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Chemicals in Statistics – Method Development

2009:4

Regional- och miljöstatistik

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Preface

This work has been done within Statistics Sweden (SCB) financed by a temporary grant for material flow statistics from Swedish Ministry of Finance.

Responsible for the work is Tomas Öberg, University of Kalmar, Sweden. Louise Sörme, Statistics Sweden, at the Unit of environmental economy and natural resources, ordered the study, ordered data from Swedish Chemical Agency and gathered data from Statistics Sweden and read and commented on the report. Christian Surtin, Statistics Sweden, Foreign trade statistics has validated data and commented the report. Anders Wadeskog, Statistics Sweden, Unit of environmental economy and natural resources has done some data compilation. Some data in the report is from the the Swedish Chemical Agency. The persons responsible for the withdrawal of data there were Åsa Almqvist and Carl-Henrik Eriksson at the Product Register. Maria Ujfalusi at the Swedish Environmental Protection Agency has given valuable expert comments.

Statistics Sweden, May 2009

Inger Eklund

Viveka Palm

A note of thanks
We would like to express appreciation to our survey respondents – the people, enterprises, government authorities and other institutions of Sweden – with whose cooperation Statistics Sweden is able to provide reliable and timely statistical information meeting the current needs of our modern society.

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A separate text in Swedish is provided at the end of the publication, on page 35.

Summary

Statistics on import, manufacture, and export of chemicals can be an important information source to follow up the results of environmental policy and management decisions. In this pilot study we evaluate the use of the official trade and manufacture statistics for the purpose of screening for bioaccumulating and persistent compounds of a particular environmental relevance. An impact index to measure these properties is applied to chemical groupings in the trade statistics. Furthermore, data from the trade statistics for selected chemicals is compared to corresponding data from the Swedish Products Register, at the Swedish Chemical Agency.

The results show that the level of detail in the trade statistics does not permit estimation on the impact index using a compound specific index for environmental impact. In the trade statistics, a substantial number of chemicals with different properties are often grouped with the same identifier. However, this study shows that it is possible to use the same index to identify the groups containing the most problematic chemicals.

The 100 chemicals identified to rank highest with regard to the potential environmental impact index belong to several groups, but 94 of these were halogenated. The two dominating groups in the trade statistics were halogenated aromatics and hydrochlorofluorocarbons (HCFC), with 25 and 20 members, respectively.

A more detailed study of the trade statistics for these high-impact groups revealed substantial deviations between data from Statistics Sweden and Swedish Chemical Agency. Anomalies and an outlier were also observed and some misclassifications discovered. The self-reported statistics thus seems to need further validation to improve their usability for chemical policy purposes. Suggestions are made for further comparisons of databases, but tracing back to primary sources may also prove necessary to ensure relevance and good quality.

Introduction

A non-toxic environment is one of Sweden's 16 environmental objectives (Swedish EPA; 2008). The fulfillment is closely linked to the success by the chemicals policy, implemented in legislation and decisions at the national and the European level. The REACH legislation is then presumed to have a great impact. However, voluntary substitution and active work by companies and industry is another and perhaps as important contribution to this objective.

The success in reducing pollution and emissions of chemicals to the environment can partly be followed by monitoring programs. However, the number of substances used are greater than what can be targeted in a monitoring programme. Another important source of information is the statistics on import, manufacture, and export of chemicals. The net use of chemicals can be assumed to provide an indication of potential emissions. Specific chemicals, nevertheless, differ substantially in properties and effects. Summation of turnover for all chemicals does therefore not provide the information needed, to indicate the direction of development with regard to the environmental objective. Chemicals are reported on an individual basis through the statistics from the Products Registry of the Swedish Chemicals Agency, but some kind of aggregation is necessary to get an overview.

The statistics for chemical products in Sweden classified as hazardous to humans provide one such indicator. According to this statistic, the net use in recent years (excluding petroleum fuels and export) has been fairly stable (SCB 2008). However, these figures do not account for the large substance flows from imported goods or commodity groups.

Detailed information on chemicals use, like the Swedish Products Registry, is not available in most countries. Commercial confidentiality also severely limits the use of this information in Sweden. An exposure index has therefore been developed by the Swedish Chemicals Agency. The index estimate the likelihood of exposure of different environmental compartments, incl. the human society. It is based mainly on the used quantity and the use pattern (Fischer et al. 2005). The index exclude quantities for export and also when chemicals during use transforms into other chemicals (e.g. fuels and raw material for synthesis). This exposure index has been applied in the screening and selection of substances for the Swedish national environmental monitoring program.

Yet another source of information is the official trade and manufacture statistics based on the Combined nomenclature eight digit codes (CN) of the European Union for groupings of chemicals (EU 1987). The CN is comprised of the Harmonized System (HS) nomenclature with further subdivisions. Each CN code for chemicals is linked to a number of Chemical Abstract (CAS) registry numbers, which provides unique identifiers for the specific compound in question (ECICS 2007).

The previously mentioned exposure index and the trade statistics does not directly link to an impact index assessment. Another obstacle is that many toxic and other dangerous properties are not additive and can thus not be

summarised. However, baseline toxicity (related to bioaccumulation) and a measure of persistence could serve such a purpose, since these properties are indeed additive (Öberg, 2006).

Baseline toxicity (narcosis) is the minimum nonspecific toxicity exhibited by an organic compound (Schwarzenbach et al. 2002). Most industrial chemicals, with different sizes, shapes, and functional groups, express only baseline toxicity. Baseline toxicity results from the accumulation of chemicals and the ensuing disruption of normal functions in biological membranes, and it is thus closely related to other forms of bioaccumulation. Baseline toxicity is therefore also a measure of bioaccumulation.

Toxicity itself does not constitute an environmental risk without exposure. Exposure for chemical hazards is determined by release into the environment and removal by physical, chemical and biological processes. The degradation varies considerably between different environmental media, with air being the most reactive one (Gouin et al. 2000). Reaction with hydroxyl (OH) radicals in the troposphere is a dominant removal pathway for many industrial chemicals (Atkinson & Arey 2003). The rate constants for this gas-phase reaction can therefore be used as an indicator of environmental persistence.

It was recently suggested to use the ratio of the atmospheric persistence (half-lives) to the baseline toxicity – expressed as median lethal concentrations (in water) (LC_{50}) – to provide a continuous scale to rank and summarize the incremental environmental impacts from the simultaneous exposure to many chemicals (Öberg 2006). The toxic persistence rating (TPR) is expressed as:

$$TPR = Atmospheric\ half\text{-}life\ (days) / LC_{50}\ (mg\ L^{-1})$$

Two validated structure-activity relationships (SAR), for baseline toxicity and hydroxyl radical reaction rate constant, form the basis for these calculations (Öberg 2004; Öberg 2005). These two statistical models describe the correlation between the two properties and a set of molecular descriptors for the investigated compounds.

This index of persistence and bioaccumulation properties can thus serve both as weighting scheme for exposure and as a screening tool to prioritize substances of particular environmental relevance.

The purpose of this investigation is to evaluate the use of trade statistics and the suggested toxic persistence rating to estimate the chemical net use in Sweden over time and to screen for chemical groupings of particular interest.

