

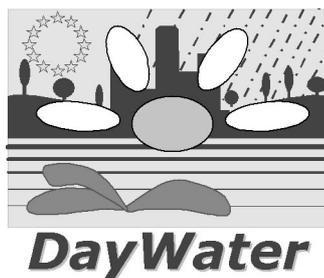
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Adaptive Decision Support System (ADSS) for the Integration of Stormwater Source Control into Sustainable Urban Water Management Strategies

Methodology for evaluating and prioritising environmental risks associated with chemical constituents in stormwater

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1 Introduction

There are a number of initiatives for finding alternative handling strategies for stormwater runoff. Driving forces are water and energy savings, reduction of combined sewer overflows and flooding, water utilisation for recreational purposes, improved recipient quality, etc. The main idea is to make a change from the traditional handling principle in most developed countries, where all types of wastewaters are mixed and thereafter treated at a wastewater treatment plant, followed by discharge to the environment, towards more sustainable and in most cases decentralised strategies. For instance, stormwater can be used locally for toilet flushing or laundry after some low- or high-tech treatment, used outside for irrigation or in daylighting such as fountains etc.

It is necessary to assess potential hazards and problems related to e.g. chemicals, when these alternatives for handling of stormwater, are considered. The types of hazards and problems that should be taken into account are related to the selected strategy for handling. Hazards regarding exposure of humans, livestock, aquatic and terrestrial organisms, crops and plants have to be considered, as well as technical and aesthetical problems. Hazards that are needed to be taken into account are both acute and long-term effects to living organisms e.g. toxicity, bioaccumulation, carcinogenicity, mutagenicity, reproduction hazards and endocrine disrupting effects, as well as promoting allergic reactions in humans. Precipitation of salts/minerals and corrosion of different types of installations and tubing are examples of relevant technical problems. Foul odour, frothing and discolouring are examples of aesthetical problems to be considered.

This deliverable presents a screening methodology: **CHIAT** – **C**hemical **H**azard **I**dentification and **A**ssessment **T**ool for selection of the most critical pollutants regarding different strategies for handling of stormwater. CHIAT is a procedure for identifying and assessing chemical hazards and problems. CHIAT has been developed in the European Daywater project with co-operation and partial funding from the Swedish MISTRA funded Urban Water Programme. One of the major aims in the DayWater project has been to use the CHIAT methodology to identify a set of selected stormwater priority pollutants for use in subsequent more detailed investigations.

This deliverable report consists of a short summary report describing the developed methodology and it has two appendices that illustrate the application of the method. Appendix 1 (Eriksson *et al.* 2005A) contains an already published paper describing the CHIAT methodology (Water Science & Technology, Vol. 51, No. 2, pp. 47-55), whereas appendix 2 contains a PowerPoint presentation that is thought to be a “tutorial” of the CHIAT methodology, which can be run as an “executable presentation” from the Daywater adaptive decision support system (ADSS) user interface. Further detailed discussions in the project group will determine which parts of the CHIAT methodology can be incorporated directly into the DayWater ADSS.

2 Methodology

Risk assessment of chemicals is composed of four elements: hazard/problem identification, hazard/problem assessment, risk characterisation and risk management according to the technical guidance document (TGD) for risk assessment of chemicals in EU (European Commission, 2003). In general, hazard identification serves to map the inherent properties of chemicals by collecting and comparing relevant data on e.g. physical state, volatility and mobility as well as potential for degradation, bioaccumulation and toxicity. Hazard assessment is divided between exposure assessment and effect assessment. Comprehensive model systems are available for assessing the distribution of contaminants in the environment (soil,

water, air) and in tissue (animals, humans). The next step is risk characterisation, where the potential negative effects are evaluated and, if possible, the probability of effects occurring is estimated. Finally, risk management involves a range of possible interventions, i.e. monitoring and control of emissions to reduce risk (see e.g. Mikkelsen *et al.*, 2001).

The methodology developed in the present work is inspired by the TGD (European Commission, 2003) and consists of five steps; 1) Source characterisation, 2) Recipient, receptor and criteria identification, 3) Hazard and problem identification, 4) Hazard and problem assessment and 5) Expert judgement, see Figure 1. A more detailed and visual description can be found in appendix 2.

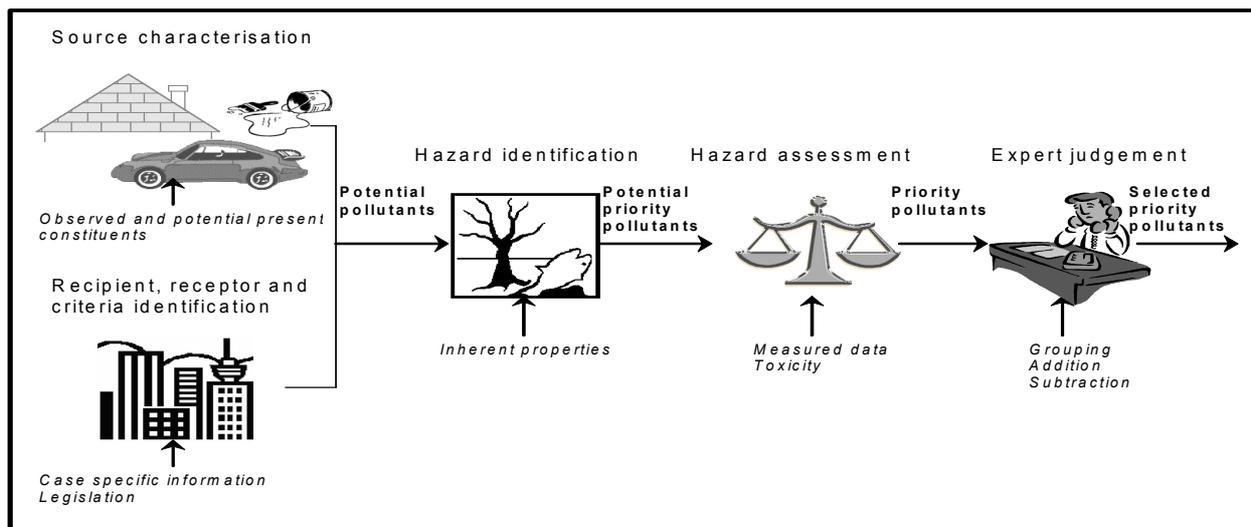


Figure 1: CHIAT – Chemical Hazard Identification and Assessment Tool

2.1 Source characterisation

Initially, information regarding the potential pollutants should be collected. This has been done for stormwater by two different approaches:

1. Searching in the open international literature regarding observations/measurements of physical and chemical constituents in stormwater. This is generating a list of observed constituents (for more details see Eriksson, *et al.*, 2005C; Ledin, *et al.*, 2004).
2. Searching in the literature regarding constituents that potentially could be present in stormwater due to (Figure 2) a) atmospheric deposition; b) releases from materials such as building and road materials, brakes and tires on vehicles; c) use of chemical products such as de-icing agents and pesticides. The aim is to identify those pollutants that have not been included in monitoring programs yet (for more details see Eriksson *et al.*, 2005A; Ledin *et al.*, 2004).

The lists generated can be used as a base for other site-specific projects. However, it should be kept in mind that some compounds may have to be added when CHIAT is applied in a case study, for example, it could be xenobiotic organic compounds (XOCs) used as de-icing agents and pesticides.

The output from step 1 is a list with all observed and potentially present pollutants: the **potential pollutants**.

