R&D PROJECT

Inventory and tracking of dangerous substances used in Ireland and development of measures to reduce their emissions/losses to the environment

Main Report

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Inventory and tracking of dangerous substances used in Ireland and development of measures to reduce their emission/losses to the environment

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Preface

The Environmental Protection Agency initiated a project under the Environmental Monitoring, R&D sub-programme of the Operational Programme for Environmental Services (1994-1999), supported by the European Regional Development Fund (ERDF). This project, entitled: ***Inventory and tracking of dangerous substances used in Ireland and development of measures to reduce their emission/losses to the environment*** was awarded on a shared cost basis to the Clean Technology Centre at Cork Institute of Technology.

The outputs from this project are represented by:

- **Main Report *(this document)***

This comprehensively reports on the conduct of the project, the methodology and the findings. It includes the conclusions and recommendations for the future based on the application of the methodology.

- **Synthesis Report**

This is an abbreviated form of the Main Report.

- **Introduction: what is BEP?**

This document introduces the origins of the project and explains the objective of a "Best Environmental Practice". It should be read as an introduction to any of the Best Environmental Practice Guidelines produced by this project.

- **Recommendations for selected substances**

This document expands on the "Introduction: what is BEP?". Recommendations for measures to be considered by policy-makers have been prepared. These recommendations range from mandatory reporting of usage and composition via a Chemical Products Registration Scheme, through the provision of research, development and demonstration measures to consideration of prohibition. They require the adoption of decisions and the provision of resources which are beyond the users of the substances alone.

- **Series of Best Environmental Practice Guidelines (BEP Guidelines)**

These are oriented to actual users and have been prepared for the following substances:

Metals	A-1	Arsenic
	A-2	Cadmium
	A-3	Lead
	A-4	Mercury
	A-5	Organo-tin compounds
Solvents	B-1	Chlorobenzene
	B-2	Dichloroethane
	B-3	Nitrobenzene
	B-4	Trichlorobenzene
	B-5	Trichloroethylene
	B-6	Xylene
Herbicides	C-1	Dichlorvos
&	C-2	Isoproturon
Pesticides	C-3	Mecoprop
	C-4	Permethrin
	C-5	Simazine
	C-6	Trifluralin
Others	D-1	Butylbenzylphthalate (BBP)
	D-2	Diethylhexylphthalate (DEHP)
	D-3	Nonyl phenol & Nonyl phenol ethoxylates (NP & NPE)
	D-4	Polycyclic Aromatic Hydrocarbons (PAH's) as in creosote
	D-5	Polybrominated diphenyl ethers (PBDEs)

These are all available from the Publications Office, Environmental Protection Agency, Regional Inspectorate, St. Martin's House, Waterloo Road, Dublin 4. Tel: +353-1-6674474; Fax: +353-1-6605848.

Executive summary

The main objectives of the project were to:

1. Prepare a preliminary priority list of dangerous substances and corresponding Best Environmental Practice Guidelines
2. Prepare a methodology to conduct an inventory of a specified dangerous substance

Preliminary priority list

Following the recommendation of the project Steering Committee, a simplified risk assessment approach, using an extended OSPAR Priority List as an initial selection of substances, was followed. In the absence of adequate monitoring data, the internationally recognised EURAM system, a model-based ranking method, was adopted. This pays particular attention to the aquatic medium.

Attempting to apply this approach, however, demonstrated the deficiencies in available data for Ireland on exposure to dangerous substances include the following:

(i) uncertainty about quantities of pure substances imported and in use;

(ii) lack of information of actual usage patterns;

(iii) absence of data on incorporation of dangerous substances in preparations and products;

(iv) inadequacy of monitoring data, due to lack of sampling and cost constraints;

(v) uncertainty in the intrinsic physicochemical and ecotoxicological properties, and

(vi) inapplicability of the model-based ranking method to metals and biocides.

They lead to the conclusion that a strictly scientific risk assessment approach could not be followed in prioritising substances for control in Ireland. An alternative method of determining a priority list for preparation of Best Environmental Practices must be adopted. An Expert Review Group was established to assist the Steering Committee. Using the information gathered in this project, it was decided to refer primarily to Ireland's international obligations and to consider substances of national or international concern, in accordance with the project specification as originally specified.

The outcome of this project is that representative substances from particular uses and potential concern were chosen, including metals, pesticides, organohalogen solvents, endocrine disrupters and substances for which daughter directives under 76/464/EEC and OSPAR action lists of priority substances were developed. This list of substances is presented overleaf. Best Environmental Practices have been developed for these.

Two major recommendations for further consideration arise from this project:

1. Data must be obtained on the identity, quantity and usage of substances applicable to Ireland. The introduction of a Chemical Products Registration scheme, similar to that in use in Norway or Sweden, must be seriously considered to achieve this.
2. Monitoring must be enhanced, but based on suspected incidence. It is not feasible from a cost or technical viewpoint to monitor for all substances or parameters. Suggestions are provided for the monitoring of the proposed priority list.

Inventory methodology

A methodology has been devised and applied with reasonable success at this initial stage. The methodology was based on substance flow analysis methods applied in Denmark, Sweden and the Netherlands. To assist its development, it was applied to four test substances: lead, dichloromethane (methylene chloride), dichloroethane (ethylene dichloride) and nonylphenol/ nonylphenol ethoxylate. Preliminary substance flow analyses were produced for lead, dichloromethane and dichloroethane. However, less comprehensive information was obtained on the use of nonylphenol/ nonylphenol ethoxylate in Ireland. The successful implementation of the proposed methodology has proved that the methodology is applicable in an Irish context.

In common with the priority listing, the deficiencies of the publicly available data have presented problems. The recording, collection and publication of specific data is widespread and engaged in by various agencies but is fragmented. It is collected for different specific purposes, and the data quality is variable. Furthermore, much of this is confidential to the specific government agency, and not available to third parties, in order to preserve commercial confidentiality. Even if it were all made available, it would be inadequate for prioritisation of substances hazardous to the environment. Industrial sources have co-operated willingly in providing further information. Introduction of a Chemical Products Registration scheme would significantly enhance risk management.

List of substances selected for development of Best Environmental Practice

Name	CAS
Arsenic	7440382
Benzylbutylphthalate (BBP)	85687
Cadmium	7440439
Chlorobenzene	108907
1,2 dichloroethane	107062
Dichlorvos	62737
Diethylhexylphthalate (DEHP)	117817
Isoproturon	34123596
Lead & organic lead compounds	7439921
Mecoprop	93652
Mercury & organic mercury compounds	7439976
Nitrobenzene	96953
Nonylphenol	25154523
Nonylphenol ethoxylate	9016459
Polycyclic aromatic hydrocarbons (PAHs)	130498292
Polybrominated-diphenylether (PBDE)	N/a
Permethrin	52645531
Simazine	122349
Tin (organic compounds)	Misc.
Trichlorobenzene	12002481
Trichloroethylene	79016
Trifluralin	1582098
Xylene, mixed isomers	1330207
m-xylene	108383
o-xylene	95476
p-xylene	106423

Structure of the report

The assessment and regulation of dangerous substances has been studied and implemented for many years, yet remains an area of active development. It poses a challenge for Ireland to use scarce resources to the maximum benefit. This project has addressed this issue, on a number of fronts. In writing this report, it is recognised that there are many possible readers: policy makers, manufacturers of products containing dangerous substances, regulators, users of such substances, importers and distributors, academic experts, and concerned citizens. The report is written both for those familiar with the topic, seeking specific information, and also those approaching it for the first time. There is therefore a danger that for some readers the material is superfluous, while for others, it is over-detailed. We have recognised that this represents an initial attempt to apply a prioritisation scheme to Ireland. It is quite likely that subsequent workers will wish to extend our findings. We have therefore attempted to convey all the essential information, assigning it to appendices as necessary to ease the flow of reading.

The Report consists of the following sections:

Section 1: Introduction

This section provides the context for the report. It indicates the primary objective of this project, and illustrates the existing chemicals control policy by referring to some of the programmes and measures already in place and the current policy direction by referring to the Water Framework Directive and the Oslo and Paris (OSPAR) Convention strategy on hazardous substances.

Section 2: Prioritisation in risk management

This provides an introduction to the topics of risk assessment, risk management and prioritisation of dangerous substances. It is not a comprehensive treatise, but again provides a context, though now with a focus on the technical approach. The overall structure of a model-based approach is provided, with more detailed consideration of the risk assessment aspects, including exposure and effects assessment, concluding with risk characterisation using a PEC/PNEC approach. Ranking methods are introduced, and the Swedish Sunset Chemicals approach is presented as an example of a semi-qualitative effects-only approach. The EURAM model-based approach is considered, along with a worked example. This forms the basis of one of the two methods elaborated in the Irish context.

Section 3: Initial application of prioritisation systems to Ireland

The appropriate criteria and the national context for Ireland are discussed here initially. Consideration was given to applying an effects-based only system to Ireland, but rejected. This was followed by an attempt to use a risk-assessment based system relying on monitoring data. The scarcity of monitoring data is discussed.

Section 4: Application of the model-based methodology to Ireland

A model-based system is then discussed in detail. This draws upon national statistics for import and export of materials. Considerable attention is given to the shortcomings in these and in the efforts to overcome these limitations. Various permutations of the underlying assumptions were attempted to provide a rational basis for prioritisation. The deficiencies of a model-based system in the Irish context are discussed.

Section 5: Use of an expert review to select a priority list of substances

Finally, an expert review approach was followed. An initial priority list of substances was developed, and the rationale for the selection of each substance is examined.

Section 6: Introduction to the Best Environmental Practice Guidelines

Best Environmental Practice (BEP) Guidelines were prepared for the selected substances, and are published separately. This section provides an introduction to the concept of Best Environmental Practice, and outlines the content of the BEP Guidelines.

Section 7: Substance Flow Analysis (SFA) – Methodology

An inventory methodology was devised to determine the flows of selected substances through the Irish economy. The potential sources of data and their relative merits are discussed, along with the need to establish a "skeleton" chain to trace the selected substances.

Section 8: Testing of the Substance Flow Analysis methodology in Ireland

The prototype methodology was tested by applying it to a limited number of substances: lead, dichloromethane, dichloroethane and nonyl phenol and nonyl phenol ethoxylate. The results of these initial flow analyses are presented.

Section 9: Recommendations

Two key recommendations are made: consideration of the introduction of a Chemical Products Register and comments on the extension of monitoring. Further elaboration is provided on a Chemical Products Register

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Section 1: Introduction

Project context

Many thousands of substances are in use. The ISIS/Riskline database contains entries for almost 180,000 substances. Of these, 100,195 are listed in the European Inventory of existing Commercial Substances (EINECS). There are 2,474 so-called High Production Volume Chemicals (HPVCs), i.e. substances produced or imported in the EU in volumes exceeding 1,000 tonnes per year. Furthermore, it is deemed that anywhere between 10,000 and 50,000 substances are used in volumes exceeding 10 tonnes per year. Each of these has an environmental impact, whether used in a pure form, or as part of a formulation. This impact may exhibit itself in any or all of the environmental compartments: water, air, soil. It may enter food chains and webs, and have an impact distant in either time or space from the initial introduction into the environment. Control of this huge number of substances is difficult. Prioritisation, or a priority setting system, is a first step in the sequential process of risk management. Faced with this large number, those that present the greatest risk to humans and the environment must be identified, to be the focus of attention. In this way, finite regulatory resources may be best applied.

In order to support this objective, the Irish Government has prepared the *Operational Programme for Environmental Services (1994-1999)*. Assisted by the European Regional Development Fund (ERDF), a number of shared-cost projects have been selected after competitive tender under the *Environmental Monitoring, R&D* sub-programme. This project, *Inventory and tracking of dangerous substances used in Ireland and development of measures to reduce their emissions/losses to the environment,* has been awarded to the Clean Technology Centre.

The primary objective of this project is "to produce a comprehensive inventory of dangerous substances used in Ireland, to track their movement from point of import to final end use and disposal and to estimate losses to the environment, particularly the aquatic environment" (1). It intends to:

- improve environmental monitoring and data collection in the interests of more detailed evaluation of the impacts of development on the environment and sustainable use of natural resources;
- encourage the production and provision of more environmentally acceptable goods and services, and
- promote better environmental quality.

It aims to provide an insight into the flows of dangerous substances in the Ireland, to prioritise those most appropriate for programmes and measures to control their use, and hence improve environmental performance.

Programmes and measures already in place

In accordance with national policy and Ireland's obligations under EU and OSPAR agreements, many steps have already been taken to control dangerous substances, a number of which may now be considered as exemplars to provide a context for this project.

In 1982, the European Commission presented to the Council of Ministers a list of 129 substances which had been selected according to their toxicity, persistence and bio-accumulation, the so-called "List I", or "black list".(2). In 1990, the Commission proposed an amendment to Directive 76/464/EEC (3) which, inter alia, contained a selection of a sub-sample of 15 substances from the above list. These substances were selected on the advice of the Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE) with particular respect to acute toxicity, persistence, bioaccumulative potential and carcinogenic or mutagenic effects. These substances were prioritised with the purpose of establishing emission limit values and quality objectives (4). This proposal was, however, withdrawn in 1993. Subsequently, on the occasion of the 19th National Experts Meeting of Directive 76/464/EEC in 1993, the application of the IPS (Informal Priority Setting) prioritisation scheme (5) to aquatic substances was presented, which resulted in two priority lists of about 230 substances based respectively on their aquatic and human risk. More recently, in preparation for the Water Framework Directive, the Fraunhofer Institute for Environmental Chemistry and Ecotoxicology in Germany presented an assessment scheme to preselect substances which have been monitored and detected in surface waters (6).

In 1967 Council Directive 67/548/EEC was adopted to provide uniform EU rules for the packaging, classification and labelling of dangerous chemicals (7). This has been amended at least twenty times since. In order to systematically evaluate the risks of the so-called existing chemicals, i.e. those substances which were deemed to be on the European Market before September 18, 1981 and, therefore, listed in the European Inventory of Existing Commercial Substances (EINECS), the EU adopted on March 23, 1993 Council

Regulation (EEC) 793/93 (8). The regulation establishes a binding framework for the data gathering, priority setting, risk assessment and proposals for the risk management of EINECS substances that are produced or imported in quantities in excess of 10 tonnes per year. Subsequent to this, two priority lists have been published (9, 10).

Authorisation of plant protection products is conducted under a framework provided by Council Directive 91/414/EEC. This requires that a risk assessment is carried out in accordance with a methodology specifically designed for active ingredients used in agriculture. In 1992, a first priority list of about 90 plant protection products, out of an estimated total of about 800 active ingredients, was adopted under Council Regulation 3600/92. A second priority list is currently under development. Recently, Council Directive 98/8/EEC, concerning the placing of biocidal products on the market, which aims to introduce a harmonised European system for disinfectants, biocides, preservatives, pest control agents and similar products has been passed.

The marketing and use of substances has been regulated under Council Directive 76/769/EEC (11). This has similarly been amended many times, including the banning of substances for particular uses, e.g. the sixteenth amendment restricted the marketing and use of hexachloroethane.

The Integrated Pollution Prevention and Control Directive (12) has, to a significant extent, been anticipated by the introduction of Integrated Pollution Control licensing by the EPA in Ireland. As well as imposing specific emission limit values on the release of substances, the obligation to prepare environmental management programmes and satisfy BATNEEC (Best Available Technology Not Entailing Excessive Costs) obliges licencees to review their operations with a major emphasis on the prevention of pollution rather than its treatment. Certain licences contain specific requirements to either reduce emissions or study the substitution of dangerous substances by less harmful ones. The “Solvents Directive” (13) aims to prevent or reduce the direct or indirect effects of emissions of volatile organic compounds to the environment, in particular to air, and the potential risks to public health.

It can be clearly seen from this small set of examples that much regulation of substances is already in place.

Policy direction

Notwithstanding the extensive regulation already applied, emphasis continues to enhance control of dangerous substances. On 26 November 1997, the Commission adopted the *Amendment to the Proposal for a Council Directive establishing a framework for Community Action in the field of Water Policy (COM(97)614, final).* Article 21 of this amendment requires the Commission to establish a list of substances prioritised on the basis of their risk to the aquatic environment and to human health via the aquatic environment. For this purpose, the Commission has proposed that the following methodologies be applied, depending on their feasibility within the chosen timescale:

1. risk assessment carried out under Council Regulation No 793/93/EEC; or
2. targeted risk assessment following the methodology of Council Regulation No 793/93 focusing on aquatic toxicology and toxicology via the aquatic medium; or
3. simplified risk assessment taking account of intrinsic hazards and environmental contamination.

It is in this context that work has been undertaken by the Fraunhofer Institute. This Directive will provide a framework to unify the various water quality Directives concerning drinking, bathing, surface, ground, etc., waters.

In addition to EU obligations, Ireland is a signatory to the OSPAR Convention for the protection of the marine environment of the north-east Atlantic, which entered into force on 25 March 1998. The objective of the OSPAR Commission with regard to hazardous substances is to prevent pollution of the maritime area by continuously reducing discharges, emissions and losses of hazardous substances with the ultimate aim of achieving concentrations in the marine environment near background values for naturally occurring substances and close to zero for man-made synthetic substances (14). There are guiding principles which involve the application of:

(i) the precautionary principle;

(ii) the polluter pays principle;

(iii) best available techniques and best environmental practice including, where appropriate, clean technology.

In addition, the principle of substitution is emphasised, i.e. "the substitution of hazardous substances by less hazardous substances or preferably non-hazardous substances where such alternatives are available, is a means to reach this objective and emissions, discharges and losses of new hazardous substances shall be avoided, except where the use of these substances is justified by the application of the principle of substitution".

This strategy has received additional political emphasis via the adoption of the "Sintra Statement" by Ministers and the European Commission. Therein it states:

"We agree to prevent pollution of the maritime area by continuously reducing discharges, emissions and losses of hazardous substances (that is, substances which are toxic, persistent and liable to bioaccumulate or which give rise to an equivalent level of concern), with the ultimate aim of achieving concentrations in the marine environment near background values for naturally occurring substances and close to zero for man-made synthetic substances. We shall make every endeavour to move towards the target of cessation of discharges, emissions and losses of hazardous substances by the year 2020. We emphasise the importance of the precautionary principle in this work.

To this end, the (OSPAR) Commission will:

(i) Implement our strategy progressively and with well-defined intermediate targets; this implementation will start from the OSPAR List of Chemicals for Priority Action which we have already agreed, included carrying forward the drawing up of programmes and measures by 2003 for the control of discharges, emissions and losses of the substances on that list, and their substitution with less hazardous or non-hazardous substances where feasible;

(ii) Develop a dynamic selection and prioritisation mechanism, in order to tackle first the substances and groups of substances which cause most concern, and use it to update the current OSPAR List of Chemicals for Priority Action;

(iii) Identify and assess substances that, although not fulfilling all the traditional criteria of a hazardous substance give rise to equivalent concern, especially those that act as endocrine disrupters;

(iv) Develop the necessary programmes and measures within three years after agreeing on the need for OSPAR action on a substance or group of substances".

Section 2: Prioritisation in risk management

Background to risk management

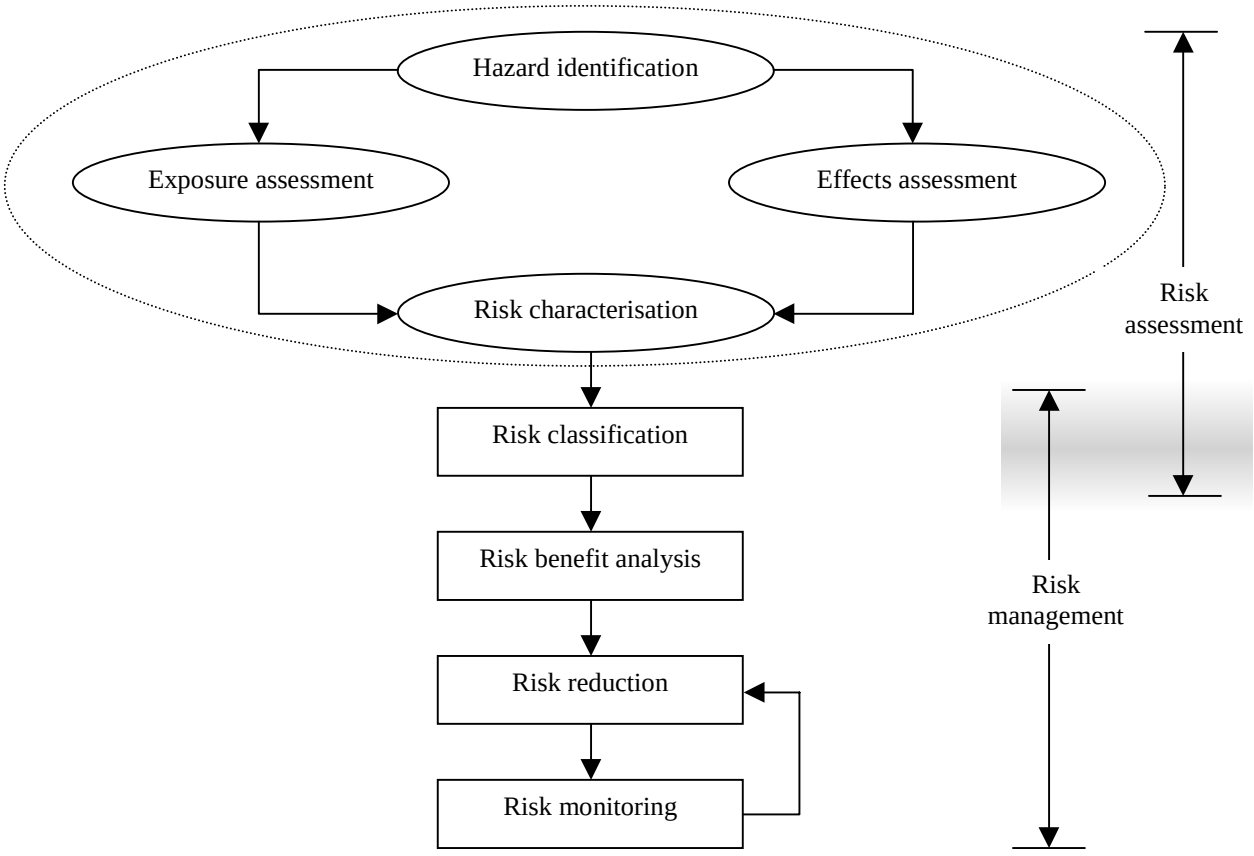
Overall structure of a model-based approach

Risk management and risk assessment are linked activities. Risk management attempts to avoid, reduce or control the risk posed by a particular dangerous substance. Management is informed by the risk assessment, which identifies the hazard, examines the mechanism whereby it causes environmental impact and considers the significance of this impact.

Risk management is considered as being composed of four elements:

- *Risk classification* is the valuation of the risk in terms of the current customs, practices and standards, which include consideration of political and social acceptability in addition to technical, scientific and economic considerations.
- *Risk benefit analysis* considers the consequences of risk reduction measures in the context of the risk presented by their absence. Feasibility, acceptability and desirability must all be considered. On occasions, financial measures are used to assist decision-making.
- *Risk reduction* entails the implementation of control measures to reduce the risk to the specified level, e.g. maximum permissible level, as low as reasonably achievable, etc.
- *Monitoring* is the final element which examines the effectiveness of the risk reduction measures, and provides input into their revision, if necessary.

Overall, the risk management process may be described as follows (15):



Risk characterisation and risk classification are the bridge between the assessment and management. They form the junction where prioritisation may be undertaken.

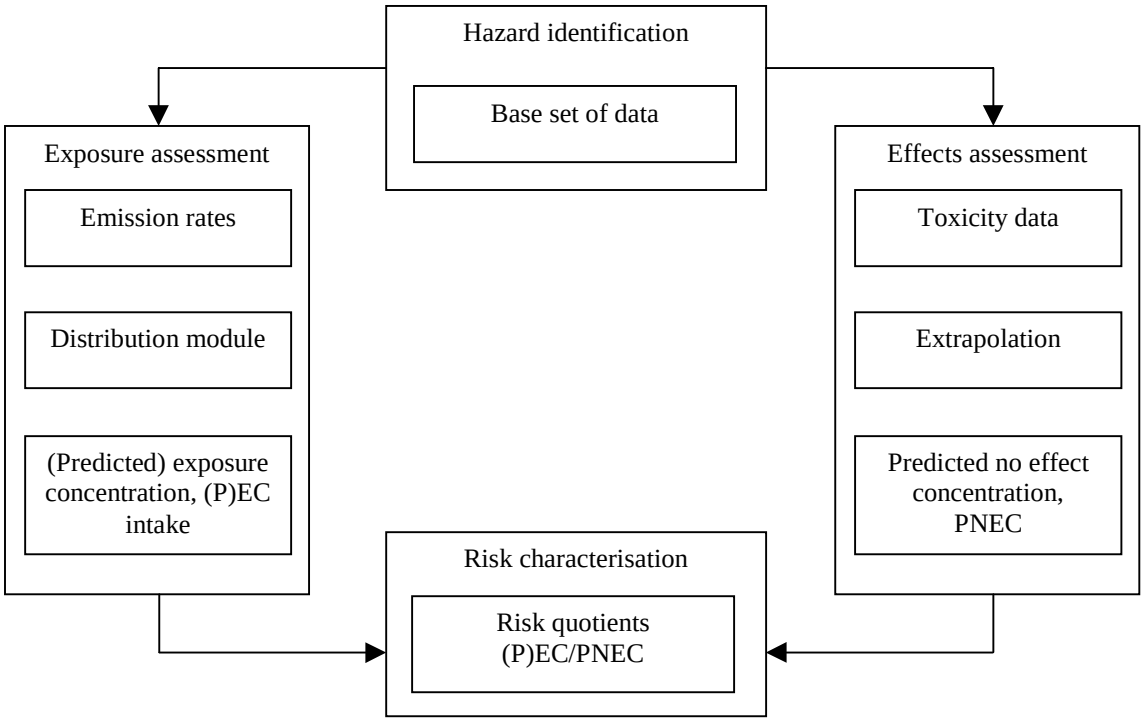
Risk assessment similarly is considered to contain four elements:

- *Hazard identification* is the identification of the adverse effects which a substance has an inherent capacity to cause, or in certain cases, the incidence and severity of an effect.
- *Effects assessment*, or more precisely, dose or response assessment, is the estimation of the relationship between dose or between level of exposure to a substance, and the incidence and severity of an effect.
- *Exposure assessment* is the determination of the emissions, pathways and rates of movement of a substance and its transformation or degradation in order to estimate the concentration/ doses to which human populations or environmental compartments are or may be exposed.
- *Risk characterisation* is the estimation of the incidence and severity of the adverse effects likely to occur in a human population or environmental compartment due to actual or predicted exposure to a substance, and may include "risk estimation", i.e. the quantification of that likelihood.

Since risk assessment provides the basis for a prioritisation, it is useful to examine this further. This "model-based" approach was initially attempted in this project.

Risk assessment

Within the EU, a model-based approach to arriving at a risk characterisation via risk assessment is currently favoured, and may be elaborated as follows:



Hazard identification is contingent on the availability of a base set of data. The content of this base set is defined for new chemicals. However, the extent of data required for the procedure in total is often in excess of that available. In this case, recourse must be made to estimated or default data. Guidelines (16) have been issued for the details of the methodology.

Exposure assessment

The assessment follows a causal chain from the origin of the substance to the place where it is available to organisms. Ideally, an exposure assessment would be performed using reliable and representative environmental monitoring data. However, this usefulness of this data is dependent on the adequacy of the number of monitoring points, monitoring frequency and monitoring techniques. Measured values can vary significantly from location to location, due to differences in production, processing, consumption and disposal and in the local environmental fate of the substance. This, in turn, varies with local environmental conditions, i.e. abiotic factors, e.g. hydrology, soil type, temperature, etc; biotic factors, e.g. differences in ecosystem structure, and on the time elapsed since the release of a substance. While such data may be available for specific cases, they are unlikely to be generally available. Hence, recourse must often be made to a model-based exposure assessment.

For a model-based approach, the following data must be available:

(i) Quantity of substance produced;

(ii) Use pattern of the substance;

(iii) Intrinsic physiochemical properties;.

(iv) Environmental fate and pathways

Equipped with this data, the following steps are applied to the modelling:

(i) Identification of emission sources;

(ii) Estimation of the quantity emitted to water, air and soil;

(iii) Estimation of the subsequent transport through and transformation in the environmental compartments;

(iv) Calculation of the resulting exposure concentrations in the compartments.

These final values are described as Predicted Environmental Concentrations (PEC), with one value for each compartment. These may be extended to estimate the daily intake rates of food and water of man and other biota.

It can be easily recognised that application of such a model requires appropriate assumptions, estimation techniques and basic data. Where available, monitoring data can validate the models.

Effects assessment

This is more precisely known as dose-response assessment. It is the estimation of the relationship between dose or level of exposure to a substance, and the incidence and severity of an effect. It involves the description of the quantitative relationship between the degree of exposure to a substance and the extent of a toxic effect or disease[15]. There are three possible sources for this data:

(i) Experimental plant and animal laboratory studies

(ii) Experimental plant and animal field studies

(iii) Epidemiological studies of ecosystems and human populations

The dose-response relationships are likely to vary for each toxic effect. From these studies, No Effect Levels (NEL) are determined. These must be derived for all the protection goals:

(i) Humans

(ii) Aquatic organisms

(iii) Terrestrial organisms

(iv) Micro-organisms in sewage treatment plants

(v) Top predators, i.e. fish-eating birds / mammals and worm-eating birds /mammals

In addition to the three primary environmental compartments, effects, not specific to a particular compartment, which are relevant to the food chain (secondary poisoning) are considered. Effects on the microbiological activity of sewage treatment plants (STP) are evaluated because their proper functioning is important for the exposure of the aquatic environment. Typically, a limited number of single species studies are the basis for further consideration. This limited data must then be extrapolated to each of the environmental compartments and for humans. Uncertainties and inadequacies in data mean that the extrapolation factors may vary from compartment to compartment and, in principle, from substance to substance. They can range between 10 and 10,000. The purpose of this extrapolation is to provide a level of confidence that no adverse effect will occur in the wider ecosystem, which can contain millions of species. This complexity is reduced to a small number of indicative measures: Predicted No Effect Concentrations (PNECs). These are concentrations below which unacceptable effects on organisms will most likely not occur.

Risk characterisation

The commonly, but not universally, accepted measure is the determination of the risk quotient for each environmental compartment (protection goal):

Risk Quotient = PEC / PNEC

If the Predicted Exposure Concentration (PEC) exceeds the Predicted No Effect Concentration (PNEC), the Risk Quotient will exceed one. Hence, the simple numerical criterion to determine if further consideration is required is:

PEC / PNEC > 1

The extent to which this exceeds one is an indicator of the degree of severity of the predicted effect.

A measure to indicate a low level of concern is:

PEC /PNEC < 0.01

To complete a risk assessment, an uncertainty analysis must be applied to the underlying assumptions and data, to determine the level of confidence in the risk quotient. Finally, the probability of an effect actually occurring may be determined, leading to a conclusion about the risk.

Risk assessment may be conducted in an iterative fashion. Ideally, all available exposure-related information should be considered. This will result in a more realistic exposure assessment. However, in the absence of this data, a "worst-case" scenario may be considered. This may place greater reliance on default values or on estimates. This is useful when there is an absence of sufficiently detailed data. If the outcome of the risk assessment based on "worst-case" assumptions for the exposure is that the substance is not of concern, the risk assessment for that substance may be stopped with regard to that compartment considered. In contrast, if the outcome is that the substance is of concern, the assessment must, if possible, be refined using a more realistic exposure prediction.

It should be apparent that the relative magnitude of the risk quotients of two or more substances will provide a measure of the relative risk. Greater confidence can be applied to the relative measures than to the absolute values of the risk. Therefore, it seems reasonable to apply the same procedure to establish a ranking, i.e. to establish a priority-setting system. However, the existence of multiple risk quotients complicates matters. Not only are these derived for the different protection goals, but they are also dependent on a number of emission characteristics with respect to time and scale, e.g. local, regional, continental. In addition, comprehensive risk assessment schemes are available for the aquatic and terrestrial compartment and for secondary poisoning, allowing a quantitative evaluation of the risk for these compartments, but the schemes for the sediment and terrestrial compartments and for secondary poisoning are currently not supported by the same level of experience and validation as available for the aquatic compartment. Further, the risk assessment for the air compartment can only be carried out qualitatively because no adequate biotic testing systems are available. If we concentrate on a single protection goal, these complications are eliminated, but may result in a narrow and inadequate consideration of the environment as a whole. Finally, the use of PEC/PNEC ratios as criteria is not universally accepted, with an alternative view that there is so much uncertainty in the method that the precautionary principle must be applied wherever there is significant cause for concern.

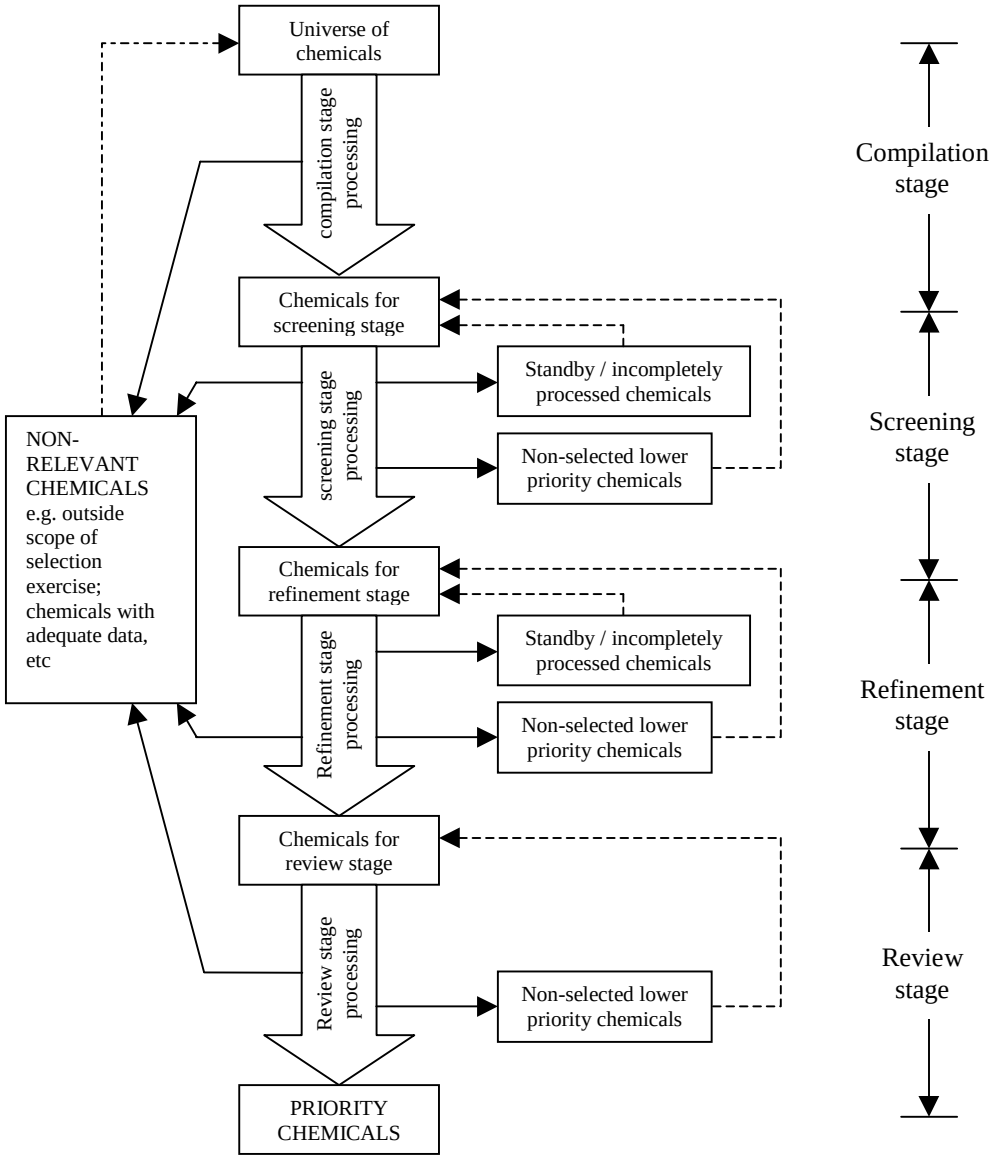
Ranking

General approach

Selecting these highest priority substances has been the subject of much investigation over the last 20 years, with increasing emphasis in the last ten. Numerous prioritisation schemes have been developed, but there has been some convergence in the generic approaches.

The OECD established the following methodology:

An initial, non-judgemental step accumulates the substances that might be of interest from the entire universe of substances. This is described as a "compilation" stage. Following this, an initial selection is conducted on the basis of readily available information, in a "screening" stage. A detailed "refinement" stage is then undertaken, where the precise ranking rules are applied. The system concludes with a "review" stage, where the recommendations from the refinement stage are examined to reach definitive conclusions. Hence, an iterative approach is required.



Priority setting according to an OECD Expert Group (OECD, 1986)

The main goal of a prioritisation strategy is to rank candidate substances with respect to relative risk, with a minimum amount of data. It is not intended to do a full risk assessment. There are three major differences between the task of carrying out the ranking leading to the priority setting and that of risk assessment (17):

(i) Focus of the evaluation

Ranking is a relative exercise. Changing the input value for one substance can change the relative ranking.

(ii) Data basis

A much smaller data set constitutes the "base set" for ranking purposes, necessitating a "global" evaluation of the substance, compared to the detailed evaluation by risk assessment.

(iii) Use of expert judgement

In principle, ranking can be applied to many more substances than risk assessment. With limited resources, less intervention by experts should be necessary for ranking, and more reliance on an automated system.

The precise ranking rules applied in the "refinement" stage are determined by the objectives and scope of the priority setting system. These systems vary in complexity, with a range of choices, not all of which are independent. Typical choices are:

(i) Ranking criteria: carcinogen/non-carcinogen; multiple factors;

(ii) Exposure consideration: intrinsic properties only / exposure related data;

(iii) Impact: human health / environmental impact / both;

(iv) Extent of quantification: integration of factor scoring / quantification / combination.

(v) Policy objectives: aquatic risk reduction / multi-media control

Choosing the carcinogenicity of a substance as the ranking criterion implies that human health protection is the objective. The intrinsic properties alone of the substance may be considered, or the likely exposure may be added to the deliberation. Considering exposure may require examination of the physical properties of the substance, e.g. vapour pressure, the mode of ingestion, e.g. oral or dermal, and the usage of the substance. Availability or reliability of data may bias the construction of the system. For example, the ready availability of monitoring data in one geographic region may lead that region to use an exposure model relying on such data. Similarly, if there is extensive research experience on the migration of substances in a particular environmental compartment, e.g. water, this may lead to a favouring of measurements from this medium. Hence availability of data may affect the setting of objectives.