One purpose of this study is to evaluate if the total TPR has changed during the years 1998-2005. Another purpose of this study is to investigate how well statistics from Statistics Sweden (trade and manufacture) is harmonized with data from the Product Register at the Swedish Chemical Agency, with a few examples of chemicals. These examples will be taken from the chemicals with highest TPR. If there are deviations, a discussion will be made about the possible reasons for the deviations. Also some trends in the use of these chemicals will be discussed.

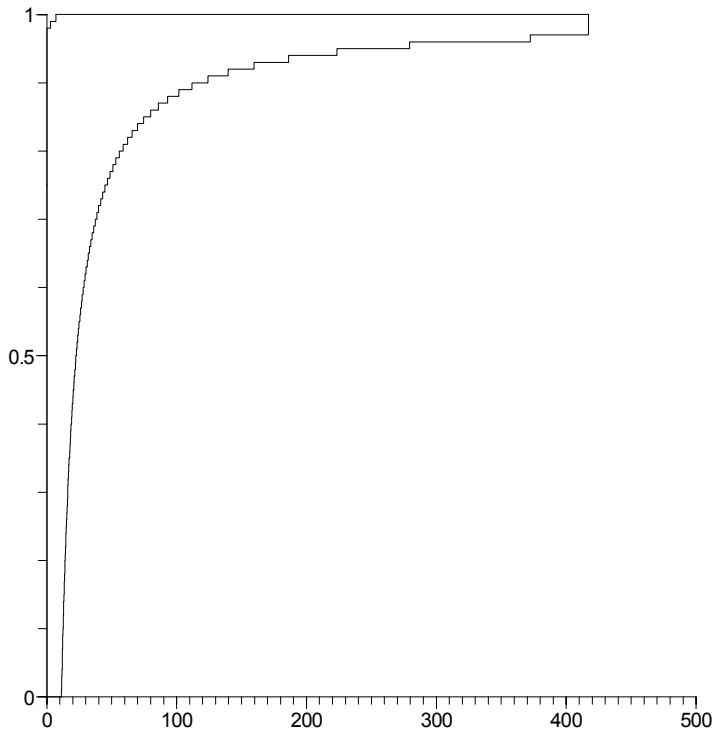
Method

Baseline toxicity, atmospheric persistence and the resulting toxic persistence ratings (TPR) have previously been estimated for a database of 50 000+ compounds using SAR models (Öberg 2006). This database was matched against 28 504 CAS registry numbers corresponding to CN codes from the ECICS database and both the SAR models for toxicity and persistence were then applicable for 10 578 compounds. However, most CN codes represent a range of chemicals (sometimes more than 100). The 10 578 compounds are thus represented by only 433 unique CN codes, out of which 269 CN represent 2 or more compounds and 164 represent only one compound. To give an estimate of toxicity and persistence for a CN code that is not unique is difficult. However, lower and upper bounds can be represented by an interval, and when more than two compounds are present it may be possible to assume some central tendency. Here we have chosen to represent those imprecise numbers by probability boxes or p-boxes for short (Ferson 2002).

A p-box is the class of distribution functions $F(x)$ bounded by two cumulative distribution functions $F_1(x)$ and $F_2(x)$ such that $F_1(x) \leq F(x) \leq F_2(x)$ for all x (Sander et al. 2006). When the precise input distribution is unknown, other available pieces of information may be put together as constraints for the class of possible distributions. The p-box becomes an interval if only a minimum and a maximum are specified. Here we have also added the mean (arithmetic average) as a third constraint for CN representing three or more compounds.

In figure 1 the TPR estimate for CN 29036990 is shown as p-box, constrained by a minimum of 0.0475, a maximum of 417, and a mean of 11.2. This CN represent 214 unique compounds (with CAS numbers) in this study.

Figure 1: Example of p-box for CN 2903 69 90 (halogenated aromatics). Probability vs. TPR-estimate (metric tons)



P-boxes can subsequently be used in a probability bounds analysis to estimate the total TPR-weighted use of chemicals. The TPR-weights given as precise numbers, intervals, and p-boxes were multiplied by the estimated net use for each CN code and each year. This yearly estimates were added together to obtain an aggregated estimate of use expressed in TPR-equivalents. Independence between factors was assumed and the calculations were performed with the software Risk Calc v4.0 (Applied Biomathematics, Setauket, NY).

Foreign trade statistics and Production of commodities and industrial services (domestic production) based on the eight digit CN codes were retrieved from Statistics Sweden, see Facts about the statistics. The net use was calculated by adding import and domestic production and subtracting the export.

The list of compounds with CN codes and toxic persistence rating was also used for screening and identification of compounds of particular environmental relevance. Six digit CN codes was used to retrieve non-confidential data from the Products Register for the purpose of comparing with the findings in the trade statistics.

Results and Discussion

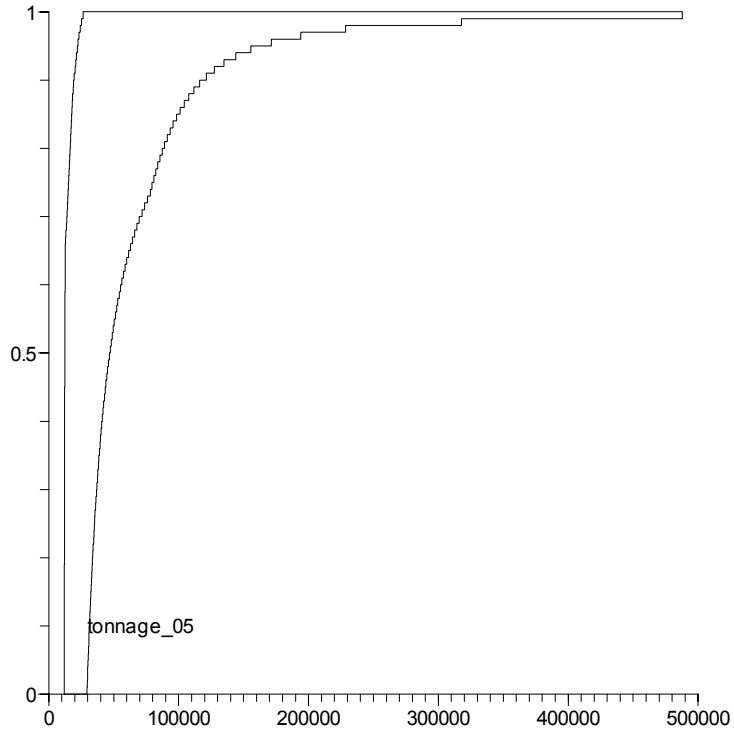
Probability bounds analysis of chemical flows

The net use of chemicals for each CN code (433 in total) was estimated by adding import and manufacture and subtracting the export. The net use was subsequently multiplied with the probability box describing its toxic persistence rating (TPR).

The net flow of chemicals, expressed in toxic persistence ratings, was estimated by adding the different compound groups. The aggregated results are similarly described by p-boxes, figure 2.

