RESEARCH ARTICLE

A source classification framework supporting pollutant source mapping, pollutant release prediction, transport and load forecasting, and source control planning for urban environments

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Abstract

Purpose Implementation of current European environmental legislation such as the Water Framework Directive requires access to comprehensive, well-structured pollutant source and release inventories. The aim of this work was to develop a Source Classification Framework (SCF) ideally suited for this purpose.

Methods Existing source classification systems were examined by a multidisciplinary research team, and an optimised SCF was developed. The performance and usability of the SCF were tested using a selection of 25 chemicals listed as priority pollutants in Europe.

Results The SCF is structured in the form of a relational database and incorporates both qualitative and quantitative source classification and release data. The system supports a wide range of pollution monitoring and management applications. The SCF functioned well in the performance test, which also revealed important gaps in priority pollutant release data.

Conclusions The SCF provides a well-structured approach for European pollutant source and release classification and management. With further optimisation and demonstration testing, the SCF has the potential to be fully implemented throughout Europe.

Keywords Priority substances · Source classification · Stormwater · Urban pollution · Wastewater · Water Framework Directive

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1 Background, aim and scope

Currently, more than half of the world's human population live in urban environments, and further urbanisation is inevitable (UNPF 2009). Numerous challenges are associated with this global trend which leads not only to the physical growth of urban areas but also to rising population density. For instance, increasing urbanisation brings increased demand for public and private transport, and the need for new roads, railways and footpaths. New buildings are required for commercial enterprises, housing and industry. Old buildings may need redeveloping or refurbishment, and pressures on key infrastructure such as

drinking water and wastewater transport networks and energy distribution schemes are intensified. Within the urban area, the use of items such as electronic equipment, personal care products and domestic and industrial chemicals is highly concentrated. Together, this concentrated use and release of goods and substances generate numerous (potential) pollution sources from a very broad range of activities and commodities. The chemical pollutants released from these sources may include a wide range of different substances, including those classed as priority pollutants, and including both inorganic and organic substances (Birch et al. 2011). These pollutants can potentially induce a wide range of negative effects on the natural environment, including both acute and chronic toxicity effects to terrestrial and aquatic organisms (Fatta-Kassinos et al. 2011). Ingestion of pollutants through the consumption of contaminated drinking water or seafood can also lead to human health effects. For instance, a number of common urban pollutants (e.g. benzene, cadmium, polycyclic aromatic hydrocarbons (PAHs)) are classed as group 1 carcinogens (WHO 2011). To mitigate the risks associated with environmental pollution, organised approaches to sustainable environmental management are required.

During the past decade, the European parliament has introduced several new legislative tools designed to focus and improve environmental management within the European Union (EU). These tools also have implications for the management and mitigation of urban pollution. For example, the year 2000 saw the introduction of the EU Water Framework Directive (WFD) (EU 2000) which focuses on obtaining good ecological and chemical status of surface waters, whilst in 2003, the Restriction of Hazardous Substances (RoHS) Directive (EU 2003a) and the Waste Electrical and Electronic Equipment (WEEE) Directive (EU 2003b) were adopted. The latter Directives focus on the use of hazardous substances such as metals and polybrominated diphenyl ethers in electrical and electronic equipment as well as the handling of such items for waste disposal and recycling. In 2008, the Marine Strategy Framework Directive (MSFD) (EU 2008b) was introduced, focusing on achieving and maintaining good environmental status of the European marine environment. The year 2008 also saw the adoption of the Environmental Quality Standards Directive (EQSD) (EU 2008a). Closely connected with the objectives of the WFD, the EQSD contains a list of priority substances (PSs) and priority hazardous substances (PHSs) selected for their persistence, and bioaccumulative and toxic properties. In this article, PSs and PHSs are collectively named priority pollutants (PPs), which is a term interchangeably used with substance and chemical. All of the abovementioned directives are available for download via http://eur-lex.europa.eu.

In order to implement and achieve the objectives of the WFD, the MSFD and the EQSD, each EU Member State must not only establish the current state of the environment with respect to the key pollutants identified in said Directives, they must also establish inventories of PP emissions, discharges and losses to demonstrate compliance with the Directives and establish monitoring programmes to track the desired improvements in environmental quality (EU 2000; EU 2008a). Typically, the implementation process involves the passing of national legislation by each individual Member State with the national legislation then being implemented on a more local scale, such as a regional or municipal level. For instance, the WFD requires the development of individual River Basin Management Plans for all natural water bodies, including a programme of action to improve water quality. Pathways to improvement may be manifold, and identifying the most suitable approach or combination of approaches requires a solid understanding of the current and local environmental situation, including the relevant sources of pollution in the target area. One of the earliest steps necessary for successful implementation of the WFD is thus the establishment of a comprehensive inventory of pollution sources for all PSs within specific management zones (e.g. urban areas, river basins, etc.). Depending on the sophistication of the source inventory and the quality of the data populating it, it can be used for many applications. For example, it may be possible to predict releases of a particular pollutant from all relevant sources, thereby allowing the relative contribution of different sources to the overall pollutant load to be determined. With this knowledge in hand, the effective targeting of pollution reduction schemes and emission control strategies becomes increasingly feasible. For example, if a single industrial facility is identified as the major source of a particular pollutant in a given river, the introduction or upgrading of on-site industrial wastewater treatment at that facility can be expected to have a major influence on the chemical status of the river system with respect to that pollutant. On the other hand, if the source inventory indicates that industrial releases for that pollutant are actually very low compared with releases from urban road surfaces, it suggests that attention would be better focussed on the implementation of structural or nonstructural stormwater best management practices (BMPs) rather than upgrading of industrial wastewater treatment. Similarly, if the inventory reveals that the major source of a pollutant is from a commercial product such as a shampoo or cleaning agent, action may be preferentially focussed on encouraging the substitution of that chemical in key products, or on designing public education campaigns to encourage informed consumer choices and correct product disposal, or even (if deemed feasible) on the introduction of new legislation to ban or limit the use of that substance in the identified products.