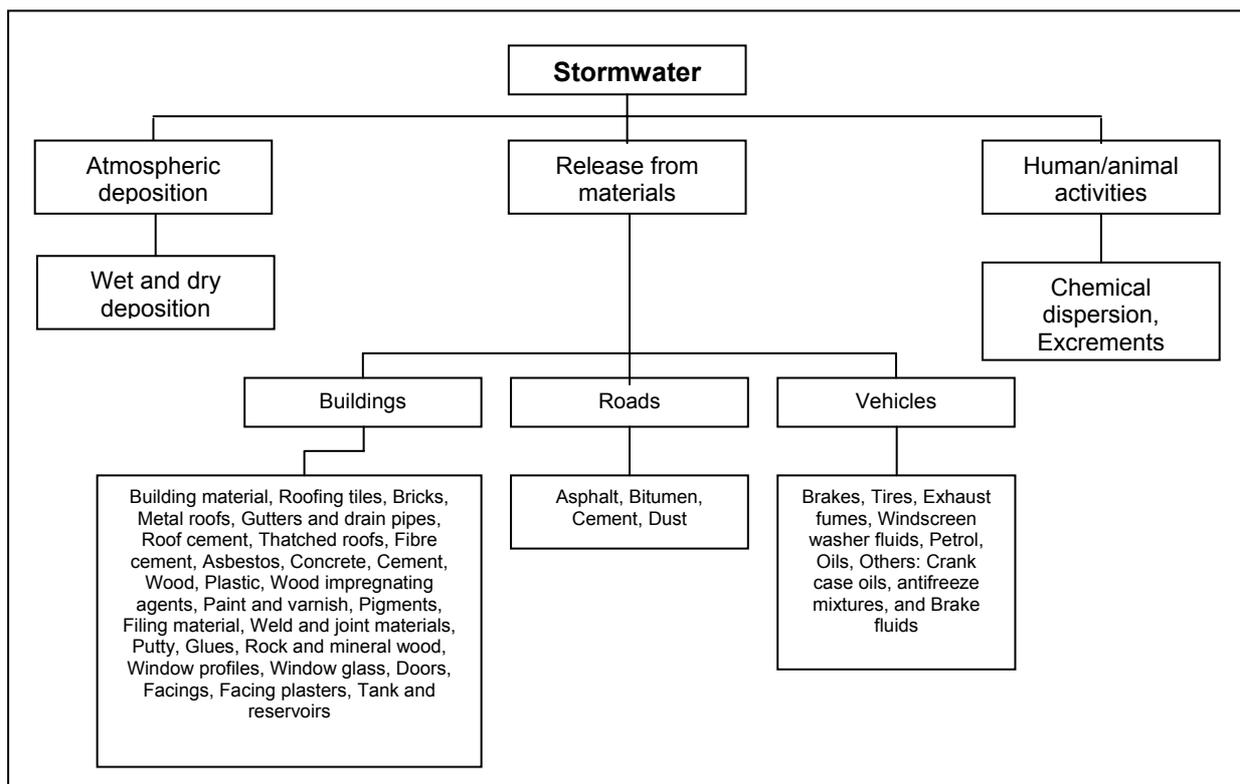


Figure 2: Sources of pollutants in stormwater

2.2 Recipient, receptor and criteria identification

In this step, the different strategies for handling of the stormwater will be evaluated with respect to potential human health hazards, technical and aesthetical problems as well as environmental hazards that could occur due to the presence of the chemical pollutants. Use, treatment or discharge scenarios will be investigated in order to identify the potential exposure routes and what or who are exposed (the receptors). Legislation is reviewed for each scenario to elucidate the quality and emission standards. Examples of recipients of relevance are water, soil and technical installations. Humans as well as aquatic and terrestrial living organisms are examples of receptors (Table 1). Human exposure routes are oral intake, inhalation of aerosols and skin contact. Continuous or pulse emissions need to be taken into account when evaluating discharges to the aquatic environment and applications to soil. The output from this step is a list with recipients, receptors and criteria for hazard assessment.

2.3 Hazard and problem identification

All constituents identified as potential pollutants in the first step of the procedure (Figure 1) are evaluated in the third step; the hazard and problem identification. The criteria for evaluation are based on environmental fate (sorption, volatilisation, persistence to degradation and bioaccumulation) short-term aquatic toxicity and long-term effects to living organisms (carcinogenicity, mutagenicity, reproduction damage, endocrine disrupting effects and promoting allergic reactions in humans).

Table 1: Examples of recipients, receptors and related criteria for hazard assessment.

Recipient	Receptor and Hazard/problem	Criteria for hazard assessment
Air	Exposure to <i>humans</i> ; allergic reactions, cancer, mutagenic effects, reproduction and toxicity	Human effect-exposure analysis
Ground water	Exposure to <i>humans</i> ; allergic reactions, cancer, mutagenic effects, reproduction and toxicity Exposure to <i>livestock</i> Effects on the <i>aquatic ecosystem</i> when groundwater infiltrate surface water	Human effect-exposure analysis and drinking water quality standards Animal effect-exposure analysis PEC/PNEC >1 in water, environmental quality standards and emission limit values
Installations	Clogging Colouring Corrosion Frothing Growth Taste and smell Precipitation	$K_s/IAP > 1^1$ $K_s/IAP > 1^1$ N&P discharge quality standards PEC/taste&smell-threshold >1 $K_s/IAP > 1^1$
Soil	Effects on the <i>soil ecosystem</i> Uptake by <i>plants</i> Exposure to <i>livestock</i> Exposure to <i>humans</i> ; when eating the crops>; allergic reactions, cancer, mutagenic effects, reproduction and toxicity	PEC/PNEC >1 in soil Soil quality standards Animal effect-exposure analysis Human effect-exposure analysis
Surface water	Effects on the <i>aquatic ecosystem</i> Exposure to <i>humans</i> ; allergic reactions, cancer, mutagenic effects, reproduction and toxicity Exposure to <i>livestock</i>	PEC/PNEC >1 in water, environmental quality standards and emission limit values Human effect-exposure analysis Drinking water quality standards Animal effect-exposure analysis

¹K_s = solubility constant for the mineral/salt

¹IAP = Ion Activity Product for the relevant ions.

The hazard and problem identification is performed according to a ranking methodology, which up to now have been developed and tested for XOCs (for more details see Baun *et al.*, 2005). The methodology consists of a decision tree in which hazardous and problematic compounds are identified. To visualize the sorting of XOCs, the decision tree can be described as a funnel fitted with several filters, see figure 3. The filters have been set according to specified criteria based on sorption, volatility, persistence to biodegradation, potential for bioaccumulation and aquatic toxicity. There are also one on/off filter for technical/aesthetical problems and a long-term chronic effects-filter considering cancer, mutagenic and reproduction hazards, endocrine disruption effects and allergenic effects. The output is a classification of the compounds in three categories (green, yellow and red) depending on their priority as possible pollutants. Green compounds are considered as non-priority pollutants, which mean that these compounds will be excluded from the fourth step in the CHIAT methodology: the hazard assessment. Yellow compounds are passed on to the next filter. These compounds may or may not be priority pollutants depending on the outcome of the following filtration. Red compounds are considered as priority pollutants.

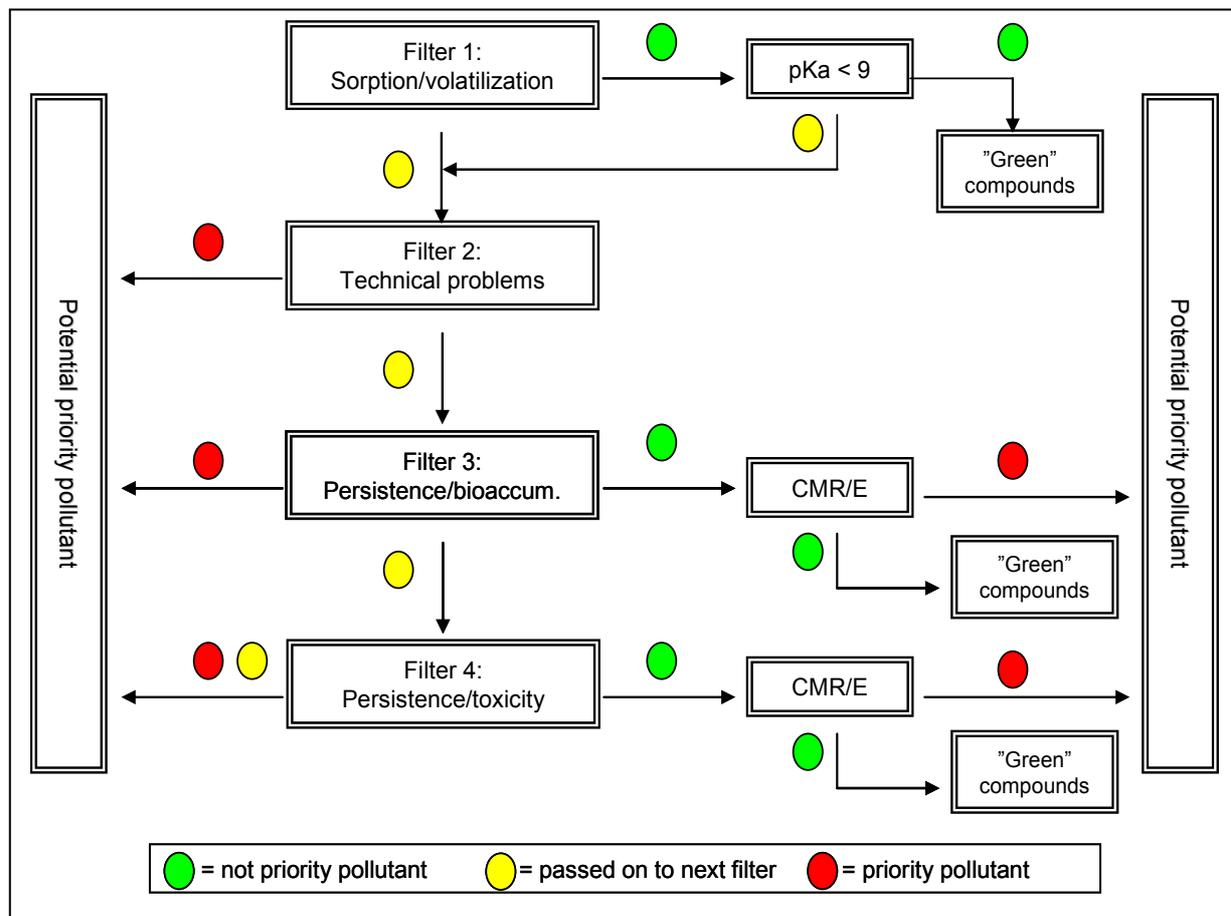


Figure 3 Decision tree used for ranking potential pollutants

The first filter is designed to separate compounds into “water phase compounds” and “solid phase compounds”. In this case the underlying assumption is that the water is transported in open systems facilitating good contact between air and water, i.e. highly volatile compounds will be identified as green compounds. It should be noted that no compound would be designated as red because of this first evaluation. The purpose with this filter is to “label” the XOCs according to their preference for the water or the solid phase (e.g. suspended solids, sediment, sludge and soil). This information will be used for the further evaluation in step 4: the hazard assessment. Information required can mainly be collected from databases and handbooks presenting the inherent properties of the XOCs (for more information and references see Baun *et al.*, 2005).

It is expected that decision trees modified for metals and other inorganic constituents will be developed in the future. Consequently, this step has been omitted in the Daywater project, and metals and inorganic constituents have been selected in the fifth step, the expert judgement.

The compounds that are identified as hazardous or problematic in this step are listed as **potential priority pollutants**.

2.4 Hazard assessment

The hazard assessment is a comparison between the effect and the exposure levels of a specific pollutant, to evaluate if there is an actual hazard under the present circumstances. The selected criteria for a hazard assessment are related to the receptor (Table 1). The exposure can be represented by predicted environmental concentrations (PEC), where the values can be based on measured data or model simulations. Evaluation of estimated concentrations for which unacceptable effects are not likely to occur can be done by estimation of predicted no effect concentrations (PNEC). The values can be found in the literature (databases and handbooks) or they can be estimated using toxicity data collected in step 3 applying recommendations from EU (2003). Comparison between the PEC and PNEC values are made in order to determine if the compound should be considered as hazardous for organisms in the environment. The pollutants for which PEC/PNEC ratios are above one ($PEC/PNEC > 1$) are classified as **priority pollutants**. A corresponding evaluation with respect to humans can be performed by e.g. using tolerable daily in-take (TDI) values, to retrieve effect-values.