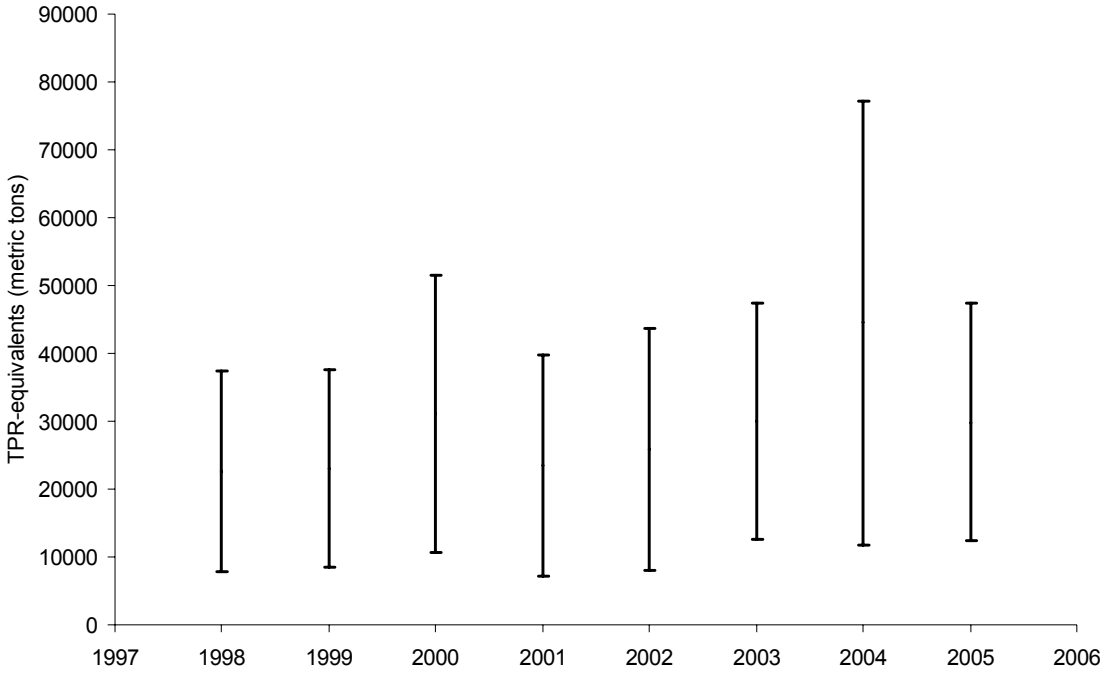
Appendix 2. Bans on HCFC in Sweden (in Swedish)

Figure 2: The probability box for the aggregated net flow of TPR (Toxic Persistence Rating)-equivalents (metric tons) in 2005



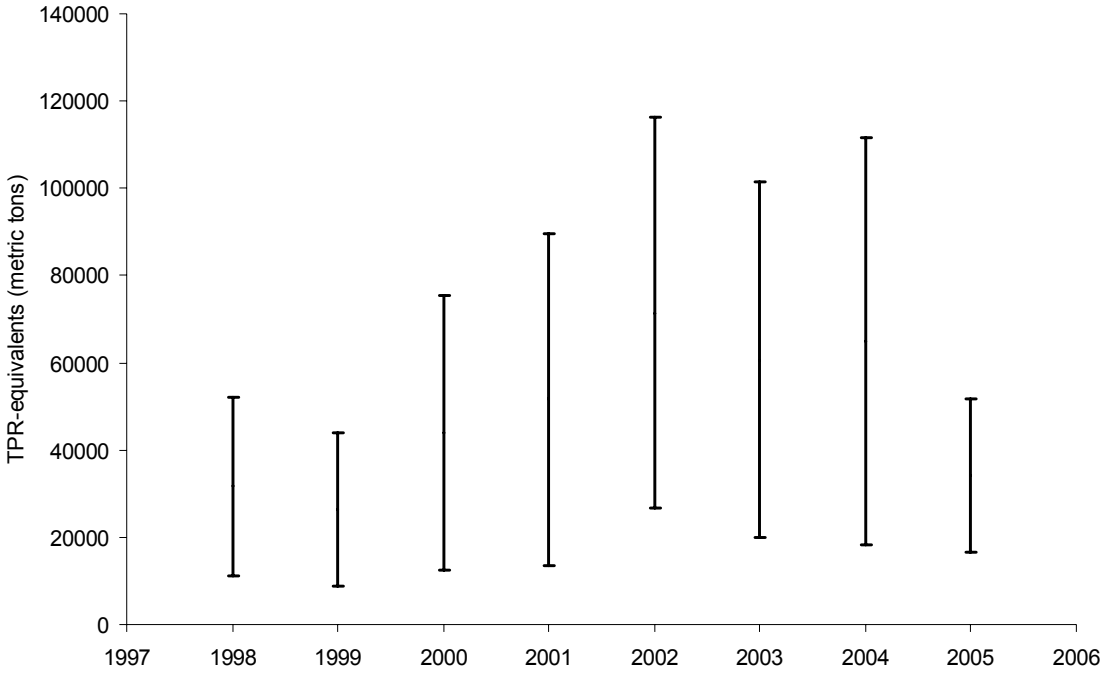
Each p-box bound the TPR-estimate with an upper and lower cumulative probability distribution. The uncertainty intervals for the medians are shown in figure 3 for each year (1998-2005). There seems to be variations between the years, but it is not possible to discern clear trends or significant differences, except that the uncertainty seems particularly pronounced in 2004.

Figure 3: Upper and lower bound in the median estimate of the net flow of TPR (Toxic persistence rating)-equivalents 1998-2005



A selection of compound groups containing more problematic compounds was evaluated separately. It was previously suggested that a TPR-value of 0.2 could be used as a cutoff for compounds possessing PBT -properties (persistent, bioaccumulating, and toxic). The number of CN-codes, groups of compounds, fulfilling this condition was 153, these are found in Appendix 3. This means that these CN codes included one substance (CAS) with a PBT value of 0.2 or higher. The same procedure of estimation of the net flows and aggregation was repeated for this subselection of environmentally relevant chemicals. The corresponding uncertainty intervals for the medians are shown for each year (1998-2005) in figure 4.

Figure 4: Upper and lower bound in the median estimate of the net flow of TPR-equivalents 1998-2005. CN-codes with at least one compound with TPR (Toxic Persistence Rating) >0.2



The outcome of the probability bounds analysis for this subselection of chemicals is similar to the previous one. There is variation between years, but no clear trend.

The CN-codes group chemicals together that possess some chemical similarity, but with widely different properties with regard to persistence, bioaccumulation and toxicity. This variation in properties is more pronounced than the changes in import, manufacture, and export. It thus seems difficult to directly use the statistics on net use to evaluate if a change in TPR (environmental impact) has occurred.

Instead this statistic can be studied at a more detailed level. One alternative is to use compound specific information, available in some countries, and the other is to identify the CN-codes carrying compound with high persistence and/or bioaccumulative and toxic properties.

Screening for substances with regard to PBT-properties

The 10 578 compounds with matching TPR-estimates were ranked and the top 20 are listed in table 1 together with their CN-codes. All top 100 of these compounds are listed in Appendix 1. Ninety-four of these compounds were halogenated.