It is clear from the examples given above that a well-designed, standardised European source classification sys-

tem is needed to support the implementation of major EU environmental legislation such as the WFD. The classification scheme should be capable of uniquely identifying pollution sources and should incorporate spatial and temporal information related to those sources, as well as quantitative data allowing the estimation of pollutant loads. A Source Classification Framework (SCF) fulfilling this need was developed in the EU-funded ScorePP (Source Control Options for Reducing Emissions of Priority Pollutants) project (see www.scorepp.eu and (Mikkelsen et al. 2008)). The SCF was developed with the aim of obtaining a system that would be both applicable to the whole EU and be dynamic in its setup, so that up to date information could be readily added and extracted. With such an ambitious aim, the use of spreadsheets or text documents was not a suitable option; thus, the SCF was developed in the form of a multifaceted relational database capable of absorbing large quantities of data in a well-organised and user-friendly manner. In order to test and demonstrate the application of the proposed SCF, the system was populated with data for a wide range of pollutants relevant to the WFD, MSFD, RoHS and WEEE directives. This paper presents an overview of the SCF and demonstrates how it can be applied throughout Europe to facilitate highly informed management of environmental pollution issues and associated challenges such as those posed by the aforementioned EU Directives.

2 Materials and methods

2.1 SCF development

The SCF was developed within the ScorePP project over a 2-year period. The multidisciplinary research team comprised academic researchers from both environmental sciences and information technology as well as industry representatives and municipal environmental authorities. The aim was to deliver a system suitable for diverse applications in the field of pollution management. Typical end-uses the team wished to support included pollutant source mapping and visualisation, pollutant release prediction, pollutant transport and load forecasts, source control planning and evaluating emission control strategies. To achieve these goals, it was evident that the SCF would need to accommodate a wide variety of qualitative discrete and quantitative information. One of the first challenges was to reach a consensus about the key components to include in the SCF to ensure that it would be sufficiently comprehensive to accommodate the mentioned needs and could easily draw on existing European data sources. Initially, a number of existing classification systems currently in use across Europe were assessed and compared for their relative strengths and weaknesses.

Table 1 summarises key classification systems that were considered during the development of the proposed SCF and shows what the classification systems cover and whether or not they are harmonised within the EU. Suitable classification schemes were then selected for total or partial inclusion in the SCF. Classification aspects which were deemed necessary but were not available or sufficiently comprehensive in existing schemes were then purposely designed to complete the SCF.

2.2 Overview of the SCF

The SCF developed through this work can comprehensively characterise and describe urban pollution sources. It is structured in the form of a relational database (Cerk et al. submitted) which, compared with the more traditional use of spreadsheets and text documents, has several advantages.

Table 1 Overview of various classification codes studied for potential inclusion in the Source Classification Framework

Code	Chemical ID	Activity	Process	Urban structure	Release dynamics	Receiving compartment	Ratio between compartments	Release factors	EU harmonised
CAS #	X								
EINECS	X								X
NACE		X							X
NOSE			X						X
USD				X					
RPD					X	X	X		
TGD		X	X			X	X	X	

The codes printed in bold make up the developed source classification framework

CAS # chemical abstracts service registry number (ACS 2008), *EINECS* European Inventory of Existing Commercial Chemical Substances (ECB 2008a), *NACE* statistical classification of economic activities in the European community (Eurostat 2008), *NOSE* standard nomenclature for sources of emissions (Eurostat 1998), *USD* urban structure descriptor developed in the ScorePP project (Vezzaro et al. 2009), *RPD* release profile descriptor developed in the ScorePP project (De Keyser et al. 2010a); *TGD* the technical guidance document on risk assessment (ECB 2003)

Firstly, it supports a standardised approach to data storage and analysis, ensuring that source and release data for different chemicals are consistently stored in the same way (Banovec et al. 2009). It also facilitates a rapid, well-organised retrieval of data via predefined database queries and output formats. The SCF approach has been designed to rely heavily on structured classification codes to minimise the possibility for subjective variation in data entry by different users. Also, as the system was designed with reference to key classification codes used throughout Europe, relevant information from large-scale data sources such as statistical bureaus (e.g. Eurostat) and national inventories as well as the European Pollutant Emission Register can easily be integrated.

During the process of conceptualising the SCF, inspiration was drawn from the United States Environmental Protection Agency Source Classification Code (US EPA SCC) (US EPA 2007). The US EPA SCC uses a multi-level classification system to denote the specific activity associated with the source (e.g. solid waste disposal at an industrial landfill site) and the specific process leading to the release of the pollutant chemical (e.g. flaring of waste gas). However, the system cannot be directly transferred to Europe as it relies on US-specific classifications for activities and emission processes that are not compatible with key European classification codes. By contrast, the SCF described here uses a similar approach for source activity and process identification as the SCC but is based directly on EU classification schemes. The SCF adopts the substance as its focal point. Other qualitative and quantitative descriptors describing the source activity and release process, environmental receiving compartment, temporal release pattern and release rate are also included as

explained below. Table 2 lists the different attributes of the SCF, whilst Fig. 1 provides a conceptual illustration of how the system works.

2.3 The qualitative components of the SCF

The proposed SCF is organised in the form of 'Release Strings' (RSs), which combine a chemical identifier with two existing classification codes and one purposely designed classification code to provide a unique identifier for each pollution source. For any given source, the RS comprises:

1. a Chemical Abstracts Service registry number (CAS#) (ACS 2008) that uniquely identifies the pollutant being released,
2. a numerical code from the Statistical Classification of Economic Activities in the European Community (NACE) (Eurostat 2008) that identifies the specific (economic) activity responsible for the release,
3. a numerical code from the EU harmonised Nomenclature for Sources of Emissions (NOSE-P) (Eurostat 1998) that specifies the process resulting in the release, and
4. a numerical code from the Urban Structure Descriptor (USD) (Vezzaro et al. 2009) identifying to which part of the technosphere the pollutant release takes place.