This step is not fully developed yet and further refinement is part of on-going research, in continuation of the Daywater activities.

2.5 Expert judgement

Finally, the expert judgement is performed. The “expert” is not necessarily a single person (e.g. an environmental chemist) but may be a group of decision-makers with different backgrounds. The idea is that the expert selects the priority pollutants for which further action needs to be taken. The evaluation may e.g. aim to reduce the number of compounds due to financial limitations in the specific project, to add compounds of special interest or to optimise a monitoring programme. Compounds may be added or removed based on use patterns in the catchments or grouped based on similarity in chemical structure and fate. In the latter case, an indicator compound may be chosen to represent the whole group. Banned compounds can be neglected unless they still represent a pollution source, e.g. when there is continuous long-term leaching from existing structures that have not been decontaminated or demolished. Legislation concerning limit values e.g. drinking water standards as well as environmental quality standards and emission limit values for watercourses, lakes or the sea, reviewed in step 2 (Figure 1 and Table 1) should be used in order to identify compounds that may need to be added to the list. Compounds may also be added if they are priority pollutants present on national/international lists (e.g. the Water Framework Directive priority substances (European Commission, 2004); the OSPAR List of Substances of Possible Concern and the OSPAR List of Chemicals for Priority Action (OSPAR, 2004)) or “special case” compounds. The output from this step is a list containing those chemical compounds and other parameters that constitute a hazard after evaluation by the expert: the **selected priority pollutants**.

3 Discussion and conclusions

CHIAT can, in a transparent way, aid the user to rank and prioritise a large number of pollutants and results in a list of case specific selected priority pollutants. Though it contains a number of limitations in its present form and currently is a so-called “expert tool” the methodology has a good potential for becoming a user-friendly tool for consultants and municipal staff. The methodology has been used within the Daywater-project to identify 25 stormwater selected priority pollutants (Eriksson *et al.*, 2005B) and 18 organic stormwater selected priority pollutants in an other study (Eriksson *et al.*, 2005A, appendix 1).

One benefit is an objective view toward the pollutants as it is not limited to merely previously measured compounds in order to state if hazard or risk is imminent. The hazard and problem identification is separated from the hazard/problem assessment, which means that an

evaluation can take place without considering concentrations. The hazard and problem assessment is flexible towards the receptors (humans, several trophic levels of organisms) and recipients (surface water, groundwater and soil). It is also very versatile as it easily can be used for other types of source waters besides stormwater (e.g. grey wastewater) as well as conveniently can implement changes e.g. in legislation. Despite being objective in the first four steps, the user is allowed to use subjective opinions in the final step.

Limitations in the present version of the methodology are that the lists of measured and potentially present constituents are not complete as the literature reviews has been limited and need continuous updating. The list of potential pollutants is also possible to further extend by updating with additional information concerning building material, transport intensity, seasonal activities etc. GIS can also improve the catchment characterisation further. The hazard identification tool is currently limited only to include XOCs and the evaluation is severely hampered by the lack of inherent properties for many compounds. The hazard assessment needs further development and the lack of monitoring data makes this step difficult to perform. Coupling this part with modelling tools that can yield PECs for different recipients and PNECs for different receptors would be beneficial for the assessment. Ways to evaluate complex mixtures and not only single compounds need to be considered. Although it as been an aim to develop an objective methodology, several choices have been made. For example, the cut-off values that determine if the compounds should be classified as hazards or not, derive from a comprehensive literature study (Eriksson *et al.*, 2005D) but choices of this type can always be discussed and priorities can be changed if new information becomes available.

To conclude, the CHIAT-tool developed was found to be very promising. The major benefits are:

- It can be used generally for identifying priority pollutants for evaluation of different strategies for handling of stormwater.
- It can be used for selection of priority pollutants to be included in monitoring programmes.
- It is transparent and flexible.
- This procedure for selecting pollutants is transparent and adaptive to the specific scenario in focus.

The major drawbacks are:

- The database generated in step 1 (source characterisation) has to include even more constituents. It is the authors strong believe that the number of compounds identified as potentially present would increase if the search for information continued. It is therefore important, that the users of CHIAT add compounds relevant for their specific case in Step 1) Source characterisation.
- The third step in CHIAT "Hazard and problem identification" is present in a β -version programmed in Excel. This needs to be improved, in order to make it available for users in the future. In addition, it needs to be further developed to apply to other chemical compounds besides xenobiotic organic compounds.
- The fourth step "Hazard assessment" needs to be developed in order to be helping the user to estimate PEC and PNEC values for different recipients and exposure-objects.

4 List of references

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5 Appendices

Appendix 1 Eriksson *et al.*, 2005: Chemical hazard identification and assessment tool for evaluation of stormwater priority pollutants. *Water, Science and Technology*, Vol. 51, No. 2, pp. 47-55.

Appendix 2 CHIAT tutorial – an executable PP-presentation describing the CHIAT methodology. The original PowerPoint file can be found on the internal Daywater website.

Chemical hazard identification and assessment tool for evaluation of stormwater priority pollutants

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Abstract Assessment of chemical hazards is a critical issue, which have to be dealt with when evaluating different strategies for sustainable handling of stormwater. In the present study, a methodology for identifying the most critical and representative chemical pollutants was developed. A list of selected stormwater priority pollutants (SSPP-list) is the out-put from the procedure. Two different strategies for handling of stormwater were considered; discharge into a surface water recipient and infiltration. However, the same methodology can be used for other types of wastewater and other strategies for handling and treatment. A literature survey revealed that at least 656 xenobiotic organic compounds (XOCs) could be present in stormwater. In the next step, 233 XOCs were evaluated with respect to the potential for being hazardous towards either aquatic living organisms or humans, or causing technical or aesthetical problems. 121 XOCs were found have at least one of these negative effects, while 26 XOCs could not be assessed due to the lack of data. The hazard assessment showed that 40 XOCs had a PEC/PNEC ratio above one., e.g. they should be considered as priority pollutants. The final step is the expert judgement, which resulted in a final SSPP-list containing 16 selected priority pollutants.

Keywords Stormwater handling; hazard identification and assessment; xenobiotic organic compounds

Introduction

There is a growing demand in society for introducing decentralised systems providing opportunities to save and reuse water. This development is driven by water shortage in several parts of the world, but also by awareness that the centralised urban water systems used for treatment of both stormwater and wastewater are expensive and resource consuming. One way to reduce the need for freshwater and at the same time reduce the urban runoff peak flows is to collect and use stormwater. Outdoors, a number of both structural and non-structural BMPs (best management practises) may be used for handling of stormwater, e.g. gullypots, retention/detention ponds, infiltration systems (porous paving and porous asphalt surfaces, swales, infiltration trenches), basins, ponds and wetlands. Most of these BMPs are constructed to reduce the risk for stormwater flooding. However, major limitations with regard to both the use of collected stormwater and treatment in BMPs are the chemical risks related to the handling of water with poor quality. The content of different types of pollutants (chemical, physical and microbiological) is largely determined by the type of surfaces the stormwater get in contact with (roofs, roads, parking lots, pavements etc.), but also by the air quality, as well as human and animal activities at a specific site. Each pollutant may lead to potential problems depending on the usage in question, either hazards regarding exposure to humans, animals, crops or plants, or technical and aesthetical problems.

The present study aims to develop a screening procedure for identification and assessment of the most critical pollutants regarding different strategies for handling of different types of storm- and wastewater, i.e. a chemical hazard and problem identification and assessment procedure aimed at identifying priority pollutants. The work presented in this paper is, due to

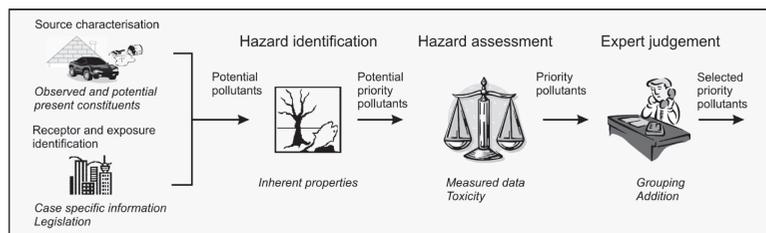


Figure 1 Approach for selecting priority pollutants based on chemical hazard identification and assessment

space limitations, restricted to one category of pollutants; the xenobiotic organic compounds (XOCs) and to two strategies for handling of stormwater; discharge of untreated stormwater to a surface water recipient and infiltration.

Methodology

Risk assessment of chemicals is composed of four elements: hazard/problem identification, hazard/problem assessment, risk characterisation and risk management according to the technical guidance document for risk assessment of chemicals in EU (TGD; European Commission, 2003). In general, hazard identification serves to map the inherent properties of chemicals by collecting and comparing relevant data on e.g. physical state, volatility and mobility as well as potential for degradation, bioaccumulation and toxicity. Hazard assessment is divided between exposure assessment and effect assessment. Comprehensive model systems have been developed to assess the distribution of contaminants in the environment (soil, water, air) and in tissue (animals, humans). The next step is risk characterisation, where the potential negative effects are evaluated and, if possible, the probability of effects occurring is estimated. Finally, risk management involves a range of possible interventions, i.e. monitoring and control of emissions to reduce risk environments (see e.g. Mikkelsen *et al.*, 2001).

The methodology developed in the present work is inspired by the TGD (European Commission, 2003) and consists of five steps; (1) source characterisation, (2) receptor and exposure identification, (3) hazard and problem identification, (4) hazard assessment and (5) expert judgement, see Figure 1.