Table 1: The 20 compound (CAS) with highest TPR-ranking, sorted by TPR

Chemical name	CAS	CN	t½ (days)	LC_{50} (mg/L)	TPR
Dichloro((dichlorophenyl)methyl)-methylbenzene	76253-60-6	29036990	13.2	0.0317	417
2,4,2',4'-Tetrachlorobiphenyl	2437-79-8	29036990	28.9	0.106	273
Polychlorinated biphenyls	1336-36-3	29036990	28.9	0.106	273
DDE	72-55-9	29036990	15.0	0.0585	257
2,2-(2-Chlorophenyl-4'-chloro-phenyl)-1,1-dichloroethene	3424-82-6	29036990	11.9	0.0618	193
DFDT	475-26-3	29036990	20.8	0.152	137
TDE	72-54-8	29036990	11.6	0.0874	132
Mitotane	53-19-0	29036990	9.29	0.0914	102
2-Butenoic acid, 2,3,4,4,4-pentachloro-, butyl ester	21824-93-1	29161980	35.9	0.447	80.3
Perthane	72-56-0	29036990	2.19	0.0298	73.6
HCFC 222	422-49-1	29034910	405	6.58	61.5
4-(Trifluoromethyl)benzophenone	728-86-9	29147000	23.5	0.389	60.4
PCB 28	7012-37-5	29036990	13.2	0.234	56.6
Decane, 1,10-dibromo-	4101-68-2	29033036	6.29	0.143	44.1
HCFC 231	421-94-3	29034910	358	8.41	42.5
2,3,4,5,6-Pentafluorobenzophenone	1536-23-8	29147000	30.1	0.776	38.8
Nonane, 1,9-dibromo-	4549-33-1	29033036	8.12	0.221	36.7
2,4,5,6-Tetrachloro-m-xylene	877-09-8	29036990	15.4	0.453	33.9
alpha,alpha,alpha-Trichloro-4-chlorotoluene	5216-25-1	29036990	25.3	0.789	32.0
Propyl 2,4,5-trichlorophenoxy-acetate	1928-40-1	29189090	8.32	0.264	31.5

Many of these environmentally relevant compounds belong to the same groups of chemicals, where halogenated derivatives of aromatic hydrocarbons (2903 69 90) was the largest with 25 members among the top 100, followed by halogenated derivatives of methane, ethane or propane (halogenated only with fluorine and chlorine) with 20 members. The 100 compounds ranked highest for baseline toxicity and persistence thus represent 22 CN numbers , table 2.

Table 2: CN-codes according to the number of compounds (CAS) that are included, chemical groups, and compounds that are members of the top 100 list

CN	Chemical Group	Compounds
29036990	Halogenated derivatives of aromatic hydrocarbons, other	25
29034910	Halogenated derivatives of methane, ethane or propane, halogenated only with fluorine and chlorine (HCFCs)	20
29033036	Bromides brominated derivatives of acyclic hydrocarbons (excl. bromomethane methyl bromide and dibromomethane)	8
29159080	Saturated acyclic monocarboxylic acids and their anhydrides, halogenides, peroxides and peroxyacids, their halogenated, sulphonated, nitrated or nitrosated derivatives, other	5
29189090	Carboxylic acids with additional oxygen function, their anhydrides, halides, peroxides and peroxyacids and their halogenated, sulphonated, nitrated or nitrosated derivatives, other	5
29269095	Nitrile-function compounds, other	5
29147000	Halogenated, sulphonated, nitrated or nitrosated derivatives	4
29173980	Aromatic polycarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their halogenated, sulphonated, nitrated or nitrosated derivatives, other	4
29031980	Saturated chlorinated derivatives of acyclic hydrocarbons, other	3
29049085	Sulphonated, nitrated or nitrosated derivatives of hydrocarbons, whether or not halogenated, other	3
29081000	Derivatives containing only halogen substituents and their salts, of phenols or phenol-alcohols	3
29159020	Chloroformates	3
29093090	Ether-alcohols and their halogenated, sulphonated, nitrated or nitrosated derivatives	2
29163900	Aromatic monocarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their halogenated, sulphonated, nitrated or nitrosated derivatives, other	2
29029080	Cyclic hydrocarbons, other	1
29029090	Cyclic hydrocarbons, other	1
29033080	Fluorides fluorinated derivatives and iodides iodinated derivatives of acyclic hydrocarbons	1
29034930	Halogenated derivatives of methane, ethane or propane, halogenated only with fluorine and bromine (excl. perhalogenated)	1
29095090	Ether-phenols, ether-alcohol-phenols and their halogenated, sulphonated, nitrated or nitrosated derivatives, other	1
29161980	Saturated acyclic monocarboxylic acids and their anhydrides, halogenides, peroxides and peroxyacids, their halogenated, sulphonated, nitrated or nitrosated derivatives, other	1
29209010	Sulphuric esters and carbonic esters and their salts, and their halogenated, sulphonated, nitrated or nitrosated derivatives	1
29309070	Organic thio compounds, other	1

The selected compound groups represent a variety of chemicals, but 95% of them are halogenated. The two dominating groups in Table 2 also represent many well-known pollutants. This screening approach can thus assist in identifying those groups of chemicals (CN codes) that could be monitored for chemical policy purposes.

Changes in use of chemicals belonging to the groups of environmentally relevant compounds

The net use of chemicals (import and domestic production minus export) in each group of chemicals can be followed in the trade statistics. Additional data was also requested from the Products Register of the Swedish Chemicals Agency. Three groups of halogenated chemicals (2903 69, 2903 49, and 2903 30) encompass 53 of the 100 top ranked compounds. Our evaluation here focuses on these three classes of compounds, to compare trends and agreement between the two data sources. However, these classes are less specific than those identified in Table 1, above. The six digit CN codes also encompass additional compound groups. The group with code 2903 69 encompasses all halogenated derivatives of aromatic hydrocarbons except chlorobenzene, hexachlorobenzene and DDT. The group with code 2903 49 encompasses not only derivatives of methane, ethane or propane halogenated with fluorine and chlorine (HCFCs), but also those halogenated with bromine and fluorine or chlorine. The group with code 2903 30 encompasses not only brominated derivatives of acyclic hydrocarbons, but also fluorinated and iodinated compounds.

The trade statistics for the three chemical groups specified both at a detailed level (eight digit CN codes) and at a higher level (six digit codes) were compared to data from the Products Register (tables 3-4). Here we have separated import and export. The reason for this separation is twofold, a comparison of net figures showed gross deviations between the two data sources and some data are not reported from the Products Register due to commercial secrecy. No domestic manufacture is reported for compound groups 2903 69 or 2903 49, and data for group 2903 30 are not reported because of secrecy. No domestic production is reported in the statistics for the three subgroups.

Table 3: Comparison of reported import (metric tons) 1998-2005. Compound groups given as six or eight digit CN-codes. The data sources are the Products Register, Swedish Chemical Agency (PR) or trade statistics, Statistics Sweden (Trade). Rounded numbers for smaller numbers

Year	290369 PR	290369 Trade	290349 PR	290349 Trade	29034910 Trade	290330 PR	290330 Trade
1998	156		129		357	772	
1999	*		118		185	678	
2000	28	13	192	189	104	1192	1079
2001	15	11	410	31	17	621	1126
2002	12	3	198	28	28	753	1035
2003	2.3	23	225	5	4.5	803	1056
2004	*	68	218	225**	24**	806	1213
2005	0.3	48	184	160	18	668	1009

* Commercial secrecy. ** Previously, an additional 2600 metric tons were erroneously reported for this CN-code.