Selecting a priority list of chemicals is based on imperfect data. Data will be missing, contradictory or of dubious quality. In addition, the significance of different impacts will be poorly understood. Consequently, a combination of pragmatism, expert judgement and consideration of the precautionary principle must provide guidance. There is a risk of "paralysis by analysis", whereby we wait until "adequate" data are available. This cannot be accepted.

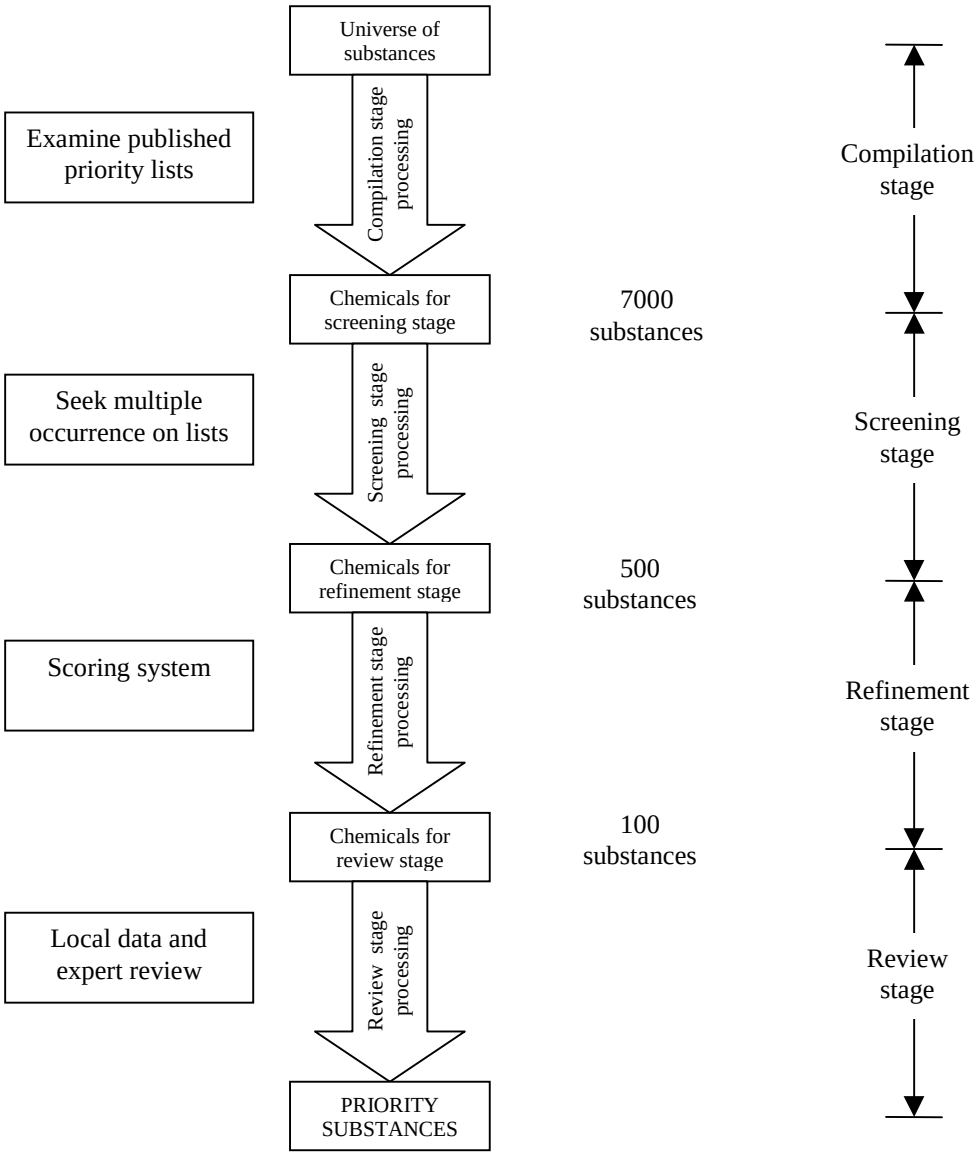
Individual countries, e.g. UK, Netherlands, Sweden, USA, Canada, Germany, Norway have produced national priority lists, with varying primary concerns. Regions, e.g. the Nordic countries, North Sea countries, have combined to produce priority lists, and international organisations, e.g. EU, OECD have also produced lists (18). A smaller number of risk reduction programmes have been developed, usually for a small number of the substances identified in the priority lists. Numerous prioritisation schemes have been developed. Most systems are semi-qualitative, assigning scores, or weightings, to the chosen factors. The weightings are then combined in some fashion to achieve an overall score. An example of this is the Swedish system, which is often cited as an example of a successful substance control policy. This will be presented by way of illustration.

Swedish Sunset system

The aims of the Swedish Sunset Project were:

1. to develop a flexible, partly computerised systematic selection procedure for hazardous chemicals
2. to identify those multi-problem chemicals which are the most crucial candidates for risk reduction measures (19).

The substances were considered as multi-problem chemicals with a high exposure potential and which are dangerous to man and the environment. The procedure may be visualised as follows:



The starting point was a database of some 70 national and international priority lists. This selection procedure was based only on existing information and did not include testing to fill data gaps. Instead, there is a reliance on evaluations and priorities made by a number of national agencies and international organisations. These lists encompassed approximately 7,000 chemicals or groups of chemicals from the entire universe of substances. They represented four major areas of concern:

(i) Environmental hazards

(ii) Health hazards

(iii) Combined environmental and health hazards

(iv) Exposure

These four major areas were then further divided into categories based on the original character or purpose of the lists. Examples of these categories are global warming, carcinogenicity, risk reduction, and chemicals released to the environment, producing a total of 19 categories. These data were then subject to a three step procedure.

Step I identify potentially hazardous chemicals

Firstly, chemicals that simultaneously occurred on lists that suggested they were harmful to human health, the environment and have a high exposure potential were identified. The number selected was reduced to 500 by imposing the condition that they should qualify under six or more unique categories.

Step II score hazardous properties in a priority setting scheme

The 500 chemicals were now reduced to 100 using data such as the published health and environmental toxicity values and classification labels. Note that up to and including this stage, all data has been based on international lists, though it may be argued that a number of these are specific to the Scandinavian region. Reduction of the 500 chemicals was achieved by applying a scoring system. However, the scoring system may be seen as providing a "qualifying" mechanism. The top 100 substances progressed to further consideration, but there was not a ranking applied between the 100 chemicals.

Step III final selection of risk reduction candidates

The selected 100 chemicals were then subject to detailed analysis, using further data relevant to Sweden and moderated by expert review. A scoring system was not employed at this point. Short hazard assessments were prepared for substances. These assessments formed the basis for review by an expert advisory group. At this point, relevance to the Swedish environment was the guiding concern. Hence, some chemicals, which were believed to be absent from Sweden, were eliminated from consideration. An outline of the use pattern was prepared for each substance. This reflected import, export, production and main uses in Sweden. Global data regarding production and main uses was also considered. The outlines of use pattern were made partly in accordance with Swedish guidelines for flow analyses of chemical substances. The main information sources were the Products Register of KemI, the Chemicals Inspectorate, Statistics Sweden and various handbooks.

Hazard assessments were not prepared for substances that:

(i) were already severely restricted in Sweden

(ii) used solely as active ingredients in pesticides

(iii) not registered in chemical products, except possibly occurring as an impurity

(iv) used solely as a raw material for synthesis, with a negligible expected exposure.

As a result, hazard assessments were prepared for a remaining 45 groups and substances from the previous 100. The main topics of the hazard assessment documents were use pattern, exposure, environmental fate and effect data, and health data.

In summary, the Sunset Project system is a multi-problem approach. It is a scoring system, using local expertise in the last stage to examine the relevance of the selected substances to the Swedish situation. It does not correspond to the EU-favoured system, which is itself being adopted by Sweden.

Common approach in EU

Considerable work has been underway in the EU over the last 10 years to provide an agreed and workable ranking system. At present, these discussions are focused on variations of the IPS (Informal Priority Setting) system (20) devised by RIVM and presented in 1993. In the context of ranking High Production Volume Chemicals under Directive 793/93, the European Chemicals Bureau has modified the IPS system to produce the so-called **EU R**isk r**A**nking **M**ethod (EURAM). The IPS (and its successor, EURAM) system is an example of a system combining scoring and quantification. Where quantification is part of the system, limitations in data availability result in the need to supply default values (typically conservative) or to resort to estimation procedures. Distortions caused by use of defaults or estimates are hopefully detected at the "review" stage. It is consistent with the risk assessment procedure recommended by the EU Technical Guidance outlined earlier. The original IPS strategy was criticised for a number of reasons. In particular, its use of default values resulted in the high ranking of substances that were considered by experts not to merit such priority. In addition, the selection was felt to be somewhat "abstract", not reflecting the actual concerns in the aquatic environment. The Fraunhofer Institute produced an amended version (21) in 1997. The basic idea of this assessment scheme was to preselect data which have been monitored and detected in surface waters. The scoring step itself was in most parts identical to the one adopted by the IPS procedure. The Fraunhofer study replaced default data by additional ecotoxicity and toxicity data taken from other databases. In these ways it was intended to overcome the short-comings of the original IPS procedure.

However, the Fraunhofer approach is heavily dependent on the availability of reliable and representative monitoring data. The Working Document (22) tabled at the National Experts Meeting on 4 February 1998 proposed a method which combines the features of both the original IPS procedure and the Fraunhofer proposal. This method, entitled **Co**mbined **M**onitoring-based and **M**odelling-based **P**riority **S**etting (COMMPS) uses both these methods in concert with a "fast-track" prioritisation of substances identified under the risk assessment procedures applicable under Regulation 793/93 for existing chemicals. Where reliable and representative monitoring data are available, exposure assessment will be determined by the Fraunhofer approach. In the absence of this data, the IPS system will be applied. Effects scoring will, in both cases, conform to the IPS approach, with the addition of ecotoxicity data and toxicity data sourced in the context of the Fraunhofer study.

The final scores are determined by using a weighting system, which differs in each of the original IPS, original Fraunhofer and COMMPS proposals.

Clearly the EURAM system has achieved some acceptance, illustrated by its use for the ranking of existing High Production Volume Chemicals and its use for ranking substances under the Water Framework Directive. Additionally, it has been accepted as a basis for progress under the OSPAR strategy for hazardous substances. However, there is still controversy attached to its use. In addition to the selection of weighting factors and combinations, there has been criticism of the Mackay Level I model. In the risk assessments for the marine environment of the OSPARCOM region conducted on behalf of EuroChlor, in referring to the model they state – "the results are valuable particularly in describing the potency of a compound to partition between water, air or sediment. Practically, it is an indicator of the potential compartments of concern" (23). However, CEFIC/EuroChlor, presenting at the OSPAR working group meeting (24) stated the following: "Modelling data at regional scale are generally unrealistic in particular if a very simple model is used like the Mackay Level I model proposed in the EURAM process", and "In many cases, a simple Mackay Level I model cannot reflect the reality and a much deeper analysis should be made." Monitoring data is preferred in determining an exposure assessment. However, this data must be representative, and is likely to be limited.

The Fraunhofer Institute sought a correlation between the substances that were subjected to both the modelling and monitoring procedures, but failed to find any. Expert opinion is divided on the significance of this. One view holds that the exclusion of outliers significantly improves the correlation. Another view maintains that since the purpose of the EURAM model is different, no correlation can be expected. A further view maintains this illustrates the inadequacies of both available monitoring results and the EURAM model.
In this project, we have taken the view that the EURAM model provides the best available model-based ranking method, in the absence of adequate monitoring data.

EURAM

The EURAM model-based approach was strictly followed in the first approach to prioritising substances for Ireland, in accordance with the recommendation of the Project Steering Committee. An overview of the method will be provided in the succeeding description, to be followed by a worked example. A full technical presentation is provided in Appendix 2. This is an unabridged presentation of the original authors.

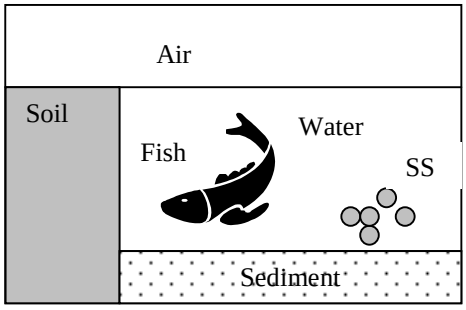
Overview

The EURAM method, as has been commented, was devised to rank the High Production Volume Chemicals recorded in EINECS. It does not use monitoring data, but instead uses a modelling approach. It is better described as a ranking algorithm or method, rather than as a model. A "model" implies an accurate representation of physical or other behaviour. The objective of the method is to rank substances relatively, rather than to precisely describe their behaviour in the environment. It relies on knowledge of the intrinsic properties of a substance, allied with a model for a substance's tendency to partition on release into the environment. It is useful to commence with a description of this partitioning model, the so-called "Mackay Level I approach".

Mackay Level I

This is a simple equilibrium model which attempts to represent the partitioning of a substance that is discharged into the environment, drawing on the intrinsic properties of the substance and the nature of the discharge environment (25). This will, of course, vary from region to region. Hence, the hypothesis is to use an "evaluative" or imaginary environment to characterise the substance's behaviour.

The evaluative environment is an area of 100,000 km^2, which is about the area of Greece. Associated with it are defined amounts of air, water, soil, suspended sediment, bottom sediment and fish.



An arbitrary quantity of 100,000 kg of substance are assumed uniformly discharged into this environment. However, the substance will preferentially migrate to the different compartments, determined by its tendency to partition between the various media. Equilibrium concentrations will be reached in each of the media. No further change is assumed to occur. This Level I model neglects the transitory migration of the substance initially and any subsequent conversion of the substance. The thermodynamic equilibrium is determined using expressions called fugacity capacities for each medium, at an assumed temperature of 25^oC. Calculating these requires data on the molecular mass, water solubility, vapour pressure and octanol-water partition coefficient. The fugacity can then be determined using the arbitrary 100,000 kg and the specified media volumes and the sum of the calculated individual fugacity capacities. Finally, the molar concentrations and amount in each medium can be calculated.

Limitations

While the EURAM approach is under development, it is currently confined to organic substances, and is not applicable to metals or inorganic metal-containing substances. Alternative models that address metals such as the COMMPS method are heavily reliant on monitoring data, which is limited in Ireland.

Hence, the criterion provided in the project specification that high priority should be given to the heavy metals can not be accommodated in the refinement stage, and must await the expert review stage.

More sophisticated models have been developed for plant protection products, and the EURAM approach is not appropriate to account for the specific use in agriculture.

The EURAM model is based on a minimum production volume of 1,000 tonnes. Since much of the Irish production volumes are less than this value, applying the model may result in a negative ranking value. The scale may still be applied to the ranking, though the negative aspect may be disconcerting.

EURAM method

The method of calculating the aquatic score is outlined on the following three diagrams:

Calculation of the environmental exposure score

Determine the usage based on production or import data	
Allocate the usage to categories with associated emission factors	
Main use category	Emission factor
Closed system	0.01
Use resulting in inclusion into or onto matrix	0.10
Non dispersive use	0.20
Wide dispersive use	1.00
Default	1.00
Calculate the emission by summing the products of individual category tonnages and associated emission factor **Emission**	

↓

Determine the distribution in the aquatic compartment by applying the Mackay Level I model **$DIST_{Env2}$**
Calculate the fugacity capacity V_iZ_i for each of the six compartments using K_{ow} and standard values and equations
Calculate substance fugacity, f, by summing the fugacity capacities and using the molecular mass & arbitrary amount of 100,000 kg
Calculate the fraction distributing into the water phase, using the water fugacity capacity, substance fugacity, hypothetical water volume and substance molecular mass
Truncate any values calculated below 0.01 to 0.01

↓

Calculate the fraction remaining after degradation, using standard OECD tests **Deg**	
OECD Biodegradability	Remaining
Ready biodegradable	0.10
Inherent biodegradable	0.50
Persistent	1.00
Default	1.00

↓

Calculate the **E**nvironment **EX**posure **V**alue for water (this is the equivalent of a PEC) **$EEXV_2$**
$EEXV_2$= **Emission** x **Dist** $_{ENV,2}$ x **Deg**

↓

Calculate the **E**nvironmental **EX**posure score for water by scaling to force into a range between 0-10 **EEX_2**
EEX_2=1.37(Log(**$EEXV_2$**)+1.301)

Calculation of the Environmental Effect Score

Gather available data from chronic (NOEC) and acute (L(E)C50) tests for different species. Preferably use chronic data. Select the lowest value. **Ecotox Test2**

↓

Determine the **A**ssessment **F**actor, based on the number of species tested **AF**

Endpoint	Number of species	Assessment factor
NOEC	>=3	10
NOEC	2	50
NOEC	1	100
L(E)C50	>=3	1000
L(E)C50	2	1000
L(E)C50	1	1000

↓

Calculate the **E**nvironmental **EF**fects **V**alue for water **$EEFV_2$**

$EEFV_2$ = Ecotox $Test_2$ / AF

Truncate the calculated value of EEFV2 at 10 ng/l if a lower value is calculated.

If no ecotoxicity data are available, use $EEFV_2$ = 10 ng/l

↓

Calculate the **E**nvironmental **EF**fects score for water by scaling to force into a range between 0-10 **EEF_2**

EEF_2 = -2 Log(**$EEFV_2$**)

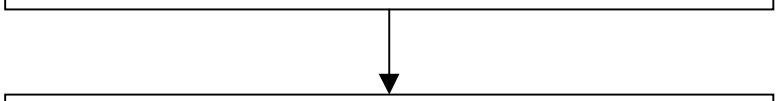
Combination of environmental exposure and effects scores for the aquatic compartment

Calculate the **A**ccumulation **P**otential from the bioconcentration factor (BCF) **AP**

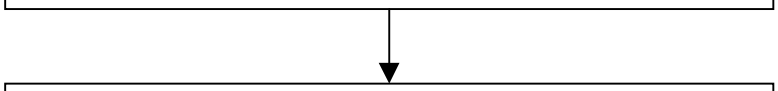
If no BCF data are available, predict using K_{ow}
Log(BCF) = -1.0+Log(K_{ow}) if MW<700
Log(BCF) = 0 if MW>700

Log(BCF)	AP
Log(BCF)<=2	0
2<Log(BCF)<=3	1
3<Log(BCF)<=4	2
4<Log(BCF)	3
Default	3

If no data are available and MW<700, set AP=3



Calculate the **A**quatic **EF**fects score **AEF**
AEF = 0.7 $\mathbf{EEF_2}$ + **AP** range: 0-10



Calculate the **A**quatic **S**core **AS**
AS = $\mathbf{EEX_2}$ x **AEF** range: 0-100

Worked example of the EURAM Method for 1,2,3-Trichlorobenzene

A worked example of the EURAM model for 1,2,3-Trichlorobenzene is outlined below. It should be noted that this example should be read in conjunction with Appendix 2 (and its associated Tables) for a full understanding of the applications and calculations involved in the model.

Section A: Environmental Exposure

Using the EURAM model, the exposure of a chemical to the environment is approximated by simple exposure models which include three factors:

1. Emissions, based on tonnage produced or imported and use patterns;
2. Distribution, based on a Mackay Level I model for the environment;
3. Degradation, based on aquatic biodegradation

A.1 Emissions

Step A1.1: Production/Import

The EURAM initially estimates the tonnage of a chemical, which could potentially be available to expose either man or the environment.

In this example, figures for imports and exports for 1995, 1996 and 1997 were used to determine the average usage of 1,2,3-Trichlorobenzene in Ireland for the period.

$$\frac{(\text{Imports (1995)} - \text{Exports (1995)}) + (\text{Imports (1996)} - \text{Exports (1996)}) + (\text{Imports (1997)} - \text{Exports(1997)})}{\text{No. of years}}$$

$$\frac{(14665 - 120508) + (92470 - 0) + (96223 - 680)}{3} = 27{,}390 \text{ kg} = 27.39 \text{ tonnes}$$

Step A1.2: Main Use Categories

Then, the main use category table (Table 1) is consulted to give an indication of the main use of a substance and can be used to estimate the emission of the substance from that use to man or the environment. In the case of 1,2,3-Trichlorobenzene the fraction and percentage of the substance emitted from different use categories is unknown and therefore the default value of 1.0 is used to reflect the worst case scenario situation.

A.2 Distribution

Step A2.1: Fugacity Capacities for Water

The fraction of the emission which partitions into the different environmental "compartments" is calculated by the Mackay Level I Model.

The fugacity capacity or Z value ($mol/m^3.Pa$) for water is calculated as follows:

$Z_2 = C^S/VP^S$ where C^S = Water Solubility(mol/m^3)

VP^S = Vapour pressure (Pa)

Therefore, the Z value for 1,2,3-Trichlorobenzene is calculated as follows:

$C^S = 31 g/m^3$

MW = 181.46

Therefore, $C^S = \frac{31 g/m^3}{181.46 g/mol} = 0.1708365 mol/m^3$

$Z_2 = \frac{0.1708365 mol/m^3}{133 Pa} = 1.2844853 \times 10^{-3} mol/m^3.Pa$

Step A2.2: Fugacity

The fugacity in units of Pa common to all media is deduced as:

$f = \frac{M (mol)}{\Sigma V_i Z_i}$ where, M is the total amount of chemical (mol)

V_i is the volume of water (m^3)

Z_i is the corresponding fugacity capacity (mol/m^3 Pa) for the chemical in that medium

The V_iZ_i calculation can be determined using Table 2 and Equations 2 to 7, the results are summarised below. **(**$K_{oc} = 0.41 (10^{\log Kow})$ ∴ for 1,2,3-Trichlorobenzene K_{oc} =5161.5942**)**

	Equation (to calculate Z)	Z (mol/m^3.Pa)	Volume (m^3)	V_iZ_i (mol/Pa)
Air	$Z_1 = 1/RT$	4.0362096×10^{-4}	10^{14}	4.0362096×10^{10}
Water	$Z_2 = C^S/V^P$	1.2844853×10^{-3}	2×10^{11}	2.56897060×10^{8}
Soil	$Z_3 = Z_2 \rho_3 f_{oc3} K_{oc}/1000$	0.3182396	9×10^{9}	$2.864156400 \times 10^{9}$
Sediment	$Z_4 = Z_2 \rho_5 f_{oc4} K_{oc}/1000$	0.6364792	10^{8}	6.3647920×10^{7}
Suspended Sediment	$Z_5 = Z_2 \rho_5 f_{oc5} K_{oc}/1000$	1.9889976	10^{6}	1.9889976×10^{6}
Fish	$Z_6 = Z_2 \rho_6 L K_{ow}/1000$	1.6170712	2×10^{5}	3.2341424×10^{5}
Total				$4.3549109792 \times 10^{10}$

Therefore, the fugacity for 1,2,3-Trichlorobenzene is determined as:

$f = \frac{(100{,}000 \times 10^3 / 181.46)}{(4.3549109792 \times 10^{10})}$

$= 1.2654349 \times 10^{-5}$ Pa

Step A2.3: Environmental Distribution

The Environmental Distribution ($Dist_{ENV2}$) denotes the fraction of the chemical which partitions at equilibrium, according to the Mackay model, into the water compartment. $Dist_{ENV2}$ can be calculated as follows:

$Dist_{ENV2}$ =**(**Z_2 (mol/m3.Pa)**) (**f(Pa)**) (**V (m3)**) (**MW(g/mol)**) (**1×10^{-3} (kg/g)**) (**1×10^{-5} (^{A})**)**

When the values for 1,2,3-Trichlorobenzene are inserted, $Dist_{ENV2}$ can be calculated as:

$$Dist_{ENV2} = (1.2844853 \times 10^{-3}) (1.2654349 \times 10^{-5}) (2 \times 10^{11}) (181.46) (1 \times 10^{-3}) (1 \times 10^{-5})$$

$$= 5.8990199 \times 10^{-3}$$

[A]: The Level I calculation describes the equilibrium partitioning of a given amount (an arbitrary 100,000 kg) which is incorporated in this equation.

In order to limit the influence of the Mackay distribution in the overall exposure score, any value of $Dist_{ENV2}$ of less than or equal to 0.01 will be set to $Dist_{ENV2} = 0.01$. Therefore, the $Dist_{ENV2}$ value for 1,2,3-Trichlorobenzene is set to 0.01.

A.3 Degradation

Degradability denotes the fraction of the chemical remaining in the environment for different levels of biodegradability (See Table 3). In the case of 1,2,3-Trichlorobenzene the fraction of emitted substance biodegraded in the aquatic environment is unknown and therefore the default value of 1.0 is chosen.

A.4 Environmental Exposure Scoring

Step A4.1: Environmental Exposure Value

The **E**nvironment **EX**posure **V**alue for Water ($EEXV_2$) is calculated as follows:

$EEXV_2$ = Emission x $Dist_{ENV2}$ x Degradability

= 27.390 t x 0.01 x 1.0

= 0.2739

Step A4.2: Environmental Exposure Score

The **E**nvironment **EX**posure Score for Water (EEX_2) is calculated as follows:

$$EEX_2 = 1.37 (\log (EEXV_2) + 1.301)$$

$$= 1.37 (\log (0.2739) + 1.301)$$

$$= 1.0118711$$

Section B: Environmental Effects

B1: Chronic and acute toxicity results

In order to calculate the **E**nvironmental **EF**fects **V**alue ($EEFV_2$) for water, several steps must be followed. Initially, the data available from acute and chronic tests for different species must be determined. If chronic NOEC (No Observable Effects Concentration) values are available for one or more species, then these data are used and the acute data neglected. However, if no NOEC values are available, then the acute data must be used.

The NOEC values for 1,2,3-Trichlorobenzene were derived from the Fraunhofer database (STOFFNAME) as 0.169 mg/l. From Table 5, an assessment factor (AF) was derived using the NOEC value and the number of species tested. The AF for 1,2,3-Trichlorobenzene is 10.

B2: Environmental Effects Value Scores

The **E**nvironmental **EF**fects **V**alue ($EEFV_2$) for the water compartment is calculated as follows:

$$EEFV_2 = \frac{\text{Ecotoxicity Test}}{\text{Assessment Factor}}$$

$$= \frac{0.169 \text{ mg/l}}{10} = 0.0169 \text{ mg/l}$$

In some cases, in order to restrict the possible range of EEFV, the EEFV is truncated at values below 10 ng/L. This does not apply to the value for 1,2,3-Trichlorobenzene. The logarithm of EEFV is normalised to between 0-10 as follows:

$$EEF_2 = -2 \log (EEFV_2)$$

$$= -2 \log (0.0169)$$

$$= 3.544$$

Section C: Environmental Combined Exposure and Effects Scoring

C1: Environmental Score

The Environmental score (ES_2) for the water compartment is calculated as follows:

ES_2	=	EEX_2	x	EEF_2
	=	1.0118711	x	3.544
	=	3.5860711		

C2: Aquatic Effects Score

Step C2.1 Calculation of BCF

The environmental score for the aquatic compartment can be used directly for ranking. However, as BCF is not used in calculating the environmental score for the aquatic compartment, but is generally available, the final score for the aquatic environment can be improved by combining both ES_2 and BCF. This combination of two scores is done so that maximum use can be made of generally available data.

The calculation for BCF is determined by the MW of the substance,

If MW < 700 then	log BCF = -1.0 + log (K_{OW}),
if MW > 700 then	log BCF = 0

Since 1,2,3-Trichlorobenzene has a MW of 181.46, the BCF can be calculated as follows:

Log BCF =	-1.0 + 4.1
=	3.1

Step C2.2: Calculation of Accumulation Potential (AP)

The Accumulation Potential for 1,2,3-Trichlorobenzene can then be calculated using Table 4. In this instance the log BCF value lies between 3 and 4 and therefore the Accumulation Potential is 2.

Step C2.3: Calculation of Aquatic Effects Score and Aquatic Score

The Aquatic Effects Score (AEF) is thereby calculated as:

AEF	= 0.7 EEF_2	+ AP
	= 0.7 (3.544)	+ 2
	= 4.4808	

The weighing of the two factors is not based on scientific arguments, but on the political relative relevance of the two factors (toxicity versus persistence) in determining risk reduction needs.

The Aquatic Score is the product of the EEX_2 and the AEF:

AS	= EEX_2	x AEF
	= 1.0118711	x 4.4808
	= 4.533992	

Section 3: Initial application of prioritisation systems to Ireland

Devising the potential approaches

In devising an appropriate system, it is useful to identify the criteria that such a system must satisfy, and also the context in which it must operate. A methodology was established, and a number of approaches were considered. As will be seen, use of an effects-only based system and a monitoring based risk assessment system were examined, but rejected as inappropriate.

Context for an Irish system

Key national policies must be respected by any chosen system. The major elements of these policies are:

- Precautionary principle;
- Polluter pays;
- Prevention of pollution;
- An integrated media approach.

The relatively recent affirmation of these policies in the national strategy for sustainable development has implications for existing strategies which have evolved over many years. For example, the adoption of Integrated Pollution Control (IPC) Licensing and the expression of the Prevention Principle in both the EPA Act and Waste Management Act alter the emphasis of regulation. The existing Water Pollution Act and Air Pollution Act have a distinct single medium emphasis. In addition, prevention does not receive the same stress. The application of the Polluter Pays Principle is receiving greater attention, e.g. charges for IPC licensing, and while the Precautionary Principle has under-pinned Irish policy for some time, it has now received further consideration.

Any system devised for Ireland should satisfy the following criteria:

1. conform to national policies;
2. consider substances that are nationally relevant;
3. be flexible to accommodate substances new to Ireland;
4. be systematic;
5. be transparent ;
6. reflect current international practice;
7. have regard to international obligations.

Prioritised substances must be relevant in an Irish context. Hence the focus which might be applied to particular substances at an OSPAR or EU level might not be appropriate. Both of these bodies are concerned with larger geographic areas. OSPAR is considering the entire north-east Atlantic, and the EU may decide that substances must have been detected in three or more member states to warrant consideration. It is a waste of resources to apply monitoring and risk management activities to substances that are unlikely to arise. Furthermore, this would distract from the significance of the substances that do merit control. Industrial acceptance will be necessary for any proposed measures. This will be more difficult to achieve if the priority list contains irrelevant substances.

A priority list will not be a static policy tool, but should evolve. Substances may become less significant if, for example, they have been phased out. Alternatively, substances new to Ireland or used in increased quantities might be re-categorised.

The system must be systematic and transparent to allow peer review, identification of its strengths and weaknesses and to facilitate discussions with industry and commerce. It should reflect current international practice, to add credibility to the system, and avoid inconsistencies in the treatment of substances.

Major factors that would assist or inhibit an effective ranking system in Ireland are:

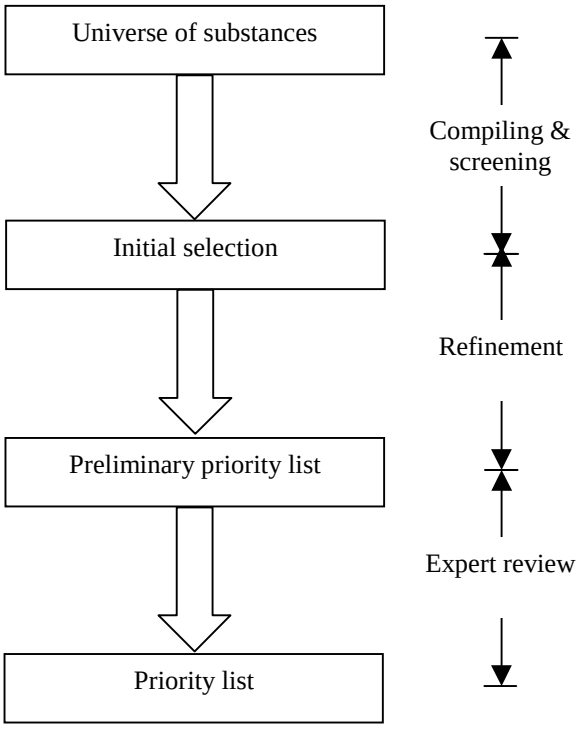
Advantages	Disadvantages
Integrated Pollution Control Licensing is in place for the major consumers of chemicals.	There is not a Chemical Products Register, which would assist the determination of the content of preparations (formulations) or artefacts, and their use patterns.
Polluting Emission Registers are obligatory for IPC licensed companies, though the accumulation of this data is at an early stage, and the specification of priority substances is dependent on the particular licence.	Environmental monitoring data is very limited.
Substances in use must conform to the Classification, Packaging and Labelling Regulations to satisfy occupational exposure requirements.	There is no central register of substances used in the workplace from an occupational control viewpoint. There is limited experience with substance control from an environmental regulation viewpoint.
All substances imported into the country must conform to Customs & Excise regulations, which already require reporting of the nature of the substances in accordance with Customs classification. In addition, the initial receiver is reported. Production data is also reported to the Central Statistics Office.	The reporting system is established for economic, primarily fiscal, measurement purposes. Precise data is not available to other Government agencies where the information is considered commercially sensitive.
Pesticides are regulated by the Pesticides Control Unit, which has data on the magnitude of quantities used.	Pesticides quantities are only available as ranges of magnitude, to protect commercial sensitivity. Products classified as veterinary medicines, e.g. sheep dip, are regulated by the Irish Medicines Board, and quantities in use are not reported.

Recognising these factors, we can turn to the adopted methodology.

Adopted methodology

There are three stages to the adopted methodology. This broadly follows the approach of the OECD methodology.

Stage	Activity	Output
1	Compiling & screening	Initial selection
2	Refinement	Preliminary priority list
3	Expert review	Priority list



Compiling & screening: initial selection

Following the recommendation of the Steering Committee, an extended OSPAR list of 381 substances, as presented in Appendix 1 has been chosen. This list reflects the substances which have been of international concern historically, and also substances which are considered suspect or of potential concern more recently.

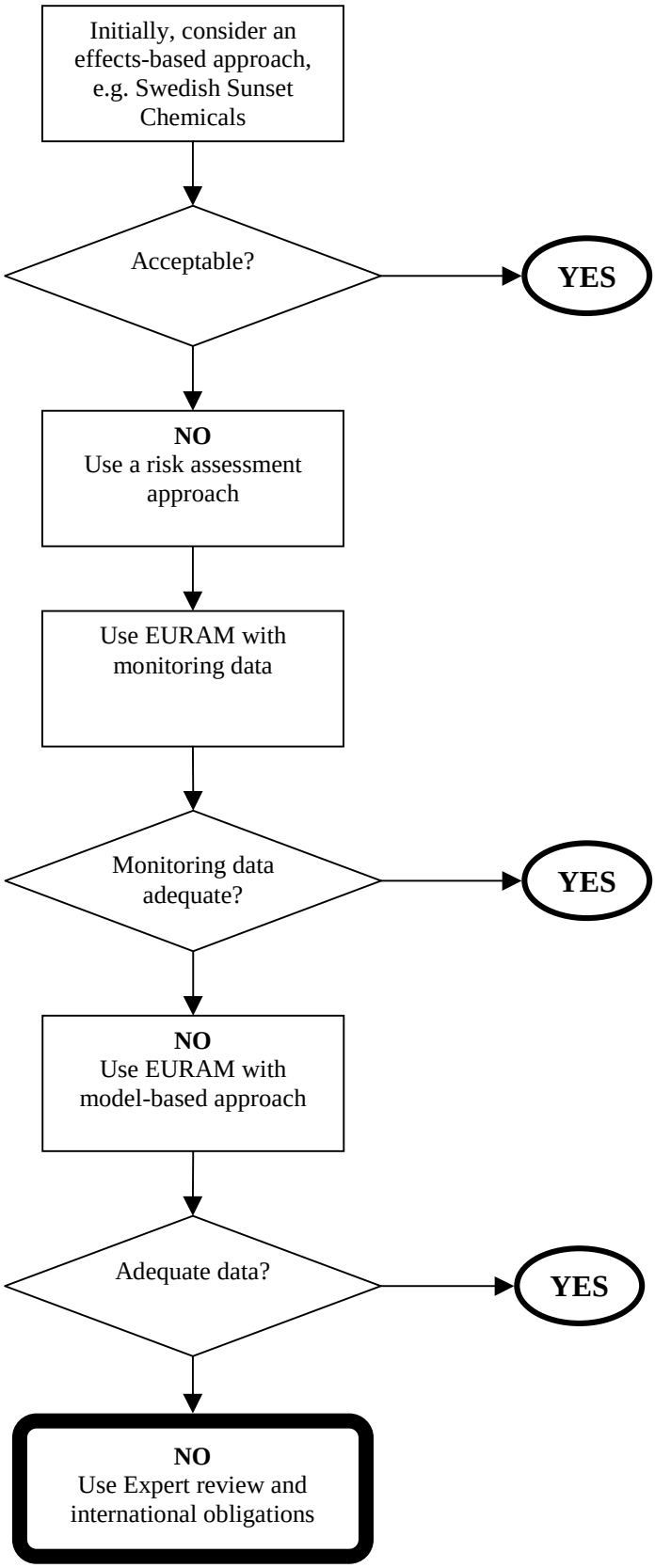
It should be emphasised that the methodology will accept the addition of any number of substances.

Refinement: preliminary priority list

A number of approaches were applied. Initially, a risk assessment type approach was considered. At first, an effect-only approach was considered. This was then altered to consider exposure also, using a EURAM based system. Preference would be given to using monitoring data if it were available, however, this proved not to be the case for Ireland. Hence, a model-based approach was followed in detail. An aquatic priority score was sought, to reflect the project specification. Unfortunately, this again failed, primarily due to lack of data. Finally, and expert review and consideration of international obligations led to the proposed priority list.

The decision sequence is outlined in the following diagram. Each approach will be considered.

Decision sequence for prioritisation system for Ireland



Experience in considering an effects-based approach for ranking

An extensive review was undertaken of the priority lists which have been devised world-wide. Most of these existing lists have been based on the effects of dangerous substances. These effects arise from the intrinsic properties of the substances. Actual exposure may not be considered. Of course, without exposure, there is no impact. Looking at these lists in more detail, the Swedish Sunset Chemicals system appeared to be very attractive, since the Swedish list linked with subsequent risk management.

The research team initially recommended the adaptation of the Swedish system as the preferred starting point for a prioritisation strategy (26). However, after extensive discussion with the Steering committee, it was agreed that it would be more appropriate to adopt a risk assessment-based system. The following table outlines the factors considered:

Comparison of the Swedish system and a risk-assessment based system

Comment	**Adaptation of the Swedish system**	**Risk assessment-based system**
Positive features	Multi-problem oriented. This conforms with the Irish integrated media approach "New" substances may be accommodated, assuming they have been assigned the appropriate Risk phrases, etc. National substance usages, if known, may be used to modify any ranking.	Conformity with EU direction; a variant will be adopted under the Water Framework Directive. Conformity with OSPAR direction. Sunset Chemicals system is being reviewed by Sweden, itself.
Negative features	Scientific basis less valid, relying on pre-existing priority lists. Lists may be deficient, outdated or irrelevant.	Single-medium approach. Aquatic focus, primarily freshwater. Reliant on relatively more data and acceptance of estimates.
Assessment	This is relatively easy to apply, builds on experiences with both the Irish regulatory framework and the Swedish Sunset Project.	This is likely to be the ultimate EU selection system, but is primarily single-medium, and has numerous underlying approximations, which are not apparent on the surface. A significant amount of data is required.