Source characterisation

Initially, information regarding potential pollutants (metals, inorganic trace elements and XOCs) is collected. This is performed by two somewhat different approaches in the present study.

- (1) Searching in the open international literature regarding observations/measurements of XOCs in stormwater collected from roofs, parking lots, roads and pavements. This is generating a list of observed constituents (for more details see Eriksson *et al.*, in preparation).
- (2) Searching in the literature regarding XOCs that potentially could be present in stormwater due to e.g. contact with surfaces or human activities (car driving, gardening, etc.) i.e. potentially present constituents. Four major sources for pollutants in stormwater were considered; atmospheric deposition, releases from materials, human activities and excretion from animals (Figure 2). The international literature and material databases (e.g. BPS-Centret, 1998) were searched for information regarding the presence of XOCs that potentially could be released from these sources (for more details see Ledin *et al.*, 2004).

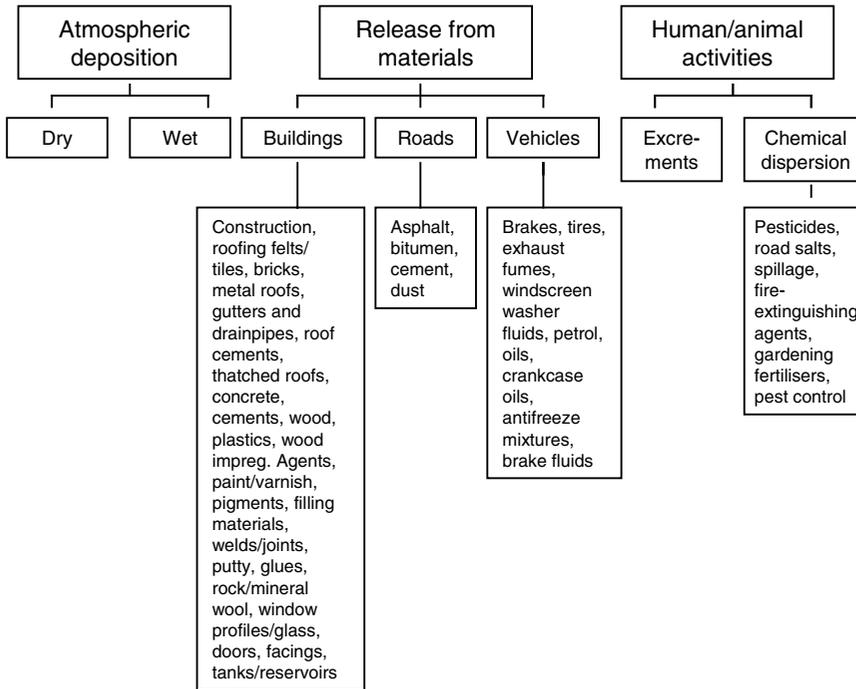


Figure 2 Examples of sources that potentially are contributing to pollutants in stormwater

All observed and potentially present constituents are listed as *potential pollutants* and evaluated in the third step: hazard identification (Figure 1).

Receptor and exposure identification

In this step the different strategies for handling of the selected type of waste- and/or stormwater will be evaluated with respect to potential human health hazards, technical and aesthetical problems as well as environmental hazards that could occur due to the presence of the chemical pollutants. Use, treatment or discharge scenarios will be investigated in order to identify the potential exposure routes and what or who are exposed. Legislation is reviewed, for each scenario, to elucidate the quality and emission standards.

Examples of receptors of relevance are humans as well as aquatic and terrestrial living organisms. Exposure route for humans' are oral intake, inhalation of aerosols and skin contact. Continuous or pulse emissions need to be taken into account when evaluating BMPs and discharges to the environment. In technical installations problems like precipitation, corrosion and clogging are identified, i.e. technical installations have to be considered as receptors as well.

Hazard and problem identification

All constituents identified as potential pollutants in the first step of the procedure (Figure 1) are evaluated in the third step; the hazard and problem identification. The criteria for evaluation are based on environmental fate (sorption, volatilisation, persistence to degradation, bioaccumulation and toxicity) and long-term chronic effects to living organisms (carcinogenicity, mutagenicity, reproduction hazards and endocrine disrupting effects) as well as promoting allergic reactions in humans. Precipitation of salts and corrosion of different types of installations and tubing are examples of relevant technical problems that

should be included if inorganic constituents are considered in the study. Bad odour and colouring of clothes and toilet bowls due to the presence of e.g. Fe- and Mn-precipitates or humic and fulvic acids are examples of aesthetic problems to be considered.

The hazard and problem identification is performed according to a ranking methodology, which is described in detail in Baun *et al.* (in preparation). The methodology consists of a decision tree in which hazardous and problematic compounds are identified. To visualize the sorting of XOCs the decision tree can be described as a funnel fitted with several filters. The filters have been set according to specified criteria based on sorption, volatility, persistence to biodegradation, potential for bioaccumulation and toxicity. There are also one on/off filter for technical/aesthetic problems and a long-term chronic effects-filter considering cancer, mutagenic and reproduction hazards, endocrine disruption effects and allergenic effects. The output is a classification of the compounds in three categories (white, grey and black) depending on their priority as possible pollutants. White compounds are considered as non-priority pollutants, which means that these compounds will be excluded from the fourth step; the hazard assessment. Grey compounds are passed on to the next filter. These compounds may or may not be priority pollutants depending on the outcome of the following filtration. Black compounds are considered as priority pollutants.

The first filter is designed to separate compounds into “water phase compounds” and “solid phase compounds”. In this case the underlying assumption is that the water is transported in open systems facilitating good contact between air and water, i.e. highly volatile compounds will be identified as white compounds, which is an acceptable assumption when evaluating stormwater. It should be noted that no compound would be designated as black as a result of this first filtration. The purpose with this filter is to “label” the XOCs according to their preference for the water or the solid phase (e.g. suspended solids, sediment and soil). This information will be used for the further evaluation in step 4; the hazard assessment.

Information required, in the present study, can mainly be collected from databases and handbooks presenting the inherent properties of the XOCs, since only hazards towards aquatic and soil living organisms are considered. The following references were used; Hazardous Substances Database (2003); CCRIS (2003); Chemfinder (2003); Danish EPA (2000); US EPA ECOTOX (2003); US EPA EPISUITE (2003); GENE-TOX database (2003); IUCLID (2000); NOVA (2003); OSPAR (2003); Rippen (2003) and Verscheuren (1996). The compounds that are identified as hazardous or problematic in this step are listed as *potential priority pollutants*.

Hazard assessment

The exposure can be represented by predicted environmental concentrations (PEC), where the values can be based on measured data or model simulations. Evaluation of the effects can be relied on predicted no effect concentrations (PNEC). These represent estimated concentrations for which unacceptable effects are not likely to occur, and they can be found in the literature (databases and handbooks). Comparison between the PEC and PNEC values are made in order to determine if the compound should be considered as hazardous for organisms in the environment. The pollutants that receive a PEC/PNEC ratio above one (1) are classified as priority pollutants. A corresponding evaluation with respect to humans can be performed by e.g. using acceptable daily in-take values, to retrieve effect-values. Possible oversaturation of metal salts can be estimated by geochemical modelling (e.g. PHREEQC; Parkhurst and Appelo, 2001). The pollutants that receive a saturation index above one (oversaturated) are classified as priority pollutants. This step is not fully developed yet and further refinement is part of on-going research.

As basis for a preliminary assessment measured concentrations found in the review by Eriksson *et al.* (in preparation) were used in the present study to represent PEC-values.

A dilution factor of 100 is used for the surface water discharge scenario according to the suggestions in the TGD (European Commission, 2003). An assessment factor of 1000 (EU Commission, 2003) is used when estimating PNEC values to the natural environment and to compensate for transferring from laboratory tests and for inter-species variations of the test organisms used. $PNEC_{soil}$ are calculated for each compound based on the Henry's law constant, the organic carbon-water partition coefficient (K_{oc}) and the $PNEC_{water}$.

Expert judgement

Finally, the expert judgement is performed. The "expert" is not necessarily a single person (e.g. an environmental chemist) but may be a group of decision-makers with different backgrounds. The idea is that the expert selects the priority pollutants for which further action needs to be taken. The evaluation may e.g. aim at reducing the number of compounds due to financial limitations in the specific project. Compounds may be removed based on use patterns in the catchments or grouped based on similarity in structure and fate. In the latter case, an indicator compound may be chosen to represent the whole group. Compounds that are banned can also be removed unless certain reasons exist.

Legislation concerning limit values e.g. drinking water standards as well as environmental quality standards and emission limit values for watercourses, lakes or the sea, reviewed in step 2 (Figure 1) should be used in order to identify compounds that may need to be added to the list. Compounds may also be added if they are priority pollutants present on national/international lists or "special case" compounds. Compounds deriving from specific anthropogenic sources e.g. car catalysts may also be added. Furthermore, high content of easily degradable organic matter can cause odour, due to oxygen depletion and anaerobic conditions, may require the presence of summary parameters as BOD and COD. Physical parameters such as turbidity and temperature may also be needed in order to make complete monitoring programme. The output from this step will be a list containing those chemical compounds and other parameters that constitute a hazard after evaluation by the expert: the selected priority pollutants.

Results and discussion

Source characterisation

The literature survey regarding observations and measurements of pollutants in stormwater clearly showed that a large number of constituents have been identified and quantified. In total, 173 publications were found in the open international literature (including e.g. the review by Makepeace *et al.*, 1995), which report all together 514 different constituents (Eriksson *et al.*, in preparation). In order to illustrate the diversity within the group of XOCs, a division in subgroups, is given in Table 1. It should be mentioned that the searching carried out within the project was limited (for more details see Ledin *et al.*, 2004). Therefore, the number of pollutants that potentially could be present would probably increase if the searching was extended. There were a relatively limited number of compounds that belonged to both groups, i.e. compounds that have been identified in stormwater and pointed out as potentially present (Table 1). This observation indicates that although a large number of organic compounds have been observed in stormwater, there could be at least as many other compounds present, that no one has tried to analyse for yet.