The data reported in table 3 is to some extent difficult to interpret. The data from the Products Register seem to indicate that the import of halogenated aromatics (CN290369) has dropped from a level of 160 t/y in 1998 to below 1 in 2005, while the data from the trade statistics indicated much less variation, no clear trend and higher tonnage at the end of the period. The difference between the trade statistics and the Products Register is substantial in the period 2002-2005.

There are inconsistencies in data for the group 290349 and sub-group 29034910 (HCFCs), and the import figure from the trade statistics in 2004 was initially a gross outlier. A direct contact with an importing company, however, revealed this to be a reporting error (wrong CN-code). There is no clear trend in the main group, but a decreasing trend in the subgroup. This would be expected, since there are no possibilities for legal use in Sweden after 1 January 2002, except for specific military applications, see Appendix 2 for list of the bans of HCFC.

There are some but less pronounced deviations between the trade statistics and data from the Products Register in the group 290330.

In a statistical report from Statistics Sweden and Swedish Chemical Agency similar data of some other chemicals are compiled annually (SCB, 2008). In that report there are also differences in data from Statistics Sweden and Swedish Chemical Agency. Since the trade statistics have other cut-off criteria than the product register, and the data collection is made differently some variations are anticipated.

Table 4: Import and export of some chemicals (CN codes 29036990, 29034910, 29033036) 1998-2005 (metric tons). The data source is trade statistics, Statistics Sweden. Rounded numbers

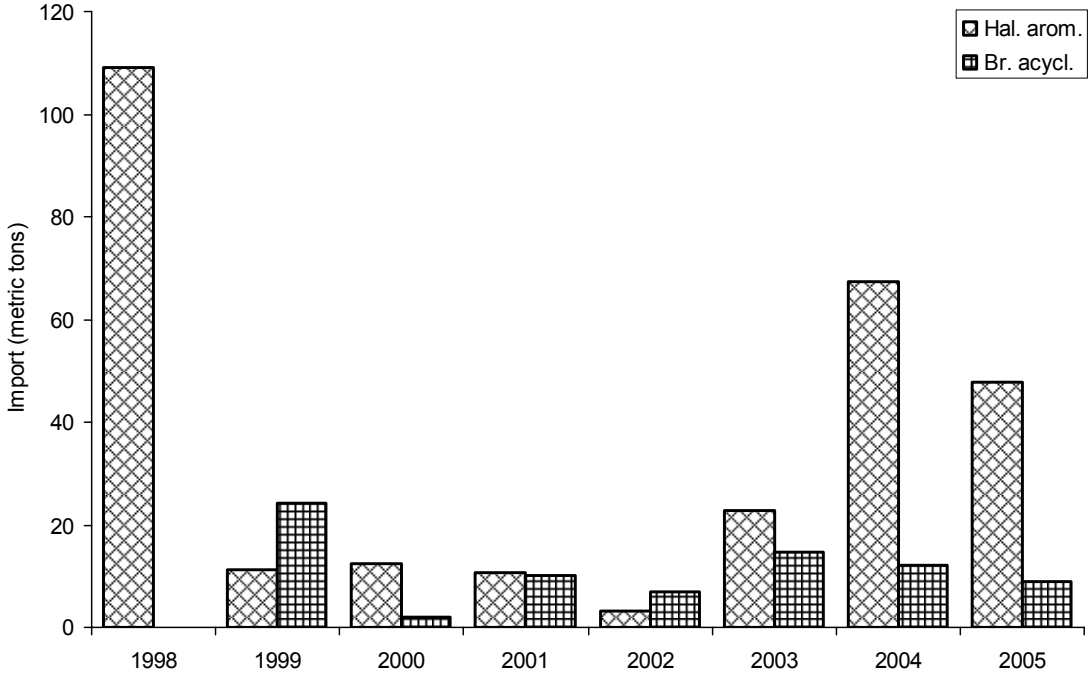
Year	29036990 Import	29036990 Export	29034910 Import	29034910 Export	29033036 Import	29033036 Export
1998	110	0.2	360	170		0.07
1999	11	2.5	190	210	24	0.005
2000	12	1.1	100	270	2.0	0.2
2001	11	0.007	17	190	10	0
2002	3.1	0.05	28	75	6.9	0.6
2003	23	11	4.5	190	15	0.001
2004	67	0.3	24*	190	12	
2005	48	0.2	18	210	9.0	0.07

* Previously, an additional 2600 metric tons were erroneously reported for this CN-code.

The relatively large export of compounds in group 29034910 is also interesting to note. This export is much higher than the import and no manufacture is reported. A possible explanation could be that this export is due to re-export of previously imported HCFCs to final treatment (destruction) outside Sweden.

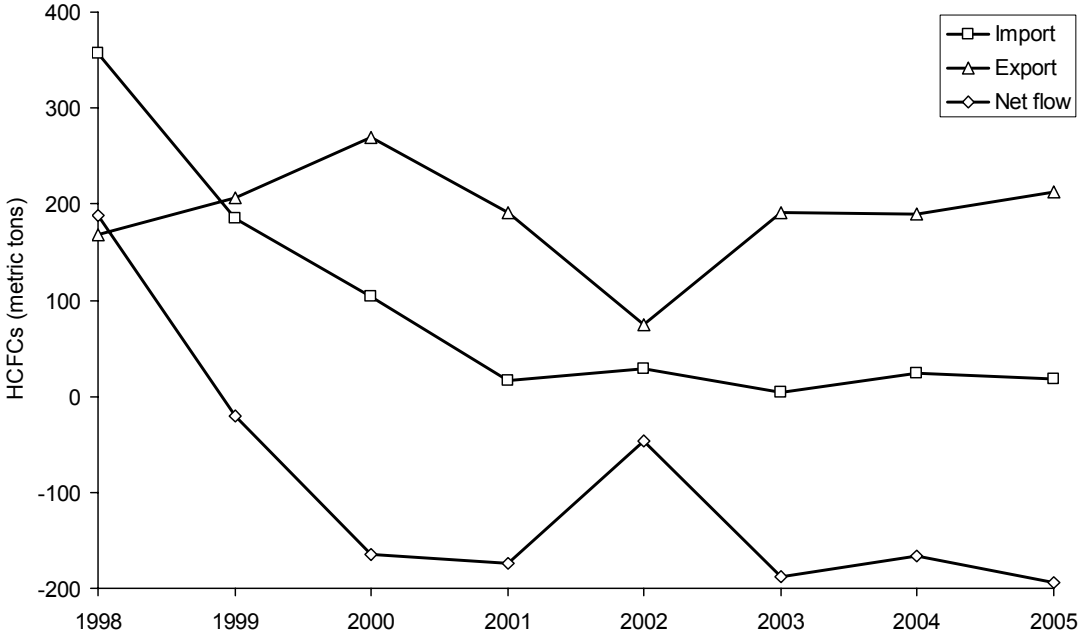
The export is relatively small for halogenated aromatics (29036990) and brominated acyclic compounds (29033036). The development over time for these two environmentally relevant compound groups can therefore be evaluated from import alone, figure 5.