CONCLUSIONS

1. A multi-factor effects-only approach does not match the current EU direction.
2. It does not conform with the project specification, which emphasises an aquatic focus.
3. A risk assessment based approach, combining exposure as well as effects, should be followed.

Experience in considering a risk-assessment approach relying on monitoring data

Introduction

Monitoring data reflects actual exposure to hazardous substances. However, to be useful, it must be representative, accurate and reliable. Prior to applying a prioritisation scheme using such data, the availability and adequacy of the data must be considered.

This review of aquatic monitoring data in Ireland focuses on the following issues and factors:

- The regularity of monitoring
- The parameters considered in the monitoring
- The aquatic environments monitored
- How localised or widespread were the areas monitored

These data are listed by the authorities or agencies that produced them.

REGULAR MONITORING OF AQUATIC ENVIRONMENTS

Regular monitoring data regarding the incidences of hazardous substances are vital for any aquatic-based prioritisation programme. Incidence rates and trends are essential if substances are to be highlighted and chemical programmes are to be introduced in Ireland. There are three regular current monitoring activities of Irish aquatic environments - carried out by the EPA and the Department of the Marine/Fisheries Board/Marine Institute.

Environmental Protection Agency

Quality of Drinking Water in Ireland

These surveys extensively monitor the nation's drinking water supplies annually. Their parameters include: aluminium, ammonium, coliforms, colour, fluoride, heavy metals (cadmium, copper, lead, zinc), iron, manganese, nitrates, nitrites, odour, pH, taste, turbidity. Some of these substances, especially the metals, may be of relevance to this project.

Water Quality in Ireland 1991 - 1994

This is the most recent report on water quality data that is regularly gathered (currently by the EPA, previously by the ERU). In its statistical compendium, it gives tabulated data for synoptic chemical and biological data for the 1170 rivers and streams monitored. It focuses on three main aquatic environments:

i) rivers and streams - this section surveys biotic indices (Q values) and allocates value of Q1 (very low community diversity) to Q5 (high community diversity). It then allocates one of four classes, A (unpolluted), B (slightly polluted), C (moderately polluted) and D (seriously polluted) to the waters. Parameters include: biological assessment - determines how faunal groups are affected; physico-chemical assessment - DO, BOD, Ammonia, Chlorine, Oxidised Nitrogen (Nitrates and Nitrites), 'ortho Phosphate' and colour. Some of these substances are of obvious relevance to this project.

ii) lakes - eutrophication: concentrates on phosphorus and nitrogen. These parameters are of little value to this project.

iii) estuarine and coastal waters - mostly organic wastes also: DO, BOD, ammonia, oxidised nitrogen and phosphate; heavy metals noted due to mercury, copper or arsenic based paints on the hulls of ships and other craft. These substances are hazardous and may form special attention in any Chemicals Programme. This information is therefore of value.

The Marine Institute, Department of the Marine

Monitoring of shellfish growing areas - 1993, 1994, 1995

These studies examined sites all around the coast over these three years. The parameters considered were: Aluminium, Cadmium, Chromium, Copper, Lead, Mercury, Zinc, chlorinated hydrocarbons such as: CB Congeners, DDD, DDE, DDT, Lindane, Chlordanes, Dieldrin, HCB etc. Findings showed a low level of contamination, both of heavy metals and organics. These reports are of special interest since metals and other seriously hazardous substances were monitored on a regular basis. Since this monitoring is ongoing annually, valuable trends may be identified that could help in the development of hazardous substances prioritisation.

IRREGULAR, ONCE-OFF, OR LOCALISED MONITORING DATA

While data that is gathered irregularly, on a once-off basis or in localised aquatic environments may be useful and may provide information of value to this project, they do not allow the analysis of trends in the incidence of

hazardous substances. If incidence of hazardous substances is high, however, then any such study is of value since it highlights a real problem that should be of relevance in any prioritisation decisions. The parameters of some of the studies below are also relevant to prioritisation of hazardous substances.

Cork County Council (CCC)

Annual Environmental Reports, 1993-1995:

Water Supply Monitoring - this section of these reports looks at the following parameters: total coliforms, faecal coliforms and conductivity, chlorine, aluminium, fluoride, ammonia, nitrate, nitrite, pH, turbidity total bacteria. Details of EPA reports on rivers and drinking is usually given. This data obviously focuses on water in the County Cork region although other local authorities produce similar reports. Some of the parameters may be of use.

Environmental monitoring of Industry Reports

These reports look at discharges by companies (data given by companies themselves) and can give information of substances considered in this project but there is no ongoing monitoring of waters.

Environmental Research Unit (ERU)

Cork Harbour Water Quality (1989)

This is a detailed study of water in Cork Harbour. Parameters include temperature, salinity, pH, dissolved oxygen, biochemical oxygen demand (BOD), nutrients, turbidity, and contaminants. In the sedimentary study, parameters include: organic content, nutrients, BOD, pH and eH, iron, copper, lead, zinc, manganese, chromium and nickel, cadmium, mercury, vanadium, arsenic and tin, aluminium, organic compounds including organochlorides.

While many of these substances are under scrutiny in this project, this once-off report is 10 years' old now and current figures may be much different. Also the report is very localised in a region with specific factors that are not relevant elsewhere.

Water Quality in Ireland - A review of water resources, water supplies and sewerage services (1991)

The chapter on Water Quality and Pollution gives an overview of the 1991 situation regarding: nature and magnitude of waste sources, assessment of water quality, river water quality, nitrate concentrations in river waters, contamination of water by toxicants, short term pollution events, acidification of surface waters, lake water quality, and estuarine and coastal water quality. All sections report low levels of contamination except for some areas of Liffey and Lee estuaries near sewage system out-falls from Dublin and Cork respectively. Parameters noted in toxicants section: metals: cadmium, chromium, copper, lead, mercury and zinc; and pesticides. Low levels of found except for copper, zinc and cadmium in the Avoca River due to leachate from former mining activities. Since this report is not localised and gives data on waters around the country, its figures are of interest, as are some of its parameters. But it was a once-off study some years ago.

Dublin Bay water quality management plan: technical report no. 5: water quality surveys (1991)

Water quality survey of Liffey estuary and Dublin Bay and of freshwater inflows based on surveys from 1986-1988. Parameters: DO, BOD, Ammonia, Oxidised Nitrogen (Nitrate and Nitrite), Phosphates, Faecal Coliforms, Total Coliforms, Enterococci, Chlorophyll, Transparency. Results show some localised problems especially: organic contamination in the lower reaches of the inflows; some high incidences of chemicals near the Ringsend discharge and lower estuary. Some anomalies due to infrequent testing are apparent. Again this report gives once-off and localised data only, though some parameters are of interest.

Environmental Protection Agency (EPA)

State of the Environment (1996)

No detailed new data was produced for this report, 2 relevant chapters in inland water and estuarine/coastal waters, refer mostly to the 1991-1994 survey of water quality (see above).

Pesticides in Drinking Waters: results of a preliminary survey December 1994 - December 1995

Samples from 27 Sanitary Authorities were taken, at least 5 supplies from each authority. Parameters: 9 groups of target compounds: BHC isomers; aldrin, dieldrin, eldrins, isodrin; Heptachlor and heptachlor epoxide, DDT and related compounds, Endosulfan group; organophosphorus pesticides; triazine herbicides; other pesticides analysed by GC; acid herbicides and pentachlorophenol analysed by HPLC. No significant background levels of

any of these compounds were found. Since pesticides are not of specific interest for this project, this report is not of significant value, but in a chemicals programme that would included these substances, it would be of interest.

Trace Chemicals Survey, 1994

Sampling of rivers downstream of towns for a range of target compounds. Parameters: 13 metals, 13 pesticides, 51 VOCs, 14 substances of which are List 1 substances. Data for all 76 substances is given in the three groups. Results for List 1 substances also given separately and compared to Environmental Quality Standards. The quality standards are achieved for 8 of the List 1 compounds, for 6 others the limits of analysis need to be lowered and 3 compounds were not covered in this survey. This is a significant study since so many parameters are hazardous substances. The somewhat localised area surveys (downstream of towns and compounds) detract from the value, as does the fact that it was a once-off study. Further similar studies would however be of value since trends could be identified.

Environmental Quality Objectives and Environmental Quality Standards: the aquatic environment, a discussion document (1997)

No data of incidence are given here. EQOs and EQSs are given for several substances, however. Useful details of Irish obligations under international laws and regulations are also highlighted.

Lough Ree : an investigation of eutrophication and its causes 1996

Survey of Lough Ree between June 1993 and October 1994. Physico-chemical and biological examinations performed on 16 occasions at 18 locations, and chemical examinations for the main rivers in the catchment area. Principle parameters: Dissolved Oxygen (DO), Biochemical Oxygen Demand (BOD), Total Phosphorus, Molybdate Reactive Phosphate (MRP), Morgans Soil Phosphorus Test, Oxidised Nitrogen (Nitrate and Nitrite), Chlorophyll "a", Water Transparency. Findings indicate the lake is now eutrophic, significant increases since 1979-82 survey of total phosphorus, molybdate reactive phosphate and chlorophyll, a reduction in water transparency and oxidised nitrogen. While this study does indicate a problem widespread in Ireland, its parameters are not of significant value for this project.

Urban Waste Water Discharges in Ireland: A report for the years 1994 and 1995

Data supplied by sanitary authorities with populations greater than or equal to 2,000 on the quality of effluents being discharged from treatment plants, sewers or drainage pipes under their control. 151 discharges tested from a variety of treatments and no treatment (41%). Parameters: BOD_5, Chemical Oxygen Demand (COD), Total Suspended Solids, Total Phosphorus and Total Nitrogen. Results indicated that in many cases, further treatment is recommended.
Sewage sludge was also tested. Parameters for sewage sludge: Cadmium, Copper, Nickel, Lead, Zinc, Mercury. Levels all below recommended limits. Again the data is useful since it focuses on areas of widespread concern and its parameters include some heavy metals that are classified as hazardous. Follow up similar surveys are necessary.

Department of the Marine/Fisheries Board/Marine Institute

Levels of metals and organic contaminants in mussels Mytilus Edulis from Cork Harbour - 1989

200 mussels tested from a site in the outer part of Cork Harbour. Parameters: mercury, cadmium, lead, copper and zinc, and a range of organochlorine compounds including pesticides and polychlorinated biphenpyls (PCBs, IUPAC congeners nos. 28, 52, 101, 118, 1153, 138, 180). Levels of contaminants of both heavy metals, organic contaminants and pesticides generally well within the ranges found in North Atlantic Shelf area and other studies. Some levels of zinc were found to be high. Very useful figures for some hazardous substances, but the localised and once-off nature of the study detract from their relevance for the national prioritisation of such substances.

Mercury concentration in fish from Irish waters in 1992, 1993, 1994

Mercury concentrations taken in fish and shellfish. Parameter: Mercury. Overall, low levels of contamination confirming previous studies. Useful data presented on mercury.

Chemical contaminants in Irish estuarine and coastal waters, 1978 to 1988

Mussels and oysters from 26 estuarine and coastal locations studied as well as fin fish landed from all coasts. Data on heavy metals and nutrients in sea water and heavy metals in sediments for 9 estuaries also reported. Parameters included: Mercury, Cadmium, Lead, Copper and Zinc, Chromium and Nickel, Chlorinated

Hydrocarbons and Nutrients. Four cases of elevated concentrations of cadmium, two each of copper, zinc and mercury and one of lead were reported with the overall trend for stability. The degree of organochloride contamination was low in all estuaries. Exceptionally low levels of contamination overall. This is a very useful study since so many relevant parameters were considered and the data locations are widespread. Follow-up studies would give very worthwhile trends in this aquatic environment.

Metal levels in Cork Harbour Mussels - 1993

Several sites in Cork Harbour and a background site in Roaringwater Bay were considered. Parameters include: Mercury, Cadmium, Lead, Zinc, Chromium, Copper. Apart from high levels of lead in Cork Harbour, levels of metals have remained fairy constant over the 8 or 9 years preceding this study. Since this study gives data over a number of years, trends for metals in mussels can be identified, but the location is too localised for general use.

Contaminants in marine biota 1990 monitoring programme

Shell and fin fish were studied from a wide variety or sources. Two levels of analysis were undertaken: human health and environmental health. Parameters: Heavy Metals: Cadmium, Copper, Lead, Mercury, Zinc; Chlorinated Hydrocarbons: HCB, A-BHC, Lindane, Dieldrin, DDTs, PCBs. Again some useful parameters were covered and from a variety of locations. But follow-up and more recent data would be necessary.

Greenpeace

The Dirty Dozen: the top dozen chemical and pharmaceutical plants licensed by the Irish state to discharge toxic waste into Irish water, 1994

This study of the pollution licenses of 12 of the 'worst' companies in Ireland details the hazardous substances that they are allowed to use. Paris Convention black and grey list chemicals are listed. Details of the substances given for each company but no specific data on the aquatic environment given.

Department of the Environment / K.T. Cullen & Co.

Trace Organic Contaminants in Irish Groundwaters 1994

Study of trace organics in Irish groundwaters from 91 wells and springs. Trace organics divided into VOCs and SOCs. 75 VOCs were identified as priority pollutants and analysed for. Most priority pollutant SOCs subdivided into phenolics, polynuclear aromatics, PCBs, and agricides. Priority Pollutant List of trace organics produced listing 63 VOCs, 9 acid extractable SOCs, 20 Base/Neutral Extractable SOCs, and 32 PCB and Agricide SOCs. Other parameters: Inorganic: pH, conductivity, temperature, nitrate, lead, manganese, ammonia ; Organic: total coliforms, e-coli, faecal streptococci etc.

CONCLUSIONS

The following conclusions may be drawn from this overview of aquatic monitoring data in Ireland:

1. The current levels of data are an inadequate basis for an exposure assessment element of a prioritisation system based on risk assessment, due to the irregularity and scarcity of monitoring.
2. Many surveys of a wide range of waters are of some use and can be built upon to draw a more complete picture.
3. Many localised surveys are also relevant but such surveys need to be extended to a wider area to get a broader Irish picture.
4. Current monitoring parameters concentrate on metals but the incidence rates of many other hazardous substances are not monitored and hence are not known.
5. This data will serve to inform any expert review of a proposed priority list.

Section 4: Application of the model-based methodology to Ireland

Introduction

Having demonstrated the inappropriateness of using monitoring data to assess exposure to the selected dangerous substances, the alternative approach in the EURAM model, i.e. the use of a model-based approach was examined.

A significant number of substances have been excluded from the automatic ranking, because of the inapplicability of the EURAM method. While the method is under development, it is currently confined to organic substances, and is not applicable to metals. Hence classes of metal and metal containing inorganic substances on the expanded OSPAR list are not addressed. There are 22 metals in addition to metal oxide and organo-metal compounds. Organo-metallic compounds may be addressed, because they exhibit properties similar to non-metallic compounds. It may be further remarked that alternative models that address metals such as the COMMPS method are heavily reliant on monitoring data. Previous reports for this project have pointed out the inadequacy of such data in Ireland. Hence, the criterion provided in the project specification that high priority should be given to the heavy metals – copper, lead, zinc, nickel, chromium and arsenic can not be accommodated in the refinement stage, and must await the expert review stage.

The project specification excludes “agrochemical pesticides”, i.e. that are used solely for agricultural use, but includes such substances if they are used outside of agriculture, e.g. gardening, parks maintenance, golf courses, animal health, roads and railway maintenance. However, the EURAM method, as explained earlier, is not appropriate to this type of substance. There are 98 pesticides on the list of 381 substances. Consideration of these must also await the expert review stage.

The environmental effect score is based on data from chronic (NOEC) and acute (L(E)C50) tests for different species. These data are subjected to an assessment factor, based on the number of species tested and the nature of the tests, whether chronic or acute. The environmental effects value is truncated at 10ng/l if a lower value is calculated. If no eco-toxicity data are available, this value of 10 ng/l is applied as a default.

An exposure score is calculated. This requires adequate usage/production data and information on the emissions likely to arise from the use patterns. The usage/production data was determined from the import-export data reported by the Central Statistics Office. This was assumed to be correct, and an average value was calculated for the years 1995-1997. A widely dispersive use was assumed in each case, the environmental distribution calculated with the Mackay model and the degradation scored from the results of standard testing.

Exposure score

Usage / Production data

Import / export data has been based on the data recorded according to the tariff classification system operated by the Revenue Commissioners in accordance with the European Customs Inventory of Chemicals. Under this system, a large number of substances are assigned a Combined Nomenclature - “CN” - number. This forms the basis for recording the flow of these substances, from the viewpoint of assessing the economy in general, but more particularly for fiscal purposes. While there are over 100,000 substances, there are only between 10,000 and 20,000 CN numbers allocated. The latest printed version of the inventory was issued in 1997, but the 1998 inventory has been consulted with the co-operation of the competent authorities in Brussels.

If a substance does not possess a CN number, we may validly conclude that it has not entered EU trade in pure form. Where a substance possesses a CN number, and this CN number is recorded as having zero imports or exports, we may validly conclude that this substance has not been used in pure form in Ireland in the period 1995-1997.

While internationally used, this classification system presents some difficulties for the task in hand. This system refers only to defined chemical products. The inclusion of a substance in a product is not subject to registration. Hence accounting for substances incorporated in products requires a detailed inventory study for that particular substance. It has not been possible to conduct these inventories for all substances on the extended OSPAR list with the personnel and financial budget available in this project. Lead was chosen as an example in developing the inventory methodology. This demonstrated the extent of investigation required. It is recognised that this is a significant deficiency in the study at this stage, but correction of this is only possible with a significant commitment of resources.

The limited number of CN reference numbers introduced considerable uncertainty. A substance may be considered as belonging to one of four categories from the viewpoint of this study:

(a) Possessing a unique CN number;

There are 55 substances on the list conforming to this category. These are identified in Appendix III. For these, it is possible to obtain exact import / export data, presuming the CSO data is correct.

The remaining 326 substances share a CN number. It is not, at present, realistic to reference from CN number to CAS number, hence the precise nature of the sharing may be unclear. Examining the description assigned by the Combined Nomenclature may give some clarification of this ambiguity. These shared numbers correspond to one of the following three categories.

(b) Sharing a CN number solely with other substances on the list;

CN 29029010 is an example of category (b). It is described as "naphthalene and anthracene". Hence, only these two substances, both of which are on the extended OSPAR list used for this study, are assigned this number.

(c) Sharing a CN number with other substances on the list, and more unlisted substances;

There are numerous examples of category (c). For example, CN 29011090 is described as "saturated acyclic hydrocarbons (excl. for use as power or heating fuels)", and contains both pentane (CAS 109660) and octane (CAS 111659), which are on the list, but also may be expected to contain hexane and heptane.

(d) Sharing a CN number with unlisted substances.

Category (d) is illustrated by CN 29031600 which is described as "1,2-Dichloropropane "propylene dichloride" and dichlorobutanes". 1,2-Dichloropropane (CAS 78875) is on the list, but dichlorobutanes are not. A further example is CN 29033031. This is described as "Dibromoethane and vinyl bromide". 1,2-Dibromoethane is on the list, but vinyl bromide is not. However, the sharing of the CN number is explicit, which removes uncertainty.

Grouping of substances

The number of substances described by the CN number may be large. For example, CN 29081090 describes "Derivatives containing only halogen substituents and their salts, of phenols or phenol-alcohols (excl. brominated derivatives)" and contains 10 substances on the list:

CAS	Substance	CAS	Substance
59507	Chlorocresol	108430	3-Chlorophenol
87865	Pentachlorophenol	120321	2-Benzyl-4-chlorophenol
95578	2-Chlorophenol	120832	2,4-Dichlorophenol
95954	2,4,5-Trichlorophenol	576249	2,3-Dichlorophenol
106489	4-Chlorophenol	1570645	4-Chloro-o-cresol

Even larger groups exist. CN 29036990 is described as "Halogenated derivatives of aromatic hydrocarbons excluding, chlorobenzene, o-dichlorobenzene, p-dichlorobenzene, hexachlorobenzene, DDT "1,1,1-trichloro-2,2-bis[p-chlorophenyl]ethane", etc" and contains 19 listed compounds. It may, of course, also be applicable to an unknown larger number of substances.

This grouping of substances has both advantages and disadvantages. Typically, substances with similar properties or uses are grouped. Adopting a "grouped" or "clustered" approach to control may be very sensible. On the other hand, it may result in anomalous recommendations. CN 29310080 is described as "Separate chemically defined organo-inorganic compounds, not elsewhere specified". It contains the following listed substances:

CAS	Substance	CAS	Substance
56359	Bis(tributyltin) oxide	683181	Dibutyltindichloride
76879	Triphenyl-tin hydroxide	818086	Dibutyltinoxide
77587	Dibutyltindidodecanat	1461252	Tetrabutyltin
78002	Lead tetraethyl	13463393	Tetracarbonylnickel
639587	Triphenyltin chloride		

While most of these are organo-tin compounds with applications as pesticides, the tetraethyl lead is used to add the anti-knock agent into petrol. These uses are quite different. Further substances could also be included under this CN number.

Where a CN number is shared, it is not possible to determine which substance or substances have actually been traded. For example, if CN 29310080 is examined, the following data is found:

95 Imports (kg)	95 Exports (kg)	96 Imports (kg)	96 Exports (kg)	97 Imports (kg)	97 Exports (kg)
139,089	0	2,798,681	2,473	2,980,021	11,278

This indicates that a total of 139,089 kg was imported in 1995, but it not possible to allocate this amount to the individual substances. It could be evenly divided, or a single substance could be responsible for all. Indeed, another substance, not included in this OSPAR extended list, could be the primary material imported.

In this study, each substance is assigned the total traded figure. This is a "worst case" assumption. Due to the inadequacies of the CN system, this cannot be improved, without doing a substance flow analysis on the various substances.

Another example illustrating the inadequacies of the reporting system, which might be detected on examination, are the import / export values for CN 29329990, which includes Carbofuran (CAS 1563662) and TCDD, PCDD, PCDF (CAS 1746016):

95 Imports (kg)	95 Exports (kg)	96 Imports (kg)	96 Exports (kg)	97 Imports (kg)	97 Exports (kg)
0	0	2,825,124	2,765	2,661,909	330,760

This CN describes heterocyclic compounds with oxygen hetero-atom(s) only, with some exclusions. It is unlikely that such a large quantity of carbofuran or TCDD, etc. has been imported.

Yet another example of results that are likely to be anomalous is CN 28443019, which describes "Uranium depleted in U 235; alloys, dispersions, ceramic products and mixtures, containing uranium depleted in U 235 or compounds of this product (excl. cermets)":

95 Imports (kg)	95 Exports (kg)	96 Imports (kg)	96 Exports (kg)	97 Imports (kg)	97 Exports (kg)
	0	11	4,887		5,219

However, this might have a sensible explanation, again only to be discovered on investigation.

Accuracy of the statistics

It has been assumed that the reported statistics are accurate. International experience indicates this may not always be correct. Indeed, the detailed inventory of dichloroethane conducted for this study indicated the CSO values are in error. However, the CSO values have been uniformly applied, since it is not possible to conduct a substance flow analysis for each substance.

Averaging of production volumes

Production volumes have been based on the average of the differences between imports and exports for the years 1995-1996-1997. This simple averaging approach has been selected in preference to a weighted average or single year. It may be argued that certain substances are being phased-out by users and this is better reflected by using the latest data, or by an average biased towards later years. However, the usage of substances may fluctuate from one year to the next. An example of this, demonstrated by the investigations into the inventory methodology, is dichloroethane (ethylene dichloride, CAS 75343). This substance is now used in Ireland as a solvent in the pharmaceutical synthesis industry. Its usage in a given year is dependent on the production campaign plan for a very small number of companies. The need to produce a particular product by one company may cause 100% swings in the annual production volume.

Validity of using import-export value as production volume

It has been assumed that none of the substances are produced in Ireland, hence any export values represent trans-shipment. The conveyance of these substances, while presenting a risk in the event of spillage, is not considered as production. Therefore the "production" volume used in the EURAM method is based on the difference between imports and exports, and is, in fact, a "usage" value.

Usage = Import – Export

This approach neglects internal recycling. Recycling is only possible if there is some degree of closure in a system. This will be common for solvents in the pharmaceutical industry. For example, 100 tonnes of imported solvent may be used multiple times before replacement. Hence "usage" is not the same as "throughput".

Ireland is a major chemical exporter, but primarily in the field of pharmaceuticals. Hence the assumption that all exports of the 381 listed substances are transhipments appears valid. However, a number of substances contradict this, as illustrated by the following tables.

There are a number of substances which possess a unique CN number, with an excess of export over import:

Unique CN number, excess of export over import, values in kg

CAS	CN	Substance	1995		1996		1997	
			Import	export	Import	export	Import	export
110827	290211..	Cyclohexane	0	0	9,555	0	14,080	180,786
76131	29034300	1,1,2-trichloro-trifluoroethane	0	0	4,527	6,260	271	1,826
81141	29147010	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitro-acetophenone	12,765	0	14,861	16,050	5,400	26,830
100970	29336920	Methenamine	0	0	400	7,200	6,400	0

The cyclohexane values are most surprising, because of their magnitude. This may represent waste shipment.

There are other examples, where the CN number is not unique:

Aggregated CN number, consistent excess of export over import, values in kg

CAS	CN	Substance	1995		1996		1997	
			Import	export	Import	export	Import	export
79061	29241000	Acrylamide	78257	1372562	868203	9050608	747798	13754743
148798	29341000	Thiabendazole	0	1953619	87680	117336	5425	72353
108918	29213010	Cyclohexyl-amine	0	0	81	38834	1549	6820
123911	29322980	Coumaphos	0	0	0	0	42204	1525564

Ireland apparently exports more of each of these substances than it imports. This might imply manufacture. However, the CN number is not unique. One substance might be imported, and a quite different substance exported, but both classified according to the same CN number.

There are many other examples where there may be an excess of export over import in a single year.

In spite of these difficulties, there is not an alternative to using the CN system, except a detailed investigation of each selected substance.

Using additional information obtained from the Irish Chemical Suppliers Association and Irish Pharmaceutical & Chemical Manufacturers Federation

In an effort to narrow the uncertainty about the usage data, the Irish Chemical Suppliers Association, ICSA, surveyed their members on the substances that were believed to be traded in Ireland. This reduced the number of substances relevant and rankable to 76.

However, an examination of this list demonstrated that materials that cannot be traded, e.g. TCDD are included. While individual errors can occur in the course of surveys, this casts sufficient doubt upon the validity of all the data.

Further information was later received from the Irish Pharmaceutical & Chemical Manufacturers Federation, IPCMF, which added further substances to the list.

The inclusion of "false positives" undermined the usefulness of this survey information. These surveys must be considered an unreliable source of information to use as a basis for a prioritisation system.

Use of a default emission category

The EURAM method requires specification of the use distribution of each substance, e.g. whether used solely in a closed system (with associated limited emissions) or having a widely dispersive use (resulting in the emission of all the substance), or an intermediate usage. Each of which has an associated emission factor:

Fraction of substance emitted from different use categories

Main use category		Fraction
I	Used in closed systems	0.01
II	Use resulting in inclusion into or onto a matrix	0.10
III	Non-dispersive use	0.20
IV	Wide dispersive use	1.00
	Default	1.00

A conservative approach, to rank the inherent hazard potential of each substance, has been applied at this phase of the project. In this study, all usage has been allocated to the default category, i.e. an emission factor of 1.00, corresponding to wide dispersive use. This is justified for two reasons:

(i) There is always a risk, albeit small, that a well-managed highly-hazardous substance will be emitted as a result of an accident. Applying the factors for closed system use obscures this potential. It is more appropriate to apply these factors at the expert review stage, where the downgrading of the risk is transparent.

(ii) Secondly, the perceived usage may be incorrect. Referring again to dichloroethane (ethylene dichloride, CAS 75343, 107062), this is widely reported as used as a grain steriliant – clearly a widely dispersive use. However, investigations as part of this project revealed that its use is banned in Ireland. Checking with prospective users indicated that the ban had been effective, with the restriction no longer remarked upon, rather that the use dichloroethane was no longer practised. However, the material is used as a solvent in the pharmaceutical industry.

Nonyl phenol (CAS 25154523) was also subject to detailed examination in developing the inventory methodology. This material is associated with surfactants. One company in Ireland had used it in large quantities some years ago. This company is generally associated with surfactant manufacture. However, the use of the substance in Ireland was concerned with the manufacture of a metal extracting solvent, a completely different application. It was merely co-incidental that the company was also a surfactant manufacturer. Nevertheless, it was discovered that a completely different company uses very large quantities. This would not have been revealed without detailed examination.

CAS	CN	Substance	1995 kg		1996 kg		1997 kg	
			Import	export	Import	export	Import	export
75343	29031990 (shared)	1,1-dichloro-ethane	0	0	3,458	0	1,378	0
107062	29031500 (unique)	1,2-dichloro-ethane	0	0	17,150	0	0	0
25154523	29071300 (shared)	Nonylphenol	113,433	0	1,101,577	0	3,940,897	0

It appears the import masses for nonylphenol (which are aggregated with “Octylphenol, nonylphenol and their isomers; salts thereof”), may not apply to pure substances, considering the magnitude.

Environmental distribution

The Mackay Level I model has been applied to the substances. This has a minimum, or truncated, value for distribution into the aquatic environment of 0.01, i.e. at least 0.01 of the substance will enter the water compartment, even if the model calculated a lower value, or even zero.

Degradation

Where data is available, the substances have been classified in accordance with standard OECD degradability tests. In the absence of this data, a default value assuming the substance is persistent has been applied.

Results from application of the EURAM model

Applying the various exclusion criteria and sourcing data or defaults, as appropriate, the following table illustrates the final number of substances rankable. Appendix III "Guide to CN classification of substances" may be used to identify the substances which have been excluded.

There are still a considerable number of substances without necessary data. However, should this data become available, or indeed should other substances be of concern, they can be easily incorporated into the spreadsheet to determine the scores and ranking.

	Metals	Pesticides	Other	Total
Initial list of substances	22	97	262	381
Substances excluded due to No CN or CN=0	3	12	59	74
Substances imported into IRL	19	85	203	307
Substances excluded: Metals/Pesticides	19	85	0	104
Substances Rankable	0	0	203	203
Substances excluded: Exports>Imports			13	13
BALANCE			190	190
Substances Missing Data			101	101
Final Number Rankable			89	89

Analysis of ranking

A total of 89 substances have been rankable, after deduction of substances that are not imported into Ireland, and those for which the EURAM model is inappropriate.

Using the OSPAR classification, these substances fall into the following categories:

Category	Number	Description
1	7	Alkanes
2	6	Alkenes
3	2	Anilines
4	10	Benzenes
8	8	Organic nitrogen compounds
9	10	Organic oxygen compounds
10	3	Organic phosphorous compounds
12	1	Organometallic compounds
14	8	Pesticides
16	2	PAH's
18	10	Toluenes and Xylenes
N/c	29	Not classified

The following table of ranked substances presents the following information:

Rank	This is the ranked position in accordance with the aquatic score
CAS number	This is the unique international identifier for the substance
ID number	This is a reference number used in the project. It may be used to cross reference to the input data, calculations and output values within the spreadsheet
Name	This is the IUPAC name of the substance
Unique CN	This indicates whether the substance has a unique CN number. If it has, precise import and export values are available. If not, the import and export values assigned are the total for the CN number, but may be only partly attributable to the particular substance. A total of 20 of the ranked substances have unique CN numbers.
Emission (tonnes)	This is determined using the default assumption that all usage is emitted. In addition, it represents the three-year average of the excess of imports over exports for the appropriate CN number
EEX_2	This is a measure of the environmental exposure of the substance in the aquatic medium. It is a combination of factors due to the estimated emission, the distribution of the substance among the environmental compartments, and its tendency to degrade.
EEF_2	This is a measure of the environmental effects of the substance, in the aquatic medium. It is based on eco-toxicity data and an assessment factor dependent on the number of species tested.
Score	This is the final aquatic score. It combines the environmental exposure and effect scores, with a modification to reflect the bioconcentration factor.
Type of chemical	This indicates the chemical type in accordance with the original OSPAR list.

Further permutations have been considered:

Usage: based on a standard 1000t value as well as the CN derived value;

Emission: considering alternative emission factors – 0.01, 0.1 as well as the worst case assumption of 1.

Finally, the substances identified by the Irish Chemical Suppliers Association have been assessed.

This information is presented in Appendix V.

Table of ranked substances

RANK	CAS NO	ID No.	Name	Unique CN	Emission (tonnes)	EEX_2	EEF_2	Score	Type of Chemical
1	75058	210	Acetonitrile		693.26	5.32	14.00	52.12	N/c
2	56359	229	Bis-(tributyltin) oxide		1968.01	4.75	11.59	43.29	N/c
3	1461252	236	Tetrabutyltin		1968.01	3.56	10.09	35.78	12
4	26444495	333	Cresyldiphenylphosphate		113.17	2.58	14.00	27.86	10
5	25154523	115	Nonylphenol		1718.64	4.82	6.64	27.24	N/c
6	140669	117	4-(1,1,3,3-tetramethylbutyl)phenol		559.51	3.53	7.83	26.39	14
7	120127	35	Anthracene		234.97	2.96	9.44	22.53	16
8	25339177	107	Isodecanol		204.30	3.66	6.44	20.18	9
9	121142	94	2,4-Dinitrotoluene		84.68	4.37	6.19	18.96	18
10	79118	148	Chloroacetic acid		14.69	3.38	7.87	18.62	9
11	102090	171	Diphenyl carbonate		560.54	4.95	3.83	18.22	9
12	121733	101	1-Chloro-3-nitrobenzene		59.26	4.04	5.77	16.34	4
13	28553120	155	Di-'isononyl'phthalate		479.90	2.72	6.94	15.90	N/c
14	62533	176	Aniline		29.07	3.77	5.59	14.76	N/c
15	77781	170	Dimethyl sulphate		560.54	4.86	4.25	14.45	N/c
16	98544	116	Butylphenol	X	197.45	2.89	5.59	14.20	14
17	98511	40	4-tert.-butyltoluene		66.24	2.36	5.40	13.61	18
18	122394	291	N,N-Diphenylamine		20.33	2.77	5.59	13.60	8
19	97007	99	1-Chloro-2,4-dinitrobenzene		59.26	4.12	4.60	13.27	4
20	1330207	368	Xylene, mixed isomers	X	465.21	2.70	6.44	12.17	N/c
21	117817	289	Bis (2-ethylhexyl) phthalate (DEHP)		5101.90	3.71	2.99	11.47	9
22	1570645	127	4-Chloro-o-cresol		9.46	1.87	7.08	11.13	N/c
23	95578	120	2-Chlorophenol		9.46	2.99	5.17	10.81	14
24	100447	84	Benzyl chloride		27.39	2.57	5.77	10.38	18
25	106489	122	4-Chlorophenol		9.46	2.94	4.99	10.27	14
26	131099	141	2-Chloroanthraquinone		806.13	3.21	3.05	10.06	16
27	99650	283	1,3-Dinitrobenzene		84.68	4.39	3.17	9.74	4
28	26761400	154	Di-'isodecyl'phthalate		479.90	1.35	6.00	9.69	N/c
29	95487	279	2-Methylphenol		4.05	2.56	5.40	9.66	14
30	76039	147	Trichloroacetic acid		14.69	3.37	4.00	9.43	9
31	120821	88	1,2,4-Trichlorobenzene		27.39	1.60	5.19	9.01	N/c
32	101779	189	4,4'-Methylenedianiline		2.05	2.19	5.65	8.68	N/c
33	110850	244	Piperazine		446.58	5.32	2.29	8.54	N/c
34	80057	273	2,2-Bis-(4-hydroxyphenyl)-propane		47.97	4.01	2.99	8.38	14
35	107028	140	Acrylaldehyde		68.09	1.55	6.00	8.08	N/c
36	95476	28	o-Xylene	X	97.71	1.77	4.99	7.95	18
37	120832	125	2,4-Dichlorophenol		9.46	2.49	4.47	7.80	14
38	106898	137	Epichlorohydrin	X	5.18	2.67	3.95	7.38	9
39	98953	92	Nitrobenzene		84.68	4.26	2.44	7.29	4
40	106467	93	1,4-Dichlorobenzene		84.68	1.85	4.11	7.18	4

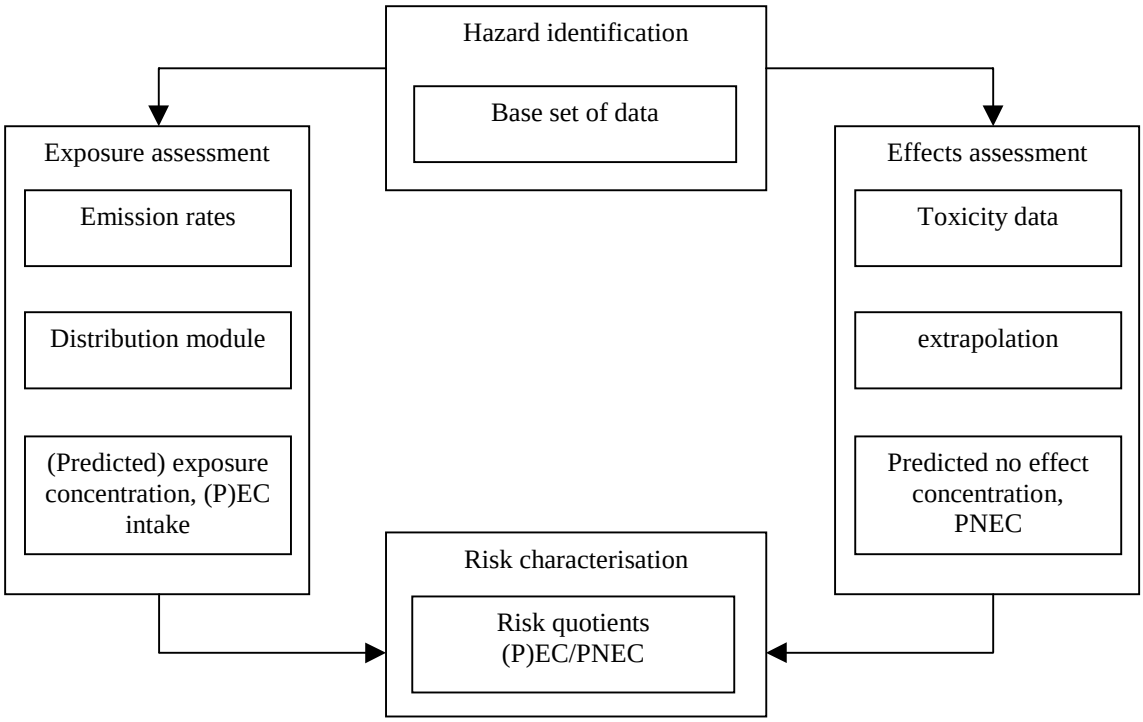
Table of ranked substances continued

RANK	CAS NO	ID No.	Name	Unique CN	Emission (tonnes)	EEX_2	EEF_2	Score	Type of Chemical
41	108952	114	Phenol		15.27	2.01	4.99	7.02	N/c
42	88733	97	2-Chloronitrobenzene		59.26	3.94	2.47	6.82	4
43	98464	100	alpha,alpha,alpha-Trifluoro-3-nitrotoluene		59.26	3.32	2.91	6.77	18
44	1817476	96	4-Nitrocumol		84.68	1.68	4.00	6.40	4
45	98873	83	a,a-Dichlorotoluene		27.39	2.35	2.12	5.84	18
46	79414	152	Methacrylic acid		12.47	1.90	4.24	5.64	N/c
47	75092	43	Dichloromethane	X	2434.14	3.58	2.25	5.63	1
48	108054	143	Vinyl acetate	X	124.83	1.88	4.00	5.26	N/c
49	71432	366	Benzene	X	161.93	2.10	3.54	5.20	4
50	87616	79	1,2,3-Trichlorobenzene		27.39	1.01	3.54	4.53	N/c
51	84742	276	Phthalic acid dibutylester (DBP)		82.09	0.93	3.90	4.38	9
52	111875	105	Octan-1-ol		1.02	1.24	3.59	4.35	9
53	95498	81	2-Chlorotoluene		27.39	1.01	4.54	4.22	18
54	103117	151	2-Ethylhexyl acrylate		15.98	1.18	3.52	4.07	N/c
55	115968	162	Tris(2-chloroethyl)phosphate		6.06	1.97	2.84	3.92	N/c
56	126738	292	Tributyl phosphate		6.06	1.47	3.17	3.27	10
57	59507	358	Chlorocresol		9.46	1.33	3.40	3.17	14
58	79016	272	Trichloroethene	X	209.09	2.22	2.02	3.14	2
59	541731	89	1,3-Dichlorobenzene		27.39	1.34	3.05	2.85	4
60	67721	48	Hexachloroethane		1.61	0.44	6.14	2.78	1
61	109660	23	Pentane		24.08	0.94	4.02	2.63	1
62	115866	288	Phosphoric acid triphenyl-ester		6.06	0.24	9.71	1.86	10
63	78875	46	1,2-Dichloropropane		10.08	0.86	2.78	1.68	N/c
64	67663	359	Trichloromethane	X	75.58	1.88	1.17	1.54	1
65	71556	47	1,1,1-Trichloroethane	X	27.98	1.02	1.77	1.27	1
66	95512	178	2-Chloroaniline		0.08	0.23	7.05	1.11	3
67	106434	85	4-Chlorotoluene		27.39	1.01	0.00	1.01	18
68	104767	104	2-Ethyl-1-hexanol	X	0.44	0.34	3.88	0.92	9
69	100425	32	Styrol	X	18.02	0.19	6.40	0.86	N/c
70	79005	52	1,1,2-Trichloroethane		1.61	0.46	2.44	0.79	1
71	95761	179	3,4-Dichloroaniline		0.08	0.04	6.99	0.19	3
72	112345	133	2-(2-butoxyethoxy)ethanol		179.81	3.50	0.00	0.00	N/c
73	80626	153	Methyl methacrylate	X	135.07	3.51	0.00	0.00	N/c
74	111159	144	2-Ethoxyethyl acetate	X	0.10	-0.98	0.44	-0.30	N/c
75	79209	145	Methyl acetate		83.09	3.97	-0.16	-0.44	N/c
76	75456	68	Chlorodifluoromethane		63.95	1.52	-0.43	-0.46	N/c
77	90040	190	o-Anisidine		0.07	-0.25	4.33	-0.76	N/c
78	79345	53	1,1,2,2-Tetrachloroethane		1.61	-0.65	3.11	-1.41	1
79	75014	56	Vinyl chloride	X	0.15	-2.08	1.36	-1.97	2
80	108883	367	Toluene	X	4383.22	2.66	-1.20	-2.24	18
81	1634044	318	Tert.-butyl methyl ether		101.54	2.77	-1.34	-2.60	N/c
82	126998	61	Chloroprene		0.01	-3.86	1.22	-3.30	2
83	127184	57	Tetrachloroethene	X	406.02	2.62	-1.82	-3.34	2
84	106423	31	p-Xylene	X	1.03	-0.94	5.40	-3.56	18
85	101848	130	Diphenyl ether	X	4.83	-0.73	5.54	-3.57	9
86	141979	157	Ethyl acetoacetate		83.72	4.40	-1.40	-4.31	N/c
87	107051	60	Allychloride		0.01	-3.86	2.40	-6.48	2
88	75354	58	1,1-Dichloroethylene		0.01	-3.73	3.87	-10.12	2
89	100414	33	Ethylbenzene	X	0.00	-5.72	5.49	-21.98	4

Discussion of the application of a model-based prioritisation mechanism to Ireland

Implications of selected mechanism

As previously discussed, it was decided to apply a risk assessment mechanism to prioritisation, as shown in the following figure:



This is consistent with current international practice, and requires an assessment of both effects and exposure. Once a decision has been taken to adopt a system that relies on risk assessment, an effects-only approach, e.g. Swedish Sunset Chemicals, is inadequate.