The CAS# was chosen as the chemical identifier in preference to other identification numbers (e.g. the European Inventory of Existing Commercial Chemical Substances number) as the CAS# is highly comprehensive and widely used in databases, dictionaries and other inventories employing chemical identification numbers. The NACE code comprises 18 main classes and approximately 850 subclasses, whilst the NOSE-P code comprises 14 main classes and about

Table 2 Overview of the different attributes of the source classification framework

Attribute	Description
Chemical	The name of the chemical
CAS#	The Chemical Abstracts Service registry number of the particular chemical
RSS	A textual description, using the researchers' own words, of the particular pollution source
NACE	Detailed classification according to NACE
NOSE-P	Detailed classification according to NOSE-P
USD	Urban structure (e.g. roads, sewers, construction yards) the pollutant is released to
COMP	Environmental compartment (e.g. urban permeable surface etc.) the pollutant is released to
RATIO	Estimated fraction of the pollutant released to the specified compartment (e.g. 70% to air)
RPD	A combination of daily, weekly and yearly release profiles for the specified source
RF	Release factor including units
References	All relevant literature references
Comment	Any comment related to the RS that might be of relevance but does not fit in the other categories

RSS release string sentence, *NACE* statistical classification of economic activities in the European Community, *NOSE*-P nomenclature for sources of emissions, *USD* urban structure descriptor, *COMP* compartment, *RPD* release profile descriptor, *RF* release factor, *RS* release string
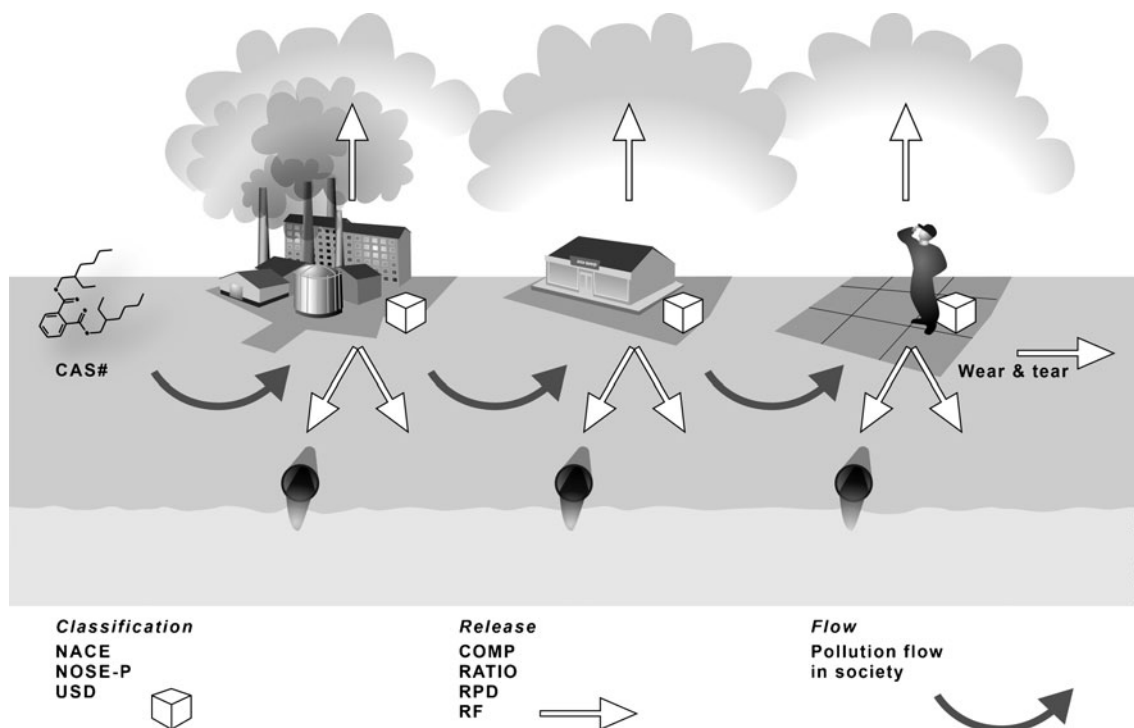
Fig. 1 Illustration of the Source Classification Framework. *Cubes* mean that the activity or commodity must be classified according to the different classification codes used, *straight arrows* mean that release information need to be assigned and *bent arrows* illustrate a flow in the urban environment. *CAS#* chemical abstracts service registry number of the particular chemical, *NACE* statistical classification of economic activities in the European Community, *NOSE-P* standard nomenclature for sources of emissions, *USD* urban structure descriptor developed in the ScorePP project, *COMP* compartment, *RATIO* ratio, *RPD* release profile descriptor, *RF* release factor

750 subclasses. Together, these codes facilitate very precise classification of a wide variety of source activities and processes. Statistical data from Eurostat are also compatible with these systems, as is the European Pollutant Release and Transfer Register (E-PRTR). The E-PRTR is a valuable source of emissions data that also contains geographical coordinates for major point sources such as industrial facilities.

The USD was developed specifically for use in this SCF. It describes 15 types (including an undefined structure named 'other') of urban structures associated with the pollutant release. Examples of urban structures delineated by the USD include 'roads', 'buildings', 'waste disposal', 'facilities' and 'households'. The structure 'facilities' covers for instance industrial production sites, dentists, slaughterhouses, etc. This code can be used to associate pollution sources with spatial data. For example, the USD can be used to link geographical information system (GIS) data to the pollution source database, thereby facilitating source mapping and visualisation. This purposely designed classification code was developed in parallel with the EU directive Infrastructure for Spatial Information in the European Community (INSPIRE) (EU 2007) having a similar aim, though not identical. However, it is likely that the USD in the future may be linked with the INSPIRE classification.

Due to the 'string' design of the SCF, it is also possible for additional qualitative data to be linked to the SCF as required. This may include information on legislation, treatment options for different source types, as shown in the developed ScorePP database including references to economic and legal dimensions of the priority substances, or even substance substitution options for specific activities/processes (Lecloux 2008; Seriki et al. 2008; Atanasova et al. 2009; Banovec et al. 2010). Finally, text information may also be linked to the RS where additional written notes for explanation and clarity are desired.

2.4 The quantitative components of the SCF

In order to *quantify* and *model* pollutant releases, it is necessary to document information about the characteristic release dynamics of each pollutant source. This is achieved by coupling each RS with several quantitative descriptors. These are denoted in the SCF structure as the environmental compartment descriptor (COMP), the environmental compartment release ratio (RATIO), the Release Profile Descriptor (RPD) and the Release Factor (RF). The COMP attribute is applied to specify the pollutant-receiving environment. COMP categories were derived with a view to their potential usefulness for pollutant fate and transport modelling applications and include categories such as air, surface water (direct), surface water (indirect), urban permeable surface, urban impermeable surface and groundwater. The direct and indirect releases to water indicate whether the chemical is being released directly to surface

water or via an on-site treatment plant. As this will affect the load released, it is important information to include when using the SCF to support quantitative applications. The RATIO attribute designates the proportion of the pollutant release load received by the relevant environmental compartments (e.g. 30% to air, 70% to permeable urban surfaces). The RPD assigns a 'release profile' to each RS, thereby documenting the temporal variation in the release on a daily, weekly and yearly basis. For instance, the release profile of a pollutant from a traffic source (e.g. a car) could reflect daily peaks during morning and afternoon rush hours on weekdays, differences between weekday and weekend traffic loads, as well as any seasonal differences such as school holidays. The RPD comprises 24 daily, 10 weekly and 13 yearly release profiles and is explained in detail by De Keyser et al. (2010a). The release profiles are suitable for covering a range of different types of releases, e.g. from the immediate release following application of a pesticide in the garden or a spill on the street to the continuous release from the evaporation of chemicals from building materials. An integrated urban wastewater system model has been designed to incorporate these data from the SCF. The model is described in detail in De Keyser et al. (2010b) and takes into account the various releases within the urban catchment as well as inputs from the surrounding environmental compartments (e.g. long-range atmospherically transported pollutants). This model also estimates the fate of the studied chemical in terms of resulting pollutant concentrations in the receiving environmental compartments.