Receptor and exposure identification

Two different scenarios for handling of stormwater were evaluated in the present study; discharge to a surface water recipients and infiltration in the ground, i.e. the receptors for consideration were surface water and soil. Accordingly, aquatic living organisms as well as

Table 1 Number of compounds that have been identified in stormwater, number of potentially present constituents, and the number that have been found in both categories

Compound group	Compounds identified in stormwater "observed constituents"	Potentially present pollutants	Number of constituents present in both categories
Alkanes	19	17	15
Benzenes	19	37	8
Dioxins	31	9	4
Ethers	8	7	1
Halogenated aliphates	27	25	8
Organotin compounds	0	9	0
Organolead compounds	9	0	0
PAHs	58	51	27
PCBs	14	0	0
Pesticides	115	64	26
Phenols	32	36	20
Phthalates and adipates	8	7	5
Miscellaneous	26	149	7
Total no. of constituents	366	411	121

soil organisms are going to be exposed to the pollutants. Groundwater quality was not considered in this study.

Hazard and problem identification

It was found that at least 656 XOCs could potentially have an impact on the water quality (Table 1). 233 XOCs (Baun *et al.*, in preparation) have so far been evaluated according to the hazard and problem identification procedure described above; 72 of these 233 XOCs were classified as hazardous with regard to the water phase, whereas 88 were classified as hazardous with respect to the solid phase (sediment, suspended solids or soil); 39 compounds were overlapping between the two groups, which means that in total 121 XOCs are so far identified as potentially hazardous. It should be noted that 26 XOCs could not be assessed due to lack of data, either basic physical chemical data or environmental fate data. These compounds require further data searching, testing or estimation by e.g. QSAR, in order to be classified. The hazardous compounds in the solid phase mainly belonged to four different groups: polycyclic aromatic hydrocarbons (PAHs), dioxins, chlorinated pesticides and PCBs. The XOCs identified as hazardous in the water phase are more evenly distributed over the 13 groups presented in Table 1. However, the major contribution is from the group with pesticides.

Hazard assessment

In the hazard assessment, PEC-values for the 121 XOCs identified in the hazard and problem identification step were compared with their corresponding PNEC-values. The XOCs are considered as priority pollutants if the ratio exceeds 1. It was found that 99 of the potential priority pollutants had been measured in stormwater according to the review by Eriksson *et al.* (in preparation) and that the PEC/PNEC ratio exceeded one for 40 of them. The majority were pesticides/herbicides, but a number of PAHs were also pointed out (e.g. anthracene, benzo[a]pyrene, chrysene, naphthalene, pyrene and triphenylene), two phthalates (DBP and DEHP), a polychlorinated biphenyl (PCB-153) as well as pentachlorophenol (PCP).

More information regarding concentrations in stormwater, efficiency of treatment methods, fate in receiving waters and soils, data for the effect analysis (human acceptable daily doses and PNECs for ecosystems) is needed in order to refine this step.

Table 2 List of selected stormwater priority pollutants: SSPP

Type of pollutants	This study	DayWater (excluding step 4)
General		BOD, COD, suspended solids, pH, nitrogen and phosphorus
Metals		cadmium, chromium, copper, nickel, lead, platinum and zinc
XOCs		
Pesticides/ Herbicides	acrolein, dichlorprop, dichlorvos, diuron, hexachlorocyclohexane (HCH), metazaklor, metoxyklor, propiconazol and terbutylazine	glyphosate, pendimethalin, phenmedipham and terbutylazine
PAH	naphthalene, pyrene and benzo [a] pyrene	naphthalene, pyrene and benzo [a] pyrene
PCB	PCB-153	PCB-28
Miscellaneous	nonylphenoethoxylates and nonylphenol, pentachlorophenol, di (2-ethylhexyl) phthalate and methyl tert-butyl ether,	nonylphenoethoxylates and nonylphenol, pentachlorophenol, di (2-ethylhexyl) phthalate and methyl tert-butyl ether

Expert judgement

Finally, the most important XOCs will be selected from the list with 40 XOCs identified in the fourth step and other relevant XOCs can be added according to the judgement from the experts involved. Among the herbicides/pesticides acrolein, dichlorprop, dichlorvos, diuron, hexachlorocyclohexane (HCH), metazaklor, metoxyklor, propiconazol and terbutylazine were selected (Table 2). The presence of these XOCs on EU Water Framework Directive list "Priority substances in the field of water policy" (European Commission, 2004) was the major reason for selecting these pesticides as they act as a representatives for groups of pesticides, e.g. dichlorprop as a representative of fenoxo acids and correspondingly metoxyklor for the chlorinated pesticides in use today. Naphthalene and benzo[a]pyrene were selected among the PAHs. This grouping of PAHs was based on their ring structure in order to ensure including a PAH present in both the aqueous phase and solid phase as well as PAHs primarily found in the solid phase. Criteria such as high persistence, bioaccumulation, and long-term chronic effects were also used in this evaluation. The other XOCs were selected since they can act as indicator compounds of different pollutant groups (Table 2). Long-term chronic effects, persistence and bioaccumulation as well as aesthetical problems like odour were taken into consideration. Some of these are also on the list of priority substances within EU's Frame Water Directive (nonylphenol and DEHP). Among these were NPEO, NP and MTBE added although they did not have PEC/PNEC ratios above 1. It was, however, judged that compounds with this property are needed in order to be able to evaluate the impact from discharging or infiltrating stormwater.

This can be compared with the results from a corresponding work carried out for the DayWater project (see the acknowledgement), where the major focus was to identify a list of pollutants suitable for comparing different BMPs. Step 4 was excluded in this work, due to the present limitations in this step (see above). The expert judgement was applied to the list with 151 potential priority pollutants. After evaluation 3 PAHs, 4 herbicides, 1 PCB and 4 other XOCs as well as 13 physical/chemical parameters, metals and inorganic trace elements were selected (Table 2). The evaluation was performed according to the following criteria. Herbicides were selected from the list with potential priority pollutants based on use statistics in Europe as well as observed presence in plants, animals and food products (Nordlander, 2003; Andersson *et al.*, 2003; Danish EPA, 2003; Swedish Chemicals Inspectorate, 2003; European Commission, 2004). Grouping of PAHs and selection of the other XOCs were based on the same arguments as for the present study. The metals were selected to cover both cationic and anionic species within the pH-range relevant for stormwater. Some

highly sorbing metals were included as well as non-sorbing ones. Specific sources (e.g. car catalysts; and high observed loads in stormwater were also used as criteria for selection. BOD, COD, suspended solids, pH and the nutrients are included since the general physical/chemicals parameters are needed to e.g. evaluate technical/aesthetical problems.

Conclusions

The methodology developed within this study was found to be very promising. It can be used generally for identifying selected priority pollutants (SSPP lists) for evaluation of different strategies for handling of storm- and wastewater and for selection of priority pollutants to be included in monitoring programmes. This procedure for selecting pollutants is transparent and adaptive to the specific scenario in focus.

The study also showed that the number of XOCs that could be expected to be present in stormwater is large (656 XOCs). However, it also illustrated that the XOCs that have been identified and quantified in stormwater is probably only a fraction of those compounds that are present; 366 have been observed by measurements and 411 have been identified as potentially present, with an overlap of only 121 XOCs.

The hazard and problem identification carried out as a filtering further reduced the number of relevant XOCs to 121, i.e. this is the potential priority pollutants. This part of the study was hampered by the lack of inherent data for some of the potential pollutants. The hazard assessment further reduced the number of relevant XOCs to 40. However, this step is very preliminary, due to lack of data and procedures for exposure and effect assessment.

Finally, 16 XOCs were selected during the expert judgement. These have all inherent properties that makes them potentially hazardous. Furthermore, some of them have been observed in the environment in concentrations that could be critical for aquatic and soil living organisms.

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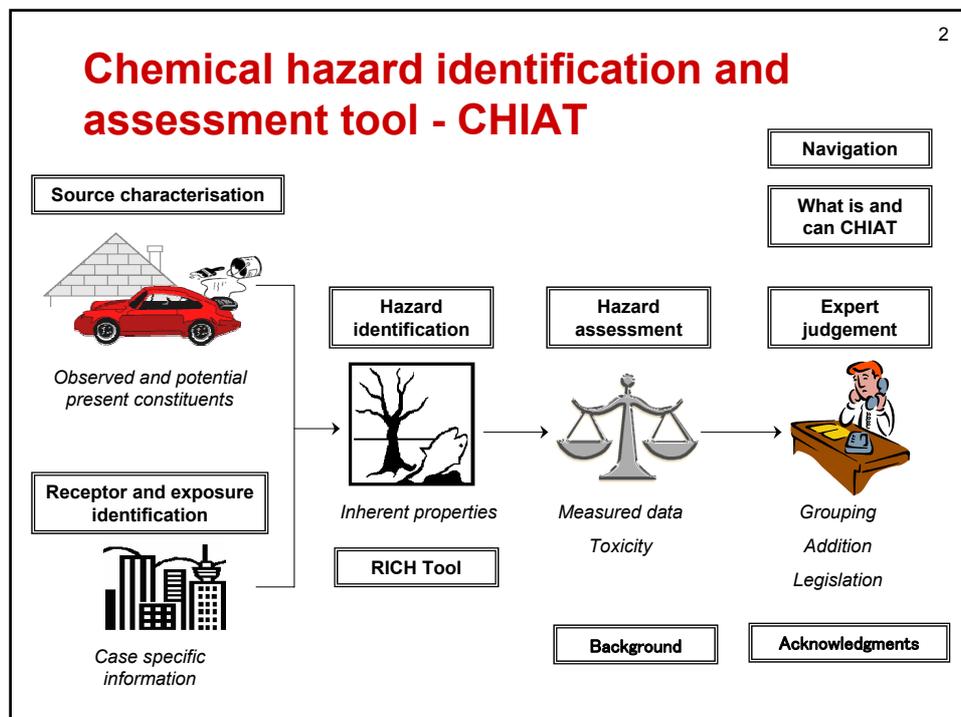
D4.2