Effects assessment

This requires values for the eco-toxicological properties of the substances, determined either experimentally or derived from predictions based on the structure of the substances (QSARs). At first sight, experimentally derived data are preferable, and one would expect they are available, however, this is not always the case. Due to the very large number of substances in existence, not all have been tested, particularly for their effects in the marine environment. Recourse may then be made to QSAR predictions. Again, validation of these predictions in the marine environment is limited, but the accuracy may, in some cases, be comparable with the accuracy of experimental values. Hence, while subject to uncertainty and incomplete validation, the determination of effects is, in principle, feasible. This project has attempted, where possible, to use experimental data.

Exposure assessment

Determination of exposure in the aquatic environment is dependent on either experimental values, or predictions from modelling. Experimental values are, again, preferred, but there is an international scarcity of data in the marine environment. Furthermore, there is a severe lack of such data for Irish waters. Hence it was concluded that this absence of monitoring data inhibits the use of experimental data for exposure assessment.

In its absence, recourse was made to what might be described as a model-based approach, but would be better described as a model-based ranking approach. Modelling demands an accurate mathematical description of the behaviour of substances in the marine environment. Such models must also be validated by adequate monitoring data. Neither a comprehensive model for Irish waters, nor, as we have seen, adequate validating monitoring data are available. In these circumstances, the model-based ranking method known as EURAM (27) was adopted.

The EURAM method was devised to rank the High Production Volume Chemicals recorded in the European Inventory of Existing Commercial Substances (EINECS). It does not use monitoring data, but instead uses a "modelling" approach. It is better described as a ranking algorithm or method, rather than as a model. A "model" implies an accurate representation of physical or other behaviour. The objective of the method is to rank substances relatively, rather than to precisely describe their behaviour in the environment. It relies on knowledge of the intrinsic properties of a substance, allied with a model for a substance's tendency to partition on release into the environment. This partitioning model follows the procedure known as the so-called "Mackay Level I approach". This is a simple equilibrium model which attempts to represent the partitioning of a substance that is discharged into the environment, drawing on the intrinsic properties of the substance and the nature of the discharge environment (28). The EURAM method uses only the aquatic compartment, and potentially human health effects (using recognised risk phrases) for ranking purposes. This emphasis on the aquatic compartment conforms to the project specification, but does not address air emission matters such as ozone depletion or global warming or multi-media issues.

Use of this method automatically presents some limitations, and requires certain data:

(i) Quantity of substance produced;

(ii) Use pattern of the substance;

(iii) Intrinsic physiochemical properties;

(iv) Environmental fate and pathways.

The method was devised for organic substances and may not be applied to:

(i) Pesticides, which are the subject of special assessment measures (29, 30).

(ii) Metals or metal-containing substances, which do not behave as organic compounds

Hence these were excluded from consideration using an automatic ranking method. Their inclusion may be considered at the expert review stage.

Intrinsic physiochemical properties

It would appear that physicochemical properties should be readily available. However, this is not the case. Even for High Production Volume Chemicals, the database (IUCLID) provided by the Joint Research Centre at Ispra is missing certain data for some substances, presents a range of recorded values, even for pure substances, and contains data that has not been validated. Predictive measures may be used to estimate properties, but the choice of method is a significant task, and normal engineering practice when this is undertaken is to validate the predictions. Comprehensive searches of databanks failed to obtain all the necessary data, and the project scope did not extend to estimation of missing data, at the appropriate level of sophistication. This is of concern, in light of the sensitivity of the distribution model within the EURAM system to key data.

Quantity of substance produced

It was assumed that the substances of concern were not produced in Ireland, and reference was made to the Import / Export statistics to estimate usage. While a flawed assumption, it is a valid approximation. It was then learned that the statistical classification system, while presumably adequate for economic and revenue purposes, is insufficiently precise to determine the actual quantities of all required substances. In some cases, a substance is allocated a unique "CN – Combined Nomenclature" number, in which case a value may be obtained for the substance alone. In many other cases, the allocated number could be shared with tens or even a hundred other substances. Furthermore, the work conducted to establish an inventory methodology had demonstrated that the Irish trade statistics were inaccurate in some cases. This problem is not unique to Ireland, and has been reported elsewhere. Faced with this difficulty, assistance was sought from industry to refine the estimates of usage, by identifying the substances actually imported, or not imported, in the opinion of the industry. Excellent support was provided by the industry representatives, but the results of the survey indicated that the responses could refer to historical practice, or were in error, or did not have sufficient confidence in the reliability of the results. At this stage, the only option was to assign a common usage figure to each substance sharing a CN-Combined Nomenclature number.

Use pattern of the substance & environmental fate and pathways

The ranking method requires a classification of the usage pattern of each substance, and assigning a "representative" emission factor to the substance. The default usage assumes widespread dispersion of the substance. Without undertaking an inventory tracking of each and every substance, there is little data, other than judgement, that might be applied to usage in an Irish context.

Incorporation of dangerous substances into preparations and products.

Dangerous substances may be used in the pure state, e.g. as solvents, but they may also be incorporated in mixtures, i.e. preparations. The composition of these preparations may not be immediately apparent, and will not necessarily be reflected in the trade statistics usage. Hence, a dangerous substance may not enter the country in pure form, but may be extensively used as a constituent of a preparation. Common practice might lead one to suspect the presence of dichloromethane in a paint-stripper preparation, but detailed knowledge would be required to determine if a metal working fluid were to contain chlorinated paraffins, and whether these were short, medium or long-chained. Dangerous substances may also be incorporated into or onto a solid matrix, i.e. a solid "product". Examples of these would be the use of heavy metals as plasticisers or brominated substances as flame retardents in polymers.

Conclusion

The deficiencies in available data for Ireland on exposure to dangerous substances include the following:

(v) uncertainty about quantities of pure substances imported and in use;

(vi) lack of information of actual usage patterns;

(vii) absence of data on incorporation of dangerous substances in preparations and products;

(viii) inadequacy of monitoring data, due to lack of sampling and cost constraints;

allied with:

(v) uncertainty in the intrinsic physicochemical and ecotoxicological properties, and

(vi) inapplicability of the model-based ranking method to metals and pesticides

lead to the conclusion that a strictly scientific risk assessment approach could not be followed in prioritising substances for control in Ireland. Consequently, recourse was made to an expert review method.

Section 5: Use of an expert review to select a priority list of substances

Final adopted methodology

Due to the difficulties outlined earlier, a strictly scientific risk assessment approach could not be applied in conducting the tasks to prioritising substances for control. The severe limitations of accurate knowledge and data on substances precluded ranking based on an automated model. Such a ranking would be of dubious credibility and inappropriate as a basis for making decisions on programmes for monitoring or for control and reduction of use. In consultation with the Steering Committee and Expert Group, it was decided to refer primarily to Ireland's international obligations and to consider substances of national or international concern, in accordance with the project specification as originally specified.

Since the scale of the project demands that the selection be restricted to a small number, a wide range of substances should be considered in addition to respecting international or national concerns. Representative substances from particular uses and potential concern should be chosen, including metals, pesticides, organohalogen solvents, endocrine disrupters and substances for which daughter directives under 76/464/EEC and OSPAR action lists of priority substances were developed. Hence, the exemplary nature of some of the substances in their particular application or sector should be a factor in their selection.

Following this approach and with further consultation with the Steering Committee and Expert Group, the following substances were selected for development of Best Environmental Practice. It must be emphasised that this priority list represents a first attempt that has been hampered by the lack of data. Prioritisation should be seen as a dynamic process, with the list of priority substances changing as information about the usage of the substances becomes better known and as the effects of recommendations to reduce or eliminate their threat to the environment or human health take effect.

Reasons for inclusion of individual substances

Name	CAS	Reason for inclusion	BEP
Arsenic	7440382	Arsenic is a List II substance of Directive 76/464/EEC. It is also present on Annex 1A of the North Sea Declaration. This substance is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive. Arsenic compounds are classified as dangerous to the aquatic environment. Arsenic is subject to extensive regulation and is widely used in Ireland in wood preservation.	A-1
Butylbenzylphthalate (BBP)	85687	Butylbenzyl phthalate is a suspected endocrine disrupter, though not regulated. This substance is also expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	D-1
Cadmium	7440439	Cadmium is a List 1 substance of Directive 76/464/EEC and has an associated daughter Directive (83/513/EEC). It is also present on Annex 1A of the North Sea Declaration. Cadmium has been selected for priority action by OSPAR. This substance is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive. Cadmium compounds are classified as dangerous to the aquatic environment. Cadmium is thought to be an endocrine disrupting substance.	A-2
Chlorobenzene	108907	Chlorobenzene is a candidate List I substance of Directive 76/464/EEC. It is also present on Annex 1D of the North Sea Declaration and is on the OSPAR list of candidate substances. It is classified as dangerous to the aquatic environment and is an example of a chlorinated aromatic compound.	B-1
1.2-Dichloroethane	107062	1,2 Dichloroethane is a List 1 substance of Directive 76/464/EEC and has an associated daughter Directive (90/415/EEC). It is also present on Annex 1A of the North Sea Declaration. It has been chosen on the basis of international obligations rather than a current threat to the Irish environment.	B-2
Dichlorvos	62737	Dichlorvos is a candidate List I substance of Directive 76/464/EEC and is present on Annex 1A of the North Sea Declaration. It was used in a dispersive manner in the marine environment.	C-1
Diethylhexylphthalate (DEHP)	117817	Diethyl hexyl phthalate is a suspected endocrine disrupter, though not regulated. DEHP has been selected for priority action by OSPAR. This substance is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	D-2

Reasons for inclusion of individual substances, continued

Name	CAS	Reason for inclusion	BEP
Isoproturon	34123596	Isoproturon is classified as dangerous to the aquatic environment. Isoproturon has high usage quantities in Ireland. This substance is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	C-2
Lead & Organic lead compounds	7439921	Lead is a List II substance of Directive 76/464/EEC and is present on Annex 1A of the North Sea Declaration. Lead and organo-lead compounds have been selected for priority action by OSPAR. This substance is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive. Lead is classified as dangerous to the aquatic environment. Lead is subject to extensive regulation and is in widespread usage in Ireland. Lead is thought to be an endocrine disrupting substance.	A-3
Mecoprop	93652	Mecoprop is a candidate List I substance of Directive 76/464/EEC and was selected on the basis of its high usage quantities.	C-3
Mercury & organic mercury compounds	7439976	Mercury is a List 1 substance of Directive 76/464/EEC and has associated daughter Directives (82/176/EEC and 84/156/EEC). It is also present on Annex 1A of the North Sea Declaration. Mercury and organo- mercury compounds have been selected for priority action by OSPAR. Mercury and organic compounds of mercury are classified as dangerous to the aquatic environment. Mercury is thought to be an endocrine disrupting substance.	A-4
Nitrobenzene	96953	Nitrobenzene is present on Annex 1D of the North Sea Declaration and is on the OSPAR list of candidate substances for priority. It is classified as dangerous to the aquatic environment. Nitrobenzene is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	B-3
Nonyl phenol & Nonyl phenol ethoxylates	25154523 9016459	Nonylphenol ethoxylate is a suspected endocrine disrupter. It has been selected for priority action by OSPAR. Nonylphenol ethoxylates may have dispersive usage. Nonylphenol ethoxylate will degrade to nonyl phenol.	D-3
Permethrin	52645531	Permethrin was chosen as an example of a pyrethroid insecticide. It is available in a wide range of products which have biocidal properties.	C-4
Polybrominated diphenyl ethers (PBDEs)	N/a	Brominated flame retardants are listed on the OSPAR list for priority action. Brominated diphenyl ether is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	D-5

Reasons for inclusion of individual substances, continued

Name	CAS	Reason for inclusion	BEP
Polycyclic Aromatic Hydrocarbons (PAH's) - creosote	130498292	Some PAHs are List 1 substances of Directive 76/464/EEC. PAHs are listed on the OSPAR list for priority action. PAHs are expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	D-4
Simazine	122349	Simazine is a candidate List I substance of Directive 76/464/EEC and is also present on Annex 1A of the North Sea Declaration.. It is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	C-5
Tin (organic compounds)	Misc	Organo-tin compounds are categorised as List 1 substances of Directive 76/464/EEC and are listed on the OSPAR list of chemicals for priority action. Tributyltin and triphenyltin compounds are present on Annex 1A of the North Sea Declaration. Tributyltin and triphenyltin compounds are classified as dangerous to the aquatic environment. Tributyltin is a suspected endocrine disrupter. Organotin compounds are subject to regulation in Ireland.	A-5
Trichlorobenzene	12002481	Trichlorobenzene is a List 1 substance of Directive 76/464/EEC and has an associated daughter Directive (90/415/EEC). It is also present on Annex 1A of the North Sea Declaration. Trichlorobenzene is expected to be included on a list of dangerous substances under the proposed EU Water Framework Directive.	B-4
Trichloroethylene	79016	Trichloroethylene is a List 1 substance of Directive 76/464/EEC and has an associated daughter Directive (90/415/EEC). It is also present on Annex 1A of the North Sea Declaration. Trichloroethylene is commonly utilised and its usage is dispersive.	B-5
Trifluralin	1582098	Trifluralin is a candidate List I substance of Directive 76/464/EEC. It is also present on Annex 1A of the North Sea Declaration.. Trifluralin is expected to be included on a list of dangerous substances. under the proposed EU Water Framework Directive.	C-6
Xylene, mixed isomers m-xylene o-xylene p-xylene	1330207 108383 95476 106423	Xylenes are candidate List I substances of Directive 76/464/EEC. Xylene was further chosen as an aromatic hydrocarbon with large usage in Ireland.	B-6

A concise list of the selected substances is presented on the following page:

List of substances selected for development of Best Environmental Practice

Name	CAS
Arsenic	7440382
Benzylbutylphthalate (BBP)	85687
Cadmium	7440439
Chlorobenzene	108907
1,2 dichloroethane	107062
Dichlorvos	62737
Diethylhexylphthalate (DEHP)	117817
Isoproturon	34123596
Lead & organic lead compounds	7439921
Mecoprop	93652
Mercury & organic mercury compounds	7439976
Nitrobenzene	96953
Nonylphenol	25154523
Nonylphenol ethoxylate	9016459
Polycyclic aromatic hydrocarbons (PAHs)	130498292
Polybrominated-diphenylether (PBDE)	N/a
Permethrin	52645531
Simazine	122349
Tin (organic compounds)	Misc.
Trichlorobenzene	12002481
Trichloroethylene	79016
Trifluralin	1582098
Xylene, mixed isomers	1330207
m-xylene	108383
o-xylene	95476
p-xylene	106423

Section 6: Introduction to the Best Environmental Practice Guidelines

Introduction

In addition to this project Main Report and associated Synthesis Report, a number of Best Environmental Practice (BEP) Guidelines and associated Recommendations have been prepared. The BEP Guidelines are oriented to actual users and have been prepared for each of the selected substances. The Recommendations are oriented to policy-makers. These recommendations range from mandatory reporting of usage and composition via a Chemical Products Registration Scheme, through the provision of research, development and demonstration measures to consideration of prohibition. They require the adoption of decisions and the provision of resources which are beyond the users of the substances alone. "Best Environmental Practice" and the content of the BEP Guidelines are explained in the following sections.

What is "Best Environmental Practice"?

The phrase "Best Environmental Practice" has been interpreted in accordance with the OSPAR Convention, to which Ireland is a signatory.

1. "Best Environmental Practice" means the application of the most appropriate combination of environmental control measures and strategies. In making a selection for individual cases, at least the following graduated range of measures should be considered:

   (a) the provision of information and education to the public and to users about the environmental consequences of choice of particular activities and choice of products, their use and ultimate disposal;

   (b) the development and application of codes of good environmental practice which covers all aspects of the activity in the product's life;

   (c) the mandatory application of labels informing users of environmental risks related to a product, its use and ultimate disposal;

   (d) saving resources, including energy;

   (e) making collection and disposal systems available to the public;

   (f) avoiding the use of hazardous substances or products and the generation of hazardous waste;

   (g) recycling, recovery and re-use;

   (h) the application of economic instruments to activities, products or groups of products;

   (i) establishing a system of licensing, involving a range of restrictions or a ban.

2. In determining what combination of measures constitute best environmental practice, in general or individual cases, particular consideration should be given to:

   (a) the environmental hazard of the product and its production, use and ultimate disposal;

   (b) the substitution by less polluting activities or substances;

   (c) the scale of use;

   (d) the potential benefit or penalty of substitute materials or activities;

   (e) advances and changes in scientific knowledge and understanding;

   (f) time limits for implementation;

   (g) social and economic implications.

3. It, therefore, follows that "Best Environmental Practice" for a particular source will change with time in the light of technological advances, economic and social factors, as well as changes in scientific knowledge and understanding.

4. If the reduction of inputs resulting from the use of "Best Environmental Practice" does not lead to environmentally acceptable results, additional measures have to be applied and "Best Environmental Practice" redefined.

Considering the situation in Ireland, the following concepts exist in Irish law:

(a) Best Practicable Means, BPM, as defined by the Air Pollution Act of 1987;

(b) Best Available Technology Not Entailing Excessive Cost, BATNEEC, as defined by the Environmental Protection Agency Act of 1992; and

(c) Best Available Technique, BAT, as defined by Council Directive 96/61/EC concerning integrated pollution prevention and control.

Best Practicable Means, BPM, is confined to machinery, plant, equipment, appliances, apparatus, buildings and other structures. The use of BATNEEC is construed in the EPA Act to mean the provision and proper maintenance, operation, use and supervision of facilities which are the most suitable for the purposes. The manner in which this is to be achieved is wide-ranging, but with the overall objective that BATNEEC will be used to prevent, eliminate or, where that is not practicable, limit, abate, or reduce an emission from an activity. It is used as a basis for setting emission limit values. Consequently, the focus is on defined activities, typically manufacturing, though also addressing areas such as treatment of waste. "Best Environmental Practice" is more comprehensive, addressing the entire product life-cycle through a combination of practices. These practices may involve producers, importers, distributors, commercial users and the general public, as well as those engaged in the collection, recovery or disposal of the substance when it enters the waste stream. These Best Environmental Practice Guidelines, prepared in the context of this EPA R&D project, should be seen as complementary to the published BATNEEC Guidelines. However, it should be recognised that the requirement for BATNEEC in a particular activity may be a statutory obligation, whereas these Best Environmental Practice Guidelines do not have a similar standing.

Description of the content of the BEP Guidelines

The BEP Guidelines have been written to be consistent with the definitions of BATNEEC, BAT and BPM and reflect national policy on the waste management hierarchy (prevention, minimisation, reuse, recycling, energy recovery and disposal) [13]. Emphasis is placed, where possible, on pollution prevention techniques rather than end-of-pipe treatment. Where a substance is used in a widely dispersive function, preference is given to minimisation or reduction. While the focus of this project has been on aquatic effects, a hazardous substance should not be removed from water, only to be transferred to air, or soil. Impacts on all media have been considered, consistent with the concept of integrated pollution prevention and control.

Quantified determination of "best" in a particular set of circumstances would require a detailed life cycle assessment of all the significant environmental impacts for the specific application, which is outside the scope of a BEP Guideline. The costs and advantages must therefore be considered for each individual case.

If applicable standards exist for the receiving environmental medium, whether general or local, these must be respected. In the absence of a specified standard, due regard should be had for the precautionary principle, i.e. taking preventive measures where there is reason to assume that substances introduced, directly or indirectly, into the environment may cause pollution or create hazards to human health, or harm ecosystems, even where there is no conclusive evidence of a cause-and-effect relationship between inputs and their impacts.

The Guidelines as presented are intended to reflect the current level of technology and control. They have been written with current and likely potential users in mind. Their application will contribute significantly to reduction in emissions of the substances of concern. In a number of cases, usage is largely confined to activities that are subject to Integrated Pollution Control licensing, and this control instrument, together with the application of BATNEEC, is currently the primary control mechanism. In other cases, the application of the Guidelines as presented will have a limited effect. There may be considerable uncertainty about the scope of emissions, due, for example, to the substance being primarily used in consumer products or the major usage may be subject to over-riding controls such as pharmaceutical product authorisation. In other cases, the substances may be pervasive, and it is only possible to address specific uses. Within the confines of this project, not all Best Environmental Practice Guidelines have been developed to the same extent.

The Best Environmental Practice Guidelines for each of the 22 selected substances is presented according to a standardised format, divided into six separate sections, namely:

- General information,
- Best environmental practice,
- Trade statistics,
- Potential uses
- Information relating to the aquatic environment,
- and Legislation.

Each of these sections is divided into a number of sub-sections as described below.

Section 1: General Information

This section consists of identification information relating to the substance, including:

- Name of the substance,
- CAS number,
- Chemical formula,
- Molecular structure,
- Common synonyms,
- Class of material,
- Physical state
- Reason for substance selection and
- Applicability.

Section 2: Best Environmental Practice

This section is divided into a number of sub-sections: public information; labelling; reduce use; re-use, recycle and recover; codes of practice and disposal.

- *Public Information* identifies measures which could be taken to increase public awareness about the substance, where relevant to public uses.
- *Labelling* outlines the current EU status with regard to the classification, packaging and labelling of the substance.
- *Reduce use* identifies various substitution or minimisation options for the substance.
- *Re-use, recycle and recover* describes various recovery options for the substance.
- *Codes of Practice* lists various operating practices which would reduce the environmental impact of the substance.
- *Disposal* identifies the options available for the disposal of the substance (and identifies possible EWC codes where appropriate).

Section 3: Trade Statistics

The CN number and CN description for the substance is identified and the import and export figures are listed for 1995-1998 inclusive. Note that in only some instances is there a unique substance allocation of CN number. Hence, reported trade statistics may refer to a group of chemicals, not solely the chemical of interest. The pesticide usage (as reported by the Pesticides Control Service) is listed where applicable.

Section 4: Potential Uses

The potential uses of the substance are listed in this section. This is comprehensive, including uses that are not known, or are unlikely, to occur in Ireland. A further section entitled *Irish Situation* outlines the current uses of the substance in Ireland and identifies current developments with regard to the substance in Ireland.

Section 5: Information Relating to the Aquatic Environment

Since the BEPs have been prepared in the context of concern for the aquatic environment, aquatic impacts alone are addressed.

This section summarises the environmental data (with particular reference to the aquatic environment) available for this substance. This section includes a number of sub-sections including:

- Release route to the environment,
- Water solubility,
- Distribution and persistence in the aquatic environment,
- Bioaccumulation in aquatic organisms and
- Any other relevant information.

There is also information concerning *Irish Aquatic Data* for this substance (when available).

Section 6: Legislation

This section outlines the current international, European and national agreements and legislation relating to the substance. This section is divided into four different sub-sections, as outlined below:

- The *Agreements* section outlines the international agreements under which this substance is addressed (including OSPAR, OECD, North Sea Declaration and so on).
- The *European Legislation* section identifies the European Directives that apply to the substance
- The C*ontrols in Ireland* section outlines the Irish legislation and controls (such as IPC licensing) which apply to this substance.
- The *Controls in other Countries* section summarises the bans, restrictions and current situation with regard to the substance in a number of other countries.

A number of herbicides and insecticides were chosen for this study and the BEPs for these substances have the above headings expanded under general and specific legislation. The general legislation is common to all the herbicides and to all the insecticides. The specific legislation refers to specific agreements, European legislation and controls for the particular substance.

References

A full reference list for the substance including books, journals, web addresses and personal communication is given at the end of each substance.

Section 7: Substance Flow Analysis (SFA) - Methodology

Introduction

The basis for a substance flow analysis is the development of a flowchart (chain) for a given substance, which details all the stocks, flows and processes related to that substance within the selected boundary. Once the "bare" flowchart (skeleton chain) has been drawn up for the substance, empirical data are collected and attributed to the stocks and flows. Statistical data on production, consumption, waste management and trade are linked to data on the content of the substance in products and materials. Monitoring data are preferably used for emissions to the environment. In their absence, emission factors, particular to the substance, process and sector may be applied. The unit processes within the chain serve as points for the redistribution of flows, and the input and output flows to each process are balanced unless accumulation occurs.
There are a number of stages in applying this methodology, described in the following sections.

Skeleton Chain

Initially, a skeleton chain gives an overview of the chains of use for each substance. To generate a skeleton chain therefore, the uses of each substance have to be determined. This first stage serves a number of purposes:

- it allows for cross-checking of information
- it identifies gaps in the data
- it can highlight present or future problem flows

There will be gaps in the data but these gaps cannot be identified until a detailed substance chain is drawn up. Therefore, the next stage is to carry out a detailed substance flow analysis.

Detailed Substance Flow Analysis

This requires that a large amount of data be collected from a variety of sources. It may also be found that a significant amount of data may be lacking.

System boundary

The system boundary is dependent on the scope of the substance flow analysis. Substance flow analyses can be carried out on a regional, national or international scale. Decisions need to be made about which chains should be followed and which should not. For example, the environmental burden of goods produced abroad but imported into Ireland could be ignored.

Streams to be quantified:

The following streams should be quantified for the most important or most representative substance sub-chains and/or product chains:

- import
- export
- production
- emission
- waste flow

Sequence to be followed:

1. Identification of the general uses of the substance.
2. Confirmation of the Irish uses of the substance.
3. Determination of the imports and exports of the substance from trade statistics.
4. Identification of user companies.
5. Confirmation of import and export figures by contact with distributors / suppliers / user companies.
6. Identification and quantification of waste streams from information obtained from the user companies.
7. Identification and quantification of streams where the substance is a natural contaminant.
8. Product information obtained where available.
9. Identification and quantification of accumulations within society.

Sources of Data[1]:

• CSO trade statistics	• User Companies
• Technical and Trade Publications	• Sector Federations
• Industrial contacts	• Suppliers / Distributors /Agents
• Environmental Protection Agency	• Health and Safety Authority (HSA)
• IPC licences and Polluting Emissions Registers (PER)	• National Waste Database (NWD)

Table 1. Summary of Information Sources

	Sources of Information
1. Substance Uses	Priority Substances Reports e.g. KEMI Literature Reviews Internet Searches Suppliers / Agents / User Companies
2. Imports / Exports	CSO Trade Statistics Major Importers / Exporters (Suppliers) User Companies
3. Users	EPA Inspectors IPC Licences and PER's Kompass Business Directory for Ireland Industrial and Commercial Contacts Sector Federations / Associations
4. Product	Manufacturers / Suppliers / Agents
5. Waste	PER for IPC-licensed companies User Companies National Waste Database (NWD) Other Substance Flow Analyses Sector Federations / Associations

Commentary on Data Sources

Determination of substance usage

Information can be obtained from reports published by other countries. Relevant sources include:

1. Swedish National Chemicals Inspectorate Sunset Project: Hazard Assessments - Chemical Substances Selected in the Swedish Sunset Project, KemI report no. 12/95
2. Revision of the Priority Substances List, no. 1994/24**,** VROM (Dutch Ministry of Housing and the Environment)
3. Priority Hazardous Substances in Norway. SFT (Norwegian Pollution Control Authority) report no. 94:03.

Literature reviews and Internet searches can also provide information on general usage. Irish usage can then be determined from information obtained from suppliers, agents and companies operating in a particular sector combined with trade statistics.

Trade statistics

The primary source of information for import / export figures are the trade statistics gathered by the Central Statistics Office. The Trade Statistics provide detailed information on imports and exports classified by country and commodity. These statistics are compiled from a combination of customs returns and the Intrastat survey of traders and are collected using the eight-digit Combined Nomenclature (CN) - the EU's tariff and statistical nomenclature. The CN contains between ten and twenty thousand sub-headings.

It will be necessary to obtain the import and export figures for a substance in its pure and compound form and for products and substances in which it is present as a certain percentage. The relevant trade statistics can be obtained once the CN code for an item is known. However, if a substance does not have a CN code of its own, and is grouped with similar substances, the figures for this substance cannot be directly obtained. Customs and

[1] Other statutory bodies (Customs and Excise/Revenue Commissioners) collect relevant information which is not accessible at present.

Excise provide specific information on imports and exports to the CSO. However, information on the consignee for a particular import, also gathered by the Customs and Excise, is not accessible.
It is well recognised that statistical information on trade can be unreliable and that it should be cross-checked with information from other sources. For this reason, import and export figures should also be obtained from suppliers / distributors and user companies.

Identification of user companies

This information will provide a further cross-check of the information obtained earlier. Once the user companies have been identified they can be contacted and requested to provide information on actual usage, waste streams and product streams.

IPC-licensed sector

Information on usage and emissions of substances from companies covered by IPC licence is readily accessible. At the moment, the licensing schedule has not been completed and the majority of companies in this sector are only beginning on the route to the production of a Polluting Emissions Register (PER). However, once the system is fully functional, information on substance usage and substance emissions in this sector should be comprehensive. The only drawback to the system is that the user of a substance has to be known before the relevant information can be obtained. In the situation where a PER has yet to be produced by a company, they should be contacted directly to obtain the required information.

Non IPC-licensed sector

Companies in this sector can be identified in a number of ways. Firstly, the Kompass Business Directory contains a comprehensive listing of companies operating in the Irish market. Once the uses of a substance are known, users can be identified from the relevant sections of the directory. This method may also be applied to the identification of companies operating in the IPC-licensed sector if required. Secondly, companies operating in a particular sector may be able to identify other companies operating in the same sector.

Products

At present, Ireland does not have a products register. This means that it will require a large number of man-hours to track down every product containing a substance and to determine the amount of the substance present in each particular product. Information on products containing a substance of interest may be available from substance flow analyses carried out in other countries. It may prove to be necessary to calculate a theoretical figure for some/all product streams in the event of a complete lack of information.

Waste

A number of sources of information for waste streams have already been mentioned. These are the PER's in the case of users operating in the IPC-licensed sector, and the companies themselves in the case of users outside the IPC-licensed sector. Substance flow analyses carried out for a substance in other countries may provide useful information if waste streams are to be determined on a more theoretical level.

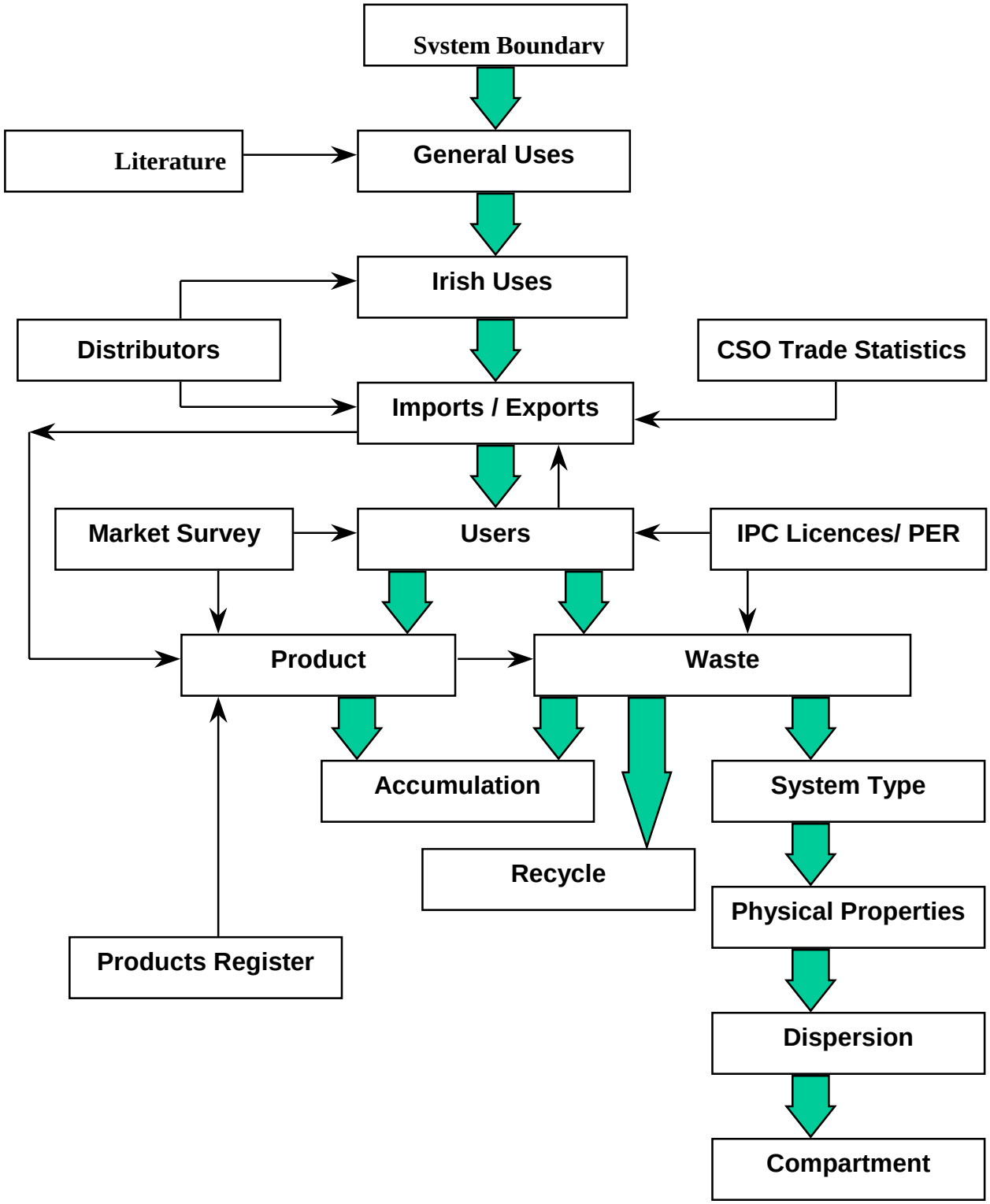
Determination of the Fate of a Substance

Until the uses and users of a particular substance have been identified it is difficult to determine the fate of a substance. Several questions need to be asked.