Table 1 shows that of the existing (EU) classification codes; only the EU Technical Guidance Document on Risk Assessment (TGD) (ECB 2003) addresses the quantitative aspects of source classification. The TGD was thus used as inspiration for the RF approach which has been adopted here. A pollutant RF can be defined in many ways and can have different units. For example, considering a traffic-related source, several types of release can be identified. Most traffic will be in the form of combustion vehicles driven by fuels that release pollutants such as PAHs, benzene and nickel during combustion (Kawashima et al. 2006; Geller et al. 2006). The quantity released is dependent on engine efficiency, which is actually a function of time. For instance, engine efficiency has been noted to increase following start-up as the engine progressively warms, and efficiency also differs if the vehicle is accelerating, driving uphill or maintaining a constant speed on the flat (Wallington et al. 2006). Local climatic conditions and seasonal weather effects may also play a role. Hence, in this example, the RF for a specific pollutant may be reported using the unit 'milligrams chemical per kilometre driven per vehicle' but will be dependent on the circumstances mentioned above. Furthermore, this is only one of the potential RFs for this source. In addition to the

releases due to the vehicle combustion process, there will also be releases of metals such as nickel and cadmium from items such as brake pads (Sörme and Lagerkvist 2002; Månsson and Bergbäck 2007). These releases can be described by the unit 'milligram chemical per braking time/braking distance', but once again, numerous factors will affect the magnitude of pollutant released during braking events, and a range of RFs could be given depending on these additional factors (e.g. the speed of the vehicle at the time of braking). Even relatively continuous releases such as the release of diethylhexylphthalate (DEHP) from the undercoating of vehicles will vary over time, being dependent on climatic conditions and the age and condition of the vehicle (Sandström 2002). As a further example, consider the release of a pollutant from urban surfaces such as 'buildings'. Here, the abrasion of the building will lead to chemical releases. A wall or roof coated with a paint that contains biocide to prevent biofouling (e.g. diuron (Burkhardt et al. 2007)) will continuously release that substance. In dry weather conditions, this will occur through simple partitioning between the wall and the air as the substance is released from the paint. The dynamics of the release will be affected by the physicochemical properties of the wall, the air and the chemical pollutant, and the RF unit could be given as 'milligrams chemical per unit time'. By contrast, the release during wet weather may be better quantified as 'milligrams chemical per millimetre rainfall'. Other variables affecting the RF are likely to include the brand of paint and the time elapsed since its application.

2.5 SCF performance and usability test

A broad range of chemicals with widely differing physico-chemical properties and urban source characteristics were used to test and refine the prototype SCF. The selected test chemicals (also known as priority substances, as used in the EU legislation, chemical substances, micropollutants and microconstituents, involving both heavy metals and organic substances) have all been characterised as priority pollutants throughout Europe and are the focus of current EU legislation such as the WFD, MSFD and EQSD. The test chemicals [CAS#] have a wide range of primary uses and include: heavy metals—cadmium [7440–43–9], lead [7439–92–1], mercury [7439–97–6], nickel [7440–02–0]; intermediates—anthracene [120–12–7], benzene [71–43–2], nonylphenol [25154–52–3]; biocides—atrazine [1912–24–9], chlorpyrifos [2921–88–2], diuron [330–54–1], endosulfan [115–29–7], endrin [72–20–8], hexachlorocyclohexane [608–73–1], tributyltin [688–73–3]; trifluralin [1582–09–8], impurities, by- and combustion products—benzo[a]pyrene (B[a]P) [50–32–8], hexachlorobenzene [118–74–1], hexachlorobutadiene [87–68–3], pentachlorobenzene [608–93–5]; sol-

vents—methylene chloride [75–09–2], trichloroethylene [79–01–6]; flame retardants—C$_{10–13}$ short-chain chloroparaffins [85535–84–8], pentabromobiphenylether [32534–81–9]; a plasticiser—DEHP [117–81–7]; and an anti-knocking agent—tetraethyl lead [78–00–2].

Information about all aspects of these chemicals and their urban sources was obtained from a combination of on-line databases, industry and government sources, and peer-reviewed journal articles. Databases consulted for this task include the Household Products Database (US NLM 2011), Hazardous Substances Data Bank (US NLM 2010), European Pollutant Emission Register (EEA 2008), Kirk-Othmar database (Wiley 2008), The Merck Index (O'Neil et al. 2006), Online European Risk Assessment Tracking System (ECB 2008b) and electronic compilations such as the e-Pesticide Manual (Tomlin 2005) and Umweltchemikalien (Rippen 2005). The approach taken was to use the literature to comprehensively identify potential sources for each of the target chemicals (Holten Lützhøft et al. 2008a) before assigning temporal release profiles (Gevaert et al. 2008) and quantitative release factors (Holten Lützhøft et al. 2008b).

3 Results and discussion

In the following paragraphs, the main results from testing the developed SCF will be presented and discussed. The actual SCF development has been presented and addressed in the Section 2. More detailed results like the pollution resulting from transport or formulating and assessing emission control strategies for a single substance have been

obtained and are or will be published elsewhere (Holten Lützhøft et al. 2009; Eriksson et al. 2010).

3.1 SCF performance and usability test

The SCF was tested and refined by populating the database with source and release data for a broad range of environmental pollutants. A wide variety of urban sources were identified for the selected test substances, but considering that these substances are all identified as EU priority pollutants, quantitative RFs were surprisingly difficult to acquire. In view of the scarcity of measured RFs, data pertaining to estimated releases or other indicative releases (e.g. in the form of loads, chemical content of commodities, pesticide dosing regimes, etc.) were also compiled.