Figure 5: Import of halogenated aromatics and brominated acyclic compounds 1998-2005. (data from Statistics Sweden, CN 29036990, 29033036)



In contrast, the reported export of HCFCs (29034910) is substantial and will determine the net flow, which is negative after 1998, figure 6.

Figure 6: Import, export, and net flow (import – export) of HCFCs (CN 2903 49 10) 1998-2005. Data from Statistics Sweden



In an attempt to clarify the deviations for groups 2903 30 and 2903 49, we also reviewed which compounds make the major contribution to these two groups in the Products Register. These six compounds are listed in table 5.

Table 5: Compounds that make a major contribution to groups 2903 30 and 2903 49 in the Products Register

CN	CAS	Name
2903 30	811-97-2	Ethane, 1,1,1,2-tetrafluoro-
2903 30	75-37-4	Ethane, 1,1-difluoro-
2903 49	354-33-6	Ethane, pentafluoro-
2903 49	420-46-2	Ethane, 1,1,1-trifluoro-
2903 49	75-10-5	Methane, difluoro-
2903 49	811-97-2	Ethane, 1,1,1,2-tetrafluoro-

This simple validity check seems to indicate that some of the deviations and inconsistencies may be due to classification errors at the information supplier level (the companies delivering the primary statistics). All compounds above are fluorinated acyclic hydrocarbons and should be classified with CN 2903 30. However, four of the six compounds are misclassified as other halogenated derivatives of acyclic hydrocarbons containing both fluorine and chlorine (CN 2903 49). One can also notice that 1,1,1,2-tetrafluoroethane is classified into both of the two mutually exclusive groups.

Conclusions

The purpose of this investigation was to evaluate the use of trade statistics and a toxic persistence rating (TPR) to estimate the chemical net use in Sweden over time and to screen for chemical groupings of particular interest.

The trade statistics is organised by the combined nomenclature (CN) and an individual CN code often represents two or more specific compounds. The 10 578 compounds included in this investigation were thus represented by only 433 "unique" CN codes, or 24 compounds per CN code on average. The variability in environmental characteristics between compounds adds substantial uncertainty to the estimates for each CN. This additional uncertainty makes it difficult to discern any clear trends from the trade statistics with regard to the development of the evaluated environmental indicator (toxic persistence rating).

An alternate approach is to use the TPR-concept to screen the CN codes for compounds of particular environmental relevance. The one hundred compounds that ranked highest with regard to potential environmental impact were mostly halogenated (94/100) and many of these environmentally relevant compounds belong to the same group of chemicals. Halogenated derivatives of aromatic hydrocarbons (29036990) was the largest with 25 members, followed by halogenated derivatives of methane, ethane or propane (halogenated only with fluorine and chlorine) with 20 members.

The trade statistics for the three CN codes with the highest impact compounds were studied in more detail. Additional supporting statistics were retrieved from the Products Register of the Swedish Chemical Agency. This study revealed some interesting details. First, substantial differences were observed between the foreign trade statistics and the Products Register. Parts of these will depend on the different system boundaries and cut-off criteria in the data compilation. Secondly, anomalies and an outlier were observed in the foreign trade statistics data. Further investigations showed that the outlier was due to a reporting error. Thirdly, the reported export of compounds classified as HCFCs (CN 29034910) was not equalled by import or domestic manufacture. The reason for this mismatch remains open, but re-export for final destruction is one possibility. And lastly misclassifications with regard to CN codes could be frequent in both the trade statistics and the Products Register.

An important conclusion from the pilot study is that the self-reported statistics seem to need further validation to improve its usability for evaluating the accomplishment of the environmental objectives concerning chemicals. The two data sources, foreign trade statistics and the Products Register, offer an excellent opportunity for validation studies by joining the data bases. For compounds and compound groups of particular environmental relevance it is also necessary to trace the statistics back to the primary source to clarify possible reporting errors. Further analysis of the CN codes with assumed PBT properties is recommended.

Misclassifications with regard to six CN codes in the Products Register can similarly be detected and corrected by further comparison with the ECICS database. A more detailed study of the net chemical use expressed in TPR-units can be achieved by directly linking the TPR-estimates to the net use for individual compounds (from the Products Register).

Facts about the statistics

Data presented in this report is a result of a method developing project and all data are coming from other statistical sources.

Statistics Sweden - Foreign Trade Statistics and Production of Commodities and Industrial Services

Data is based on Foreign Trade Statistics, Production of Commodities and Industrial Services, Statistics Sweden. Information from the statistics on foreign trade in goods is not revised for non-response and reduced coverage. The degree of coverage in 2005 was 97 percent when calculated in the total value of exports and imports. Of course, non-response can be greater for certain groups of goods. The information from the statistics on Industrial production of goods is revised for non-response and reduced coverage.

To calculate the domestic usage at the most detailed level, as was done in this report, is uncertain. Measurement errors arise to a certain extent, primarily when the respondent reports net weight or another quantity, where the occurrence of rough estimates and erratic figures is not impossible. Respondents' uncertainty in classifying goods with the right goods code is due cause to assume that some percentage is made up of misclassified goods (Statistics Sweden, 2008).

For Foreign Trade Statistics, see:

http://www.scb.se/Pages/ProductDocumentations____17842.aspx (Swedish)

http://www.scb.se/Pages/Product____7232.aspx (English)

For production of Commodities and Industrial Services, see:

http://www.scb.se/Pages/ProductDocumentations____19165.aspx (Swedish)

http://www.scb.se/Pages/Product____11292.aspx (English)

Swedish Chemicals Agency

The product register is a national register maintained by the Swedish Chemical Agency. The register contains information about approxiamtely 120 000 chemical products and biotechnical organisms. Information is submitted to the register by approximately 2 500 companies that are legally bound in their reporting and provide an image of how chemical substances and products are used in Sweden. More information about the statistics is available at the Product Register, www.kemi.se.

www.kemi.se

http://www.kemi.se/templates/Page____2833.aspx (Swedish)