1. What are the physical properties of the substance. In particular, how volatile is the substance and how soluble is it? This will indicate in which environmental compartment (air, water or soil) the substance is likely to end up.
2. What is the use pattern of the substance? Is the substance used in a closed system (recycling of the substance) or an open system (no recycling)?
3. Is the emission source a point source, a dispersive source or a widely dispersive source?

The final fate of a substance cannot be truly identified until all the use patterns of the substance have been identified. Determination of the distribution between environmental compartments is dependent on the physical properties of the substance and its sectoral usage.

The various steps may be illustrated by the following diagram:



List of Suppliers and Distributors

ACI Ltd.
Allegro Ltd.
BASF IRL Ltd.
Bayer Ltd.
BP Chemicals IRL Ltd.
Chemicals and Plastics Ltd.
Chemtek Sales Ltd.
Corcoran Chemicals Ltd.
Degussa Ireland
Dow Chemical Company Ltd.
FSW Coatings Ltd.
Hays Chemical Distributors
Heterochem Ltd.
Hoescht IRL Ltd.
Lennox Laboratory Supplies
PK Chemicals Ltd.
Shell Chemicals IRL Ltd.
The National Chemical Company Ltd.
Zeneca IRL Ltd.

Section 8: Testing of the Substance Flow Analysis methodology in Ireland

Proposed Methodology

The proposed methodology was as follows:

- 1. Production of a skeleton chain for each of the four substances selected
- Sources of information would include previously published and technical literature. No figures would be included at this stage.
- 2. Initial Quantification
- Sources of information would include CTC partner companies and the National Chemical Company.
- 3. Market Survey
- Information from contacted companies would provide further data and allow refinement of the preliminary substance flow analyses.

Proposed sources of data included:

- Central Statistics Office (CSO) data for imports/exports
- Statistical data from the main supply countries
- PER (Polluting Emissions Register) / AER from EPA IPC-licensed companies
- Permitted emissions from EPA IPC-licensed companies (PER not yet produced)
- CTC data on solvent usage in partner companies
- National Waste Database
- Local Authority trans-shipment records
- HSA data
- National Hazardous Waste Management Plan (NHWMP)

These data sources are similar to those used in other SFA studies. It was expected that there would be some gaps in the data which would not be identified until a detailed substance chain was drawn up.

Application of the methodology to the Irish situation

This section describes how the methodology was actually applied and details problems that were encountered due to the level of data collection and data availability in Ireland. The year chosen was 1996 as it was assumed that more information would be available for that year. This assumption proved to be correct.

System boundaries:

The requirement of this phase of the project was to apply the proposed methodology to the Irish lead, dichloromethane, dichloroethane and nonylphenol ethoxylate chains. In other words, the environmental burden of goods produced with each substance and its compounds abroad was ignored but exports were included.

Steps taken to fulfil the methodology:

- Identification of both the general and the Irish uses of the four substances chosen.
- Determination of the imports and exports for each substance.
- Contact made with manufacturers / suppliers / users.
- Product information obtained where relevant
- Identification of waste streams with a focus on the aqueous environment.

Table 1. Summary of the Information Sources Used

	Sources of Information
1. Substance Uses	Priority Substances Reports e.g. KEMI Literature Reviews Internet Searches Suppliers / Agents / Companies
2. Imports / Exports	CSO Trade Statistics Major Importers / Exporters (Suppliers)
3. Users	CTC Partner Companies IPC Licences and PER's EPA Inspectors Compass Business Directory for Ireland Sector Federations / Associations Industrial and commercial contacts
4. Product	Manufacturers / Suppliers / Agents
5. Waste	PER for IPC licensed companies Companies themselves Sector Federations / Associations National Hazardous Waste Management Plan (NHWMP) Other substance flow analyses

Substance Usage

Initially information was obtained from reports published by other countries. The reports used were listed earlier. The Norwegian report was the only one of the three to include nonylphenol ethoxylate and classed it as a substance about which important information is lacking. Other sources of information used were literature reviews and Internet searches carried out by the Clean Technology Centre. This was combined with information from suppliers, agents and companies operating in the relevant sector. The latter sources along with the trade statistics defined what substances were actually in use in Ireland.

General Uses of Lead:

a) Batteries

b) cable coverings

c) ammunition

d) trace components in copper concentrate, zinc concentrate, coal, oil

e) stabilisers

f) semi-finished products

g) paints

h) Solders

i) glass and ceramics

j) others including fishing industry

Uses of lead in Ireland:

All of the above apart from item g.

General Uses of Dichloromethane (Methylene chloride, DCM):

a) Degreasing agent in mechanical and electrical engineering industry

b) dry cleaning

c) pharmaceutical industry

d) foodstuffs industry

e) chemical industry

f) paint removers

g) adhesive products

h) aerosols

Uses of DCM in Ireland:

Dichloromethane is used as a process chemical in the Pharmachem sector and in the production of paints, paint strippers and adhesives. It is also used as a degreasing agent. It does not appear to be used in the dry cleaning sector and is not used in the food industry.

General Uses of Dichloroethane (Ethylene Dichloride, EDC):

a) chemical industry as intermediary in vinyl chloride production

b) pharmaceutical industry (drugs and bandages)

c) rubber industry

d) used for cleaning electronic components until recently

e) used as a soil sterilising agent (nematicide)

f) used as a scavenger in leaded petrol (use falling)

Uses of EDC in Ireland:

It would appear that EDC is only used in the PharmaChem sector in Ireland. It was difficult to find any other information on the use of this substance in Ireland

General Uses of Nonylphenol Ethoxylate:

a) used mainly in cleaning agents

b) detergents

c) humidifying agents

d) emulgants

e) dispersants

f) paint and varnish

g) pesticides

Uses of Nonylphenol Ethoxylate in Ireland:

This substance is used in the detergent and paints sector in Ireland.

Uses of Nonylphenol in Ireland:

The nonylphenol chain was also followed. This substance is used in the manufacture of adhesives in Ireland.

Import / Export

The first source of information for import / export figures was the trade statistics gathered by the Central Statistics Office. The method used to collect the statistics is described below.

Statistical information

The Trade Statistics provide detailed information on imports and exports classified by country and commodity. Trade statistics are compiled from a combination of customs returns and the Intrastat survey of traders.

EU and Non-EU Trade

Intrastat is used to collect statistics on trade with EU member states. Traders whose annual imports from EU countries exceed £100 000 must make a detailed import return each month and traders whose exports exceed £500 000 must make a detailed export return each month. Statistics from non-EU states are collected from customs documentation.

Intrastat EU Trade

The information gathered under this heading is made up of two components:

1. Intrastat survey
   This is used to provide detailed monthly returns. Information on the quantity and value of imports and exports is reported. Intrastat covers about 95% of Irish trade with EU countries with a response rate of approximately 85%, covering about 88% of the total value of intra-EU trade.
2. Regular VAT returns are used:
   - for traders below Intrastat levels
   - for estimating trade for non-respondents above the thresholds
   - for maintaining the VIMA trade register of EU traders
   - for identifying those traders exceeding the thresholds

Non-EU Trade

Statistics are compiled mainly from documents supplied by importers and exporters or their agents to customs. The document used to collect the data is known as the Single Administrative Document (SAD) which is used for customs clearance. The information on the SAD is transferred to the VIMA for processing.

Data Processing

The basic data are collected and edited by the Office of the Revenue Commissioners (The VIMA Office in Dundalk). For Intrastat this work includes the maintenance of a trade register (a register of all known Inter-EU traders), the processing of returns, data validation and editing. For non-EU trade, the work involves editing and validation. VIMA passes the edited data to the CSO. The CSO checks the data for consistency and prepares estimates for each trader who has not been included (Intrastat non-respondents and traders below the Intrastat thresholds).

Commodity Classification

Statistics are collected using the eight-digit Combined Nomenclature (CN) - the EU's tariff and statistical nomenclature. The CN contains over 10 000 sub-headings. Data classified by CN code are further aggregated and classified according to the United Nations Standard International Trade Classification, SITC, which contains around 3100 basic headings of 5-digit numbers.

Difficulties encountered with the CSO data:

Classification

There were a number of immediate problems with the information initially available. Substances were classified by their SITC code in the published version of the Trade Statistics. Dichloromethane can be taken as an example of the problems encountered. In the published statistics it was not listed as a discrete entity but was included under the grouping "Other saturated chlorinated derivatives of acyclic hydrocarbons" (SITC 511.36). Once the CN code for dichloromethane had been determined, the imports and exports could be easily provided by the CSO. Imports and exports by CN code are not given in the published version of the trade statistics and have to be obtained from the CSO directly.

As it was required to obtain the imports and exports for a large number of items it was decided to purchase the information in disc format from the CSO. This then meant that the CN classifications had to be determined for each item of interest before the import / export figures could be found. Figures for nonylphenol ethoxylate have been impossible to obtain as it may be grouped with other substances ("octylphenol, nonylphenol and their isomers; salts thereof"). No CN code exists for nonylphenol ethoxylate on its own. It may well be included with a surfactant grouping or a detergent grouping.

Reliability of Data

It is internationally recognised that statistical information on trade can be unreliable and that it should be cross-checked with information from other sources. Table 2 gives the import and export figures for dichloromethane (DCM), dichloroethane (EDC) and the grouping "octylphenol, nonylphenol and their isomers; salts thereof" for the years 1993 to 1996. Lead was not included, as there were too many items. A figure for one year should not

be considered in isolation, as the trend over a number of years will give some hint as to whether the substance usage has increased or decreased. This trend provides a starting point when looking for the number of users of a substance.

The imports of both DCM and EDC increased significantly in 1996 from 1995 levels. DCM is the only substance of the three to be exported from 1994 to 1996. Indeed the exports of DCM increased dramatically in 1996 from 9 tonnes in 1995 to 133 tonnes in 1996. It is a possibility that the export may well have been to Northern Ireland but this would have to be checked. Imports can be broken down on the basis of country of origin and exports by country of destination.

Table 2. Trends in Imports and Exports over the Years 1993 - 1996.

Year	Imports Tonnes			Exports Tonnes		
	DCM	EDC	Octyl/Nonyl[2]	DCM	EDC	Octyl/Nonyl
1993	2686	1.6	1442	30	2.4	0
1994	3459	7	2764	6	0	0
1995	3433	0	113	9	0	0
1996	4156	17	1102	133	0	0

Importers and exporters

51 companies were initially contacted by letter. Of these companies, 19 operate as suppliers/distributors of bulk chemicals in Ireland. Each letter was followed up by a minimum of two phone-calls. Initially quite a number of companies requested that the letter be sent again. Once the letter had been received and the objectives in contacting them had been explained in detail, companies were generally willing to co-operate. At the end of this phase of the project only 4 of the 19 suppliers/distributors contacted had not provided the figures requested. This represents a success rate of approximately 80%.

Each supplier/distributor was asked:

1. if they used any or all of the four substances
2. to provide figures for the relevant substances (if they dealt with them) for 1996
3. to identify the destination of the substance

The information gathered has been included in the substance flow analysis for each substance. As two of the major suppliers did not provide figures, comment cannot be made on the reliability of the CSO data. User companies should be contacted to retrace the chain back to the suppliers as a further cross-check. A supply source has stated that the market for DCM is 3000 tonnes and not the 4000 tonnes given in the CSO data. However, this statement may be based on 1994 / 95 import levels which were approximately 3000 tonnes. In the case of EDC it would appear that the import figures are inaccurate based on the usage figures gathered.

Other possible sources of information on imports, exports and the final destination of goods

The next possible source of information explored was the information collected by the Revenue Commissioners. From the 1st May 1996 Customs and Excise introduced a further development of automated entry processing known as the "Paper-less Declaration". This electronic system, or Direct Trader Input (DTI), records the importer under both VAT number and trader account number (TAN). The data input, under the CN code classification, is instant and immediately accessible but is not available to third parties.

Imports and exports by sea

All movements of Dangerous Substances into and out of Irish parts are advised to the relevant Harbour Master prior to unloading and loading, respectively. The information provided details the following:

- Container number
- IMDG number
- UN number
- Technical name of substance
- Quantity
- Details of storage
- Port of loading
- Port of Discharge (if route ongoing)
- Consignor
- Consignee

This degree of recorded detail would be extremely useful but the port authorities will not provide any information to third parties on the grounds of confidentiality and to ensure that no action would be taken against them for breach of confidence.

[2] The figures for Octyl/Nonyl are for the CN group Octylphenol, nonylphenol and their salts; isomers thereof.

The port authorities differentiate between the different types of shipments, which are, full or part tanker loads (500-1,500 tonnes), 20' ISO bulk containers (20+ tonnes), 20'/40' dry containers drained of logged products and "less than full" container loads (LCL) of mixed cargo.
The port authorities primary concern is that, in the event of an incident the consignee, their agent, warehouse/store-tank operator, carrier and the emergency services have accurate, up-to-date information enabling them to deal safely, quickly, readily and adequately with the incident. Captain Faruan, Habour Master, Cork, commented that their greatest concerns centre on the exports of "waste chemicals/products" because of the unclear, insufficient and/or inaccurate information provided by waste disposal operators.
Even though a "Products Register" or "Dangerous Substances Inventory" does not currently exist in Ireland, the recording, collection and publication of specific import/export data is widespread and engaged in by various agencies but is not coordinated in one integrated readily accessible, easy-to-use medium. The following is a list of the principal sources of data:

- Manufacturer (Consignor)
- Shipping company
- Shipping and forwarding agents
- Customs clearance agent
- Local haulier or carriers
- Port authorities
- Warehousing or bulk storage operator
- Consignor's Irish subsidiary, agent or distributor
- Revenue Commissioners (Customs)
- Central Statistics Office (CSO)
- End-user (Consignee)

The range and detail of the data which any of these agencies receive, use and file, is directly related to their specific functions and their relationship with their correspondent agencies and their (the agents) particular needs. For example, the Revenue Commissioners record trader account and VAT numbers whereas the CSO has no need of such information. Similar information priorities exist across the entire paper-trial. The isolation and identification of particular information is not difficult but it does assume unrestricted access to the various data sources, which is not possible at this time.

Documentation associated with the importation of goods into Ireland

Due to the comprehensive detail of the "official", as distinct from the "commercial", data recorded by Customs and Excise it was decided to comment on the procedures at point of import, in some detail.

1. The supplier, or more usually the importer, appoints a licensed Customs Clearance Agent (CCA), who will receive all of the relevant documentation associated with the particular consignment.
2. The use of the hard-copy Single Administrative Document (SAD) in intra-community trade is normally no longer required except in particular circumstances and at the request of the Customs Authorities. However, the format of the SAD document is used as the basis of the Direct Trader Input (DTI) declaration.
3. By means of the DTI facility the CCA inputs the Trader Account Number (TAN) and the VAT Number of both the Consignee and the declarant. Both of these reference numbers are the primary identification indicators held on the customs database.
4. The CCA inputs the necessary data in the appropriate "boxes" of the SAD format. Most importantly, from the viewpoint of conducting a substance flow analysis, is that this data includes:
    - Consignee's Name
    - Product Name
    - Commodity Code
    - Invoice Number

The Consignor's name does not always appear in this format but it is obviously on their own invoice, a copy of which must be held on file for two years by the CCA along with all of the other shipping documents.
Every month the Customs Stations return the previous months import/export data to the CSO who update their records and the Monthly/Annual Trade Statistics, accordingly.
It can be concluded that there is a wealth of information available regarding the transit of goods across the national boundary, including information on the final destination of said goods. Unfortunately at present it is not possible to access this information.

Users

The next step in the methodology was to identify the actual end-users of the substances. This information would provide a further cross-check for the information obtained in the earlier steps. Secondly, once the users had been identified and contacted, information on waste emissions could also be obtained. It took a significant amount of time to identify the end users of each substance. Initially IPC licence applications, and PER's where available, were read to identify user companies. Personal contacts and CTC data were also used. The Kompass Business Directory was used to identify a further 24 possible user companies. Letters identical to those sent to the suppliers/distributors were sent out to these companies.

At this stage it was decided to concentrate on the starting point of each substance sub-chain. It was felt that if too much information were requested initially, companies would be unwilling to provide any information.

The companies were asked:

1. if they used any or all of the four substances
2. to provide figures for the relevant substances (if they dealt with them) for 1996
3. to identify the destination of the substance
4. where relevant, further information was required with respect to the presence of a substance in a manufactured product

Companies contacted in relation to Lead

15 companies were contacted, the majority of whom dealt in scrap metal or metal processing. Of these companies, 5 did not produce the figures requested. This represents a success rate of approximately 66%.

Companies contacted in relation to DCM , EDC and Nonylphenol / Nonylphenol Ethoxylate

As these substances are used mainly in the PharmaChem sector, IPC Licences were read on the EPA Internet site and a preliminary list of potential users was drawn up. The CTC had already produced Polluting Emissions Registers (PER's) for several of its partner companies. It was therefore possible to determine the purchase orders and aqueous effluent figures for DCM for those companies. It then proved necessary, to go to EPA headquarters to look at the files of those companies on the list for which no information had yet been obtained. Figures were obtained for those companies, which had produced a PER in 1996. Unfortunately only a small percentage of the companies on the list were required to produce a PER in 1996. However, there was enough information on file to confirm whether a company on the list was a user of DCM or EDC along with an annual usage figure.

Nine further potential users of these three substances were identified and contacted, only two did not produce the figures requested. This represents a success rate of approximately 78%. Initial identification of nonylphenol users was also achieved through contact with an EPA inspector.

Sector Federations / Associations

IPCMF - Irish Pharmaceutical and Manufacturers Federation (IBEC)

A contact in SIFA informed us that companies make annual returns to IPCMF. This information was followed up. It appears that the Federation is in the process of setting up a database for emissions from allied companies for the years 1992 to 1996. The Federation had undertaken to provide the information if its members were prepared to permit it. No information was received from this quarter.

Products

Some information on products containing the four substances, was obtained from the companies contacted. For example, the percentage of dichloromethane present in certain branded paint strippers was obtained. EDC appears only to be used as a process chemical in Ireland. Some information on the amount of nonylphenol ethoxylate in detergents and paint was also obtained.

The main drawback in the analysis of products containing the selected substances is the fact that there is no products register in Ireland. It would require a large number of man-hours to track down every product containing a substance and to determine the amount of that substance present in said product.

Waste

A number of sources for information on aqueous waste have already been mentioned. These are the PER's produced by the companies in the IPC-licensed sector , IPCMF and the companies themselves. The information given in the PER's has been obtained but would need to be cross-checked with information from the companies themselves. The information from the IPCMF was not obtained. Preliminary information on the waste produced by some of the companies contacted was obtained. The final source of information on waste and emissions was the National Hazardous Waste Management Plan. This source was used to find information on lead-acid battery waste and the recycling of lead-acid batteries. It also provided some information on chlorinated solvents. Substance flow analyses carried out for the substances selected in other countries were also useful sources of information.

Summary

Production of a skeleton chain for each of the four substances selected

A skeleton chain gives an overview of the chains of use for each substance. To generate a skeleton chain therefore, the uses of each substance had to be determined. It was possible to obtain information on the general uses of each of the four substances from technical literature, searches and so on. However, at times it proved to be quite difficult to confirm substance uses in Ireland (uses of EDC and nonylphenol / nonylphenol ethoxylate).

Initial quantification

At this stage the uses of each substance in Ireland had been determined but no figures had been obtained. Figures were required for imports, exports, production and emissions along with information on products. The proposed sources of information were :

1. CTC partner companies
2. National Chemical Company
3. CSO data for imports and exports
4. Statistical data from the main supply countries
5. PER/AER reports from IPC licensed companies
6. the National Waste Database
7. Local Authority trans-shipment records
8. HSA data
9. National Hazardous Waste Management Plan

The sources of information actually of use were items 1, 2, 3, 5, and 9.

Statistical information (Items 3 and 4):

It was necessary to obtain the import and export figures for the substances in their "pure" form and in commodities in which they were present as a certain percentage (products). The CSO statistics were accessible once the CN code for an item had been obtained. If a substance is classified under a general grouping it is extremely difficult to obtain figures for that substance on its own. This was found to be the case for nonylphenol/nonylphenol ethoxylate. The reliability of these import and export figures has yet to be fully determined. However, it is suspected that the figures may be erroneous in some cases (dichloromethane and dichloroethane). Suppliers were contacted with the aim of corroborating the figures, however some suppliers did not supply the information requested. Statistical information from the main supply countries was not required as the CSO provided a breakdown on commodity by country of origin. This information could only be considered useful if the environmental burden of a substance in its country of origin was to be considered. It did provide a rough guide as to which supplier was importing it.

IPC-Licensed sector (Items 1 and 5):

The IPC licensed sector was a sector which was relatively easy to obtain information on. It was assumed that the majority of the usage of DCM, EDC and nonylphenol ethoxylate (or nonylphenol) would be in this sector. EPA files either contained information on the usage figure for a substance, or a PER, which detailed the purchase orders and emission figures for that substance. There were several drawbacks encountered. The first was that the EPA itself did not have a list of users of a particular substance. EPA inspectors did however respond to a query sent out to them. This provided a starting list for DCM only. The second drawback was that the PER system is not yet fully operational, in that companies have agreed a schedule with the EPA but may not have to produce a PER until some time in the future. It was not always possible to determine which companies used a particular substance from its licence alone, as solvents can be reported as Luft Organic Classes.

A minor problem in relation to the methodology was that some information was obtained from the CTC partner companies and other contacts. However, the advantage of using these contacts was that information was obtained quickly. This should be balanced by the fact that these companies would have responded to either direct contact, or contact by mail, had they been approached in this manner.

Non IPC-Licensed sector:

Companies outside of this sector were initially more reluctant to provide information and in certain cases did not provide information which they had agreed to send. These companies were contacted by mail to assure them that the inquiry was legitimate and that the information they provided would be treated as confidential information. In general, this produced a positive response.

Products containing the four substances were not considered to any great extent. This was due to the fact that Ireland does not have a Products Register or Chemical Products Register, unlike Denmark for example, which would be a major source of this type of information. It would require a large amount of research to track down all the products containing a particular substance. This problem is particularly relevant to lead in that it is present in a diverse number of products.

Waste (Item 9):

The National Hazardous Waste Management Plan was of some use in relation to the waste arisings of lead and DCM. It is possible that the IPCMF may be a source of information on emissions from companies who are members of this federation.

Conclusions

The proposed methodology has been applied with reasonable success at this initial stage. The methodology was based on substance flow analysis methods applied in Denmark, Sweden and the Netherlands. It was applied to four test substances; lead, dichloromethane, dichloroethane and nonylphenol ethoxylate. Preliminary substance flow analyses were produced each substance (the nonylphenol chain was also traced). The successful implementation of the proposed methodology has proved that the methodology is applicable in an Irish context. The majority of the sources of information suggested in conjunction with the proposed methodology were valid sources. These sources were:

- CSO trade statistics
- Technical and Trade Publications
- CTC partner companies and other industrial contacts
- EPA
- IPC licences and PER's
- User Companies themselves
- Sector Federations
- Suppliers / Agents (Importers and Exporters)
- National Hazardous Waste Management Plan (NHWMP)

The CSO data on imports and exports can be obtained once the CN code of a commodity is known. However, if a substance does not have a CN code of its own, and is grouped with similar substances, the figures for this substance cannot be obtained directly. The CSO data may be unreliable in a certain number of cases. This is a common finding for trade statistics used in substance flow analyses carried out in other countries. Therefore, it is imperative that import and export figures are cross-checked with information from other sources. These other sources would be suppliers, agents and the user companies.

Customs and Excise provide specific information on imports and exports to the CSO. However, information on the consignee for a particular import, also gathered by the Customs and Excise, is not accessible. This information would be extremely useful in the tracking of hazardous substances through Ireland.

Information on usage and emissions of substances from companies covered by IPC licence is readily accessible. At the moment, the licensing schedule has not been completed and the majority of companies in this sector are only beginning on the route to production of a PER. However, once the system is fully functional, information on substance usage and substance emissions in this sector should be comprehensive. The only drawback to the system is that the user of a substance has to be known before the relevant information can be obtained.

Contacts in CTC partner companies and other contacts within this sector were utilised to identify other companies using a particular substance, and to obtain figures on usage and emissions quickly. This approach could be considered outside the scope of the methodology. However, a reasonable number of companies in this sector were either contacted directly or by mail. Most companies contacted directly required some proof of legitimacy and were subsequently mailed. This approach was very successful in eliciting information. The only drawback was the time scale required to actually obtain the information promised.

Information retrieval from companies outside of the IPC-licensed sector was also very successful. Only one company actually refused to provide the information requested. The reason given was that they were a small company and it would require a large amount of man-hours to produce the information. Initial contact by phone, only was not found to be successful, as companies were suspicious of the motives behind the project and were not aware of our credentials. The effect of contact by mail, which included the request from the EPA for information, was successful as long as the request was followed up by a number of phone-calls.

A large number of companies in this particular sector manufacture or supply products containing the substances of interest. At present no products register exists in Ireland, which means that a substantial number of man-hours would be required to identify all products containing a substance of interest. Once the range of products had been identified a breakdown of the constituents of each product would then have to be obtained.

The waste streams for each substance have not been fully quantified at this stage. In the IPC-licensed sector the majority of user companies had to be contacted directly, due to the relatively small numbers of PER's produced in 1996. As stated earlier, this will not be a problem once the system is fully functional. A second source of information on waste streams was the NHWMP. Another possible source on emissions may be the IPCMF.

Preliminary Substance Flow Analysis for Lead 1996

The two tables given below indicate the percentage of total consumption made up by the various uses of lead in Denmark and Finland respectively. The population of Denmark is 5.3 million and the population of Finland is 5.1 million. This compares with a population of 3.6 million in Ireland.
These served as initial indicators of the identity and scale of uses in Ireland.

Table 1. Danish SFA on Lead (Lassen and Hansen 1996) [3]

Use	**Consumption Tonnes / annum**	**% of Total Consumption**
Metallic Lead:		
Batteries	8 100 - 8 900	48
Building Materials	2 800-4 100	20
Cable Sheaths	2 000 - 2 300	12
Fishing Tackle and weights	380 - 730	3
Ammunition	350 - 465	2
Keels	50 - 150	0.6
Other	700 - 1 200	5
Chemical Compound:		
Glass	620 - 990	5
PVC stabilisers	300 - 400	2
Pigment in plastics / paints	35 - 110	0.4
Other	60 - 240	0.9
Natural Contaminant:		
Fuels	40 - 130	0.5
Other	24 - 60	0.2
Total	**15 500 - 19 800**	**100**

[3] ***Danish EPA Miljoprojekt no. 327***

Table 2. Use of lead in Finland 1990 (Mukherjee 1993)[4]

Use	Consumption Tonnes / annum	% of Total Consumption
Batteries	9 500	43
Cable Coverings	1 830	8
Ammunition	2 740	12
Trace Components:		
- Cu concentrate	1 300	6
- Zn concentrate	4 360	20
- Coal	130	<1
- oil	1	<1
Stabilisers	740	3
Semi-finished products	420	2
Paints	190	1
Solders	130	<1
Nuclear Power Plant	200	<1
Glass and Ceramics	<10	<1
Others (fishing weights etc.)	400	2
Total	**21 950**	**100**

Lead in cables

Lead sheathed cables are considered to be an accumulation or stockpile within Ireland for the substance flow analysis. Leaded sheath cables were and still are being installed in Ireland. The lead is not in direct contact with the soil. Older cables had a protective layer of jute/pitch, modern cables have a protective layer of polyethylene. In the past, 10 kV and 38 kV cables would have had lead sheaths, but this has not been the case for the last 15 years. Most 110 kV, 220 kV and 400 kV cables have lead sheaths. The volumes of cables are expressed in terms of circuit length. The total length of 10 kV and 38 kV cables installed is approximately 4 200 km, most of which does not consist of lead sheathed cabling. The total lengths of 110 kV, 220 kV and 400 kV cables installed is approximately 65 km. Most of the original cables installed are still in service. More information can only be obtained by contacting the ESB office in a specific location. However, according to the ESB it would be quite difficult to determine the exact location of each lead sheathed cable and its length.

Lead ore and concentrates

Ireland ranks as the tenth largest producer in the world of lead concentrates and is the second largest producer in Europe. An estimated 50 000 tonnes per annum of lead concentrate is produced[5]. Therefore, exports of lead ore make up the biggest outflow from Ireland for this substance flow analysis.

There are three Lead-Zinc mines in Ireland : Tara , Lisheen and Galmoy (Arcon). Of these only Tara mines was in production in 1996. This information was obtained from The Geological Survey of Ireland (Department of Transport, Energy and Communications). This mine confirmed that the CSO export figure for lead ores for 1996 was correct and that the metal content would be of the order of 45 000 - 48 000 tonnes. At this stage of the project no waste stream information has been obtained from the mine.

According to the CSO figures, 48 tonnes of lead ore and concentrates were imported. Information on the importer has not been obtained so the lead content of this import, its end use and any associated waste streams cannot be ascertained.

Lead-acid batteries

A typical lead-acid accumulator consists of 30% lead, 49% lead oxide, 12% sulphuric acid and 9% plastics. The CSO imports of lead-acid accumulators in 1996 were 9 963 tonnes. It is possible that the batteries imported with motor vehicles are not included in this import figure but this was not confirmed. The lead content of each accumulator type has not been ascertained. If it is taken that the lead content of any accumulator type is 79% (lead plus lead oxide) then the total "pure" lead imported for this chain segment is 7 870 tonnes.

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[4] *Mukherjee A.B. Emissions of lead and its Fate in the Finnish Environment, In: Proc. Int. Conf. Heavy Metals in the Env., Toronto, pp254-257, 1993*

[5] *Tobin, T. , "Ireland - A World Class Zinc and Lead Producer", The Engineers Journal, vol. 52 no.1, pp 23-25, 1998*

There was no data available in the trade statistics for lead-acid battery exports in 1996. However, according to the NHWMP there were 4 375 tonnes of waste lead-acid batteries exported and 170 tonnes of lead-acid batteries recycled in 1996. This recycle figure is projected to increase to 1 020 tonnes per annum. According to these figures this leaves 5 318 tonnes of lead-acid batteries unmanaged (this is based on an import figure of 9 863 tonnes). If a lead content of 79% is assumed, this equates to 4 201 tonnes of lead. The figures given in the NHWMP have yet to be cross-checked, however, there appears to be an error for the figure quoted for CSO imports. One scrap merchant confirmed that his company exported 247.4 tonnes of waste lead-acid batteries in 1996. No other figures were obtained for waste lead-acid batteries.

Table 3. Flow Analysis Figures for Lead-Acid Batteries 1996

	Lead-Acid Accumulators	**Approximate Lead Content**
Imports	9 963 tonnes	7 871 tonnes
Recycle	170 tonnes	134 tonnes
Exports	4 375 tonnes ?	3 456 tonnes ?

The figures for lead consumption in Denmark and Finland were given in Tables 1 and 2. Only the figure for battery imports to Ireland, which are assumed to be entirely "consumed", is reasonably comparable. In Denmark and Finland, the consumption of batteries equated to 43-48% respectively of the total consumption of lead. This would imply that the total consumption in Ireland should be approximately 22 937 - 20 548 tonnes. The total imports of "pure" lead to Ireland were 27 635 tonnes. However, considerable cross-checking and further quantification would have to be carried out to directly compare the figures obtained for Ireland with these studies.

Table 4. Comparison of Battery Consumption

Ireland 1996	Denmark 1996	Finland 1993
9863 tonnes	8900 tonnes	9500 tonnes

Articles of pure lead

Lead can be used in many forms as a building material as shown in Table 5. Refined lead and articles of lead have been included in this figure as the refined lead (99.9% lead) and the articles of lead (this is lead that is not specified elsewhere in the trade statistics - possibly used as radiation shields) are taken to be pure lead. Therefore, imports of substances made up of pure lead were 812 tonnes and exports of these items were 18 887 tonnes in 1996. The largest metal processor in Ireland processed 11 500 tonnes of lead, in the form of lead sheet in 1996. This lead was obtained by the company from metal merchants, who in turn received it from the demolition of buildings (lead roofing and pipes). According to the company, the majority of this processed lead was returned to the domestic market. The other two major companies in this sector did agree to provide the information requested, but it was not received. This meant that the large export figure could not be corroborated.

Table 5. Imports and Exports of Lead used for Building Material and Other "Pure" Lead Items

	SITC	**Imports (tonnes)**	**Exports (tonnes)**
lead bars, rods, profiles etc.	685.21	62	7
lead plates, sheets, strip etc.	685.22	726	18866
lead tubes, pipes and fittings	685.24	24	-
refined lead	685.12	Ö	14
articles of lead	699.76	29	17
Total		**812**	**18887**

Unrefined lead and lead alloys

4 tonnes of unrefined lead and lead oxide were imported in 1996. There were no exports under this heading. Information regarding the percentage lead content in this category was not obtained.

Lead waste and scrap

9 977 tonnes of lead waste and scrap were imported in 1996. Data was required from the various scrap-merchants to corroborate this figure. Only 71 tonnes was accounted for. This lead scrap was processed in Ireland. Exports of lead waste and scrap were 1404 tonnes according to the CSO but again it was not possible to corroborate this figure. For the purposes of the analysis, lead waste and scrap was taken to be pure lead.

Lead used in the fishing industry

The figures for this sector were not quantified. Accumulation of fishing weights in the aquatic environment can be significant. However, this sector is not yet regulated with regard to waste.

Lead used in glass

Lead is present in glass crystal, Waterford Crystal for example has a 33% lead oxide content. There were three main categories of leaded crystal under the CN system as described in Table 5. The total imports for leaded crystal in 1996 were 889 tonnes. This figure needs to be adjusted for lead only. To carry out this calculation a large amount of information on the various types of glass and their lead content would have to be gathered. The total amount of lead crystal exported from Ireland in 1996 was 5 451 tonnes. The largest leaded crystal manufacturer in Ireland produced approximately 14 000 tonnes of glass. Approximately 85% of this figure would be exported. However, a sizeable proportion of this figure would first enter the domestic market before being exported. So the export tonneage by this route cannot be obtained from CSO statistics. Lead is also present in the glass used in computer monitors and television screens to shield the user from radiation. This chain segment was not followed.

Lead oxides

Lead monoxide (litharge, massicot) is imported for use in the glass industry in Ireland. The total imports of lead oxide and red and orange lead for 1996 were 2 881 tonnes and the total exports were 119 tonnes. This information was obtained using the SITC code. The CN classification is broken down into separate substances. Three leaded glass manufacturers were contacted of which two have provided information at this stage. These companies used approximately 4 267 tonnes of litharge. It is obvious that this figure does not correspond with the CSO figures. Suppliers were contacted to corroborate this figure. One company dealt with litharge in but proved reluctant to provide such commercially sensitive information.

Leaded petrol

Lead is present in petrol in the form of tetraethyl and tetramethyl lead. The use of leaded petrol is being phased out. The total imports of leaded petrol in 1996 were 305 075 litres and exports were 1 351 litres. This figure would have to be adjusted to give the approximate lead content only.

Lead in ammunition

The import / export figures were only taken for shotgun cartridges. Imports were 3 843 tonnes and there were no exports in 1996. Again, a figure has not been obtained for the percentage lead present in a shotgun cartridge. A company was contacted but they were not prepared to provide any information. Lead accumulates in the aquatic environment in the form of lead shot and other leaded ammunition due to the pursuit of hunting. No figures are available to indicate the level of lead waste due to this source.

Lead stabilisers in PVC

No figures were obtained for this chain due to the lack of information on the percentage of lead present in the PVC imported into Ireland and the PVC which has accumulated within Ireland. PVC stabilisers were also not considered.

Ash and residues containing mainly lead

Imports in this category were 1 tonne and exports were not considered. The use of this import in Ireland has not been quantified due to its relative insignificance. According to the NHWMP 141 tonnes of tin ashes containing lead constituted a waste stream. This figure was not checked. According to the largest metal processor in Ireland, approximately 5% of lead processed will be in the form of waste ash or residue. This waste is not treated.

Lead used for soldering

Imports of rods, electrodes etc. for soldering for 1996 were 4 229 tonnes and exports were 2 580 tonnes. Information was obtained on the export of lead solder. One company exported approximately 22 tonnes of waste lead solder for recycle. This is equivalent to a lead content of 5-6 tonnes. Companies using lead solder as part of their processes should be contacted to identify the destination of their waste solder.

Lead in fertilisers

Phosphate fertilisers made from phosphate rock contain trace lead. This chain was not quantified.

Lead carbonate

This chain was not quantified.

Paint and ink

This chain was not quantified.

Coal

The emission of trace amounts of lead is associated with the combustion of coal in power plants. As this is a gaseous emission this chain was not quantified.

Summary:

- Not enough information was obtained to quantify all the elements of each chain segment.
- Only chains for pure lead were quantified to any reasonable degree.
- Waste streams and accumulations in society were not quantified.
- It was not possible to cross-check figures due to the non-response of several companies.

Table 6. Preliminary Substance Flow Analysis for Lead 1996[6]

Category	Import tonnes	Accumulation tonnes	Recycle tonnes	Export tonnes
Articles of pure lead	8 212	??? society	11 500+ scrap?	18 887
Batteries[7]	(9 963) 7 871	??? landfill	(170) 134	(247) 196
Lead ores	(48)	??? reserves	???	48 000
Cable sheaths	???	??? soil deposition	none	none?
Unrefined lead	(4)	??? society / landfill	scrap?	0
lead waste and scrap	9 977	all recycled? soil	???	1 404
fishing	???	??? aquatic	???	???
glass	(889)	??? society landfill?	0	(5451) + other exports
lead oxides	(2 881)?	air-born?	???	(1 185)
leaded petrol (litres)	(305 075)	??? air-born soil deposition?	0	(1 351)
ammunition	(3 843)	??? aquatic	???	0
PVC stabilisers	not followed	??? landfill/society	0	not followed
ash	(1)	(141) soil?	???	not followed
solders	?	?	?	(22) 5-6
fertilisers	not followed	not followed	not followed	not followed
lead carbonate	not followed	not followed	not followed	not followed
paints and inks	not followed	not followed	not followed	not followed
Total Pure Lead	**?**	**?**	**?**	**?**

[6] ***Figures in parentheses indicate "impure" lead chains.***

[7] *Pure figures are based on a 79% lead content (lead + lead oxide)*

Preliminary Substance Flow Analysis for Dichloromethane (DCM) 1996

The chain segments of this substance were a lot easier to follow than for lead. This was due to the fact that the majority of dichloromethane imported into Ireland is used in the PharmaChem sector. The majority of companies operating in this sector are regulated by the EPA and will have obtained, or have applied for, an IPC licence. It was possible to obtain varying degrees of information on usage and emissions depending on whether a company had produced a PER or not.

CSO imports and exports

Table 1 gives the figures for the imports and exports of dichloromethane from 1993 to 1996. The import figures for both imports and exports were the highest in 1996.