Figures 2 and 3 show results extracted from the test database. Figure 2 shows that although the number of RSs identified for the different chemicals varied, potential urban pollution sources were identified for all test substances. Looking at the pollutant RSs on the basis of major use groupings (i.e. heavy metals, intermediates, biocides, impurities, by- and combustion products, solvents and miscellaneous), it is clear that some groupings tend to have a greater number of RSs than others. For example, relatively few RSs were established for the majority of biocides (5–10, except tributyltin with 93 RSs) and impurities, by- and combustion products (5–13, except benzo[a]pyrene with 72 RSs), whereas between 44 and 133, RSs were identified for the various heavy metals. This is not surprising given the extremely wide range of uses that metals are put to for industrial purposes, building and

Fig. 2 Number of release strings (RSs) with and without quantitative release information for each chemical. ■: Number of RSs with *release factors*; ▓: Number of RSs with *loads* meaning a measured quantity per unit (e.g. person or city) in e.g. waste water; ▒: Number of RSs with *miscellaneous* data meaning for instance a pesticide dosing regime or a product content and □: Number of RSs with no data. Chemicals are presented in groups: heavy metals, intermediates, biocides, impurity, by- and combustion products, solvents and the group of miscellaneous functional chemicals. Within each group, chemicals are ranked according to how many pollution sources were identified
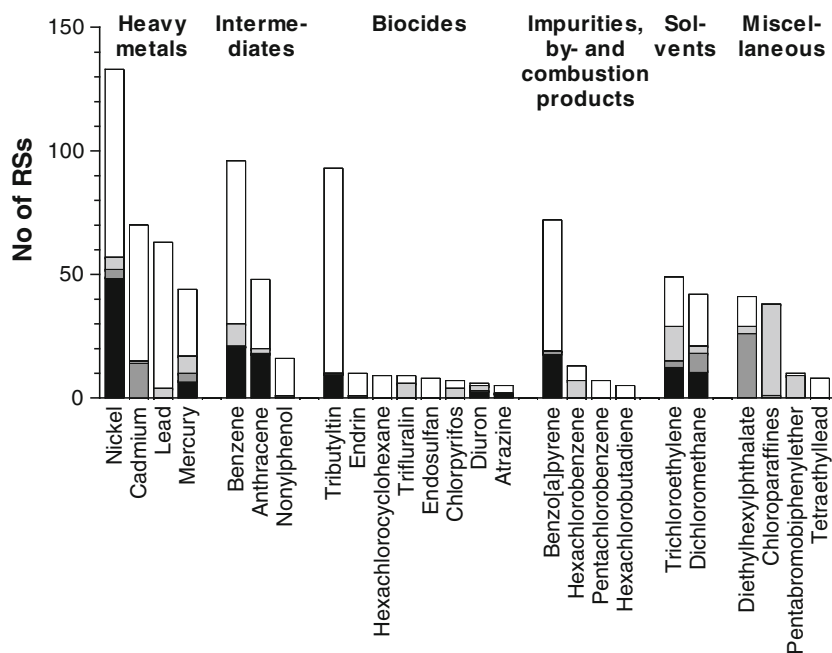
Fig. 3 Number of release strings (RSs) with and without quantitative release information classified according to urban structure. ■: Number of RSs with *release factors*; ▨: Number of RSs with *loads* meaning a measured quantity per unit (e.g. person or city) in e.g. waste water; ▨: Number of RSs with *miscellaneous* data meaning for instance a pesticide dosing regime or a product content and □: Number of RSs with no data. Urban structures are grouped with respect to categories representing a production activity in society (industries), belonging to people and buildings including households (people & households), structures on the edge of the urban environment (extra urban) and transport. Please note the broken *y*-axis!
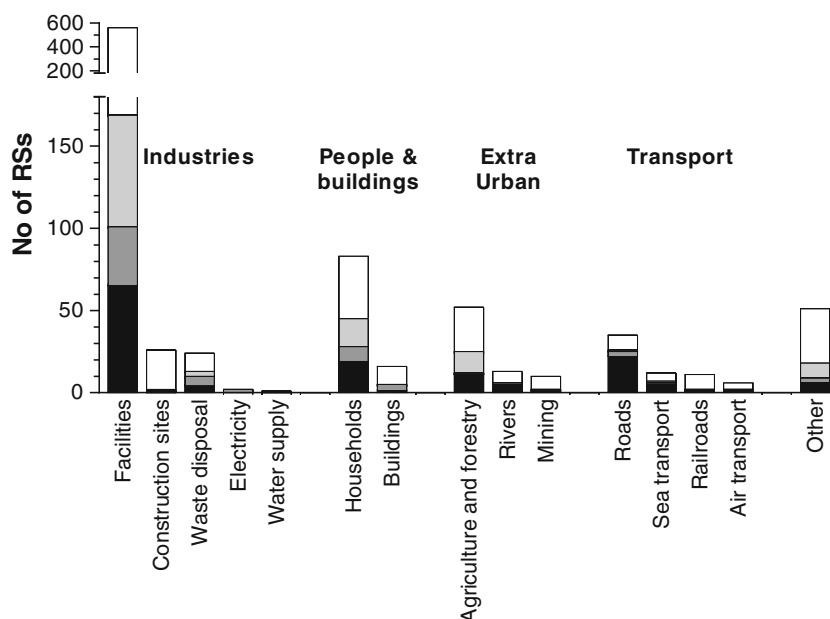
construction, manufacturing and so on. By contrast, biocides are often designed or chosen for their specific mode of action, and therefore may have relatively few but very specific applications. This is reflected by a low number of RSs. Figure 3 shows the total number of RSs associated with the different urban structures. Overall, it can be seen that RSs are associated with all 15 urban structures included in the USD. The figure also indicates that a large majority of the RSs are associated with industrial 'facilities', 'households', 'agriculture and forestry' and 'roads'. As this could be taken to indicate the importance of these categories in terms of managing environmental pollution, it must be recalled that the number of RSs does not necessarily indicate the most important pollutant source category. For example, some facilities may have source control measures in place to limit releases or to prevent emissions via treatment, in which case these facilities may in fact be relatively small sources in a quantitative sense. Moreover, the facilities being well identified as point sources and having been intensively scrutinised by the regulators, it is much easier to discriminate between many different types of releases. On the other hand, a continuous small release from an RS associated with households could equate to a major point source when viewed on a quantitative basis.