CHIAT tutorial an executable PP- presentation describing the CHIAT methodology

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Chemical hazard identification and assessment tool - CHIAT

This guide is prepared by the Danish Daywater team: Mikkel Boye Hauger, Eva Eriksson, Anna Ledin, Anders Baun and Peter Steen Mikkelsen

From the Technical University of Denmark

The content of this guide is based on the content of Daywater deliverables:

D4.2 Methodology for evaluating and prioritising environmental risks associated with chemical constituents in stormwater

D4.3 Selected stormwater priority pollutants (SSPP)

D4.4 Database of SSPP

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About the Daywater project

Acknowledgement

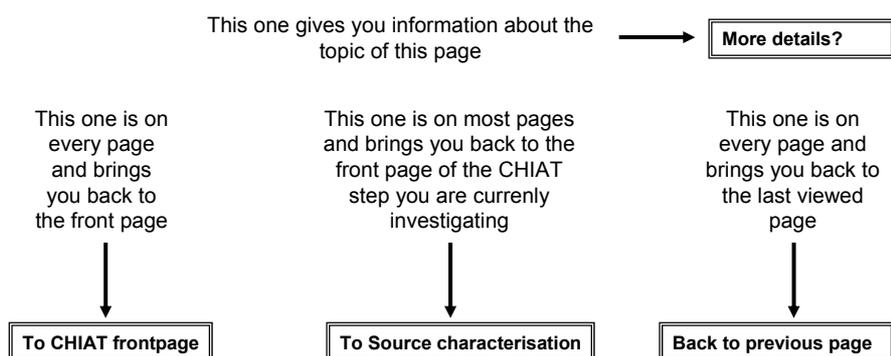
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This project is organised within the "Energy, Environment and Sustainable Development" Programme in the 5th Framework Programme for "Science Research and Technological Development" of the European Commission and is part of the CityNet Cluster, the network of European research projects on integrated urban water management.

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Navigation in the CHIAT Guide

In the CHIAT guide you will find a lot of clickable boxes!
Click and learn!



What is CHIAT and what can CHIAT do?

CHIAT is: A tool that helps the user of the ADSS to select priority pollutants.

The version demonstrated in this guide have main focus on organic compounds.

CHIAT can:

- Identify selected priority pollutants (SPP) for source control of stormwater
- Identify SPP's relevant to be included in a monitoring programme in a specific project
- Identify SPP for evaluation of different strategies for stormwater handling, e.g. selection of BMP's in a specific project

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Source characterisation

CHIAT step 1



Observed and potential present constituents

Source characterisation is a collection of:

Those compounds that have been identified in stormwater

Those compounds that potentially are present in stormwater

How are compounds identified ?

What does potentially present mean?

[Currently not active](#) [Characteristics paper?](#)

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[Download Daywater report on source characterisation](#)

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How are compounds identified?

The compounds identified in urban stormwater runoff in connection with WP4 were collected from the open international literature (articles, reports, conference proceedings as well as public available reports) from 1980 to the beginning of 2004.

Information regarding physical, and chemical contaminants, both individual compounds as well as summa parameters was collected from unmixed stormwater runoff. Information originating from combined sewer overflows (CSO) or surface water recipients, or that had been diluted by treated wastewater, were not included.

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Identified compounds -details

CHIAT step 1



Observed and potential present constituents

The compounds found in runoff varies a lot depending on the type of area where the runoff is collected

Airport runoff

Parking lot runoff

Recreational runoff

Road runoff

Roof runoff

Unspecified or mixed urban runoff

Yard runoff

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Identified compounds – Airport runoff

CHIAT step 1



Observed and potential present constituents

Sources: main terminal, inflow to stormwater pond, runway, unspecified airport runoff

Explanation and or examples:

Airport runoff has been found to contain different types of anti-icing fluids due to aircraft deicing

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Identified compounds – Parking lot runoff

CHIAT step 1



Observed and potential present constituents

Sources: parking lot with different surfaces e.g. asphalt, concrete and stone. Different use suburban shopping plaza; commercial, industrial, and residential parking area, car park.

Explanation and or examples:
The types of compounds found in parking lot runoff depend partly on the surface material used, for example can asphalt surfaces leach organic compounds deriving from bitumen whereas concrete work of all types tends to cause elevated pH.

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Identified compounds – Recreational runoff

CHIAT step 1



Observed and potential present constituents

Sources: landscaped areas, golf courses, green areas, green house area, and field.

Explanation and or examples:
Green areas in cities e.g. golf courses, sports fields and parks requires maintenance in form of fertilizers and pesticides which can be found in the runoff

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Identified compounds – Road runoff

CHIAT step 1



Observed and potential present constituents

Sources: Street, highway, freeway, motorway and trunk roads, suburban roads, industrial, residential, commercial, different surface structures e.g. asphalt, concrete

Explanation and or examples:
Runoff quality from roads highly depends on the traffic intensity and vehicle type as well as the applications used on the road and the road sides e.g. de-icing and weed control.

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Identified compounds –Roof runoff

CHIAT step 1



Observed and potential present constituents

Sources: concrete tile, pan tile, fibrous cement, tar felt, tile roof, polyester roof, flat gravel roof, combined roof system, domestic residence, galvanized iron, residential area, commercial, industrial, galvanized roof, tar coated, aluminium, asbestos cement, zinc sheet, slate, gravel

Explanation and or examples:
The type of roofing material is the one of source of compounds in roof runoff and for example are metal roofs leaching metal ions whereas felt and thatched roof has been impregnated with pesticides to avoid unwanted growth, which can be found in the runoff.
Atmospheric deposition both long-range and local e.g. from the local industries affects the roof runoff quality.

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Identified compounds Unspecified or mixed urban runoff

CHIAT step 1

Sources: industrial, commercial and residential districts, stormwater sewers, separate sewer systems, urbanised areas



Observed and potential present constituents

Explanation and or examples:

The runoff deriving from these types of catchments receives input from atmospheric deposition, materials in the buildings as well as the human activities including traffic in the studied area. Industrial areas have a high ratio of trucks compared to cars, which is reflected in the runoff. Residential areas contribute with compounds deriving from car washing and gardening as well as organic material from defoliation

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Identified compounds –Yard runoff

CHIAT step 1

Sources: courtyards, residential, concrete, pavement, gravel



Observed and potential present constituents

Explanation and or examples:

The material used in the yard has an effect on the runoff volumes. Porous pavement allows rain and snowmelt to pass through it, thereby reducing the runoff from a site and surrounding areas. Permeable pavement systems, e.g. gravel allow water to seep through the surface, so that natural filtration can still occur. Conventional hard asphalt surface does not allow seepage and result in surface runoff ending up in storm drains or in puddles.

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What does potentially present mean?

CHIAT step 1



Observed and potential present constituents

The substances that can be potentially present in stormwater are dependent on what the runoff have been in contact with on its way.

The three main sources of substances in runoff are atmospheric deposition, material release and human/animal activities

More details on Sources?

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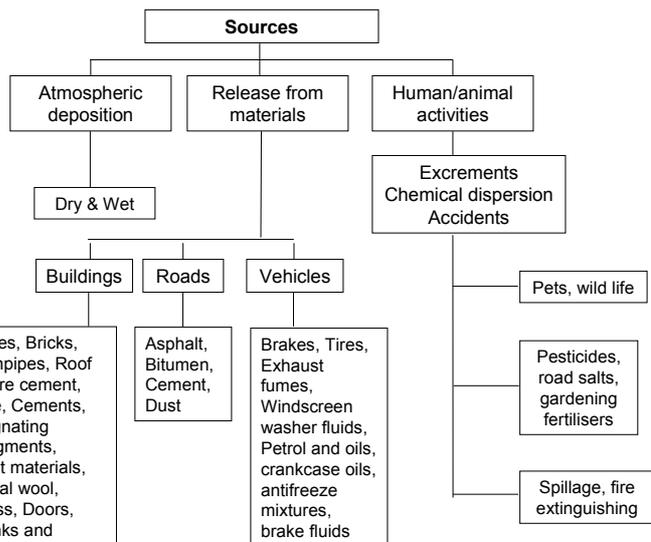
Potential substances

CHIAT step 1



Observed and potential present constituents

Building materials, Roofing tiles, Bricks, Metal roofs, Gutters and drainpipes, Roof cements, Thatched roofs, Fibre cement, asbestos free roofs, Concrete, Cements, Wood, Plastics, Wood impregnating agents, Paint and varnish, Pigments, Filling material, Weld and joint materials, Putty, Glues, Rock and mineral wool, Window profiles, Window glass, Doors, Facings, Facing plasters. Tanks and reservoirs



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To Identified compounds

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Receptor and exposure identification

CHIAT step 2



Case specific information

See a list with sets of receptors, exposure-objects and criteria

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Receptor and exposure identification is

1. Collection of specific information about the project in focus like
Type of runoff (roof, road etc.)
Selected strategies for handling (BMP's, reuse etc.)
2. Identification of the receptors (Surface water, soil, groundwater)
And the exposure objects (Humans, aquatic ecosystem)
3. Identification of criteria for hazard assessment (used in CHIAT step 4)
4. Collection of local, regional and EU legislation (used in CHIAT step 5 expert judgment)

All this is used in specific scenarios



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Receptors, exposure-objects and criteria