Table 1. Import and Export Trends for DCM

Year	Imports Tonnes	Exports Tonnes
1993	2685.451	30.373
1994	3458.574	6.199
1995	3432.522	9.329
1996	4155.909	132.761
Average	3433.11	44.67
Std Dev	600.58	59.70

Figures for paint thinners, varnish and paint removers, aerosols and adhesive products were not obtained. This was due to the fact that a products register does not exist in Ireland and it would have taken a considerable amount of time to quantify the percentage of dichloromethane in each substance concerned. The dry cleaning sector was not investigated.

Use of Dichloromethane

The CSO statistics were cross-checked with figures from companies operating in this sector, with 838 tonnes remaining unaccounted for. An attempt was made to cross-check these figures with those of suppliers. This approach accounted for some 2156 tonnes, however, two of the major suppliers did not provide the information requested. It became clear that a small, yet significant, amount of DCM was being used by smaller operators outside of the PharmaChem sector. For example, one supplier quoted a figure of 100 tonnes being sold outside of this sector.

Table 2 details the usage of dichloromethane in Ireland by company. Some companies were only able to provide annual usage figures rather than amount bought in so this will affect the balance. However, it was assumed that most companies would not hold a large amount of dichloromethane in stock.

Waste Dichloromethane - NHWMP

According to the NHWMP it can be expected that 15-30% of the amount of dichloromethane used in Ireland will arise as chlorinated waste (recycled). This figure is based on an extrapolation of Dutch data which may not be applicable. It was estimated in the NHWMP that 500 - 1000 tonnes of pure dichloromethane would be disposed of as waste. If this stream were contaminated it follows that this figure may be several times higher. It is generally assumed that approximately 15% of paint remover used is released as waste residue. These figures cannot be substantiated without further research.

Aqueous emissions of Dichloromethane

It can be reasonably assumed that the majority of dichloromethane used in the PharmaChem sector will be within a closed system and that most emissions will be to air. Emissions to water have yet to be completely quantified.

Summary:

- CSO data was obtained.
- A preliminary cross-check of the CSO data was carried out. 52 percent of this figure was cross-checked using information provided by suppliers. However, several large suppliers did not supply the information requested.
- Due to that fact that most dichloromethane is used in the IPC - licensed sector information was accessible.
- 20 percent of the CSO import figure was not accounted for using information obtained from user companies (probably outside the PharmaChem sector).
- Waste streams were not quantified for those companies who had not completed a PER.

Table 2. Breakdown of DCM usage by Company

Company	Usage 1996 (tonnes)
A	701.0
B	7.5
C	716.0
D	565.0
E	0.2
F	39.0
G	498.0
H	140.0
I	7.0
J	2.2
K	0.2
L	69.0
M	46.0
N	250.0
O	32.0
P	20.0
Q	3.0
R	82.0
S	0.2
T	6.6
Export	**133.0**
Total	**3317.9**
Unaccounted	**838.1**

Preliminary Substance Flow Analysis for Dichloroethane (EDC) 1996

As this substance was another solvent used in the Pharmachem sector information was also readily accessible. From the investigations carried out it would appear that the only use of EDC in Ireland is as a process chemical. There appears to be only two or three main users of EDC in the country. From information obtained from EPA records and the user companies themselves, only one company used a significant amount of EDC in 1996. One other company used an amount of 0.08 tonnes in that year.

CSO imports / exports

Table 1 gives the trends in imports and exports from 1993 to 1996. 1996 saw a huge increase in the amount of EDC imported into the country. To cross-check these figures, user companies were contacted. One user received 23 tonnes in 1995. This figure was not consistent with the CSO figure. The main user of EDC in 1996 used a quantity of 30 tonnes. Again this was not consistent with the CSO figure. Companies generally do not hold a large amount of this solvent in stock so it was assumed that the amount received was the amount imported for use. This would imply that the CSO data for this particular substance is unreliable.

Table 1. Import and Export Trends for EDC

Year	Imports Tonnes	Exports Tonnes
1993	1.628	2.388
1994	7.018	0.000
1995	0.000	0.000
1996	17.150	0.000
Average	6.45	0.60
Std Dev	7.74	1.19

Use of EDC in the IPC-Licensed sector

User companies were identified from EPA files. As stated above, it appears that there was only one main user in 1996. Emission figures were not obtained. However, the company reports a recycle rate of 79%. Information from the suppliers of EDC was not received so it was not possible to corroborate the import, export and usage figures.

Summary:

- The main users of EDC in Ireland were identified. One other small user was also identified.
- The CSO data on imports were cross-checked with figures provided by the main user companies and there would appear to be a discrepancy between the two sets of figures.
- Information from suppliers, which would corroborate the CSO data, was not received.
- Information on emissions was not obtained.

Preliminary Substance Flow Analysis for Nonylphenol/ Nonylphenol Ethoxylate 1996

Information was obtained on the use of both nonylphenol and nonylphenol ethoxylate in Ireland in 1996. Nonylphenol ethoxylate is used by three companies in Ireland, and nonylphenol by one. It was impossible to determine import or export figures from the CSO trade statistics because nonylphenol and nonylphenol ethoxylate do not have their own CN code. Three supplier /distributors were identified for nonylphenol ethoxylate and only one provided the information requested. This company supplied 48 tonnes in 1996.

Use in detergents

Two companies in Ireland used nonylphenol ethoxylate as a constituent of a detergent in 1996. One company, which formulates detergents, used 7 tonnes as part of their detergent mixing and blending process. Another company, which uses a detergent containing nonylphenol ethoxylate for cleaning purposes, did not provide the information requested.

Use in paints

Nonylphenol ethoxylates are used in the formulation of paints. One paint manufacturer used 11.5 tonnes in 1996. According to this company the percentage of this substance present in their product is generally in the range of 0.2 to 0.3%, but can vary in the range of 0.05 to 0.5%. This product was supplied to the domestic and trade markets in Ireland in 1996.

Use in adhesives

One company used 383 tonnes, and purchased 416 tonnes, of nonylphenol in 1996. This substance was used on its own but was also mixed with dinonylphenol.

Use in pesticides

This stream was not quantified.

Summary

- CSO data was not readily available for this substance.
- Four user companies were identified. Three companies used nonylphenol ethoxylate and one used nonylphenol.
- Some product information was obtained.

Section 9: Recommendations

Data must be obtained on the identity, quantity and usage of substances applicable to Ireland. The introduction of a Chemical Products Registration scheme must be seriously considered

While there are "Product Registers" in most EU countries, their purpose is largely confined to poisoning response, outside of the more comprehensive Nordic registers. The EU Commission is presently reviewing its chemicals control policy, and initiatives have been undertaken by the German government to study the potential for a Chemical Products Register in Germany.

These Chemical Product Registers have proven to be very effective in the Nordic countries, and are felt in some quarters to be indispensable to proper risk management. Such information would be beneficial not only for environmental risk management, but also occupational health risk management and emergency response.

Having such data available to decision makers would allow a rational basis for policy development. In examining such a scheme, consideration should be given to ensuring the protection of commercially sensitive data, minimising the administrative burden on data supplier and analyst alike, and maintaining a database that is relevant and properly reflects current practice.

While the trade statistics data provided based on the CN-Combined Nomenclature system are internationally comparable, they do not provide sufficient precision for decision making, except in limited cases. In addition, they may not reflect the actual use practice in Ireland. Without this detailed information, it may be quite inappropriate to adopt a default position which assumes wide dispersion of a substance, when actual usage may be confined to a tightly regulated closed system.

This current study has been confined to pure substances. The collected data must extend to the use of dangerous substances in preparations. Lack of knowledge of the composition of preparations is a serious problem. This presents greater difficulty in terms of obtaining data which may not be readily available to the importer or supplier. However, it should be recognised this difficulty has been overcome in some of the Scandinavian countries. Chemical Product Registers have been established in Sweden, Norway and Denmark where commercial confidentiality has been respected and adequate data has been provided, to the satisfaction of both data supplier and user.

Dangerous substances in products present a more difficult problem. This has been addressed elsewhere through narrow, targeted enquiries, but has not been amenable to a general Products Registration scheme. This difficulty is not unique to Ireland. The establishment of a Chemical Products Register should be initially confined to pure substances and preparations.

Monitoring must be enhanced, but based on suspected incidence

While monitoring is favoured as the absolute indication of exposure in the environment, the experimental difficulties of obtaining representative, reproducible, validated data for the marine environment is difficult. It is necessary to examine the incidence of selected chemicals, rather than to attempt to screen for all existing substances. A comprehensive screening programme to cover the entire country is hardly feasible, and certainly expensive. Without guidance on the likely occurrence of specific substances, it would be difficult to design an effective programme.

As limits of detection move lower and lower, it becomes more likely to detect particular substances, but more difficult to attribute their origin, whether natural or man-made, or degradation products of man-made emissions. Further consideration must be given to improved monitoring, but in view of the expense associated with this, prioritisation must be based on suspected incidence and must be justified.

Further consideration of a Chemical Products Register

What is a Chemical Products Register?

A Chemical Products Register is a database, or collection, of information on chemical products. Typically, the chemical products are pure substances, e.g. organic solvents, or mixtures known as preparations, e.g. paint, detergent. A register may be relevant to an industrial sector, activity, region or, as is most common, a country. The extent of information registered may range over the following:

Class of information	Description
Intrinsic properties	Properties such as the physical, chemical, human and ecotoxicological inherent to the product. The extent of these can be very wide-ranging
End uses	Which chemical products are used by industry, commerce and the general public. Where they are used, for what purpose, in what manner and in what quantities. Details of the composition of the products are necessary for adequate insight.
Safe handling	Conditions and practices necessary for the safe storage, transport and use of the chemical product. These may refer to industrial, commercial or public handling of the materials. Proper labelling and provision of material safety data sheets are necessary.
Accident & emergency	Response to poisoning incidents. In such cases, knowledge of the composition may be desirable, but knowledge of the necessary medical response is more important. Responses to spills, fires, explosions or releases to the environment may be registered to assist emergency services and land-use planning.

Who are the users?

Chemical Product Registers may be used to protect human health and the environment. Registers have been established in most European countries. The majority of these are concerned with poisoning response and/or occupational health and safety and confine their information gathering to safe handling and accident and emergency response, supported by international databases or user-supplied values for intrinsic properties where necessary [17, 18]. Many registers seem to have been established to fulfil the obligations of Article 12 of the Council Directive 88/379/EEC, the "Preparations Directive" [19]. This obliges Member States to "appoint the body or bodies responsible for receiving information on dangerous preparations, including their chemical composition, placed on the market". Restrictions are placed by the Directive on the use such bodies may make of the information they receive:

- "Member States shall take the necessary steps to ensure that the appointed bodies provide all the requisite guarantees for maintaining the confidentiality of the information received"
- "Such information may only be used to meet any medical demand by formulating preventive and curative measures, in particular in emergencies".
- "Member States shall ensure that the information is not used for other purposes".

Moreover, important classes of product i.e. those that would be considered medicinal, veterinary, or cosmetic products, or pesticides are excluded from the Directive. These "Article 12" registers may be described as Poison Information Centres or Safety Data Sheet centres. However, the Nordic countries (Denmark, Finland, Norway & Sweden) have, for nearly two decades, gathered more extensive data to include details of end use [20].

The information gathered is intended to be used to protect human health and safety or to protect the environment, or both. There is an important link between the information gathered, the users, and the uses to which it is put. Chemical Product Registers extend across a spectrum of uses from poisoning response, through occupational health and safety to environmental management. Their existence provides knowledge and guides response to health and emergency situations and assists risk management, assessment and prevention.

The potential range of users, uses and their information needs (in an Irish context) are illustrated in the Table overleaf.

User	Information need				Use
	Inherent properties	End use	Safe handling	Accident & emergency	
Policy makers, e.g. national & local authorities		X X			Prepare aggregated statistical data for reporting nationally or internationally Acquire insight prior to intervention with new policy initiatives, e.g. regulations, taxes
Research, e.g. research or educational institutes, consultants to authorities	X X X X	X X X X X	X		Assessment of chemicals Determination of emission inventories Conduct of material and substance flow analyses Direct and support impact studies, e.g. incidence in the environment or workplace disease Support life cycle assessment of substances and products
Policy implementation					
Environmental protection e.g. local authorities, Environmental Protection Agency (EPA)	X X X	X X X X			Preparation and control of environmental hazard classification and labelling Risk management Assessment of effectiveness of substitution policies Direct monitoring of potential emissions
Workplace protection, e.g. Health & Safety Authority (HSA)	X X	X X X X	X X	X X	Preparation and control of workplace hazard classification and labelling Risk management Assessment of effectiveness of substitution policies Direct and support surveys of workplace hazard control
Public safety, e.g. Fire services, HSA	X X	 X	X X	X X	Emergency response to spills, fires, etc. Assessment of risk to public presented by industrial activities
Public health, e.g. hospitals, poisons centre	X			X	Medical response to individual or large scale poisoning incidents. This may be confined to symptomatic, non-specific treatment.
Public	X X	X	X	X	Information on correct handling and disposal of chemical products Awareness information on the state of the environment
Enterprises	X	X	X	X	Information on the correct labelling of a chemical product

Scope of data to be collected

The primary objective of a Chemical Products Register is to assist in the management of risk, whether environmental or human. This distinguishes the data needs from economic or fiscal requirements. There is a cost associated with data reporting, borne by both the reporter and the receiver. This cost is only justifiable where the benefits are adequate. The advantages and disadvantages of such Registers are:

Advantages	Disadvantages
• Better knowledge of what's being used, in what quantities and by whom • Potential to measure the effectiveness of new policies and technological advances • Potential to streamline data collection • Better emergency response • Potential to study occupational health hazards	• Costs must be borne by both reporter and receiver. Data must be collected, input, analysed and reported. • Data quality may be questionable • Security of confidentiality requires significant precautions • Data will be deficient on the health or environmental effects of certain chemicals.

Where a Register is established, data reporting should be streamlined to avoid duplicative reporting. Information which is available from technical databases should not be requested. Ecotoxicological, environmental impact or human toxicological properties should be requested only where these are not otherwise available. The primary concern should lie with gathering data on quantities in use and the usage patterns, e.g. activities and sectors using the chemicals, and details of the manner in which they are used. This latter point refers to determining whether the usage is in a closed system, or dispersive, or somewhere in between. Detailed compositions must be provided for preparations.

Criteria for inclusion on a Register

Quantity may be considered as a threshold for reporting. For example, the Swedish and Norwegian Registers have a threshold of 100 kg per annum, whereas the Danish Register requires reporting of all dangerous substances. The introduction of an Irish Chemical Products Register could be phased in accordance with decreasing thresholds.

The Nordic Registers use either a list of substances or preparations specified by their classification under the Combined Nomenclature, or the risk phrases specified in accordance with classification and labelling requirements.

A comparison of these suggests:

Combined Nomenclature	Risk phrases
Advantages • Substances which are not yet allocated a risk phrase, but are of concern, are reportable • Determination by an importer or distributor of the need to report does not require technical expertise • Data reported under this system may be cross-checked with import-export data.	*Advantages* • The existence of an agreed risk phrase for substances or preparations is a clear indication of hazard • Manufacturers and importers have an obligation to know these phrases and to make them available
Disadvantages • There will be a larger number of substances reported. • Some of the reportable substances will not present any hazard, due to the coarseness of the CN system	*Disadvantages* • The risk phrases are biased towards human health and safety, with the allocation of aquatic risk only recently introduced.

Risk phrases will provide a suitable criterion for substances that have been historically recognised as presenting a risk, but will be of less use in managing substances of emerging concern, e.g. phthalates. Alternative criteria such as sectoral usage, e.g. wood-working, vehicle maintenance, or activity, e.g. painting, adhesives, are possible, but importers of a product may be unaware of all the uses to which it is put. Some of the Nordic Registers originated as targeted studies of particular sectors or activities but have since changed.

Establishment

Using the Swedish Register, which is dependent on the Combined Nomenclature, provides an indication of the scale of undertaking likely if a Chemical Products Register were introduced in Ireland. This Register includes 90-95 per cent of the products on the market and 100 per cent of products used for occupational purposes. It contains information on 58,000 products, containing over 11,000 chemicals and collects data from 2,100 companies. There is significant annual turnover of products. For example, in 1998, 7,450 products were added and 5,130 products withdrawn. The staff required to operate a Chemical Products Register are likely to be small in number, possibly approximately 10, composed of clerical, computer support and technical specialists. A crude annual budget estimate of £500,000 - £600,000 is indicative. Again referring to the Swedish Registry, they have 6.5 whole-time equivalents, but are supported by being related to the Chemicals Inspectorate.

The strict confidentiality requirements result usually in the registry staff operating as a closed unit. Commercially valuable information will be collected by any Chemical Products Register. Extreme care to preserve confidentiality is necessary. Detailed measures have been put in place in each of the Nordic Registers to ensure this. This extends from physical security of data, through restrictions on sharing the data with other government agencies. Product Registers tend to operate on a segregated basis, even while part of larger agencies. Data flow into a registry is not limited, but passing data out is rigorously examined. However, it may be convenient for administrative, computer support and technical assistance reasons to attach the unit to a larger entity. Since the outputs a Chemical Products Register have policy implications across a wide range of interests, there are a number of candidate support frameworks in Ireland: EPA, HSA, Enterprise Ireland, Department of Environment & Local Government, etc. Trade statistical data is already collected by the Customs & Excise personnel. Pesticides are reported to the Pesticides Control Unit, and pesticides for animal use are regulated by the National Medicines Board. Detailed information is provided to EPA by IPC licensed companies, and safety related information is provided to HSA for large-scale plants. The trade data will provide some insight into diffuse as well as potential point sources of emission, whereas the EPA and HSA are primarily concerned with potential point sources.

Funding for a Chemical Products Register may be provided by the exchequer, or via registration fees, or via a combination. Charges may be based on the number of products, the total quantity a company reports and on the initial registration of a product. The major benefit of an annual charge is to provide an incentive to reporters to ensure their information is current. Denmark, which does not have an annual charge, has a Register which is believed to contain much obsolete information.

Elaboration of the major recommendation

The major recommendation to consider the introduction of a Chemical Products Register in Ireland may be elaborated into the following key points:

1 A Chemical Products Register should be established.

Without this data, it is not possible to arrive at a rational basis for the assessment of risk presented by exposure to hazardous substances.

2 The criteria for reporting should be: Risk phrase and quantity.

Risk phrases should be available for all substances and preparations, and are relevant indicators of risk. Quantity is a fundamental measure of potential exposure. This approach is the less onerous and less progressive than using a specified list based on the Combined Nomenclature classification. Fewer substances will be registered and products of potential concern may be missed. However, mandatory reporting of this information will be more acceptable and have more immediate benefits.

3 The introduction of a chemical products register should be phased.

Phasing may be based on a number of criteria:

decreasing quantity

pure substances, followed by preparations.

Artefacts, i.e. products incorporating hazardous substances into or on to a matrix, should not be part of the regular register, but subject to targeted investigation.

Once a system is active, after some years, it could be extended to be based on a specified list of categories under the Combined Nomenclature system.

4 Usage by sector and activity should be reported, but not be a basis for selection.

Usage information is highly desirable, but there is potential for considerable uncertainty in the knowledge of importers and manufacturers as to all the use of a particular product. Confining the Register to certain sectors will not be appropriate.

5 Intrinsic properties should not be criteria for selection.

Ecotoxicological properties, human toxicity and other environmental impacts are highly relevant, but may be relatively inaccessible to small scale importers. However, much of this data may be determined or estimated by experts. Risk phrases are adequate indicators.

6 Data reporting should be obligatory and the minimum necessary data are:

Name of product

Composition, defined by CAS number of constituent substances, and fractional content by mass.

Quantity in use, categorised by sector and activity

Identity and contact details for importer or manufacturer.

7 The Chemical Products Register should be established as an autonomous activity, linked to a larger entity

The Register should be supported by a larger organisation, e.g. national agency or government department. The registry itself is likely to require approximately 10 people, with an annual budget of £0.5-£0.6 million, based on experience in the Nordic countries.

8 Annual reporting and charges should be required

Costs of operating the Register may be shared by the exchequer and producers, particularly in the initial establishment phase. Annual charges, based on the number of products and quantity of usage should be imposed, both to off-set the operational costs, but more importantly to ensure updating of the data.

9 Strict provisions must be introduced for confidentiality

Notwithstanding any obligation, the operation of the register will be dependent on co-operation from business. This can be achieved only if confidentiality is assured. This has been achieved in the Nordic countries.

10 A firm and clear legal basis must be established

The obligations and rights of data providers must be clearly established in law. Risk phrases must be available. Obtaining precise quantities, composition and expected uses may require a legislative provision. An obligatory requirement to report is preferable to a voluntary system, as there is a potential for “free-riders” that refuse to disclose. A duty should be imposed on manufacturers and importers to report.

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30. Directive 98/8/EC concerning the placing of biocidal products on the market (OJ L 123, 24.4.98, p1)
31. Report of the European Workshop on National Registers of Chemical Products, Ministry of Labour, Finland, 1996
32. Andersen, P.& Nielsen, S. (Eds), European Product Registration: a review of information systems for chemical products. Publication EF/96/26/EN, European Foundation for Living and Working Conditions, 1996.
33. Council Directive 88/379/EEC on the approximation of the laws, regulations and administrative provisions of the Member States relating to the classification, packaging and labelling of dangerous preparations.
34. Kraft, J., Nordic Product Registers, Nordic Council of Ministers, 1999.

Appendix I: Extended OSPAR list of chemicals used in the project

Notes on following table

[A] Modelled by Fraunhofer

[B] No CN or CN = 0 (which indicates zero usage in pure form in Ireland)

[C] As classified by Fraunhofer

[D] Listed by Department of Agriculture marked with X

[D] Also listed by OSPAR (code 13) marked with (X)

[E] Codes for types of chemicals (as classified by OSPAR):

1. Alkanes
2. Alkenes
3. Anilines
4. Benzenes
5. Hormones
6. Inorganic Compounds
7. Metallic Compounds
8. Organic Nitrogen Compounds
9. Organic Oxygen Compounds
10. Organic Phosphorus Compounds
11. Organic Compounds
12. Organometallic Compounds
13. Pesticides
14. Phenols
15. Polycyclic Aromatic Compounds
16. PAH's
17. Products
18. Toluenes and Xylenes

n/c. Not Classified

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
3327228	(3-chloro 2-hydroxypropyl) Trimethylammonium chloride	X	X						X	29239000		X				n/c
71556	1,1,1-Trichloroethane	X	X		X	X		X		29031910	X					1
79345	1,1,2,2-Tetrachloroethane	X	X		X		X	X		29031990						1
79005	1,1,2-Trichloroethane	X	X		X		X	X		29031990		X				1
76131	1,1,2-Trichlorotrifluoroethane	X	X		X		X	X		29034300	X	X				1
75343	1,1-Dichloroethane	X			X		X	X		29031990		X				1
75354	1,1-Dichloroethylene	X	X		X		X	X		29032900		X				2
78999	1,1-Dichloropropane									29031990						1
563586	1,1-Dichlorpropene									29032900						n/c
3389717	1,2,3,4,7,7-Hexachloro-norbornadiene						X	X		-			X			16
87616	1,2,3-Trichlorobenzene	X		X						29036990		X				n/c
95943	1,2,4,5-Tetrachlorobenzene				X		X	X		29036990						4
120821	1,2,4-Trichlorobenzene	X	X	X					X	29036990						n/c
33855479	1,2,-N(4-bromophenyl)methyl-ethanediamine						X	X		-			X			8
68515480	1,2-Benzenedicarboxylic acid, di-C6-10 branched alkyl esters, C9-rich	X	X						X	-		X	X			n/c
68515491	1,2-Benzenedicarboxylic acid, di-C7-11-branched alkyl esters, C10-rich	X	X						X	-		X	X			n/c
106934	1,2-Dibromoethane	X	X		X					29033031					X	n/c
95501	1,2-Dichlorobenzene	X	X		X		X	X		29036100						4
107062	1,2-Dichloroethane	X	X	X		X		X		29031500	X	X			X	1

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
540590	1,2-Dichloroethene				X		X	X		29032900						2
78875	1,2-Dichloropropane	X			X		X	X		29031600						n/c
108703	1,3,5-Trichlorobenzene			X						29036990						n/c
96231	1,3-Dichloro-2-propanol		X		X		X	X		29055010						9
541731	1,3-Dichlorobenzene	X			X		X	X		29036990		X				4
542756	1,3-Dichloropropene	X			X		X	X		29032900		X			X	2
99650	1,3-Dinitrobenzene	X					X	X		29042090		X				4
106467	1,4-Dichlorobenzene	X	X		X		X	X	X	29042090						4
123911	1,4-Dioxane	X	X						X	29329930		X				n/c
2163000	1,6-Dichlorohexane		X					X		29031990						1
57636	17-Ethynylestradiol		X					X		29379200						5
97007	1-Chloro-2,4-dinitrobenzene	X			X		X	X		29049080		X				4
121733	1-Chloro-3-nitrobenzene	X			X		X	X		29049080						4
544105	1-Chlorohexane							X		29031990						1
90131	1-Chloronaphthalene				X					29036990						n/c
88120	1-Vinyl-2-pyrrolidone	X	X						X	29337900		X				n/c
112345	2-(2-butoxyethoxy)ethanol	X	X						X	29094300		X				n/c
111773	2-(2-methoxyethoxy)ethanol	X	X						X	29024200			X			n/c
80057	2,2-Bis-(4-hydroxyphenyl)-propane	X	X				X	X	X	29072310						14
75990	2,2-Dichloropropionic acid						X	X		29159080						9
576249	2,3-Dichlorophenol						X	X		29081090						14

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
78886	2,3-Dichloropropene				X		X	X		29032990			X			2
602017	2,3-Dinitrotoluene						X	X		-			X			18
3033770	2,3-Epoxypropyltrimethylammonium chloride	X	X						X	29239000		X				n/c
25167708	2,4,4-Trimethylpentene	X	X						X	29012990		X	X			n/c
95954	2,4,5-Trichlorophenol							X		29081090						14
93765	2,4,5-Trichlorophenoxy acetic acid				X			X		29189090					(X)	13
94757	2,4-D	X	X		X		X	X		29181990		X			X	13
53190	2,4'-DDD			X						29036990						n/c
13312588	2,4'-DDE			X						-			X		X	n/c
789026	2,4'-DDT			X						29036990					X	n/c
120832	2,4-Dichlorophenol	X	X		X		X	X		29081090						14
121142	2,4-Dinitrotoluene	X	X				X	X		29042090		X				18
95852	2-Amino-4-chlorophenol				X		X	X		29222900						14
120321	2-Benzyl-4-chlorophenol		X				X	X		29081090					X	14
615656	2-Chloro-4-methylaniline				X					29214390						n/c
95512	2-Chloroaniline	X	X		X		X	X		29214210						3
131099	2-Chloroanthraquinone	X					X	X		29147090		X				16
107073	2-Chloroethanol	X			X		X	X		29055010		X				9
88733	2-Chloronitrobenzene	X			X		X	X		29049080						4
95578	2-Chlorophenol	X			X		X	X		29081090						14
95498	2-Chlorotoluene	X			X		X	X		29036990						18

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
110805	2-Ethoxyethanol	X	X						X	29094400		X				n/c
111159	2-Ethoxyethyl acetate	X	X						X	29153500	X					n/c
104767	2-Ethyl-1-hexanol	X	X				X	X		29051610	X					9
103117	2-Ethylhexyl acrylate	X	X						X	29161290						n/c
98011	2-Furaldehyde	X	X						X	29321200	X	X	X			n/c
97541	2-Methoxy-4-propenyl-phenol		X				X	X		29095090						14
110496	2-Methoxyethyl acetate		X						X	29153990						n/c
95487	2-Methylphenol	X	X				X	X		29071200						14
95761	3,4-Dichloroaniline	X	X					X	X	29214210						3
3452979	3,5,5-Trimethyl-1-hexanol	X	X				X	X		29051990		X				9
108429	3-Chloroaniline		X		X		X	X		29214210						3
108430	3-Chlorophenol				X		X	X		29081090						14
108418	3-Chlorotoluene				X		X	X		29036990						18
140669	4-(1,1,3,3-tetramethylbutyl)phenol	X	X				X	X		29071990		X				14
14861177	4-(2,4-dichlorophenoxy)aniline	X					X	X		29222900		X				3
101779	4,4’-Methylenedianiline	X	X						X	29215990						n/c
72548	4,4'-DDD			X						29036990						n/c
72559	4,4'-DDE			X						29036990						n/c
50293	4,4'-DDT	X		X		X		X		29036200		X			X	13
92875	4,4'-Diaminobiphenyl		X		X		X	X		29215990						8
81141	4’-tert-butyl-2’,6’-dimethyl-3’,5’-dinitroacetophenone	X	X						X	29147010	X					n/c

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
89634	4-Chloro-2-nitroaniline				X		X			29214210						3
89598	4-Chloro-2-nitrotoluene		X		X					29049080						n/c
106478	4-Chloroaniline		X		X		X	X		29214210						2
100005	4-Chloronitrobenzene	X			X		X			29049085		X	X			4
1570645	4-Chloro-o-cresol	X	X						X	29081090		X				n/c
106489	4-Chlorophenol	X			X		X	X		29081090						14
106434	4-Chlorotoluene	X			X		X	X		29036990						18
1544689	4-Fluorophenylisothiocyanate						X	X		29309070						4
95807	4-Methyl-m-phenylenediamine								X	29215119						n/c
1817476	4-Nitrocumol	X					X	X		29042090		X				4
104405	4-Nonylphenol		X				X	X		-		X	X			14
98544	4-tert-butylphenol	X	X					X		29071910	X	X				14
98511	4-tert-butyltoluene	X					X	X		29029080		X				18
14678058	5-Isoxazolamine						X	X		-			X			8
98873	a,a-Dichlorotoluene	X			X		X	X		29036990		X				18
83329	Acenaphthene	X	X				X	X		29029080		X				16
75058	Acetonitrile	X	X						X	29269080		X				n/c
107028	Acrylaldehyde	X							X	29121900		X				n/c
79061	Acrylamide	X	X						X	29241000		X				n/c
79107	Acrylic acid	X	X						X	29161110	X	X				n/c
107131	Acrylonitrile	X	X						X	29261000	X	X	X			n/c

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
319846	a-Hexachlorocyclohexane			X						-			X			n/c
15972608	Alachlor	X						X		29242990		X			(X)	13
116063	Aldicarb						X	X		29309070					X	13
309002	Aldrin			X		X		X		29035990			X		X	13
85535859	Alkanes, C14-17, chloro	X	X						X	-		X	X			n/c
107051	Allychloride	X	X		X		X	X		29032900		X				2
98464	Alpha,alpha,alpha-trifluoro-3-nitrotoluene	X					X	X		29049080		X				18
61790338	Amines, tallow alkyl	X	X						X	-		X	X			n/c
61825	Amitrole	X	X				X	X		29339095					(X)	13
7789095	Ammonium dichromate	X	X						X	28415000			X			n/c
62533	Aniline	X	X						X	29214100		X				n/c
120127	Anthracene	X	X		X		X	X	X	29029010		X				16
7440360	Antimony (Sb)		X		X					811000..	X			X		n/c
7440382	Arsenic		X		X	X		X		28048000	X					7
1912249	Atrazine	X	X		X	X		X		29336910		X			X	13
384225	a-Trifluoro-2-nitrotoluene						X	X		29049085			X			18
402540	a-Trifluoro-4-nitrotoluene						X	X		29049085			X			18
2642719	Azinphos-ethyl				X	X		X		29339095					(X)	13
86500	Azinphos-methyl	X	X		X	X		X		29339095		X			X	13
7440393	Barium (Ba)	X	X		X					28052200			X			n/c
25057890	Bentazone		X		X		X	X		29349098					X	13

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
71432	Benzene	X	X		X		X	X	X	290220..	X					4
67774747	Benzene; C10-13 -alkyl derivs.	X	X						X	-		X	X			n/c
56553	Benzo-a-anthracene		X		X					29029080						n/c
50328	Benzo-a-pyrene		X		X					29029080						16
205992	Benzo-b-fluoroanthene		X		X					29029080						n/c
191242	Benzo-g,h,i-perylene				X					29029080						n/c
207089	Benzo-k-fluoroanthene		X		X					29029080						n/c
85687	Benzyl butyl phthalate	X	X				X	X	X	29173400			X			9
100447	Benzyl chloride	X	X		X		X	X		29036990						18
7440417	Beryllium (Be)		X		X					81121...	X					n/c
319857	b-Hexachlorocyclohexane							X		-			X		(X)	13
92524	Biphenyl	X	X		X		X	X		29029030		X	X			16
39368329	Bis(2-chloroisopropyl)-ether									-			X			9
117817	Bis(2-ethylhexyl) phthalate	X	X					X	X	29173200		X				9
10039540	Bis(hydroxylammonium)sulphate	X	X						X	28251000		X				n/c
1163195	Bis(pentabromophenyl)ether	X	X						X	29093038		X				n/c
56359	Bis(tributyltin) oxide	X	X		X	X				29310080						n/c
7440428	Bromium (Br)		X		X					28045010	X					n/c
1715408	Bromocyclene							X		29035990			X			18
110656	But-2-yne-1,4-diol	X	X						X	29053980		X				n/c
106990	Buta-1,3-diene	X	X						X	29012410			X			n/c

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
25013165	Butylhydroxyanisole		X					X		29095090						14
7440439	Cadmium (Cd)	X	X	X		X		X	X	8107...	X			X		7
1306190	Cadmium oxide	X	X						X	28259060	X		X			n/c
86748	Carbazol	X	X				X	X		29339095		X			(X)	13
1563662	Carbofuran		X				X	X		29329990					X	13
302170	Chloral hydrate		X		X		X	X		29055099						9
57749	Chlordane				X			X		29035990			X		X	13
143500	Chlordecone (Kepon)							X		29147090						13
85535848	Chlorinated paraffins, short chained	X	X					X	X	-		X	X			1
7782505	Chlorine	X	X						X	28011000	X	X				n/c
79118	Chloroacetic acid	X	X		X		X	X	X	29154000		X				9
108907	Chlorobenzene	X	X		X		X	X		29036100						4
59507	Chlorocresol	X	X		X		X	X		29081090						14
75456	Chlorodifluoromethane	X	X						X	29034910		X				n/c
25567673	Chlorodinitrobenzene						X	X		-			X			4
25586430	Chloronaphthalene				X		X	X		-			X			16
126998	Chloroprene	X	X		X		X	X		29032900		X				2
15545489	Chlortoluron	X	X					X		29242190		X			X	13
1333820	Chromium trioxide	X	X						X	28191000	X				X	n/c
7440484	Cobalt (Co)	X	X		X					8105....	X					n/c
7440508	Copper (Cu)	X	X		X	X		X		74.....				X		7

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
56724	Coumaphos				X		X	X		29322980						13
26444495	Cresyldiphenylphosphate	X	X				X	X		29190090		X				10
7440473	Cromium (Cr)	X	X		X	X		X		811220...				X		7
21725462	Cyanazine		X					X		29336980					X	13
461585	Cyanoguanidine	X	X				X	X		29262000	X	X				8
108771	Cyanuric chloride				X		X			29336980						8
110827	Cyclohexane	X	X				X	X	X	290211...	X	X				1
108918	Cyclohexylamine	X	X				X	X		29213010						8
57966957	Cymoxanil	X								-		X	X			n/c
112301	Decanol	X	X				X	X		29051991		X	X			9
298033	Demeton						X	X		29309070					(X)	13
919868	Demeton-s-methyl				X		X			29309070					X	n/c
319868	d-Hexachlorocyclohexane			X						-			X			n/c
26761400	Di-'isodecyl'phthalate	X	X						X	29173410		X				n/c
28553120	Di-'isononyl'phthalate	X	X						X	29173410		X				n/c
1327533	Diarsenic trioxide	X	X		X					28112910						n/c
683181	Dibutyltindichloride	X	X		X					29310080		X			(X)	13
77587	Dibutyltindidodecanat		X				X	X		29310080						12
818086	Dibutyltinoxide		X		X		X	X		29310080					(X)	13
1194656	Dichlobenil		X				X	X		29269080					X	13
27134276	Dichloroaniline (all isomers)							X		29214210						3

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108601	Dichlorodiisopropylether				X		X	X		29091900						n/c
75092	Dichloromethane	X	X		X		X	X		29031200	X	X				1
120365	Dichlorprop	X	X		X		X	X		29189090		X			X	13
62737	Dichlorvos		X		X	X		X		29190090					X	13
115322	Dicofol (Kelthane)	X	X				X	X		29062990		X			X	13
60571	Dieldrin			X		X		X		29109000					X	13
109897	Diethylamine	X	X		X		X	X		29211200		X				8
56531	Diethylstilbestrol							X		29072990						5
13464807	Dihydrazine sulfate						X	X		28251000					(X)	13
60515	Dimethoate	X	X		X		X	X		29309070					X	13
68783788	Dimethyl ditallowalkylammoniumchloride		X					X		-			X			11
77781	Dimethyl sulphate	X	X						X	29209010						n/c
124403	Dimethylamine	X	X		X		X	X		29211110					X	8
61789808	Dimethylbis(hydrogenated tallowalkyl)ammoniumchloride	X	X					X		-		X	X			11
107642	Dimethyldistearylammoniumchloride	X	X					X	X	29239000						11
1335859	Dinitro-2-methylphenol						X	X		-			X		(X)	13
117840	Di-n-octylphthalate		X				X	X	X	29173200						9
88857	Dinoseb		X				X	X		29089000					X	13
102090	Diphenyl carbonate	X					X	X		29209010		X				9
101848	Diphenyl ether	X	X				X	X		29093010	X					9
32536520	Diphenyl ether, octabromo derivative	X	X						X	29093038		X				n/c

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
32534819	Diphenyl ether, pentabromo derivative	X							X	29093031		X	X			n/c
712481	Diphenylchloroarsene						X	X		-			X			12
101815	Diphenylmethane		X				X	X		29029080						1
65996921	Distillates (coal tar)		X						X	-			X			n/c
298044	Disulfoton				X		X	X		29309070					X	13
148185	Dithiocarbamate		X				X	X		29302000						13
330541	Diuron	X	X					X		29242190		X			X	13
534521	DNOC							X		29089000						14
27193868	Dodecylphenol	X	X				X	X		-		X	X			14
115297	Endosulfan	X	X		X	X		X		29209080		X			X	13
72208	Endrin			X		X		X		29109000					X	13
106898	Epichlorohydrin	X	X		X		X	X		29103000	X					9
13194484	Ethoprophos									29309070					X	n/c
141979	Ethyl acetoacetate	X	X						X	29183000		X				n/c
100414	Ethylbenzene	X	X		X		X	X	X	29026000	X					4
598141	Ethyldichloroarsine						X	X		29310095			X			12
60004	Ethylenediaminetetraacetic acid (EDTA)	X	X						X	29224970		X				n/c
25550145	Ethyltoluene		X				X	X		-			X			18
122145	Fenitrothion		X		X	X		X		29201000					X	13
55389	Fenthion	X			X	X		X		29309070					X	13
900958	Fentinacetate				X	X				29310095			X		X	n/c