To illustrate further the potentials of the SCF, the plasticiser DEHP was chosen as an example. Data on urban releases of DEHP have been compiled for the city of Stockholm (Sandström 2002). As data on release factors for nonindustrial sources in the open literature were scarce, the load data from Sandström (2002) were recalculated to give updated release data in the form of estimated releases per

person from different activities and commodities. Table 3 shows that seven RSs have been identified for the 'households' and 'roads' USDs. The RF column shows that 'indoor electrical cables' contribute with 0,046 g DEHP per person per year, whereas 'floor and wall covering' contribute with 10 g DEHP per person per year. As seen from the COMP column, DEHP is released to both air, water and urban surfaces, and according to the RATIO column, the estimated ratios between the compartments vary from 100% release to air for 'indoor electrical cables' to a split between 5% to air and 95% indirectly to surface water for 'coated textiles'. Also, the dynamics in the releases have been described by the RPD, where for instance the releases from 'indoor electrical cables' are continuous throughout the year due to a passive release, and the releases from 'tubes and profiles used for construction' are also continuous but with higher releases during rainy periods. As indicated in Table 3, such knowledge allows the suggestion of different potential source control options. For instance, in the case of 'clothing and footwear', the release of DEHP from washing clothes and wear and tear of shoes are estimated to be equal between urban surfaces and water. To reduce the emissions to surface waters, it is therefore suggested to improve municipal wastewater treatment or to establish a suitable stormwater BMP or even to ban some of the concerned commodities.

The SCF works well from a standardised classification perspective and is able to store and manage large amounts of data. General data such as larger categorisations, groupings and trends are easily retrieved. The system also supports a wide range of applications by facilitating flexible

Table 3 Release strings for DEHP from the 'households' and 'roads' urban structure descriptor, including release factors (RFs), receiving compartment (COMP), in what ratio (RATIO) the release distributes between COMPs, the daily, weekly and yearly dynamics of the release as well as suggested potential source control option

Description	RF, g/year/person	COMP	RATIO, %	RPD[a]	Potential source control option
Undercoating of motor vehicles	0,26	U	25	1,1,1	Stormwater BMP,
		W	75		chemical substitution in the undercoating
Indoor electrical cables	0,046	A	100	1,1,1	
Floor and wall covering	10	A	50	1,5,1	Municipal WWTP
		WI	50		
Other building installation, coated metal sheets	1,2	U	50	1,1,5	Stormwater BMP,
		W	50		municipal WWTP
Tubes and profiles used for construction	0,075	U	50	1,1,5	Stormwater BMP,
		W	50		municipal WWTP
Coated textiles	1,1	A	5	1,5,1	Municipal WWTP
		WI	95		
Clothing and footwear	0,19	U	50	1,5,1	Stormwater BMP,
		W	50		municipal WWTP

Data originates from Stockholm (recalculated from Sandström (2002)) and could thus be representative for a city with similar way of life, building habits and uses of DEHP

RF release factor, *COMP* compartment, *RPD* release profile descriptor, *BMP* best management practice, *WWTP* wastewater treatment plant

[a] The three numbers represent different temporal daily, weekly and yearly, respectively, variations of the release; *1* continuous, *5* a low continuous release with certain periods of increased release

data extraction routines and queries. For example, an overview of potential pollutant sources for a specific chemical can quickly be extracted, as can a summary of the different chemicals emitted by a single source category or group of sources. In addition, as classification elements linking pollutant sources to economic activities (e.g. type of industry), national employment statistics, and trade data have also been included (e.g. the NACE code), the potential socioeconomic impacts of possible pollutant control measures may be investigated.

As the SCF is designed to be a comprehensive system that identifies all potential sources, users must select the relevant sources for their particular management area (e.g. city or river basin) before extracting the relevant data. This may be done by linking to a local GIS system or by manually selecting the relevant RSs for the pollutant of interest. The SCF can then be used to support pollution management planning, for example, by indicating where best to focus available resources. For example, a large number of RSs with no RFs for a given category, such as 'construction sites' or 'households', would indicate the need for further quantitative release data for these sources. This may help prioritise the use of limited funds for emission monitoring. Alternatively, a well-managed system with relatively comprehensive and reliable quantitative data would rapidly reveal the main pollutant sources and priorities for additional source control measures. Unfortunately, the test exercise revealed significant data gaps in the quantitative priority pollutant release data that are presently available. Further efforts are required to fill this data gap. Considering that the selected test chemicals were all priority pollutants and relatively well studied, it is easy to imagine how difficult it will be to find data for the majority of chemicals not listed in this category and hence subject to less intensive investigation.

3.2 Drawbacks and benefits

From the work with the SCF, we have discovered some drawbacks and benefits. The SCF is populated with literature data, and as time progresses, these data need to be updated. The SCF is organised in the RSs, which in most cases can be directly translated into a pollution source (activity or commodity). In some cases, several RSs may in fact represent one activity or commodity. In this way, it may look like a given substance has many pollution sources, where a range of the RSs actually cover a single activity. This is for instance the case with benzene releases from the combustion of fuel in vehicles, where there are RSs for both gasoline and diesel as well as for cars equipped with or without a catalytic converter. As different researchers have the opportunity to feed the SCF with data, there are chances for slight differences in the various classifications. However, as the SCF is based on standardised entries, such variations have been minimised compared with similar work where information is stored either as text or spreadsheet documents. The benefit is at the same time that the information that is retrieved for each substance is of the same type, due to the

standardised entries. This makes further work with establishing emission loads easier and more comparable from substance to substance. For the purpose of formulating emission control strategies, the work is also made more feasible as the SCF for instance may reveal all the potential pollution sources for a given substance or it may reveal all potential pollutants within a given urban structure. In this way, a much better overview is given enabling a better prioritisation to find the most appropriate mitigation options to minimise the releases of pollutants.

3.3 Recommendations and perspectives

Good quality pollutant source and release data are needed for the implementation of EU Directives such as the WFD, and the SCF described in this paper is an ideal tool for organising this information. Nevertheless, the SCF is still in the demonstration phase, and the conducted performance and usability test highlighted some potential areas for further research and development. For example, it is structurally possible for pollutant source control information to also be included in this framework. Initial work has been undertaken in this direction with promising results, but further development work is needed (Vezzaro et al. 2009). If the SCF incorporated this type of information, sources could be linked explicitly with source control/treatment options.

