn;R22 C;R34	N;R50/53	13
Nonylphenol di ethoxylate (NPEO2)	-									
Nonylphenol mono ethoxylate (NPEO1)	9016-45-9			6.6	5	1.3	5			
4-Nonylphenol	104-40-5			0.18	5	0.13	10			
PCB 28	7012-37-5			0.16	6	0.16	6	R33	N;R50/53	6
Pendimethalin	40487-42-1	0.0052	6	0.08	10	0.05	6	Xn; R22, R43	R50/53	6&10
				0.0002-959	5	0.00099-64		T;R24/25 Tx;R26 Xi;R36/37/38 Carc3;R40	N;R50/53	6
Pentachlorophenol	87-86-5	0.03	1				5			
Phenmedipham	13684-63-4	0.13	6	3.2	6	1.4	6			
Pyrene	129-00-0	0.1	10	0.004	10	0.0026	6			
Terbutylazin	5915-41-3	0.016	5	5	6	1.6	5			

Compound	Cas-nr.	Carc.	Ref C.	Mut.	Ref M.	Reprod. incl endocrine	Ref R.	Tech	Ref Tech
Benzo(a)pyrene	50-32-8 117-81-7	Animal	3	Animal, human	3				
Di-(2-ethylhexyl)-phthalate						Teratogen (animal)			
Glyphosate	1071-83-6							odour	
MTBE	1634-04-4								
Naphtalene	91-20-3	Animal	3						3
Nonylphenol (NPE)	25154-52-3					endocrine disr. (animal)	1		
Nonylphenol di ethoxylate (NPEO2)	-								
Nonylphenol mono ethoxylate (NPEO1)	9016-45-9								
4-Nonylphenol	104-40-5								
PCB 28	7012-37-5								
Pendimethalin	40487-42-1								
Pentachlorophenol	87-86-5	Animal	1+10	Animal	1&3	Teratogen (animal)	1		
Phenmedipham	13684-63-4			Animal	3				
Pyrene	129-00-0		3	Animal	3				
Terbutylazin	5915-41-3			Animal	3				

1 Rippen G (1990) Handbuch Umweltschmelien 3. Auflage. Ecomed Verlagsgesellschaft, Landberg/Lech. Germany; 2 Verschueren K, (1996) Handbook of environmental Data on Organic Chemicals, 3. Edition, van Nostrand Reinhold co. Dordrecht, Holland; 3 Hazardous Substances Databank <http://www.toxnet.nlm.nih.gov/>; 4 European Commission, Joint research centre. Institute for health and consumer protection. European Chemicals Bureau. Second edition, 2000; 5 <http://www.epa.gov/ecotox/>; 6 http://ovs.dmu.dk/2NOVA_2003_ov./4datablade/; 7 BCF calculated from Kow (BCF=0.41*(10^{logKow}); 8 Reference data in EPI Suite, US Environmental Protection Agency. 2000; 9 CambridgeSoft Corporation. Chemfinder.com database. 100 CambridgePark Drive, Cambridge, MA 02140 USA. <http://chemfinder.cambridgesoft.com/>; 10 OSPAR Commission for the protection of the Marine Environment of the North-East Atlantic. <http://www.ospar.org/eng/html/welcome.html>; 11 DHI Institut for vand og miljø, Agern Alle 5, 2790 Hørsholm. Overview of water quality criteria (manuscript); 12 Modelling data out-put (EPI Suite), US Environmental Protection Agency. 2000; 13 Danish EPA list of unwanted compounds <http://www.mst.dk/>; 14 GENE-TOX database; <http://www.toxnet.nlm.nih.gov/>; 15 CCRIS database; <http://www.toxnet.nlm.nih.gov/>

6 Appendix 2 Results from the screening of the organic SSPP

Compound name		Filter 1	Filter 2	Filter 3	Filter 4	Filter 5
Compound	Step	1	2	3	4	3a, 4a
Benzo(a)pyrene	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
50-32-8	SEDIMENT	23	n	33		
			Anaerobic	33		
Compound	Step	1	2	3	4	3a, 4a
Di-(2-ethylhexyl)-phthalate	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
117-81-7	SEDIMENT	23	n	33		
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
Glyphosate	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	11	n	0	41	
1071-83-6	SEDIMENT	11				
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
MTBE	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	21	y			
1634-04-4	SEDIMENT	21				
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
Naphtalene	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	22	n	23		
91-20-3	SEDIMENT	22	n	23		
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
Nonylphenol (NPE)	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
25154-52-3	SEDIMENT	23	n	33		
			Anaerobic	33		
Compound	Step	1	2	3	4	3a, 4a
Nonylphenol mono ethoxylate (NPEO1)	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	13				
9016-45-9	SEDIMENT	13	n			
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
Nonylphenol di ethoxylate (NPEO2)	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER					
-	SEDIMENT					
			Anaerobic			
Compound	Step	1	2	3	4	3a, 4a
4-Nonylphenol	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
104-40-5	SEDIMENT	23	n	32		
			Anaerobic			

Compound name		Filter 1	Filter 2	Filter 3	Filter 4	Filter 5
Compound PCB 28	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 7012-37-5	WATER	23				
	SEDIMENT	23	n	33		
		Anaerobic				
Compound Pendimethalin	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 40487-42-1	WATER	22	n	32		
	SEDIMENT	22	n	32		
		Anaerobic				
Compound Pentachlorophenol	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 87-86-5	WATER	22	n	33		
	SEDIMENT	22	n	33		
		Anaerobic		32		
Compound Phenmedipham	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 13684-63-4	WATER	12	n	23		
	SEDIMENT	12	n	23		
		Anaerobic				
Compound Pyrene	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 129-00-0	WATER	23				
	SEDIMENT	23	n	32		
		Anaerobic				
Compound Terbuthylazin	Step	1	2	3	4	3a, 4a
	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no. 5915-41-3	WATER	12	n	23		
	SEDIMENT	12	n	23		
		Anaerobic				