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
206440	Fluoroanthene		X				X	X		29029080						16
608731	HCH, mixed isomers			X		X		X		29035190			X		X	13
76448	Heptachlor				X			X		29035990			X		X	13
36355018	Hexabromobiphenyl							X		29036990						15
25637994	Hexabromocyclododecane	X	X						X	29035990		X	X			n/c
118741	Hexachlorobenzene	X		X		X		X		29036200		X			X	13
87683	Hexachlorobuta-1,3-diene	X	X	X		X		X		29032900		X			X	13
67721	Hexachloroethane		X		X		X	X		29031990						1
1335871	Hexachloronaphtalene						X	X		-			X			16
51235042	Hexazinone		X					X		29336980					(X)	13
7664393	Hydrogen fluoride	X	X						X	28111100	X	X				n/c
7722841	Hydrogen peroxide	X	X						X	28470000		X				n/c
25339177	Isodecanol	X	X				X	X		29051990		X				9
465736	Isodrin			X		X				-			X			n/c
27458942	Isononanol	X	X				X	X		29051990						9
98828	Isopropylbenzene	X	X		X		X	X	X	29027000	X	X	X			4
34123596	Isoproturon	X	X					X		29242110	X	X			X	13
7439921	Lead (Pb)	X	X		X	X		X		78.....	X			X		7
78002	Lead tetraethyl	X	X				X	X		29310080		X				12
58899	Lindane	X		X		X		X		29035110	X				X	13
330552	Linuron	X	X		X		X	X		29280090		X			X	13

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
121755	Malathion	X	X		X	X		X		29309070					X	13
94746	MCPA	X	X		X		X	X		29189090		X			X	13
93652	Mecoprop	X	X		X		X	X		29189090					X	13
7439976	Mercury and compounds		X	X		X		X		280540...	X			X	some	7
72333	Mestranol							X		29379200						5
41394052	Metamitron	X	X							29336980		X			X	n/c
67129082	Metazachlor	X	X					X		29331990		X			X	13
18691979	Methabenzthiazuron	X	X					X		29342090		X			X	13
79414	Methacrylic acid	X	X						X	29161300						n/c
10265926	Methamidophos	X			X		X	X		29309070		X			X	13
100970	Methenamine	X	X						X	29336920	X					n/c
72435	Methoxychlor							X		29093090					(X)	13
79209	Methyl acetate	X	X						X	29153930						n/c
80626	Methyl methacrylate	X	X						X	29161410	X					n/c
108872	Methylcyclohexane		X				X	X		29021990			X			1
26447405	Methylenediphenyl diisocyanate	X	X						X	29291090		X				n/c
75569	Methyloxirane	X	X						X	29102000	X	X	X			n/c
51218452	Metolachlor							X		29242990					(X)	13
19937598	Metoxuron		X					X		29242190					X	13
7786347	Mevinphos		X		X		X	X		29190090					(X)	13
8012951	Mineral oil		X				X	X		-			X		X	17

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
2385855	Mirex							X		8102….	X				(X)	13
7439987	Molybdenum (Mo)	X	X		X					29280090						n/c
1746812	Monolinuron				X		X	X		29042090					X	13
81152	Musk xylene	X	X					X	X	29214400						18
108383	m-Xylene	X	X				X	X		29024200	X	X	X			18
122394	N,N-Diphenylamine	X	X				X	X	X	29214400		X				8
91203	Naphthalene	X	X		X		X	X	X	29029010		X			X	16
95330	N-cyclohexylbenzothiazole-2-sulphenamide	X	X						X	27074000			X			n/c
7440020	Nickel (Ni)	X	X		X	X		X	X	75…..				X		7
7786814	Nickel sulfate	X	X						X	28332400	X		X			n/c
98953	Nitrobenzene	X	X				X	X	X	29042090		X				4
25154523	Nonylphenol	X	X						X	29071300		X				n/c
9016459	Nonylphenolethoxylate		X					X		34021300					X	14
90040	o-Anisidine	X							X	29222200		X				n/c
111875	Octan-1-ol	X	X				X	X		29051680						9
111659	Octane	X	X				X	X		29011090						1
9036195	Octylphenolethoxylate		X					X		-			X			14
50282	Oestradiol		X					X		29379200						5
53167	Oestron		X					X		29379200						5
1113026	Omethoate				X		X	X		29309070					X	13
301122	Oxydemeton-methyl		X		X		X			29309070					X	13

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
95476	o-Xylene	X	X				X	X		29024100	X					18
2074502	Paraquat						X	X		29333995					X	13
56382	Parathion	X			X	X		X		29201000					X	13
298000	Parathion-methyl	X			X	X		X		29201000		X			X	13
1336363	PCBs				X			X		29036990						15
61788338	PCT (mixtures)							X		29036990					(X)	13
527208	Pentachloroaniline									29214210						n/c
608935	Pentachlorobenzene						X	X		29036990						4
76017	Pentachloroethane		X				X	X		29031990						1
87865	Pentachlorophenol			X		X		X		29081090					X	13
109660	Pentane	X	X				X	X	X	29011090		X				1
30899195	Pentanol	X	X						X	29051500		X				n/c
11138479	Perboric acid sodium salt	X	X						X	-		X	X			n/c
85018	Phenanthrene		X		X		X	X		29029080						16
13684634	Phenmedipham	X	X							29242990		X			X	n/c
108952	Phenol	X	X						X	29071100						n/c
84852153	Phenol, 4-nonyl-, branched	X	X						X	-			X			n/c
115866	Phosphoric acid triphenyl-ester	X	X				X	X		29190010		X				10
14816183	Phoxim		X		X		X	X		29280090					X	13
90193763	Phthalic acid						X	X		-			X			9
84742	Phthalic acid dibutylester (DBP)	X	X				X	X	X	29173100						9

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
84662	Phthalic acid diethyl ester (DEP)	X	X				X	X		29173400			X			9
110850	Piperazine	X	X						X	29335970		X				n/c
65996932	Pitch, coal tar, high-temp	X	X						X	-		X				n/c
7778509	Potassium dichromate	X	X						X	28414000	X					n/c
1918167	Propachlor	X	X					X		29242990		X			X	13
71238	Propan-1-ol	X	X						X	29051200		X				n/c
709988	Propanil	X			X		X	X		29242990		X			(X)	13
106423	p-Xylene	X	X				X	X		29024300	X					18
1698608	Pyrazon	X	X		X		X	X		29339095		X			(X)	13
7782492	Selenium (Se)		X		X					28049000	X			X		n/c
7440224	Silver (Ag)	X	X		X					7106…				X		n/c
122349	Simazine	X	X		X	X		X		29336910		X			X	13
7775113	Sodium chromate	X	X						X	28415000			X			n/c
10588019	Sodium dichromate	X	X						X	28413000	X				X	n/c
7681529	Sodium hypochlorite	X	X					X	X	28289000		X			X	6
100425	Styrol	X	X						X	29025000	X					n/c
1746016	TCDD, PCDD, PCDF		X					X		29329990						15
13494809	Tellurium (Te)		X		X					28045090	X		X			n/c
75912	Tert.-butyl hydroperoxide	X	X						X	29096000		X				n/c
1634044	Tert.-butyl methyl ether	X	X						X	29091900		X				n/c
64028	Tetra sodium ethylendiaminetetraacetate	X	X						X	29224970						n/c

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				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
558134	Tetrabromomethane						X	X		29033037						1
1461252	Tetrabutyltin	X	X		X		X	X		29310080		X				12
13463393	Tetracarbonylnickel		X				X	X		29310080						12
127184	Tetrachloroethene	X	X	X		X		X	X	29032300	X	X				2
56235	Tetrachloromethane	X	X	X		X		X		29031400	X		X			1
7440280	Thallium (Tl)				X					81129990						n/c
148798	Thiabendazole		X					X		29341000					X	13
7440315	Tin (Sn)	X	X		X					80				X		n/c
7440326	Titanium (Ti)		X		X					8108….	X					n/c
108883	Toluene	X	X		X		X	X	X	290230…	X					18
731271	Tolyfluanid		X							29309070					X	n/c
8001352	Toxaphene							X		38081020						13
10061026	trans-1,3-dichloropropene		X							-			X			n/c
43121433	Triadimefon	X	X							29339095		X			X	n/c
55219653	Triadimenol		X							29339095					X	n/c
24017478	Triazophos				X		X	X		29339095					X	13
75252	Tribromomethane									29033037						n/c
126738	Tributyl phosphate	X	X		X		X	X		29190010		X				10
36643284	Tributyltin (cation)									-			X		(X)	13
76039	Trichloroacetic acid	X	X				X	X		29154000		X				9
79016	Trichloroethene	X	X	X		X		X	X	29032200	X	X				2

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
52686	Trichlorofon		X		X		X	X		29310095			X		X	13
67663	Trichloromethane	X	X	X		X		X	X	29031300	X					1
1330785	Tricresylphosphate		X				X	X		29190010						10
1582098	Trifluralin		X		X	X		X		29214390					X	13
78422	Trioctylphosphate		X				X	X		29190090						10
791286	Triphenylphospinoxide (TPPO)	X	X							-		X	X			n/c
668348	Triphenyltin (cation)									-			X		(X)	13
639587	Triphenyltin chloride				X	X				29310080					(X)	13
76879	Triphenyl-tin hydroxide				X	X				29310080					(X)	13
126727	Tris(2,3-bromo-1-propyl)phosphate						X	X		29190090						10
115968	Tris(2-chloroethyl)phosphate	X	X						X	29190010		X				n/c
13775536	Trisodium hexafluoroaluminate	X							X	29224970						n/c
5064313	Trisodium nitrilotriacetate	X	X						X	29224970		X				n/c
25155231	Trixylenylphosphate		X				X	X		29190010						10
7779900	Trizinc bis(orthophosphate)	X	X						X	28352990						n/c
7440611	Uranium (U)	X			X					28443019						n/c
7440622	Vanadium (V)	X	X		X					811240…	X		X	X		n/c
50471448	Vinclozolin	X	X					X		29349098					X	13
108054	Vinyl acetate	X	X						X	29153200	X	X				n/c
75014	Vinyl chloride	X	X		X		X	X		29032100	X	X				2
1330207	Xylene, mixed isomers	X	X		X					290244..	X	X				n/c

CAS NO	Name	IUCLID	NordicPR	Directive 76/464/EEC		IIINorth Sea Conference		Candidate Substances	Council Regulation 793/93/EEC	CN	Unique CN	Modelled [A]	No CN or CN = 0 [B]	Metal [C]	Pesticide [D]	Type of Chemical [E]
				List I	List II	List 1A	List 1D	OSPAR	1-3PL							
7440666	Zinc (Zn)	X	X		X	X		X	X	79……				X		7
7646857	Zinc chloride	X	X						X	28273600	X					n/c
1314132	Zinc oxide	X	X						X	28170000						n/c
557051	Zinc stearate	X	X						X	29157030		X				n/c
7733020	Zinc sulphate	X	X						X	28332600	X					n/c
	SUM	227	256	27	133	40	161	239	109	381	57	136	73	12	98	

Appendix II: Priority setting for existing chemicals: the European Union risk RAnking Method

Priority setting for existing chemicals: the European Union risk RAnking Method

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Abstract

In order to provide a legal framework within the European Union (EU) for the evaluation of existing chemicals, i.e. EINECS substances, Council Regulation (EEC) 793/93 was adopted, in which the evaluation of the existing chemicals is carried out by four steps, namely data collection, priority setting, risk and, if necessary, risk reduction. To fulfill the priority setting step the EU Risk Ranking Method (EURAM) has been developed to produce rankings which are the basis for drawing up lists of substances, used for priority setting, among the so called High Production Volume Chemicals appearing in the database IUCLID. EURAM ranks substances on the basis of their potential risk to man and environment by using a simple exposure-effect model, containing both human health and environmental effect endpoints as well as exposure parameters. The EURAM fulfills criteria for a good chemical ranking scheme and has been applied and used as a basis for selecting substances for the second and the third list of priority substances as foreseen under council Regulation (EEC) No 793/93.

Keywords: Chemical ranking, Priority setting

INTRODUCTION

There is a large number of chemicals in use in the world. In the EU alone, there are 100,195 so-called existing substances (i.e., substances which were deemed to be on the European market before September 18, 1981 and listed in the European Inventory of Existing Commercial Substances (EINECS)). Of these, 2474 are the so-called High Production Volume Chemicals (HPVCs), i.e., substances produced in the EU in volumes exceeding 1000 tonnes per year. Furthermore, it is deemed that anywhere between 10,000 and 50,000 substances are used in volumes exceeding 10 tonnes a year, the so-called Low production Volume Chemicals (LPVCs). In recent years attention has focused in many OECD Member Countries on establishing legal mechanisms for evaluating the risk of these chemicals and as a result the OECD secretariat coordinates an OECD wide program in evaluating the risk of HPVCs. As part of this process the EU has implemented a series of legislative tools for an EU risk evaluation of chemicals, building on the experiences of the EU member states and its OECD partners, and where the outcome in turn feeds back into the OECD risk assessment activities.

In the EU the chemicals control was initiated with Council Directive 67/548/EEC [1], which was adopted in 1967 in order to provide uniform EU wide rules for the packaging, classification and labeling of dangerous chemicals. On March 23, 1993 the EU adopted Council Regulation (EEC) 793/93 [2] (hereafter referred to as the regulation) which foresees a systematic evaluation of the existing chemicals. This is carried out in four steps: (1) a data collection step, (2) a priority setting step, (3) a risk assessment step and (4), if necessary, a risk reduction step.

The regulation is initially concerned with the HPVCs. Following Article 3 of the regulation, producers and importers of substances are obliged to submit available data on end-points listed in Annex III of the regulation to the European Commission (EC). These data are stored in the International Uniform ChemicaL Information Database (IUCLID) [3]. In order to handle the mass amount of information in IUCLID, an Informal working group on Priority Setting (IPS) was developed. This Informal working group proposed to the EC a ranking method, called the IPS Method [4], which could be used by the EC as an integral part of the priority setting process. The method presented in this paper, the so-called EU Risk rAnking Method (EURAM), is the result of discussions, based on the original proposal in [4], with member states and industry and represents thereby the EU method for ranking the HPVC substances.

Several ranking systems have already been developed in the last decades to suit specific needs, to fit into specific legal frameworks and to answer specific questions [5-11]. In developing the EU system, the existing ranking systems were taken into account, but as the EU existing chemicals program has several unique (e.g. the available database, the fact that the rankings lead up to an EU risk assessment) features, it was necessary to develop a new method, in order to address these needs, fixed in a legal framework.

In order to promote consistency among current and future ranking systems a consensus framework for Chemical Ranking and/or Scoring (CRS) has been developed recently by participants in a workshop organized by the Society of Environmental Toxicology and Chemistry (SETAC)[12]. Therefore, in addition the presented EU Risk rAnking Method is evaluated in this paper according to the SETAC guidelines to show whether EURAM fulfils the consistency requirements for a CRS system.

METHODOLOGY

The EU priority setting procedure is a relatively simple procedure, where a balance is sought between the time-saving and objective, but possibly inaccurate, results of automated methods and the time-consuming and subjective, but generally more accurate, results of expert judgment. This balance is attempted by maintaining the following three parts in order to draw up priority lists: consolidate and distribute IUCLID (Part I), extract data from IUCLID, to be used as input data to the ranking method (Part IIa), rank the IUCLID substances using the automated ranking method (Part IIb) and finally introduce expert judgment and produce a proposal for a priority list (Part III). Part I is described in Heidorn et al. [3]. This paper is concerned mainly with Part IIb. Parts IIa and III will be discussed in future papers.

The three main requirements set in the development of an EU ranking method were to develop a transparent, generally acceptable and scientifically sound ranking method. Transparency is sought through Part I. In order to achieve general acceptability of the method, by the parties whose substances are ranked, and thereafter prioritized, and by those who assess the prioritized substances, the EC has used two and a half years and four Technical Meetings[8] to discuss and agree on the method. The condition of developing a scientifically sound method can be established by using as far as possible chemical risk assessment methodology. There are though three major differences between the task of carrying out the ranking leading to the priority setting and that of risk assessment:

[8]A Technical Meeting is attended by scientific experts from each of the 15 member states, EFTA, 5 Industrial Organisations, Trade Unions and organisations such as OECD and IPCS.

1. The focus of the evaluation: the ranking is concerned with the evaluation of the quantitative potential impact between all HPVCs, whereas risk assessment is concerned with the evaluation of the potential concern of single substances. For the ranking, the choice of a specific data value as the "representative" value for a given test can therefore influence the rank of another substance.

2. The data base on which the evaluations are carried out differ: both data bases for ranking and risk assessment consist of the base set (Annex VIIA of Council Directive 67/548/EEC [1]). However the data base for the risk assessments is usually more comprehensive, as extra information and testing is frequently required to assess the priority substances as foreseen under Council Regulation (EEC) No 793/93.

3. The extent to which expert judgement can be used: the risk assessment will be carried out by the member states on a limited number of substances, whereas the ranking will be carried out by the EC on all IUCLID substances. Although the judgement of experts is used already at the ranking stage, it is limited compared to the risk assessment.

The EURAM ranks substances on the basis of their potential risks to man and the environment using a simple exposure-effect model. The EURAM calculates scores, one for the environment and one for human health. For the calculation of the environmental score the Predicted Environmental Concentration (PEC) and the Predicted No Effect Concentration (PNEC) are calculated using simple models, but still fully in line with the EU risk assessment methodology as laid down in the Technical Guidance Documents (TGD) [[13]. The scaled PEC and PNEC ratios are taken to obtain the environmental score. For the calculation of the human score a more simple scoring system is used based on the most important parameters related to both human exposure and human effects. Due to the complexity of the data (e.g., the multiplicity of end-points) it is not feasible in a way similar to the environmental score to calculate the No Observed Adverse Effects Level (NOAEL) values relevant for human health risk assessment. However, the human health effects are captured to a large extent by the general classifications within the EU, the so-called risk-phrases (R-phrases), which are developed following Annex I of Directive 67/548 [1] or the provisional classification and labeling following Annex VI thereof or exactly by the lack of them.

The TGD [13] identifies five protection goals for the environmental risk assessment, namely the aquatic ecosystem, the terrestrial ecosystem, top predators, micro-organisms in Sewage Treatment Plants (STP) and the atmosphere. Due to the limited amount of non-aquatic environmental effects data in IUCLID and the need for expert interpretation of the limited available non-aquatic environmental effects data, the environmental ranking of the substances is by default based on their potential risk to the aquatic ecosystem. For other protection goals, in particular for the terrestrial ecosystem, for top predators and for micro-organisms in STPs, scores are calculated in EURAM. However, these scores can only influence the ranking at the expert judgment stage, i.e., after expert evaluation of the scores and the underlying data. Aspects such as ozone depletion are not taken directly into account in the EURAM.

Commission Regulation (EC) 1488/94 [14] requires that the risk assessment of existing chemicals for human health addresses the following specific effects: acute toxicity, irritation, corrosivity, sensitization, repeated dose toxicity, mutagenicity, carcinogenicity and toxicity to reproduction, with the last three effects being of greatest concern. Furthermore, the following three human populations are considered in the risk assessment and therefore also by the EURAM: workers, consumers and man exposed indirectly via the environment. It is difficult to establish a simple ranking method which covers each of the three populations of concern. The EURAM therefore calculates an exposure score which reflects, at a very crude level, the concern for workers and consumers, by considering the chemicals physico-chemical properties. The calculation of a score for man exposed through the environment would be too complex for a ranking method and is therefore not covered by the EURAM. The concern is however partially captured in the environmental score of aquatic environment and in the score for top predators.

ENVIRONMENTAL RANKING

Environmental exposure

The exposure of a chemical to the environment is approximated by simple exposure models which includes three factors:

[a] emissions, based on tonnage produced or imported and use patterns

[b] distribution, based on a Mackay Level I model [15] for the environment

[c] degradation, based on aquatic biodegradation

Emissions

The EURAM initially estimates the tonnage of a chemical, which could potentially be available to expose either man or the environment. This is done by determining the tonnage distribution over the different use patterns. For each of the four main use categories, which are described in Table 1, the tonnage limit value produced or imported is calculated (T_i, where i is main use category), thus obtaining four tonnage scores.

T_i will always be greater than 1000, as the method is used for HPVCs, but is set to be no more than 1.000.000 (the default). The main use category gives an indication of the main use of a given importers or producers substance and thereby can be used to estimate the emission of the substance from that use to man or the environment. The fraction of the quantity estimated to be emitted based on main use category is given in Table 1.

Table 1. Fraction and percentage of substance emitted from different use categories [3]

Main use category	Fraction	%
I Used in closed systems	0.01	1
II Use resulting in inclusion into or onto matrix	0.10	10
III Non dispersive use	0.20	20
IV Wide dispersive use	1.00	100
Default	1.00	100

The total tonnage which is potentially available to expose man or the environment is therefore:

$$\text{Emission} = 0.01T_I + 0.1T_{II} + 0.2T_{III} + T_{IV} \quad (1)$$

Distribution

The fraction of the emission which partitions into the different environmental "compartments" is calculated by a Mackay Level I model [15]. This model is described in detail in Mackay et al. [15]. The fugacity capacities or Z values (mol/m^3.Pa) in the compartments air, water, soil, sediment, suspended solids and biota are:

Air, compartment nr 1; $Z_1 = 1/RT$ (2)

Water, compartment nr 2; $Z_2 = C^S/VP^S$ (3)

Soil; compartment nr 3; $Z_3 = Z_2\ \rho_3 f_{oc3}\ K_{oc} / 1000$ (4)

Sediment; compartment nr 4; $Z_4 = Z_2\ \rho_4 f_{oc4}\ K_{oc} / 1000$ (5)

Susp. solids; compartment nr 5; $Z_5 = Z_2\ \rho_5 f_{oc5}\ K_{oc} / 1000$ (6)

Fish (Biota); compartment nr 6; $Z_6 = Z_2\ \rho_6\ L\ K_{ow} / 1000$ (7)

where R is the gas constant (8.314 J/mol K), T is the temperature (K), C^S is the water solubility (mol/m^3), VP^S is the vapour pressure (Pa), ρ_i is the density of phase i (Kg/m^3), f_{oci} is the mass fraction organic carbon in phase i, and L is the lipid content in fish (0.10). The K_{oc} is derived from K_{ow} according to Mackay et al.[16], i.e., $K_{oc} = 0.41\ K_{ow}$. The environmental parameters used in the EURAM are given in Table 2.

Table 2. Environmental parameters used for Mackay level I fugacity model [15]

Compartment (Nr)	Air (1)	Water (2)	Soil (3)	Sediment (4)	Susp. Solids (5)	Fish (Biota) (6)
Volume (m^3)	10^{14}	2×10^{11}	9×10^9	10^8	10^6	2×10^5
Depth (m)	1000	20	0.1	0.01	-	-
Area (m^2)	10×10^{10}	10×10^9	90×10^9	10×10^9	-	-
Fraction oc (f_{oc})	-	-	0.02	0.04	0.2	-
Density (kg/m^3)	1.2	1000	2400	2400	1500	1000

Let $Dist_{ENV,i}$ denote the fraction of the chemical which partitions at equilibrium, according to the Mackay model, into compartment i. From Eqs. (4)-(7), Table 2 and Mackay et al.[15] it follows that

$$V_3Z_3 = V_4Z_4\ V_3\rho_3f_{oc3}\ /\ V_4\rho_4f_{oc4} = 45\ V_4Z_4 \quad (8)$$

and therefore,

$$Dist_{ENV,3} = 45\ Dist_{ENV,4} = 1440\ Dist_{ENV,5} = 17712\ Dist_{ENV,6} \quad (9)$$

As the ranking is concerned with relative risk, it is clear that the Mackay I model is less suitable for ranking with respect to compartments sediment, suspended solids and biota. In order to limit the influence of the Mackay distribution in the overall exposure score, any value of $Dist_{ENV,i}$ of less than or equal to 0.01 will be set to $Dist_{ENV,i} = 0.01$ for i = 1,2,3.

The percentage of the substance actually in the STP is calculated using the fractions from Appendix II of Chapter 3 of the TGD [13], which is an estimate used for this purpose in the risk assessment. Denote this fraction by $Dist_{ENV,0}$ that is the STP is seen as the zero-th compartment.

Degradation

Once a substance has reached the environment or an STP (i.e., compartment nr 0), it may degrade. The data, on which the degradation is based, are the results of the OECD "ready" and "inherent" tests [17]. This is taken into account by using the result on biodegradability with the fractions indicated in Table 3.

Table 3. Fraction and percentage of emitted substance biodegraded in the aquatic environment

Biodegradability	Fraction Remaining	% Degraded
Ready biodegradable	0.1	90
Inherent biodegradable	0.5	50
Persistent	1.0	0
Default	1.0	

Let Deg. denote the fraction of the chemical remaining in the environment for different levels of biodegradability (Table 3). These fractions have been derived especially for the EURAM and are therefore to a certain extent arbitrary. The main consideration behind chosing these values was to limit the range of possible degradation (i.e., interval scaling) and to create sufficient separation between the three scores.

Environmental exposure scoring

The Environment EXposure Value ($EEXV_i$) for compartment i, which can be seen as the EURAM equivalent of the PEC_i, is calculated by (cf. (1) and Tables 3 and 4):

$$EEXV_i = \text{Emission } Dist_{ENV,i}\ Deg, \qquad i = 0,1,2 \text{ and } 3 \qquad (10)$$

The logarithm of the raw aquatic exposure score AEXV is scaled to take values between 0 and 10 to obtain the Environmental EXposure score for compartment i (EEX_i) (cf. (20):

$$EEX_i = 1.37(\text{Log}(EEXV_i) + 1.301) \qquad i = 0,1,2 \text{ and } 3;\ \text{Range: } 0 \text{ to } 10 \qquad (11)$$

In order still to produce an exposure score for top predators, the derivation following the TGD [13], where the PEC for the aquatic compartment is multiplied by the BCF, is followed. To implement this methodology in to the EURAM, it is necessary to interval scale the BCF, in order to assure that the BCF does not receive too large a weight. If the measured BCF, expressed on a lipid basis, is available, then the Accumulation Potential (AP) is determined using the score obtained from Table 4.

Table 4. Accumulation Potential (AP)

Log(BCF)	AP
Log(BCF)≤2	0
2<Log(BCF)≤3	1
3<Log(BCF)≤4	2
4<Log(BCF)	3
Default	3

If no BCF data are available in IUCLID, then the K_{OW} will replace measured BCFs using

$$Log(BCF) = -1.0 + Log(K_{ow}) \text{ if } MW < 700 \text{ and } Log(BCF) = 0 \text{ if } MW > 700 \quad (12)$$

if the measured K_{ow} are available. If no data are available and MW < 700 then the default is used. Finally, the EEX_6 is calculated by

$$EEX_6 = 0.971(Log(EEXV_3) + AP + 1.301) \quad \text{Range: 0 to 10} \quad (13)$$

Environmental effect scoring

In order to calculate the Environmental EFfects Value for compartment i ($EEFV_i$), several steps must be followed. Initially, the data available from acute and chronic tests for different species must be determined. If chronic NOEC values are available for one or more species, then these data are used and the acute data neglected. On the other hand, if no NOEC values are available, then the acute data must be used. The Assessment Factors (AF), as described in Chapter 3 of the TGD [13], listed in Table 5 and 6 are then applied to the lowest of either the NOEC (if present) or L(E)C50 (if no NOEC present), i.e.,

$$EEFV_i = (Ecotox.\ Test_i)/AF_i \quad (14)$$

Table 5. Assessment Factor (AF) [13] to derive an aquatic and terrestrial effect score

endpoint	number of species	AF
NOEC	≥3	10
NOEC	2	50
NOEC	1	100
$L(E)C_{50}$	≥3	1000
$L(E)C_{50}$	2	1000
$L(E)C_{50}$	1	1000

Table 6. Assessment Factor (AF) [13] to derive the micro-organisms effect score in sewage treatment plants

endpoint	number of species	AF
NOEC or EC10	≥3	10
NOEC or EC10	2	10
NOEC or EC10	1	10
EC50	≥3	100
EC50	2	100
EC50	1	100

In order to restrict the possible range of EEFV values, the EEFV will be truncated at values below 10 ng/L for water or micro organisms or 10 ng/kg dry soil for the terrestrial organisms and above at 1 mg/L or 1 mg/kg dry soil. Finally the logarithm of EEFV is normalized to be between zero and ten to give Environmental EFfects score for compartment i (EEF_i):

$$EEF_i = -2 \log(EEFV_i). \qquad i = 0, 2, \text{ or } 3 \qquad (15)$$

If no aquatic toxicity data are available, then the minimal cut-off value of 10 ng/L will be taken as a default.

The effects score for top predators, EEF_6 is determined by using the score obtained from Table 8 for the risk phrases: R46, R40, R47, R60, R61, R62, R63, R64, R48 (toxic) and R48 (harmful) [1]. If none of these risk phrases are in the IUCLID, then an EEF_6 of 0 is given. These risk phrases are associated with the endpoints for repeated dose toxicity, genetic toxicity and reproductive toxicity.

Environmental combined exposure and effect scoring

The Environmental Score for compartment i (ES_i) are calculated as follows: Table 8, (11) and (15)):

$$ES_i = EEX_i \times EEF_i \qquad i = 0, 2,3, \text{ or } 6; \text{ Range: } 0 \text{ to } 100 \qquad (16)$$

From the previous discussions, it follows that the environmental score for the aquatic compartment (ES_2) can be used directly for the ranking, but the environmental scores for the compartments STP, soil and biota (ES_0, ES_3 and ES_6) are not directly appropriate for an automatic ranking. These scores can though be used at a later stage, after considering the underlying data more carefully, to adjust or replace the EURAM score for the aquatic compartment.

As BCF is not used in calculating the environmental score for the aquatic compartment (ES_2), but is generally available, the final score for the aquatic environment should be improved by combining both ES_2 and BCF. This combination of two scores is done so that maximum use can be made of generally available data. The Aquatic Effects Score (AEF) is thereby calculated as (cf. Table 4 and Table 5):

$$AEF = 0.7EEF_2 + AP \qquad \text{Range: } 0 \text{ to } 10 \qquad (17)$$

The weighing of the two factors is not based on scientific arguments, but on the political relative relevance of the two factors (toxicity versus persistence) in determining risk reduction needs. The Aquatic Score (AS) is the product of the EEX_2 and the AEF:

$$AS = EEX_2 \, AEF. \qquad \text{Range: } 0 \text{ to } 100 \qquad (18)$$

Human health ranking

Human health exposure

The exposure of a chemical to man is approximated by simple exposure models which including two factors:

[a] emissions, based on tonnage produced or imported and use patters (see previous section on emissions described in the paragraph environmental exposure)

[b] distribution, based on physical chemical properties for human exposure

Distribution

The fraction ($Dist_{HH}$) of the emitted substance to which humans are potentially exposed is given in Table 7.

Table 7. Fraction ($Dist_{HH}$) of emitted substance to which humans are exposed

Physico-chemical property	Value	Fraction contribution to $Dist_{HH}$
Boiling point (°C)	b.p. ≤ 60 [a]	0.75
	60 < b.p. ≤ 200[a]	0.50
	200 < b.p. ≤ 1500[a]	0.25
	1500 < b.p.[a]	0.05
	Default	0.50
Vapour pressure (hPa)	VP ≥ 200[b]	0.75
	0.5 ≤ VP < 200[b]	0.50
	VP < 0.5[b]	0.25
	VP < 0.5 at 200°C	0.05
	Default	0.50
$LogK_{OW}$	$LogK_{OW}$ > 3	0.25
	$LogK_{OW}$ ≤ 3	0.00
	Default	0.25

[a]at 950-1050 hPa.
[b]at 20-30°C

The fraction $Dist_{HH}$ is obtained from Table 7 by taking the largest value of the two fractions obtained for b.p. or vapour pressure (VP) and then adding this largest value to the fraction obtained for $logK_{OW}$.

Human health exposure scoring

The Human EXposure Value (HEXV) is calculated by (cf. Table 7 and (1)):

$$HEXV = Emission\ Dist_{HH} \quad (19)$$

The logarithm of HEXV is then scaled to take values between 0 and 10 to obtain the Human EXposure score (HEX) by (cf. (19)):

$$HEX = 1.785(Log(HEXV) - 0.398) \quad \text{Range: 0 to 10} \quad (20)$$

Human health effect scoring

The ranking of human health effects is determined by using the R-phrases, the test results from genetic toxicity and reproductive toxicity and the presence or absence of test results for repeated dose toxicity. The Human health Effects score (HEF), tabulated in Table 8, is the maximal score the substance achieves by considering all the R-phrases and the specified test information in IUCLID for that substance.

The scores attributed to each end-point is politically driven, as they reflect the relative concern which each end-point has in terms of the need to consider risk reduction measures.

Human health combined exposure and effect scoring

The Human health Score (HS) are calculated as follows: (cf. (20), Table 8)

$$HS = HEX \times HEF \qquad \text{Range: 0 to 100} \qquad (21)$$

The HS is used directly for the ranking.

Table 8. Human health effects scoring (HEF)

Carcinogenicity	Genetic toxicity[a]	Reproductive toxicity[b]	Respiratory sensitization	Repeated dose toxicity	Acute toxicity	Irritation	Skin sensitization	HEF
R45 or R49[d]	R46[d]	R47, R60 or R61[d]	-	-	-	-	-	10
R40[d]	R40[d]	R62, R63 or R64[d]	-	-	-	-	-	9
-	Positive in at least one in vitro test but no in vivo somatic cell test conducted	Positive in an in vivo screening test but no appropriate full in vivo test conducted[c] or positive in OECD-reproductive screening test	-	-	-	-	-	8
-	No test	No test and no repeat test or positive Chernoff/Kavlock screen test	R42[d]	R48 (Toxic)[d]	-	-	-	7
-	-	No test but repeat test available or positive in screening test	-	R48 (Harmful)[d]	-	R34 or R35 or R41[d]	R43[d]	6
-	-	Negative in screening test	-	R33[d]	-	R36 or R37 or R38[d]	-	5
-	Positive in at least one in vitro test, with only one negative in vivo somatic cell test	Negative in OECD reproductive screening test	-	no test	-	-	-	4

Carcinogenicity	Genetic toxicity[a]	Reproductive toxicity[b]	Respiratory sensitization	Repeated dose toxicity	Acute toxicity	Irritation	Skin sensitization	**HEF**
-	-	Only negative in full in vivo test(s) for teratogenicity or in Chernoff/Kavlock teratology screening test	-	-	R26, R27 or R28[d]	-	-	3
-	Only negative in vitro gene mutation test(s) or only negative test(s) for chromosomal aberrations in somatic cell (in vitro or in vivo)	Only negative in full in vivo test(s) for fertility	-	-	R23, R24 or R25[d]	-	-	2
-	-	-	-	-	R20 or R21 or R22[d]	-	-	1
No R-phrase	-	-	No R-phrase[d]	No R-phrase[d] and test performed	No R-phrase[d]	No R-phrase[d]	No R-phrase[d]	0

[a]A substances scores zero for genetic toxicity if

- Test(s) for gene mutation (in vitro) and for chromosome aberrations in somatic cells (in vivo or in vitro) conducted, and all were negative;
- Possible positive in vitro test(s), but with at least two in vivo tests conducted and both were negative (i.e., no positive or ambiguous in vivo data).

[b]A substance scores zero for reproductive toxicity if full in vivo fertility and teratogenicity tests have been conducted, and only negative results obtained.

[c]For an OECD reproductive screening test, an appropriate in vivo test is a full fertility test. For a Chernoff/Kavlock screening test, an appropriate in vivo test is a full teratogenicity test.

[d]Risk phrases (R-phrases) developed following Annex I of Directive 67/548 [1] or the provisional clasification and labeling following Annex VI.

EVALUATION OF EURAM ACCORDING TO CRS GUIDELINES

The consensus framework for Chemical Ranking and/or Scoring (CRS) in order to promote consistency and harmonization so that various CRS methods used are universally recognizable and employ similar principles, should consist of four primary steps [12], namely:

1. Goal definition and scoping; what decisions are made based on the CRS results
2. Indicator selection; this involves the identification of the type and amount of data needed for the particular CRS exercise
3. Ranking and scoring; based on agreed principles
4. Output and presentation, reporting the results in a form useful for achieving the goal of the analysis

In this section the consistency of EURAM according to this framework and in particular to the ranking and scoring step, with the underlying seventeen principles, are briefly discussed.

1. The first guideline principle of the chemical ranking and scoring, namely *having a clearly defined purpose* is fulfilled by EURAM, as the purpose of EURAM is to rank HPVCs as a basis for selecting substances for risk assessment and risk management.
2. In contrary to risk assessment, which is concerned with the evaluation of the potential concern of single substances, EURAM ranks the relative potential concern between all IUCLID substances. Therefore, EURAM is *compatible with the risk assessment paradigm*, in which hazard and exposure are assessed and integrated into a characterization of risk to a certain extent, without being a risk assessment itself.
3. The third principle concerns the *acknowledgment and assessment of uncertainty;* a chemicals ranking system is by definition highly uncertain, and applications should acknowledge and communicate the uncertainty in the results [12]. In EURAM this guideline is fulfilled as after using the automated ranking method (part IIb), and before producing a proposal for a priority list (part III) an expert judgement phase is introduced.
4. The *role for professional judgment* is acknowledged in EURAM, as many European companies and organizations, and their member states have been involved through four Technical Meetings to discuss and agree on the EURAM and, as is discussed in the previous item, an expert judgement phase is introduced before the priority setting phase. Furthermore, the data selected by the automated data selection procedure of EURAM, namely the biodegradability data and the human health effects, which are used to calculate the environmental and human health scores (ES and HS), are evaluated by expert judgement.
5. *Broad consideration of effects* are taken into account in EURAM, as the recommended environmental and human health CRS-effect endpoints are mainly applied.

   The environmental effects according to CRS concern the aquatic and terrestrial environments, whereas due to the availability of toxicological endpoints, algae, invertebrates, fish, birds and domestic, laboratory mammals are the animals of interest. Also of interest are effects data relevant for the evaluation of potential impacts on terrestrial wildlife mammals, birds, reptiles, and amphibians. In EURAM, however, due to the limited amount of non-aquatic environmental effects data, only effects data for the aquatic organisms, namely fish, daphnia and algae, are directly used. Effects data of terrestrial organisms, of top predators and of micro-organisms in STP, and therefore the calculation of their scores, can influence the rankings only at the expert judgement stage. Furthermore, the measurement endpoint of primary interest according to CRS, namely the NOEC, is also the main measurement endpoint in EURAM [12].

   The human health effects endpoints, namely acute toxicity, irritation, corrosivity, sensitization, repeated dose toxicity, mutagenicity, carcinogenicity and toxicity to reproduction, used in EURAM are all the endpoints considered relevant for the risk assessment [6] and are also those required by a CRS.