Another potential improvement to the SCF would be the addition of more detailed household source categories. At present, all of the relevant classification systems (e.g. NACE, NOSE-P etc.) class household sources as a single group, without distinguishing specific household activities, commodities and pollutant release processes. In fact, these can differ considerably, and separating them into more specific categories would facilitate better source control planning. For example, biocide application in the garden would not only have a different USD to the release of a biocide from bathroom tile caulking, it would also have a very different RPD. For these types of applications, it would be interesting to analyse the various pieces of information that will be collected in the REACH dossier about the different uses of registered chemicals (EU 2006). Another example is the use of pharmaceuticals and personal care products, some of which are ingested and partly biotransformed before release to the sewer system, whilst others are released directly down the drain, e.g. shampoos, etc. in the bathroom. And further, functional chemicals, e.g. stabilisers in plastic materials, will evaporate slowly to the air from indoor installations, whereas from outdoor installations they will evaporate slowly to the air during dry weather conditions, but upon rain will be released into the stormwater and transferred to urban permeable or impermeable surfaces.

Natural sources such as forest fires and volcanic eruptions could also be more effectively classified than they are at present. For instance, there is no NACE code to cover these sources as they are not linked to economic activities. Nevertheless, they can have a significant effect on local pollution levels that should be accounted for, and classing them as 'Other', as is presently the case, is less than ideal. RFs relating to the use of commodities during their different life cycle stages were also found to be lacking, and this was identified as an area requiring further attention.

There is potential for the SCF to be used for a wide range of applications associated with pollution monitoring and management. For example, data stored in this manner could be used to explore the spatial agreement between pollution sources and predicted chemical releases and epidemiological statistics for an area. An initial attempt to compare water quality of urban stormwater runoff with predictions using the SCF has shown a broad qualitative similarity in terms of which pollutants are found within the two respective approaches (Holten Lützhøft et al. 2011). Indeed, with European companies already reporting their activities and pollutant emissions to Eurostat using the NACE and NOSE-P codes, the possibility exists for the retrieval and analysis of large amounts of harmonised data. Finally, although we were focussing on the classification of urban pollution sources for the purposes of the ScorePP project, the SCF is also potentially applicable to more rural environments. The extent of applicability would need to be tested further if transfer of the SCF is envisaged; however, the use of NACE and NOSE-P codes ensures a broad degree of relevance due to the inclusion of codes relevant to agricultural practices, forestry and other key categories.

4 Conclusions

The SCF described in this paper provides an EU-specific, well-structured approach for source and release classification and data management. The system facilitates a wide variety of environmental management planning approaches and worked well in the test case using 25 EU priority pollutants. The test case however revealed significant data gaps regarding priority pollutant releases from urban activities and commodities, as indicated by the difficulties in obtaining quantitative release factors, in particular for diffuse sources. These data gaps need to be addressed to support the implementation of current EU environmental legislation, e.g. the WFD, but when detailed data are missing, the proposed SCF will allow possible grouping of RSs to get a more global view that could however bring interesting information to the environmental management. With further optimisation, testing and demonstration, the SCF has the potential to be implemented EU-wide.

References

ACS (2008) Chemical Abstracts Service registry number. The American Chemical Society, Columbus

Atanasova N, Škerjanec M, Banovec P, Cerk M, Kompare B, Lecloux A, Eriksson E, Jamtrot A (2009) Identification of legislative and regulative measures to reduce release of priority pollutants. Deliverable report 4.3, 1–69, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark.

Banovec P, Cerk M, Atanasova N, Kompare B, Holten Lützhøft H-C, Donner E, Bessat M-C (2009) Data requirement analysis and definition of common data structures. Deliverable report 9.3, 1–40, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark.

Banovec P, Cerk M, Atanasova N, Viavattene C, Revitt M, Scholes L (2010) Economic assessment of emission control options and strategies. Deliverable report 8.5, 1–139, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark.

Birch H, Mikkelsen PS, Jensen JK, Holten Lützhøft H-C (2011) Micropollutants in stormwater runoff and combined sewer overflow in the Copenhagen area, Denmark. Wat Sci Technol 64:485–493

Burkhardt M, Kupper T, Hean S, Haag R, Schmid P, Kohler M, Boller M (2007) Biocides used in building materials and their leaching behavior to sewer systems. Wat Sci Technol 56:63–67

Cerk M, Holten Lützhøft H-C, Banovec P (2011) Classification of priority substance sources for the purpose of DSS (submitted)

De Keyser W, Gevaert V, Verdonck F, De Baets B, Benedetti L (2010a) An emission time series generator for pollutant release modelling in urban areas. Environ Model Softw 25:554–561

De Keyser W, Gevaert V, Verdonck F, Nopens I, De Baets B, Vanrolleghem PA, Mikkelsen PS, Benedetti L (2010b) Combining multimedia models with integrated urban water system models for micropollutants. Wat Sci Technol 62:1614–1622

ECB (2003) Technical guidance document on risk assessment, part II, chapter 3. Institute for Health and Consumer Protection European Chemicals Bureau, Ispra, pp. 1–328

ECB (2008a) The European inventory of existing commercial chemical substances. Institute for Health and Consumer Protection, European Chemicals Bureau, Ispra, Italy. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=ora. Accessed 29 Apr 2011

ECB (2008b) Online European Risk Assessment Tracking System. Institute for Health and Consumer Protection, European Chemicals Bureau, Ispra, Italy. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=ora. Accessed 29 Apr 2011

EEA (2008) The European Pollutant Emission Register. European Environment Agency, Copenhagen, Denmark. http://www.eea.europa.eu/data-and-maps/data/eper-the-european-pollutant-emission-register-4. Accessed 29 Apr 2011

Eriksson E, Revitt M, Holten Lützhøft H-C, Viavattene C, Scholes L, Mikkelsen PS (2010) Emission control strategies for short-chain chloroparaffins in two semi-hypothetical case cities. 10th Urban Environmental Symposium, Gothenburg, Sweden

EU (2000) Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. Official Journal of the European Communities L327/1: 1–72

EU (2003a) Directive 2002/95/EC of the European Parliament and of the Council of 27 January 2003 on the restriction of the use of certain hazardous substances in electrical and electronic equipment. Official Journal of the European Communities L37/19: 1–5

EU (2003b) Directive 2002/96/EC of the European parliament and of the council of 27 January 2003 on waste electrical and electronic equipment (WEEE). Official Journal of the European Communities L37/24: 1–15

EU (2006) Regulation EC 1907/2006 of the European Parliament and of the Council of 18 December 2008 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH). Official Journal of the European Communities L396/1: 1–846