Recipient	Exposure object	Criteria for hazard assessment
Ground water	Exposure to humans: allergic reaction, cancer, mutagenic effects, reproduction and toxicity Exposure to livestock Effects on the aquatic ecosystem when groundwater infiltrate surface water	Human effect-exposure analysis Drinking water quality standards Animal effect-exposure analysis Aquatic living organism effect exposure analysis Environmental quality standards Emission Limit values
Soil	Effects on the soil system Uptake by plants Exposure to livestock Exposure to humans; when eating crops; allergic reaction, cancer, mutagenic effects, reproduction and toxicity	Soil dwelling organism effect exposure analysis Soil quality standards Animal effect-exposure analysis Human effect-exposure analysis
Surface water	Effects on the aquatic system Exposure to humans; allergic reaction, cancer, mutagenic effects, reproduction and toxicity Exposure to livestock	Aquatic living organism effect exposure analysis Environmental quality standards Emission Limit values Human effect-exposure analysis Drinking water quality standards Animal effect-exposure analysis

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Example: Environmental discharge



Discharge of runoff to surface water

The receptor is: Surface water

The exposure objects are:

Humans

Aquatic ecosystem

Livestock

The relevant criteria are:

Human effect exposure analysis: Human exposure-effect analysis based on Tolerable Daily Intake

Livestock effect exposure analysis: Animal exposure analysis based on Tolerable Daily Intake for 1. animals and 2. humans

Drinking water quality standards: National/EU regulation for drinking water quality

Aquatic living organism effect exposure analysis: Predicted environmental concentration (PEC) / Predicted no-effect concentration (PNEC) > 1; criteria for risk

Environmental quality standards: National/EU regulation for surface water quality standards

Emission Limit values: National/EU regulation for discharge to surface waters

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Inherent properties

Hazard identification



Inherent properties

The hazard identification is based on the following properties of the substances:

Chemical properties

[Details ?](#)

Effects on humans and animals

[Details ?](#)

Concentrations

[Details ?](#)

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Hazard identification

Hazard identification
CHIAT step 3



Inherent properties

The next step is the hazard and problem identification. It has the following elements:

Inherent properties of substances

Ranking and identification of chemical hazards (RICH) tool

Cut-off values for 5 criteria

Databases with relevant properties

More details about properties

More about RICH

More about criteria

More details about databases

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Cut-off values for 5 criteria

Hazard identification



Inherent properties

Parameter	Low	Medium	High
Volatization (atm·m ³ mol ⁻¹)	$KH < 3 \cdot 10^{-7}$	$3 \cdot 10^{-7} \leq KH < 10^{-3}$	$KH \geq 10^{-3}$
Sorption (liter·kg)	1. $K_D < 100$ 2. $K_{oc} < 500$	1. $100 \leq K_D < 1000$ 2. $500 \leq K_{oc} < 5000$	1. $K_D \geq 1000$ $K_{oc} \geq 5000$
Persistence	1. Ready biodegradable 2. $T_{1/2} < 60d$ 3. Biowin 3: result "weeks" and Biowin 5 result 5: prob $\geq 0,5$	1. Inherent biodegradable 2. $60 \leq T_{1/2} < 180d$ 3. Biowin 3: result "weeks" or Biowin 5 result 5: prob $\geq 0,5$	1. Persistent biodegradable 2. $T_{1/2} \geq 180d$ 3. Biowin 3: result "months" or Biowin 5 result 5: prob $< 0,5$
Bioaccumulation	1. $BCF < 100$ 2. $\log K_{ow} < 3$	1. $100 \leq BCF < 5000$ 2. $3 \leq \log K_{ow} < 4,5$	1. $BCF \geq 5000$ 2. $\log K_{ow} \geq 4,5$
Toxicity (mg/l)	$(LC_{50} \text{ or } EC_{50}) \geq 100$	$1 \leq (LC_{50} \text{ or } EC_{50}) < 100$	$(LC_{50} \text{ or } EC_{50}) < 1$

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Databases

Hazard identification



Inherent properties

Some links to chemical databases in which inherent data from the identified chemicals can be found

Use [Chemfinder](#) to find the CAS no. of your compounds use the CAS no as input in the databases

[Toxnet](#) consists of several databases:

Hazardous substances databank (inherent properties and toxicity)

Gene-Tox (mutagenicity)

CCRIS (cancer)

[ECOTOX](#) from US. EPA contain plant and animal both aquatic and terrestrial toxicity data

[Environmental Fate Data Base](#) (CHEMFATE, fate of chemicals in the environment. BIOLOG ca also be useful)

Information on high volume produced/imported chemicals can be obtained by [European chemical substances information system?](#) and then accessing IUCLID D.S., look for the CAS no. and finally retrieve the data by downloading the chemical data sheets.

[EPI Suite](#) is a modelling tool that can model different parameters e.g. biodegradability

[OSPAR](#) contain priority pollutants and their inherent properties

National authorities e.g. [Danish EPA](#) and Swedish [Kemli \(N-Class Database\)](#) can provide data for some compounds

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Chemical properties

Hazard identification



Inherent properties

A list of chemical properties that are of included in the hazard identification

Click to see definition

Aerobic degradation

Anaerobic degradation

Boiling point Bp

Degradability

Distribution constant Koc

Henrys constant (Kh)

Melting point (°C) Mp

Molecular weight Mw

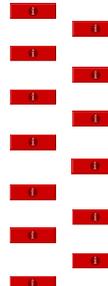
Octanol-water partitioning constant Kow

Partitioning coefficient Kd

pKa

Vapour pressure

Water solubility Ws



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Chemical properties—details on degradation

Hazard identification



Inherent properties

Biodegradability is evaluated from results of standardised biodegradations test methods as well as abiotic degradation pathways e.g. hydrolysis and photolysis. A distinction is made between:

Aerobic: Life or processes that require, or are not destroyed by, the presence of oxygen.

Anaerobic: A life or process that occurs in, or is not destroyed by, the absence of oxygen.

A distinction between three levels of biodegradability are made

- Ready biodegradability: either 70% removal of the dissolved organic substance or 60% of theoretic Oxygen consumption/CO₂-formation dependent on the test method.
- Inherent biodegradability: <70% degradation but >20%
- Persistent to biodegradation: <20% according to standardised tests.

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Chemical properties—details on boiling and melting point

Hazard identification



Inherent properties

Melting point (°C) Mp is the temperature at which a solid becomes a liquid at normal atmospheric pressure (1013 hPa).

Boiling point (°C) is the temperature at which a liquid changes to a gas (vapour) at normal atmospheric pressure

Vapour pressure A measure of a substance's propensity to evaporate, the vapour pressure corresponds to the saturation pressure above a solid or a liquid chemical substance.

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Chemical properties—details on Henrys constant (Kh)

Hazard identification



Inherent properties

Henry's law constant, K_h , is the central parameter that describes the substance's tendency or willingness to escape from an aqueous solution to the air.

Henry's law constant express the concentration in the air divided by the concentration in water

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Chemical properties—details on Partition coefficients

Hazard identification



Inherent properties

K_{oc} Distribution constant between organic carbon (organic matter of soil or sediments) and water (K_{oc}). It is expressed in L/kg

K_d Partitioning coefficient between the solid phase and water it is expressed as L/kg

Octanol-water partitioning constant (K_{ow}) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents

Octanol is interesting because it is an organic solvent with properties resembling those of the body fat in humans and animals

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Chemical properties—details on Molecular weight Mw

Hazard identification



Inherent properties

Molecular weight (g/mole) Mw; a mole is an amount of substance that contains as many objects (molecules, particles, ions, cells etc.) as the number of atoms in exactly 12 grams of 12C (carbon).

Example: Benzene C_6H_6 has a molecular weight of:
 $M_w 6 \cdot 12 + 6 \cdot 1 = 78 \text{ g/mol}$

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Chemical properties—details on water solubility (g/L)

Hazard identification



Inherent properties

Water solubility (g/L), the solubility of a substance (at room temperature) is the maximum dissolved concentration of a substance in water

Usually measured at 20°C or 25°C in distilled water

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Inherent properties – details on effects

Hazard identification



Inherent properties

The hazard identification includes a number of effects that the chemical can have on humans or animals

Acute toxicity	<input type="checkbox"/>	<input type="checkbox"/>
Bioconcentration	<input type="checkbox"/>	<input type="checkbox"/>
Carcinogenicity	<input type="checkbox"/>	<input type="checkbox"/>
Chronic toxicity	<input type="checkbox"/>	<input type="checkbox"/>
Ecotoxicity	<input type="checkbox"/>	<input type="checkbox"/>
Endocrine disrupting	<input type="checkbox"/>	<input type="checkbox"/>
Mutagenicity	<input type="checkbox"/>	<input type="checkbox"/>
Reproductive toxicity	<input type="checkbox"/>	<input type="checkbox"/>

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Effects on humans and animals – details on toxicity

Hazard identification



Inherent properties

Toxicity: The degree to which a substance or mixture of substances can harm humans or animals.

Acute toxicity involves harmful effects in an organism through a single or short-term exposure

Chronic toxicity is the ability of a substance or mixture of substances to cause harmful effects over an extended period, usually upon repeated or continuous exposure sometimes lasting for the entire life of the exposed organism.

Results from standardised ecotoxicological tests (LC50, EC50, NOEC, LOEC) for a minimum of 3 species (e.g. algae, crustaceans, and fish) are included in hazard identification in relation to aquatic organisms

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Effects on humans and animals – details on bioconcentration factor BCF

Hazard identification



Inherent properties

Bioconcentration is expressed through the bioconcentration factor BCF

The Bioconcentration factor is defined as the relationship between the concentration of a substance in the organism and the concentration in the surrounding environment at equilibrium

Compounds that are bioaccumulative are critical because that even though the exposed dose is low, the concentration in the organism can accumulate over time to a critical level, as well as accumulate in the foodchain

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Effects on humans and animals – details on Mutagenicity and Carcinogenicity

Hazard identification



Inherent properties

A carcinogen is a substance that causes cancer (or is believed to cause cancer).