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Appendix

Appendix 1. The 100 compound (CAS) with highest TPR-ranking

Chemical name	CAS	CN	t½ (days)	LC_{50} (mg/L)	TPR
Dichloro((dichlorophenyl)methyl)-methylbenzene	76253-60-6	29036990	13.2	0.0317	417
2,4,2',4'-Tetrachlorobiphenyl	2437-79-8	29036990	28.9	0.106	273
Polychlorinated biphenyls	1336-36-3	29036990	28.9	0.106	273
DDE	72-55-9	29036990	15.0	0.0585	257
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	3424-82-6	29036990	11.9	0.0618	193
DFDT	475-26-3	29036990	20.8	0.152	137
TDE	72-54-8	29036990	11.6	0.0874	132
Mitotane	53-19-0	29036990	9.29	0.0914	102
2-Butenoic acid, 2,3,4,4,4-pentachloro-, butyl ester	21824-93-1	29161980	35.9	0.447	80.3
Perthane	72-56-0	29036990	2.19	0.0298	73.6
HCFC 222	422-49-1	29034910	405	6.58	61.5
4-(Trifluoromethyl)benzophenone	728-86-9	29147000	23.5	0.389	60.4
PCB 28	7012-37-5	29036990	13.2	0.234	56.6
Decane, 1,10-dibromo-	4101-68-2	29033036	6.29	0.143	44.1
HCFC 231	421-94-3	29034910	358	8.41	42.5
2,3,4,5,6-Pentafluorobenzophenone	1536-23-8	29147000	30.1	0.776	38.8
Nonane, 1,9-dibromo-	4549-33-1	29033036	8.12	0.221	36.7
2,4,5,6-Tetrachloro-m-xylene	877-09-8	29036990	15.4	0.453	33.9
alpha,alpha,alpha-Trichloro-4-chlorotoluene	5216-25-1	29036990	25.3	0.789	32.0
Propyl 2,4,5-trichlorophenoxyacetate	1928-40-1	29189090	8.32	0.264	31.5
Sebacoyl chloride	111-19-3	29171990	6.44	0.208	31.0
2,3,4,5-Tetrachloronitrobenzene	879-39-0	29049085	55.7	1.83	30.4
1,2,3,5-Tetrachlorobenzene	634-90-2	29036990	28.6	0.940	30.4
Benzonitrile, 2,3,4,5,6-pentafluoro-	773-82-0	29269095	695	22.9	30.3
1,2,3,4-Tetrachlorobenzene	634-66-2	29036990	37.1	1.23	30.3
Propane, 2,2,3-trichloro-1,1,1,3-tetrafluoro-	139754-75-9	29034910	662	22.0	30.1
1,2,4,5-Tetrachlorobenzene	95-94-3	29036990	30.9	1.08	28.7
3,5-Dinitro-4-chloro-alpha,alpha,alpha-trifluorotoluene	393-75-9	29049085	252	9.04	27.9
2,3,5,6-Tetrachloro-p-xylene	877-10-1	29036990	15.1	0.558	27.1
HCFC 223	422-52-6	29034910	452	17.5	25.8
Propane, 1,1,1,3-tetrachloro-2,2,3-trifluoro-	422-50-4	29034910	381	15.8	24.1
1,2,4,5-Tetrachloro-3-nitrobenzene	117-18-0	29049085	52.7	2.24	23.5

(forts.)

Chemical name	CAS	CN	t½ (days)	LC_{50} (mg/L)	TPR
Benzene, 1-chloro-2-(trichloromethyl)-	2136-89-2	29036990	24.9	1.07	23.2
Undecane, 1-bromo-	693-67-4	29033036	1.80	0.0814	22.1
Octane, 1,8-dibromo-	4549-32-0	29033036	10.1	0.476	21.3
2-Bromotridecane	59157-17-4	29033036	1.57	0.0749	20.9
Propane, 1,1,3,3-tetrafluoro-1,2,2-trichloro-	422-32-2	29034910	400	19.5	20.5
Chloropentafluorobenzene	344-07-0	29036990	98.6	5.18	19.0
Propane, 1,1,1,2-tetrafluoro-2,3,3-trichloro-	422-47-9	29034910	667	35.1	19.0
Carbonochloridic acid, 2,4,5-trichlorophenyl ester	16947-69-6	29159020	15.0	0.840	17.8
Decane, 1,10-dichloro-	2162-98-3	29031980	3.07	0.184	16.7
HCFC 225aa	128903-21-9	29034910	475	29.1	16.3
HCFC 224	422-54-8	29034910	727	45.1	16.1
Propane, 1,1,1,3-tetrachloro-2,2-difluoro-	677-54-3	29034910	380	23.6	16.1
4-Hexylbiphenyl	59662-31-6	29029090	0.620	0.0394	15.7
3,4-Dichlorobenzotrifluoride	328-84-7	29036990	53.0	3.46	15.3
2-Bromododecane	13187-99-0	29033036	1.39	0.0912	15.2
4-Benzylphenyl chloroformate	74176-32-2	29159020	3.75	0.248	15.1
Dodecane, 1-chloro-	112-52-7	29031980	0.982	0.0652	15.1
2,4,5-T-isopropyl	93-78-7	29189090	8.71	0.590	14.8
1,1,1,2-Tetrachloroethane	630-20-6	29031980	187	13.0	14.4
Dodecanoyl chloride	112-16-3	29159080	2.43	0.171	14.2
Trichloroacetyl chloride	76-02-8	29159080	224	16.1	14.0
Benzonitrile, 4-(trifluoromethyl)-	455-18-5	29269095	296	21.3	13.9
Propane, 1,1,1,2-tetrachloro-2-fluoro-	3175-25-5	29034910	318	23.2	13.7
Propane, 1,1,2,3-tetrafluoro-1,2,3-trichloro-	422-42-4	29034910	455	33.3	13.7
Propane, 2,2-dichloro-1,1,1,3-tetrafluoro-	149329-24-8	29034910	568	41.9	13.6
alpha,alpha,alpha-Trifluoro-m-toluonitrile	368-77-4	29269095	288	21.5	13.4
Propane, 2,2,3,3-tetrafluoro-1,1,1-trichloro-	422-51-5	29034910	419	32.4	12.9
Benzene, 2,4-dichloro-1-(trifluoromethyl)-	320-60-5	29036990	50.1	3.88	12.9
Propane, 1,2,2-trichloro-1,1,3,3-tetrafluoro-	139754-76-0	29034910	402	31.4	12.8
2,5-Furandione, dihydro-3-(octen-1-yl)-	26680-54-6	29171990	2.84	0.224	12.7
Bis(p-chlorophenoxy)methane	555-89-5	29093090	4.64	0.371	12.5
alpha,alpha,alpha-Trifluoro-2-toluonitrile	447-60-9	29269095	334	27.1	12.3
Octanoic acid, 4-methylphenyl ester	59558-23-5	29159080	1.21	0.0988	12.2

(forts.)