EU (2007) Directive 2007/2/EC of the European Parliament and of the Council of 14 March 2007 establishing an Infrastructure for Spatial Information in the European Community (INSPIRE). Official Journal of the European Communities L108/1: 1–14

EU (2008a) Directive 2008/105/EC of the European Parliament and of the Council of 16 December 2008 on environmental quality standards in the field of water policy. Official Journal of the European Communities L348/84: 1–14

EU (2008b) Directive 2008/556/EC of the European Parliament and of the Council of 17 June 2008 establishing a framework for community action in the field of marine environmental policy (Marine Strategy Framework Directive). Official Journal of the European Communities L164/19: 1–22

Eurostat (1998) NOSE-P. Nomenclature for sources of emissions Manual. European Commission, Luxembourg, pp 1–66

Eurostat (2008) NACE Rev. 2. Statistical classification of economic activities in the European community. European Commission, Luxembourg. http://epp.eurostat.ec.europa.eu/cache/ITY_OFFPUB/KS-RA-07-015/EN/KS-RA-07-015-EN.PDF. Accessed 29 Apr 2011

Fatta-Kassinos D, Meric S, Nikolaou A (2011) Pharmaceutical residues in environmental waters and wastewater: current state of knowledge and future research. Anal Bioanal Chem 399:251–275

Geller MD, Ntziachristos L, Mamakos A, Samaras Z, Schmitz DA, Froines JR, Sioutas C (2006) Physicochemical and redox characteristics of particulate matter (PM) emitted from gasoline and diesel passenger cars. Atmos Environ 40:6988–7004

Gevaert V, De Keyser W, Benedetti L, Nilsson M-L, Jonsson A, Holten Lützhøft H-C, Donner E, Vanrolleghem PA, De Baets B, Verdonck F (2008) Development of a classification system for dynamic generic release patterns and evaluation of the pollutant's exposure potential. Deliverable report 3.3, 1–30, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark

Holten Lützhøft H-C, Donner E, De Keyser W, Gevaert V, Wickman T, Cerk M, Eriksson E, Banovec P, Lecloux A, Verdonck F, Mikkelsen PS, Ledin A (2008a) Classifying urban sources of priority pollutants: a source classification framework. Deliverable report 3.2, 1–30, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark

Holten Lützhøft H-C, Donner E, Gevaert V, De Keyser W, Wickman T, Cerk M, Eriksson E, Lecloux A, Ledin A (2008b) Quantifying

releases of priority pollutants from urban sources. Deliverable report 3.4, 1–28, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www. scorepp.eu), Technical University of Denmark

Holten Lützhøft H-C, Eriksson E, Donner E, Wickman T, Banovec P, Mikkelsen PS, Ledin A (2009) Quantifying releases of priority pollutants from urban sources. 82nd Annual Water Environment Federation Technical Exhibition and Conference, Orlando, Florida (US)

Holten Lützhøft H-C, Birch H, Eriksson E, Mikkelsen PS (2011) Comparing chemical analysis with literature studies to identify micropollutants in a catchment of Copenhagen (DK). 12th International Conference on Urban Drainage, Porto Alegre, Brazil

Kawashima H, Minami S, Hanai Y, Fushimi A (2006) Volatile organic compound emission factors from roadside measurements. Atmos Environ 40:2301–2312

Lecloux A (2008) List of possible substitutes for each defined use of priority pollutants, in particular for diffuse uses. Deliverable report 4.1, 1–37, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www. scorepp.eu), Technical University of Denmark

Månsson N, Bergbäck B (2007) Lead, cadmium and mercury—flows and stocks in Stockholm. Kalmer University, Sweden, pp 1–38, in Swedish: Bly, kadmium och kvicksilver—Flöden och lager i Stockholms teknosfär

Mikkelsen PS, Holten Lützhøft H-C, Eriksson E, Ledin A, Donner E, Scholes L, Revitt M, Lecloux A, Wickman T, Atanasova N, Kompare B, Banovec P (2008) Source control options for reducing emissions of priority pollutants from urban areas. 11th International Conference on Urban Drainage, Edinburgh, Scotland

O'Neil MJ, Heckelman PE, Koch CB, Roman KJ (2006) The Merck Index: an encyclopedia of chemicals, drugs, and biologicals. CambridgeSoft Corporation, Cambridge

Rippen G (2005) Environmental chemicals (in German: Umweltchemikalien). CD-ROM [11/2005]. Ecomed Sicherheit, Landsberg

Sandström H (2002) DEHP in Stockholm—a substance flow analysis (in Swedish: DEHP i Stockholm—en substansflödesanalys), pp. 1–42. MSc thesis, University of Umeå, Sweden

Seriki K, Gasperi J, Scholes L, Eriksson E, Revitt M, Meinhold J, Atanasova N (2008) Priority pollutants behaviour in end of pipe wastewater treatment plants. Deliverable report 5.4, 1–91, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark

Wiley (2008) Kirk-Othmer encyclopedia of chemical technology. Wiley, New York

Sörme L, Lagerkvist R (2002) Sources of heavy metals in urban wastewater in Stockholm. Sci Tot Environ 298:131–145

Tomlin CDS (2005) The e-Pesticide Manual. CD-ROM[3.2], 13th edn. British Crop Production Council, Hampshire

UNPF (2009). State of world population 2009. United Nations Population Fund. http://www.unfpa.org/swp/2009/. Accessed 29 Apr 2011

Us EPA (2007) United States Environmental Protection Agency Source Classification Code. United States Environmental Protection Agency, Research Triangle Park

US NLM (2010) Household Products Database. US National Library of Medicine, Bethesda, Maryland, US. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB. Accessed 29 Apr 2011

US NLM (2011) Hazardous Substance Data Bank. US National Library of Medicine, Bethesda, Maryland, US. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB. Accessed 29 Apr 2011

Vezzaro L, Cerk M, Viavattene C, Donner E, Scholes L, Ledin A, Mikkelsen PS (2009) Visualization elements, tools and demonstrations. Deliverable report 6.3, 1–56, within the "Source Control Options for Reducing Emissions of Priority Pollutants" project (www.scorepp.eu), Technical University of Denmark

Wallington TJ, Kaiser EW, Farrell JT (2006) Automotive fuels and internal combustion engines: a chemical perspective. Chem Soc Rev 35:335–347

WHO (2011) International Agency for Research on Cancer (IARC) list of group 1 carcinogens: carcinogenic to humans. List accessed via: www.cancer.org. Accessed 06 Sept 2011