A mutagen is a substance or agent that causes an increase in the rate of change in genes (subsections of the DNA of the body's cells). These mutations (changes) can be passed along as the cell reproduces, sometimes leading to defective cells or cancer

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Effects on humans and animals – details on Chronic toxicity

Hazard identification



Inherent properties

Chronic toxicity is the ability of a substance or mixture of substances to cause harmful effects over an extended period, usually upon repeated or continuous exposure sometimes lasting for the entire life of the exposed organism.

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Effects on humans and animals – details on Endocrine disrupting

Hazard identification



Inherent properties

An environmental endocrine or hormone disrupter is an agent that interferes with the synthesis, secretion, transport, binding, action, or elimination of natural hormones in the body that are responsible for the maintenance of homeostasis, reproduction, development, and/or behaviour.

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Effects on humans and animals – details on Reproductive toxin

Hazard identification



Inherent properties

A reproductive toxin is a substance or agent that can cause adverse effects on the reproductive system. It may include alterations to the reproductive organs and/or the endocrine system. Chemicals which affect the reproductive capabilities including chromosomal damage (mutations) and effects on foetuses (teratogenesis)."

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Inherent properties – details on toxicity measures/concentrations

Hazard identification



Inherent properties

The toxicity of a compound is expressed through different concentration levels

Effect concentration EC50	<input type="checkbox"/>
Lethal concentration LC50	<input type="checkbox"/>
Lowest Observed Effect Concentration LOEC	<input type="checkbox"/>
No observed effect concentration NOEC	<input type="checkbox"/>
Predicted Environmental Concentration PEC	<input type="checkbox"/>
Predicted No Effect Concentration PNEC	<input type="checkbox"/>

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Effects on humans and animals – details on EC50 and LC50

Hazard identification



Inherent properties

Effect Concentration EC50, the concentration that causes negative effects on 50% of the tested population (percentage that is desired to be shown)

Lethal Concentration LC50 the concentration needed to kill 50% of a group of experimental organisms in a given time. A standard measure of toxicity.

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Effects on humans and animals – details on LOEC and NOEC

Hazard identification



Inherent properties

Lowest Observed Effect Concentration LOEC is the lowest concentration, found by observation or experiment, which causes an effect.

No observed effect concentration NOEC is the highest concentration, found by observation or experiment, which causes no detectable adverse effect.

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Effects on humans and animals – details on PEC and PNEC

Hazard identification



Inherent properties

Predicted Environmental Concentration PEC, the concentration of a substance that is expected in the environment according to a defined scenario.

Predicted No Effect Concentration PNEC, the concentration of a substance that is not expected to have an effect on the ecosystem's organisms.

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Ranking and Identification of Chemical Hazards - RICH

Hazard identification



Inherent properties

RICH is a system of rules called "filters" with the purpose of identifying those substances on the long list of potentially present stormwater pollutants that could pose a hazard

The sequence of filters is referred to as funnels. The funnel applied is dependent on the selected scenario

[View drawing of filter system](#)

[More information about RICH](#)

[View example made by E&R DTU](#)

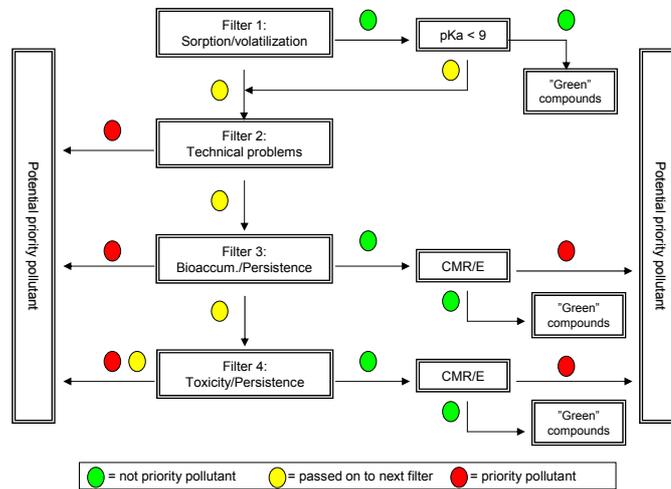
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RICH filtration in a decision tree

View specific information about RICH



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Example of “filtering” prepared by DTU

Compound/CAS no.	Step	Filter no. 1	Filter no. 2	Filter no. 3	Filter no. 4	Filter no.
		1	2	3	4	3a, 4a
Compound	Step	1	2	3	4	3a, 4a
Nonylphenol (NPE)	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
25154-52-3/104-40-5	SEDIMENT	23	n	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			
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					
Compound	Step	1	2	3	4	3a, 4a
Pentachlorophenol	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	22	n	33		
87-86-5	SEDIMENT	22	n	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		
Compound	Step	1	2	3	4	3a, 4a
PCB 28	Evaluation	Volat/sorp	Tech	Bioac/degr	Tox/degr	CMR/E
CAS no.	WATER	23				
7012-37-5	SEDIMENT	23	n	33		
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				

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Hazard assessment

Hazard assessment
CHIAT step 4



Measured data
Toxicity

After the hazard identification a hazard assessment is carried out

The hazard assessment generally deals with comparisons of predicted environmental concentrations (PEC) or measured environmental (EC) and predicted no effect concentrations (PNEC):

Details?

For assessment of hazards and problem related to inorganic substances, geochemical modelling can be applied e.g. PHREEQC

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Hazard assessment

Hazard assessment
CHIAT step 4



Measured data
Toxicity

To establish PEC the following approaches can be used:
Measured concentrations
Modelling data, e.g. using SEWSYS/STORM

PNEC are based on toxicity data collected in the hazard identification and calculated using safety factors defined by the EU Technical Guidance Document on Risk Assessment of Chemicals. The safety factors typically range from 10-1000 depending on the amount and relevance of the toxicity data.

Hazard assessment is one of the angles of approach to the risk characterisation but this is beyond the scope of CHIAT

Risk characterisation

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Expert judgement

Expert judgement



Grouping

Addition

Legislation

Lists of priority
pollutants

The following questions should be asked in the expert group

1. What was the aim and who should be protected?
2. Can any compound be excluded from the list with priority pollutants due to:
 - Legislation (banned compounds) or other agreements on phase-out.
 - Some compounds have similar properties and one compound can be chosen as representative for a group of compounds
3. Should any compound be added to the list with priority pollutants (which is the output from step 4) due to
 - Relevant legislation
 - The compound is on other relevant lists with priority pollutants. OSPAR list etc.
 - Stakeholder focus or site specific compounds

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RICH - an external tool

Hazard identification



Inherent properties

The current version of RICH allow you to search for a hazard profile for all Daywater potential priority pollutants and to create the hazard profile for your own organic compounds if you have the relevant inherent data.

The quality of the outcome from RICH depend on the quality and amount of data you feed into it.

[Profile?](#)

[Outcome](#)

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RICH - Profile

Hazard identification



Inherent properties

Compounds filtrated though RICH will receive a profile indicating which classification they have yielded in each filter

Volat/ Sorp Tech Bioac/ degr Tox/ degr CMRE

Water phase	Yellow	Yellow	Yellow	Red
Solid phase	Yellow	Yellow	Green	

Green = not a priority pollutant Yellow = passed on to next filter Red = priority pollutant



View example made by E&R DTU

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RICH - Outcome

Hazard identification

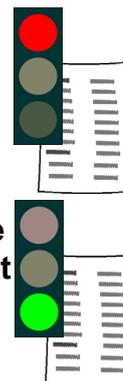
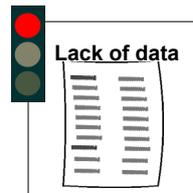


Inherent properties

List of Potential Stormwater Priority Pollutants (PSPP) to be included in hazard assessment of stormwater

Justified lists of compounds to be disregarded in hazard assessment of stormwater

Important! "A priori problematic" chemicals can be added directly to the "red list"



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RICH – How are the filters constructed?

Hazard identification



Inherent properties

Volatility/sorption – separates compounds into different phases; aqueous, solid or air.

Volat/
Sorp

Technical – are there any known technical problems such as odour, corrosion, foaming etc.?

Tech

Bioaccumulation/persistence – tests if the compounds bioaccumulates and persistence to degradation.

Bioac/
degr

Acute toxicity/persistence – tests if the compounds are acute toxic and persistence to degradation.

Tox/
degr

CMRE – tests for long-term chronic toxicity; cancer, mutagenicity, reproduction hazards, endocrine disrupting effects and allergic reactions.

CMRE

Chemical properties

Cut-off values in RICH

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RICH – Phase distribution

Hazard identification



Inherent properties

Water phase – compounds listed in this group will primarily exist in the aqueous phase.

Solid phase – compounds listed in this group will primarily exist in the solid phase i.e. sediment, suspended material and soil.

Chemical properties

Cut-off values in RICH

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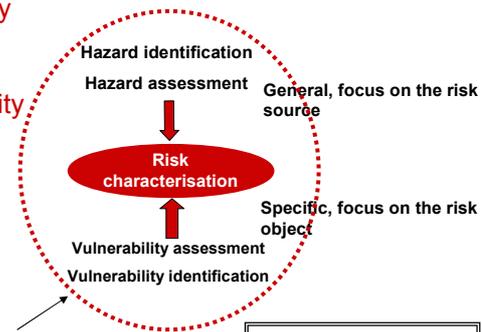
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Risk characterisation

For a full risk characterisation focuses on both the risk source and the object exposed to the risk (the vulnerability) and this is more information than included in CHIAT methodology.

Hazard information is scenario un-specific whereas vulnerability information is scenario specific. The biotest-study performed in Daywater focuses on vulnerability for aquatic organisms to stormwater discharges incl. snowmelt in Europe



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For a defined scenario

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