Chemical name	CAS	CN	t½ (days)	LC_{50} (mg/L)	TPR
Triclosan	3380-34-5	29095090	2.23	0.192	11.6
Propane, 1,1,3-trichloro-1,2,2,3-tetrafluoro-	422-53-7	29034910	436	38.0	11.5
Pentafluorobenzyl bromide	1765-40-8	29036990	108	9.42	11.4
1,1,1,3,3-Pentachloroacetone	1768-31-6	29147000	94.3	8.28	11.4
2,4-D-butyl	94-80-4	29189090	3.65	0.332	11.0
Benzene, 1,1'-(1,2-dibromo-1,2-ethanediyl)bis-	5789-30-0	29036990	6.69	0.612	10.9
Trichloroethyl chloroformate	17341-93-4	29159020	51.1	4.78	10.7
Tetrachlorophthalic acid	632-58-6	29173980	9.74	0.917	10.6
Heptane, 1,7-dibromo-	4549-31-9	29033036	10.0	0.962	10.4
Haloprogin	777-11-7	29093090	15.5	1.49	10.4
Propane, 1,1,1-trichloro-2,2,3-trifluoro-	131211-71-7	29034910	508	49.6	10.2
Chlorbenside	103-17-3	29309070	2.40	0.241	10.0
HCFC 225ca	422-56-0	29034910	806	83.6	9.6
Nonanedioyl dichloride	123-98-8	29171990	5.41	0.562	9.6
Carbonic acid, 1,1-dimethylethyl 2,4,5-trichlorophenyl ester	16965-08-5	29209010	20.0	2.10	9.5
2-Chloranil	2435-53-2	29147000	23.2	2.50	9.26
Decane, 1-iodo-	2050-77-3	29033080	1.43	0.159	9.02
4,4'-Dichlorobiphenyl	2050-68-2	29036990	7.80	0.888	8.78
Decyl bromide	112-29-8	29033036	1.93	0.222	8.71
2-Bromo-2,2-diphenylacetyl chloride	17397-37-4	29163900	12.4	1.43	8.69
HCFC-225bb	422-44-6	29034910	488	57.0	8.55
2,3,4,6-Tetrachlorophenol	58-90-2	29081000	5.22	0.616	8.47
Hexanoic acid, 1,1'-anhydride	2051-49-2	29159080	1.71	0.202	8.44
4-Bromo-2-chloro-alpha,alpha,alpha-trifluorotoluene	445-01-2	29036990	54.0	6.61	8.18
2,3,4,5-Tetrachlorophenate	4901-51-3	29081000	6.26	0.774	8.09
Benzeneacetonitrile, 3-(trifluoromethyl)-	2338-76-3	29269095	166	20.6	8.07
Decylbenzene	104-72-3	29029080	0.568	0.0711	7.99
Benzoyl chloride, 4-heptyl-	50606-96-7	29163900	2.09	0.263	7.96
2,4-D sec-butyl ester	94-79-1	29189090	3.39	0.427	7.94
Ethyl 2,4,5-trichlorophenoxyacetate	1928-39-8	29189090	7.80	0.989	7.89
HCFC 121	354-14-3	29034910	351	44.7	7.85
2,3,5,6-Tetrachlorophenate	935-95-5	29081000	5.88	0.755	7.79
Trityl chloride	76-83-5	29036990	3.00	0.387	7.74
Propane, 3-bromo-1,1,1,2,2-pentafluoro-	422-01-5	29034930	1426	188	7.60
d-Bornyl a-Bromoisovalerate	52964-40-6	29159080	2.23	0.298	7.49

Appendix 2. Bans on HCFC in Sweden (in Swedish)

Lagstiftningens område	Träder i kraft	SFS Nummer
Framställning av varor av hård skumplast (XPS) ur tulltaxenummer 39.21.110 och 29.25.900	1 jan 1997	1994:968
Framställning av varor av hard skumplast ur tulltaxenummer 84.19, 85.16, 89.01 samt 89.02	1 jan 1998	1994:968
Som arbetsmedium vid nyproduktion och nyinstallation av kyl-, värme- och andra klimatanläggningar	1 jan 1998	1995:636
För påfyllning av befintliga kyl-, värme-, och andra klimatanläggningar	1 jan 2002	1995:636

Undantag från förbudet: Försvarsmakten, Försvarets materielverk och Fortifikationsverket får använda HCFC för att fylla på en kyl-, värme- eller klimatutrustning, om utrustningen var i bruk den 1 juni 2002 och sedan dess har fortsatt och fortsätter att vara i bruk och HCFC inte kan ersättas med något annat ämne (SFS 2007:846)

Appendix 3. CN numbers which include a chemical with a PBT value above 0.2

28510080		29143900		29214980
29011000		29144090		29214990
29011090		29145000		29215190
29012900		29146990		29215990
29021930		29147000		29221980
29021980		29147090		29222900
29029010		29151300		29223000
29029080		29153990		29223900
29029090		29154000		29224970
29031600		29155000		29224995
29031910		29156019		29225000
29031980		29156090		29239000
29031990		29159010		29241900
29032900		29159020		29242990
29033036		29159080		29242995
29033080		29161290		29252000
29034590		29161910		29269095
29034910		29161980		29269099
29034930		29162000		29270000
29034980		29163100		29280090
29035990		29163210		29291090
29036100		29163500		29299000
29036990		29163900		29309070
29042000		29171100		29310095
29049020		29171290		29322980
29049085		29171310		29322985
29051700		29171390		29329980
29051900		29171910		29329985
29055020		29171990		29331990
29055910		29172000		29332990
29061900		29173940		29333920
29062900		29173980		29333945
29071300		29181100		29333995
29071900		29181980		29333999
29072900		29182390		29334090
29081000		29182980		29334990
29089000		29182990		29336980
29091900		29183000		29337900
29093038		29189090		29339050
29093090		29190090		29339095
29094990		29201000		29339190
29095090		29209010		29339930
29096000		29209085		29339990
29109000		29211190		29341000
29110000		29211200		29342080
29121900		29211980		29343090
29122900		29214210		29349096
29124900		29214300		29349990
29130000		29214400		29350090
29141990		29214500		29419000
29142900		29214600		34021300

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In Swedish

Statistiken för utrikeshandeln och industrins varuproduktion är en viktig informationskälla för uppföljning av verkan av miljöpolicybeslut och andra riskhanteringsåtgärder. I pilotstudien som redovisas i rapporten har vi utvärderat om den officiella handelsstatistiken kan användas för sållning av kemiska ämnen med särskilt miljöfarliga egenskaper. Ett effektindex för dessa egenskaper har använts för att beskriva varugrupperna i handelsstatistiken. Dessutom har handelsstatistiken för några utvalda grupper jämförts med motsvarande information från kemikalieinspektionens produktregister.

Resultaten visar att detaljeringsgraden i handelsstatistiken inte är sådan att effekterna kan skattas från ett ämnesspecifikt index. I handelsstatistiken grupperas ofta ett flertal kemiska ämnen med olika egenskaper under samma varukod. Däremot visar det sig möjligt att med samma index identifiera de varugrupper som innehåller de från miljösynpunkt mest problematiska kemikalierna.

De 100 kemiska ämnena som fick högst rang med avseende på miljöpåverkan kommer från flera olika varugrupper, men 94 av dessa var halogenerade (innehåller klor, fluor eller brom). De två dominerande varugrupperna från handelsstatistiken var halogenerade aromater och klorfluorkolväten (HCFC), representerade med 25 respektive 20 ämnen vardera.

En mer ingående granskning av handelsstatistiken för dessa grupper av miljörelevanta ämnen visade på påtagliga avvikelser med produktregistret. Dessutom upptäcktes att avvikelser och felklassificeringar kan vara frekvent förekommande. Den egenrapporterade statistiken är därför i behov av ytterligare validering för att öka dess användbarhet i uppföljningen av miljömålen. I rapporten föreslås samkörning av olika databaser, men det kan även finnas behov att i en del fall spåra uppgifterna bakåt till den primära uppgiftslämnaren.

SCB tackar
Tack vare våra uppgiftslämnare – privatpersoner, företag, myndigheter och organisationer – kan SCB tillhandahålla tillförlitlig och aktuell statistik som tillgodoser samhällets informationsbehov

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