   Other effects mentioned in CRS, such as physical/chemical effects, alteration of environmental media, waste reduction and management and material resources, energy use and land use associated with chemical production, are not adressed directly in EURAM.

6. The *role of valuation in aggregation and weighting* has been justified in terms of scientific arguments (e.g. following risk assessment methodology) and policy decisions (e.g., the weights attributed to biodegradation, aquatic effect score (AEF) or the human health scoring)

7. The *transparency of the method* is taken into account in this paper as the methodology is following the general risk assessment principles. The *transparancy of the outputs* of EURAM, however, will be descibed in a future paper.

8. EURAM cannot follow the principle of being *neutral to data availability*, as according to the regulation [1] one of the criteria for selecting priority substances is lack of data. In order for EURAM to fulfill this selection criterion substances without data are penalized.

9. EURAM *accommodates the principle extreme variability in data availability across chemicals.* The rankings, to be published in a future paper, will be separated according to their data availability, e.g. substances for which a large amount of data, only few data or no data are available.

10. *A tiered approach is practical and desirable* in a CRS ranking system. In EURAM the first tier is the ranking by applying the automatic data selection procedure for the aquatic compartment. The second and the third tier is the expert judgement on the quality of the data and on other compartments, i.e.,terrestrial compartment, top predators and microorganisms in STPs, respectively.

11. Also the guideline '*similar effects/exposure categories should be assessed across tiers'* is respected in EURAM, as the exposure- and effect data are refined as tiers increase, while the method stays the same.

12. *Critical information should be preserved. This principle is taken into account*, as in the output of EURAM a number of flags are included, the input data, e.g. critical NOECs and R-phrases, are summarized and information on data density is given.

13. *Data selection guidelines* in EURAM, in particular the automated data selection procedure, will be specified in a future paper.

14. The EURAM is developed to get a transparent, generally acceptable and scientifically sound method; the theoretical background being established by using the risk assessment methodology [13] and the data availability through IUCLID determining the input data. Therefore EURAM seems to be in agreement with the CRS guideline, namely to be *theory-driven as well as data-driven.*

15. S*ensitivity analysis* has been performed for EURAM, using the Sobol first order [17] and the Homma & Saltelli [18] total sensitivity indices. The results willl be described in a future paper.

16. The guideline *pre-selection of chemicals to be consistent with CRS* is fulfilled by EURAM, as EURAM selects consistently all HPVCs, which are listed in the EINECS and which have been imported or have been produced in quantities exceeding 1000 metric tonnes per year in the EU, at least once between March 23, 1990 and March 23, 1994 .

17. The *impact of scaling* has been considered. All scaling is interval scaling. The contributions in percentage of each input data, and thereby the impact at the scaling, to the final score is therefore relatively easy to determine.

CONCLUSIONS

The EURAM is a new method which has achieved international acceptance by 16 national authorities and several of the European industrial organizations. The EURAM as described in this paper fulfills the basic criteria recently established [12] for a good chemical ranking scheme and it has been applied and used as the basis for selecting substances for the second and third priority lists in the EU [20,21]. The result therefore of Part III of the priority setting scheme as described in section 1 is in part reflected in the substances selected for the published priority lists [20,21]. The actual results of applying the EURAM to the IUCLID data will be reported on in greater detail in the near future.

There are a number of issues, which could help in the further development and refinement of the EURAM. Two of these issues are:

1. An evaluation is needed on the usefulness to combine the environmental effect score for water (EEF_2) with the accumulation potential (AP) to calculate an aquatic effects score (AEF) (cf. (17). It might be better to use directly the environmental scores (ES), for the compartments water and biota, where biota is used for the evaluation of secondary poisoning.
2. A better usage of the IUCLID information regarding use patterns of the chemicals could be used to estimate the emissions in a more refined way.

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Appendix III: Guide to CN classification of substances

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
95330	N-cyclohexylbenzothiazole-2-sulphenamide	27074000		X			n/c	Naphthalene (excl. chemically defined)
7782505	Chlorine	28011000	X				n/c	Chlorine
7440428	Boron (B)	28045010	X		X		n/c	Boron
13494809	Tellurium (Te)	28045090	X	X	X		n/c	Tellurium
7440382	Arsenic	28048000	X		X		7	Arsenic
7782492	Selenium (Se)	28049000	X		X		n/c	Selenium
7440393	Barium (Ba)	28052200		X	X		n/c	Strontium and barium
7439976	Mercury and compounds	280540...	X		X	some	7	Mercury in flasks of a net content of 34,5 kg "standard weight", of a fob value per flask of <= ECU 224 Mercury (excl. in flasks of a net content of 34,5 kg "standard weight", of a fob value per flask of <= ECU 224)
7664393	Hydrogen fluoride	28111100	X				n/c	Hydrogen fluoride "hydrofluoric acid"
1327533	Diarsenic trioxide	28112910					n/c	Sulphur trioxide "sulphuric anhydride"; diarsenic trioxide
1314132	Zinc oxide	28170000					n/c	Zinc oxide; zinc peroxide
1333820	Chromium trioxide	28191000	X			X	n/c	Chromium trioxide
10039540	Bis(hydroxylammonium)sulphate	28251000					n/c	Hydrazine and hydroxylamine and their inorganic salts
13464807	Dihydrazine sulfate	28251000				(X)	13	
1306190	Cadmium oxide	28259060	X	X			n/c	Cadmium oxide
7646857	Zinc chloride	28273600	X				n/c	Zinc chloride
7681529	Sodium hypochlorite	28289000				X	6	Hypochlorites, chlorites and hypobromites (excl. calcium hypochlorites)
7786814	Nickel sulfate	28332400	X	X			n/c	Sulphates of nickel
7733020	Zinc sulphate	28332600	X				n/c	Sulphate of zinc
7779900	Trizinc bis(orthophosphate)	28352990					n/c	Phosphates (excl. phosphates of triammonium, monosodium, disodium, trisodium, of potassium and of calcium)
10588019	Sodium dichromate	28413000	X			X	n/c	Sodium dichromate
7778509	Potassium dichromate	28414000	X				n/c	Potassium dichromate

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
7775113	Sodium chromate	28415000		X			n/c	Chromates and dichromates; peroxochromates (excl. chromates of zinc or of lead, sodium dichromate and potassium dichromate)
7789095	Ammonium dichromate	28415000		X			n/c	
7440611	Uranium (U)	28443019			X		n/c	Uranium depleted in U 235; alloys, dispersions, ceramic products and mixtures, containing uranium depleted in U 235 or compounds of this product (excl. cermets)
7722841	Hydrogen peroxide	28470000					n/c	Hydrogen peroxide, whether or not solidified with urea kg H2O2
109660	Pentane	29011090					1	Saturated acyclic hydrocarbons (excl. for use as power or heating fuels)
111659	Octane	29011090					1	
106990	Buta-1,3-diene	29012410		X			n/c	Buta-1,3-diene for use as power or heating fuel Buta-1,3-diene (excl. for use as power or heating fuel)
25167708	2,4,4-Trimethylpentene	29012990		X			n/c	n/c
110827	Cyclohexane	290211…	X				1	Cyclohexane for use as power or heating fuel Cyclohexane (excl. for use as power or heating fuel)
108872	Methylcyclohexane	29021990		X			1	n/c
71432	Benzene	290220. .	X				4	Benzene for use as power or heating fuel Benzene (excl. for use as power or heating fuel)
108883	Toluene	290230…	X				18	Toluene for use as power or heating fuels Toluene (excl. for use as power or heating fuel)
95476	o-Xylene	29024100	X				18	o-Xylene
108383	m-Xylene	29024200	X	X			18	n/c
111773	2-(2-methoxyethoxy)ethanol	29094200		X			n/c	n/c
106423	p-Xylene	29024300	X				18	p-Xylene
1330207	Xylene, mixed isomers	290244. .	X				n/c	Mixed xylene isomers for use as power or heating fuels Mixed xylene isomers (excl. for use as power or heating fuels)
100425	Styrol	29025000	X				n/c	Styrene
100414	Ethylbenzene	29026000	X				4	Ethylbenzene
98828	Isopropylbenzene	29027000	X	X			4	Cumene
91203	Naphthalene	29029010				X	16	Naphthalene and anthracene
120127	Anthracene	29029010					16	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
92524	Biphenyl	29029030		X			16	Biphenyl and terphenyls
50328	Benzo-a-pyrene	29029080					16	Cyclic hydrocarbons (excl. cyclanes, cyclenes, benzene, toluene, xylenes, styrene, ethylbenzene, cumene, naphthalene, anthracene, biphenyl, terphenyls, vinyltoluenes and 1,3-diisopropylbenzene)
56553	Benzo-a-anthracene	29029080					n/c	
83329	Acenaphthene	29029080					16	
85018	Phenanthrene	29029080					16	
98511	4-tert-butyltoluene	29029080					18	
101815	Diphenylmethane	29029080					1	
191242	Benzo-g,h,I-perylene	29029080					n/c	
205992	Benzo-b-fluoroanthene	29029080					n/c	
206440	Fluoroanthene	29029080					16	
207089	Benzo-k-fluoroanthene	29029080					n/c	
75092	Dichloromethane	29031200	X				1	Dichloromethane “methylene chloride”
67663	Trichloromethane	29031300	X				1	Chloroform “trichloromethane”
56235	Tetrachloromethane	29031400	X	X			1	Carbon tetrachloride
107062	1,2-Dichloroethane	29031500	X			X	1	1,2-Dichloroethane “ethylene dichloride”
78875	1,2-Dichloropropane	29031600					n/c	1,2-Dichloropropane “propylene dichloride” and dichlorobutanes
71556	1,1,1-Trichloroethane	29031910	X				1	1,1,1-Trichloroethane “methylchloroform”
67721	Hexachloroethane	29031990					1	Saturated chlorinated derivatives of acyclic hydrocarbons (other than chloromethane [methyl chloride], chloroethane [ethyl chloride], dichloromethane [methylene chloride], chloroform [trichloromethane
75343	1,1-Dichloroethane	29031990					1	
76017	Pentachloroethane	29031990					1	
78999	1,1-Dichloropropane	29031990					1	
79005	1,1,2-Trichloroethane	29031990					1	
79345	1,1,2,2-Tetrachloroethane	29031990					1	
544105	1-Chlorohexane	29031990					1	
2163000	1,6-Dichlorohexane	29031990					1	
75014	Vinyl chloride	29032100	X				2	Vinyl chloride “chloroethylene”
79016	Trichloroethene	29032200	X				2	Trichloroethylene

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
127184	Tetrachloroethene	29032300	X				2	Tetrachloroethylene “perchloroethylene”
75354	1,1-Dichloroethylene	29032900					2	Unsaturated chlorinated derivatives of acyclic hydrocarbons (excl. vinyl chloride “chloroethylene”, trichloroethylene and tetrachloroethylene “perchloroethylene”)
87683	Hexachlorobuta-1,3-diene	29032900				X	13	
107051	Allychloride	29032900					2	
126998	Chloroprene	29032900					2	
540590	1,2-Dichloroethene	29032900					2	
542756	1,3-Dichloropropene	29032900				X	2	
563586	1,1-Dichlorpropene	29032900					n/c	
78886	2,3-Dichloropropene	29032990					2	
106934	1,2-Dibromoethane	29033031				X	n/c	Dibromoethane and vinyl bromide
75252	Tribromomethane	29033037					n/c	Bromides “brominated derivatives” of acyclic hydrocarbons (excl. dibromoethane, vinyl bromide, bromomethane “methyl bromide” and dibromomethane)
558134	Tetrabromomethane	29033037					1	
76131	1,1,2-Trichlorotrifluoroethane	29034300	X				1	Trichlorotrifluoroethanes
75456	Chlorodifluoromethane	29034910					n/c	Halogenated derivatives of methane, ethane or propane, halogenated only with fluorine and chlorine (excl. perhalogenated)
58899	Lindane	29035110	X			X	13	Lindane “ISO”
608731	HCH, mixed isomers	29035190		X		X	13	1,2,3,4,5,6-Hexachlorocyclohexane (excl. lindane “ISO”)
57749	Chlordane	29035990		X		X	13	Halogenated derivates of alicyclic hydrocarbons (excl. 1,2,3,4,5,6-hexachlorocyclohexane, 1,2-dibromo-4-“1,2-dibromoethyl”cyclohexane and tetrabromocyclooctanes)
76448	Heptachlor	29035990		X		X	13	
309002	Aldrin	29035990		X		X	13	
1715408	Bromocyclene	29035990		X			18	
25637994	Hexabromocyclododecane	29035990		X			n/c	
95501	1,2-Dichlorobenzene	29036100					4	Chlorobenzene, o-dichlorobenzene and p-dichlorobenzene
108907	Chlorobenzene	29036100					4	
50293	4,4’-DDT	29036200				X	13	Hexachlorobenzene and DDT "1,1,1-trichloro-2,2-bis[p-chlorophenyl]ethane"
118741	Hexachlorobenzene	29036200				X	13	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
53190	2,4'-DDD	29036990					n/c	Halogenated derivatives of aromatic hydrocarbons (excl. chlorobenzene, o-dichlorobenzene, p-dichlorobenzene, hexachlorobenzene, DDT "1,1,1-trichloro-2,2-bis[p-chlorophenyl]ethane" and 2,3,4,5,6-pentab
72548	4,4'-DDD	29036990					n/c	
72559	4,4'-DDE	29036990					n/c	
87616	1,2,3-Trichlorobenzene	29036990					n/c	
90131	1-Chloronaphthalene	29036990					n/c	
95498	2-Chlorotoluene	29036990					18	
95943	1,2,4,5-Tetrachlorobenzene	29036990					4	
98873	a,a-Dichlorotoluene	29036990					18	
100447	Benzyl chloride	29036990					18	
106434	4-Chlorotoluene	29036990					18	
108418	3-Chlorotoluene	29036990					18	
108703	1,3,5-Trichlorobenzene	29036990					n/c	
120821	1,2,4-Trichlorobenzene	29036990					n/c	
541731	1,3-Dichlorobenzene	29036990					4	
608935	Pentachlorobenzene	29036990					4	
789026	2,4'-DDT	29036990				X	n/c	
1336363	PCBs	29036990					15	
36355018	Hexabromobiphenyl	29036990					15	
61788338	PCT (mixtures)	29036990				(X)	13	
98953	Nitrobenzene	29042090					4	Derivatives of hydrocarbons containing only nitro or nitroso groups (excl. trinitrotoluenes and dinitronaphthalenes)
99650	1,3-Dinitrobenzene	29042090					4	
106467	1,4-Dichlorobenzene	29042090					4	
121142	2,4-Dinitrotoluene	29042090					18	
1746812	Monolinuron	29042090				X	13	
1817476	4-Nitrocumol	29042090					4	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
88733	2-Chloronitrobenzene	29049080					4	Sulphonated, nitrated or nitrosated derivatives of hydrocarbons, whether or not halogenated (excl. those containing only sulpho, nitro or nitroso groups and sulphohalogenated derivatives and esters of
89598	4-Chloro-2-nitrotoluene	29049080					n/c	
97007	1-Chloro-2,4-dinitrobenzene	29049080					4	
98464	Alpha,alpha,alpha-trifluoro-3-nitrotoluene	29049080					18	
121733	1-Chloro-3-nitrobenzene	29049080					4	
100005	4-Chloronitrobenzene	29049085		X			4	n/c
384225	a-Trifluoro-2-nitrotoluene	29049085		X			18	
402540	a-Trifluoro-4-nitrotoluene	29049085		X			18	
71238	Propan-1-ol	29051200					n/c	Propan-1-ol "propyl alcohol" and propan-2-ol "isopropyl alcohol"
30899195	Pentanol	29051500					n/c	Pentanol "amyl alcohol" and isomers thereof
104767	2-Ethyl-1-hexanol	29051610	X				9	2-Ethylhexan-1-ol
111875	Octan-1-ol	29051680					9	Octanol "octyl alcohol" and isomers thereof (excl. 2-ethylhexan-1-ol and octan-2-ol)
3452979	3,5,5-Trimethyl-1-hexanol	29051990					9	Saturated monohydric acyclic alcohols (excl. methanol "methyl alcohol", propan-1-ol "propyl alcohol", propan-2-ol "isopropyl alcohol", butanols, pentanol "amyl alcohol" and isomers thereof, octanol "o
25339177	Isodecanol	29051990					9	
27458942	Isononanol	29051990					9	
112301	Decanol	29051991		X			9	n/c
110656	But-2-yne-1,4-diol	29053980					n/c	Acyclic diols (excl. ethylene glycol "ethanediol", propylene glycol "propane-1,2-diol", 2-methylpentane-2,4-diol "hexylene glycol", butane-1,3-diol and 2,4,7,9-tetramethyldec-5-yne-4,7-diol)
96231	1,3-Dichloro-2-propanol	29055010					9	Halogenated, sulphonated, nitrated or nitrosated derivatives of saturated monohydric alcohols
107073	2-Chloroethanol	29055010					9	
302170	Chloral hydrate	29055099					9	Halogenated, sulphonated, nitrated or nitrosated derivatives or acyclic polyvalent alcohols (excl. 2,2-bis"bromomethyl"propanediol)
115322	Dicofol (Kelthane)	29062990				X	13	Aromatic cyclic alcohols and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. benzyl alcohol and cinnamyl alcohol)
108952	Phenol	29071100					n/c	Phenol "hydroxybenzene" and its salts
95487	2-Methylphenol	29071200					14	Cresols and their salts

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
25154523	Nonylphenol	29071300					n/c	Octylphenol, nonylphenol and their isomers; salts thereof
98544	4-tert-butylphenol	29071910	X				14	p-tert-Butylphenol
140669	4-(1,1,3,3-tetramethylbutyl)phenol	29071990					14	Monophenols (excl. phenol "hydroxybenzene" and its salts, cresols and their salts, octylphenol, nonylphenol and their isomers and salts thereof, xylenols and their salts and naphthols and their salts
80057	2,2-Bis-(4-hydroxyphenyl)-propane	29072310					14	4,4'-Isopropylidenediphenol "bisphenol A, diphenylolpropane"
56531	Diethylstilbestrol	29072990					5	Polyphenols (excl. resorcinol and hydroquinone "quinol" and their salts, 4,4'-Isopropylidenediphenol "bisphenol A, diphenylolpropane" and its salts and dihydroxynaphthalenes and their salts)
59507	Chlorocresol	29081090					14	Derivatives containing only halogen substituents and their salts, of phenols or phenol-alcohols (excl. brominated derivatives)
87865	Pentachlorophenol	29081090				X	13	
95578	2-Chlorophenol	29081090					14	
95954	2,4,5-Trichlorophenol	29081090					14	
106489	4-Chlorophenol	29081090					14	
108430	3-Chlorophenol	29081090					14	
120321	2-Benzyl-4-chlorophenol	29081090				X	14	
120832	2,4-Dichlorophenol	29081090					14	
576249	2,3-Dichlorophenol	29081090					14	
1570645	4-Chloro-o-cresol	29081090					n/c	
88857	Dinoseb	29089000				X	13	Halogenated, sulphonated, nitrated or nitrosated derivatives of phenoles or phenol-alcohols (excl. derivatives containing only halogen substitutes and their salts or only sulpho groups, their salts an
534521	DNOC	29089000					14	
108601	Dichlorodiisopropylether	29091900					n/c	Acyclic ethers and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. diethyl ether)
1634044	Tert.-butyl methyl ether	29091900					n/c	
101848	Diphenyl ether	29093010	X				9	Diphenyl ether
32534819	Diphenyl ether, pentabromo derivative	29093031		X			n/c	Pentabromodiphenyl ether; 1,2,4,5-tetrabromo-3,6-bis"pentabromophenoxy"benzene
1163195	Bis(pentabromophenyl)ether	29093038					n/c	Brominated derivatives of aromatic ethers (excl. pentabromodiphenyl ether, 1,2,4,5-tetrabromo-3,6-bis"pentabromophenoxy"benzene and 1,2-bis"2,4,6-tribromophenoxy"ethane for the manufacture of acryloni
32536520	Diphenyl ether, octabromo derivative	29093038					n/c	

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72435	Methoxychlor	29093090				(X)	13	Aromatic ethers and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. diphenyl ether and brominated derivatives)
112345	2-(2-butoxyethoxy)ethanol	29094300					n/c	Monobutyl ethers of ethylene glycol or of diethylene glycol
110805	2-Ethoxyethanol	29094400					n/c	Monoalkylethers of ethylene glycol or of diethylene glycol (excl. monomethyl ethers and monobutyl ethers)
97541	2-Methoxy-4-propenyl-phenol	29095090					14	Ether-phenols, ether-alcohol-phenols and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. guaiacol and guaiacolsulphonates of potassium)
25013165	Butylhydroxyanisole	29095090					14	
75912	Tert.-butyl hydroperoxide	29096000					n/c	Alcohol peroxides, ether peroxides, ketone peroxides and their halogenated, sulphonated, nitrated or nitrosated derivatives
75569	Methyloxirane	29102000	X	X			n/c	Methyloxirane "propylene oxide"
106898	Epichlorohydrin	29103000	X				9	1-Chloro-2,3-epoxypropane "epichlorohydrin"
60571	Dieldrin	29109000				X	13	Epoxides, epoxyalcohols, epoxyphenols and epoxyethers, with a three-membered ring, and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. oxirane "ethylene oxide", methyloxirane
72208	Endrin	29109000				X	13	
107028	Acrylaldehyde	29121900					n/c	Acyclic aldehydes, without other oxygen function (excl. methanal "formaldehyde", ethanal "acetaldehyde" and butanal "butyraldehyde, normal isomer")
81141	4’-tert-butyl-2’,6’-dimethyl-3’,5’-dinitroacetophenone	29147010	X				n/c	4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone "musk ketone"
131099	2-Chloroanthraquinone	29147090					16	Halogenated, sulphonated, nitrated or nitrosated derivatives of ketones and quinones (excl. 4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone "musk ketone")
143500	Chlordecone (Kepon)	29147090					13	
108054	Vinyl acetate	29153200	X				n/c	Vinyl acetate
111159	2-Ethoxyethyl acetate	29153500	X				n/c	2-Ethoxyethyl acetate
79209	Methyl acetate	29153930					n/c	Methyl acetate, pentyl acetate "amyl acetate", isopentyl acetate "isoamyl acetate" and glycerol acetates
110496	2-Methoxyethyl acetate	29153990					n/c	Esters of acetic acid (excl. ethyl, vinyl, n-butyl, isobutyl, 2-ethoxyethyl, propyl, isopropyl, methyl, pentyl "amyl", isopentyl "isoamyl", glycerol, p-Tolyl, phenylpropyl, benzyl, rhodinyl, santalyl
76039	Trichloroacetic acid	29154000					9	Mono- di- or trichloroacetic acids, their salts and esters
79118	Chloroacetic acid	29154000					9	
557051	Zinc stearate	29157030					n/c	Salts of stearic acid

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
75990	2,2-Dichloropropionic acid	29159080					9	Saturated acyclic monocarboxylic acids and their anhydrides, halogenides, peroxides and peroxyacids; their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. formic acid and acetic ac
79107	Acrylic acid	29161110	X				n/c	Acrylic acid
103117	2-Ethylhexyl acrylate	29161290					n/c	Esters of acrylic acid (excl. methylacrylate and ethylacrylate)
79414	Methacrylic acid	29161300					n/c	Methacrylic acid and its salts
80626	Methyl methacrylate	29161410	X				n/c	Methylmethacrylate
84742	Phthalic acid dibutylester (DBP)	29173100					9	Dibutyl orthophthalates
117817	Bis(2-ethylhexyl) phthalate	29173200					9	Dioctyl orthophthalates
117840	Di-n-octylphthalate	29173200					9	
84662	Phthalic acid diethyl ester (DEP)	29173400		X			9	n/c
85687	Benzyl butyl phthalate	29173400		X			9	
26761400	Di-'isodecyl'phthalate	29173410					n/c	Diisooctyl, diisononyl and diisodecyl orthophthalates
28553120	Di-'isononyl'phthalate	29173410					n/c	
94757	2,4-D	29181990				X	13	Carboxylic acids with additional oxygen function and their anhydrides, halides, peroxides and peroxyacids; their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. lactic acid, tartar
141979	Ethyl acetoacetate	29183000					n/c	Carboxylic acids with aldehyde or ketone function but without other oxygen function, their anhydrides, halides, peroxides, peroxyacids and their halogenated, sulphonated, nitrated or nitrosated deriva
93652	Mecoprop	29189090				X	13	Carboxylic acids with additional oxygen function, their anhydrides, halides, peroxides and peroxyacids and their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. only with alcohol,
93765	2,4,5-Trichlorophenoxy acetic acid	29189090				(X)	13	
94746	MCPA	29189090				X	13	
120365	Dichlorprop	29189090				X	13	
115866	Phosphoric acid triphenyl-ester	29190010					10	Tributyl phosphates, triphenyl phosphates, tritolyl phosphates, trixylyl phosphates, and tris"2-chlorethyl" phosphate
115968	Tris(2-chloroethyl)phosphate	29190010					n/c	
126738	Tributyl phosphate	29190010					10	
1330785	Tricresylphosphate	29190010					10	
25155231	Trixylenylphosphate	29190010					10	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
62737	Dichlorvos	29190090				X	13	Phospheric esters and their salts, incl. lactophosphates; their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. tibutyl phosphates, triphenyl phosphates, tritolyl phosphates, trixy
78422	Trioctylphosphate	29190090					10	
126727	Tris(2,3-bromo-1-propyl)phosphate	29190090					10	
7786347	Mevinphos	29190090				(X)	13	
26444495	Cresyldiphenylphosphate	29190090					10	
56382	Parathion	29201000				X	13	Thiophosphoric esters "phosphorothioates" and their salts; their halogenated, sulphonated, nitrated or nitrosated derivatives
122145	Fenitrothion	29201000				X	13	
298000	Parathion-methyl	29201000				X	13	
77781	Dimethyl sulphate	29209010					n/c	Sulphuric esters and carbonic esters and their salts, and their halogenated, sulphonated, nitrated or nitrosated derivatives
102090	Diphenyl carbonate	29209010					9	
115297	Endosulfan	29209080				X	13	Esters of inorganic acids and their salts; their halogenated, sulphonated, nitrated or nitrosated derivatives (excl. esters of hydrogen halides, phosphoric esters, sulphuric esters, carbonic esters an
124403	Dimethylamine	29211110				X	8	Methylamine or di- or trimethylamine (excl. their salts)
109897	Diethylamine	29211200					8	Diethylamine and its salts
108918	Cyclohexylamine	29213010					8	Cyclohexylamine and cyclohexyldimethylamine, and their salts
62533	Aniline	29214100					n/c	Aniline and its salts
89634	4-Chloro-2-nitroaniline	29214210					3	Halogenated, sulphonated, nitrated and nitrosated aniline derivatives and their salts
95512	2-Chloroaniline	29214210					3	
95761	3,4-Dichloroaniline	29214210					3	
106478	4-Chloroaniline	29214210					2	
108429	3-Chloroaniline	29214210					3	
527208	Pentachloroaniline	29214210					n/c	
27134276	Dichloroaniline (all isomers)	29214210					3	
615656	2-Chloro-4-methylaniline	29214390					n/c	Derivatives of toluidines and their salts
1582098	Trifluralin	29214390				X	13	
81152	Musk xylene	29214400					18	Diphenylamine and its derivatives; salts thereof
122394	N,N-Diphenylamine	29214400					8	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
95807	4-Methyl-m-phenylenediamine	29215119					n/c	o-Phenylenediamine, m-phenylenediamine, p-phenylenediamine, diaminotoluenes, and their halogenated, sulphonated, nitrated and nitrosated derivatives; salts thereof (excl. m-phenylenediamine of a purit
92875	4,4'-Diaminobiphenyl	29215990					8	Aromatic polyamines and their derivatives; salts thereof (excl. o-phenylenediamine, m-phenylenediamine, p-phenylenediamine or diaminotoluenes and their derivatives, and salts thereof, m-phenylenebis"m
101779	4,4'-Methylenedianiline	29215990					n/c	
90040	o-Anisidine	29222200					n/c	Anisidines, dianisidines, phenetidines, and their salts
95852	2-Amino-4-chlorophenol	29222900					14	Amino-naphthols and other amino-phenols, their ethers and esters (excl. those containing > one kind of oxygen function; aminohydroxynaphthalenesulphonic acids, anisidines, dianisidines, phenetidines
14861177	4-(2,4-dichlorophenoxy)aniline	29222900					3	
60004	Ethylenediaminetetraacetic acid (EDTA)	29224970					n/c	Amino-acids and their esters, and salts thereof (excl. those containing > one kind of oxygen function, lysine and its esters and salts thereof, glutamic acid and salts thereof, glycine and anthranilic
64028	Tetra sodium ethylendiaminetetraacetate	29224970					n/c	
5064313	Trisodium nitrilotriacetate	29224970					n/c	
13775536	Trisodium hexafluoroaluminate	29224970					n/c	
107642	Dimethyldistearylammoniumchloride	29239000					11	Quaternary ammonium salts and hydroxides (excl. choline and its salts)
3033770	2,3-Epoxypropyltrimethylammonium chloride	29239000					n/c	
3327228	(3-chloro 2-hydroxypropyl) Trimethylammonium chloride	29239000					n/c	
79061	Acrylamide	29241000					n/c	Acyclic amides, incl. acyclic carbamates, and their derivatives; salts thereof
34123596	Isoproturon	29242110	X			X	13	Isoproturon "ISO"
330541	Diuron	29242190				X	13	Ureines and their derivatives, salts thereof (excl. isoproturon "ISO")
15545489	Chlortoluron	29242190				X	13	
19937598	Metoxuron	29242190				X	13	
709988	Propanil	29242990				(X)	13	Amides cyclic, incl. cyclic carbamates, and derivatives; salts thereof (excl. ureines and their derivatives, salts thereof, lidocaine "INN", paracetamol "INN" and 2-acetamidobenzoic acid [N-acetylanth
1918167	Propachlor	29242990				X	13	
13684634	Phenmedipham	29242990				X	n/c	
15972608	Alachlor	29242990				(X)	13	
51218452	Metolachlor	29242990				(X)	13	

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107131	Acrylonitrile	29261000	X	X			n/c	Acrylonitrile
461585	Cyanoguanidine	29262000	X				8	1-Cyanoguanidine "dicyandiamide"
75058	Acetonitrile	29269080					n/c	Nitrile-function compounds (excl. acrylonitrile, 1-cyanoguanidine "dicyandiamide", 2-hydroxy-2-methylpropiononitrile "acetone
1194656	Dichlobenil	29269080				X	13	
330552	Linuron	29280090				X	13	Organic derivatives of hydrazine or of hydroxylamine (excl. N,N-bis"2-methoxyethyl"hydroxylamine)
2385855	Mirex	29280090				(X)	13	
14816183	Phoxim	29280090				X	13	
26447405	Methylenediphenyl diisocyanate	29291090					n/c	Isocyanates (excl. methylphenylene diisocyanates [toluene diisocyanates])
148185	Dithiocarbamate	29302000					13	Thiocarbamates and dithiocarbamates
55389	Fenthion	29309070				X	13	Organic thio compounds (excl. dithiocarbonates [xantates], thio- and dithiocarbamates, thioammono-, di- or tetrasulphides, methionine, cysteine or cystine, and their derivatives, thiodiglycol "INN" [2
60515	Dimethoate	29309070				X	13	
116063	Aldicarb	29309070				X	13	
121755	Malathion	29309070				X	13	
298033	Demeton	29309070				(X)	13	
298044	Disulfoton	29309070				X	13	
301122	Oxydemeton-methyl	29309070				X	13	
731271	Tolyfluanid	29309070				X	n/c	
919868	Demeton-s-methyl	29309070				X	n/c	
1113026	Omethoate	29309070				X	13	
1544689	4-Fluorophenylisothiocyanate	29309070					4	
10265926	Methamidophos	29309070				X	13	
13194484	Ethoprophos	29309070				X	n/c	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
56359	Bis(tributyltin) oxide	29310080					n/c	Separate chemically defined organo-inorganic compounds, n.e.s.
76879	Triphenyl-tin hydroxide	29310080				(X)	13	
77587	Dibutyltindidodecanat	29310080					12	
78002	Lead tetraethyl	29310080					12	
639587	Triphenyltin chloride	29310080				(X)	13	
683181	Dibutyltindichloride	29310080				(X)	13	
818086	Dibutyltinoxide	29310080				(X)	13	
1461252	Tetrabutyltin	29310080					12	
13463393	Tetracarbonylnickel	29310080					12	
52686	Trichlorofon	29310095		X		X	13	n/c
598141	Ethyldichloroarsine	29310095		X			12	
900958	Fentinacetate	29310095		X		X	n/c	
98011	2-Furaldehyde	29321200	X	X			n/c	2-Furaldehyde "furfuraldehyde"
56724	Coumaphos	29322980					13	Lactones (excl. coumarin, methylcoumarins, ethylcoumarins, phenolphthalein, 1-hydroxy-4-[1-"4-hydroxy-3-methoxycarbonyl-1-naphthyl"-3-oxo-1H, 3H-benzo[de]isochromen-1-yl]-6-octadecyloxy-2-naphthoic ac
123911	1,4-Dioxane	29329930					n/c	Internal ethers
1563662	Carbofuran	29329990				X	13	Heterocyclic compounds with oxygen hetero-atom[s] only (excl. compounds containing an unfused furan ring, whether or not hydrogenated, in the structure, lactones, benzofuran "coumarone", internal ethe
1746016	TCDD, PCDD, PCDF	29329990					15	
67129082	Metazachlor	29331990				X	13	Heterocyclic compounds with nitrogen hetero-atom(s) only, containing an unfused pyrazole ring, whether or not hydrogenated, in the structure (excl. phenazone "antipyrin" and its derivatives and phenyl
2074502	Paraquat	29333995				X	13	Heterocyclic compounds with nitrogen hetero-atom[s] only, containing an unfused pyridine ring, whether or not hydrogenated, in the structure (excl. pyridine and its salts, piperidine and its salts and
110850	Piperazine	29335970					n/c	Heterocyclic compounds with nitrogen hetero-atom"s" only, containing a pyrimidine ring, whether or not hydrogenated, or piperazine ring in the structure (excl. malonylurea "barbituric acid", its deriv

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
122349	Simazine	29336910				X	13	Atrazine "ISO"; propazine "ISO"; simazine "ISO"; hexahydro-1,3,5-trinitro-1,3,5-triazine "hexogen, trimethylenetrinitramine"
1912249	Atrazine	29336910				X	13	
100970	Methenamine	29336920	X				n/c	Methenamine "INN" "hexamethylenetetramine"
108771	Cyanuric chloride	29336980					8	Heterocyclic compounds with nitrogen hetero-atom[s] only, containing an unfused triazine ring, whether or not hydrogenated, in the structure (excl. melamine, atrazine "ISO", propazine "ISO", simazine
21725462	Cyanazine	29336980				X	13	
41394052	Metamitron	29336980				X	n/c	
51235042	Hexazinone	29336980				(X)	13	
88120	1-Vinyl-2-pyrrolidone	29337900					n/c	Lactams (excl. 6-hexanelactam "epsilon-caprolactam")
61825	Amitrole	29339095				(X)	13	Heterocyclic compounds with nitrogen hetero-atom"s" only (excl. compounds containing an unfused pyrazole, imidazole, pyridine or triazine ring, whether or not hydrogenated, a quinoline or isoquinoline
86500	Azinphos-methyl	29339095				X	13	n/c
86748	Carbazol	29339095				(X)	13	
1698608	Pyrazon	29339095				(X)	13	
2642719	Azinphos-ethyl	29339095				(X)	13	
24017478	Triazophos	29339095				X	13	
43121433	Triadimefon	29339095				X	n/c	
55219653	Triadimenol	29339095				X	n/c	
148798	Thiabendazole	29341000				X	13	Heterocyclic compounds containing an unfused thiazole ring, whether or not hydrogenated, in the structure
18691979	Methabenzthiazuron	29342090				X	13	Heterocyclic compounds containing a benzothiazole ring-system, whether or not hydrogenated, but not further fused (excl. di"benzothiazol-2-yl"disulphide, benzothiazole-2-thiol "mercaptobenzothiazole"
25057890	Bentazone	29349098				X	13	Heterocyclic compounds (excl. those with oxygen or nitrogen hetero-atom"s" only, compounds containing an unfused thiazole ring or a benzothiazol or phenothiazine ring-system, whether or not hydrogenat
50471448	Vinclozolin	29349098				X	13	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
50282	Oestradiol	29379200					5	Oestrogens and progestogens
53167	Oestron	29379200					5	
57636	17-Ethynylestradiol	29379200					5	
72333	Mestranol	29379200					5	
9016459	Nonylphenolethoxylate	34021300				X	14	Non-ionic organic surface-active agents, whether or not put up for retail sale (excl. soap)
8001352	Toxaphene	38081020					13	Insecticides based on chlorinated hydrocarbons, put up in forms or packings for retail sale or as preparations or articles
7440224	Silver (Ag)	7106…			X		n/c	Powder of silver, incl. silver plated with gold or platinum Silver, incl. silver plated with gold or platinum, unwrought, of a fineness of >= 999 parts per 1.000 Silver, incl. silver plated with gold or platinum, unwrought, of a fineness of < 999 parts per 1.000 Silver, incl. silver plated with gold or platinum, in the form of purls, spangles and cuttings Semi-manufactured silver, incl. silver plated with gold or platinum, of a fineness of >= 750 parts per 1.000 (excl. purls, spangles and cuttings) Semi-manufactured silver, incl. silver plated with gold or platinum, of a fineness of >= 750 parts per 1.000 (excl. purls, spangles and cuttings)
7440508	Copper (Cu)	74...			X		7	29 forms of copper from 74011000 to 74199900

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
7440020	Nickel (Ni)	75...			X		7	Nickel mattes
								Nickel oxide sinters and other intermediate products of nickel metallurgy (excl. nickel mattes)
								Nickel, not alloyed, unwrought
								Unwrought nickel alloys
								Waste and scrap, of non-alloy nickel (excl. ingots or other similar unwrought shapes, of remelted non-alloy nickel waste and scrap, ashes and residues containing non-alloy nickel, waste and scrap of p
								Waste and scrap, of nickel alloys (excl. ingots or other similar unwrought shapes, of remelted nickel alloys waste and scrap, ashes and residues containing nickel alloys)
								Powders and flakes, of nickel (excl. nickel oxide sinters
								Bars, rods, profiles and wire, of non-alloy nickel, n.e.s. (excl. electrically insulated products)
								Bars, rods, profiles and wire, of nickel alloys, n.e.s. (excl. electrically insulated products)
								Wire of non-alloy nickel (excl. electrically insulated products)
								Wire of nickel alloys (excl. electrically insulated products)
								Plates, sheets, strip and foil, of non-alloy nickel (excl. expanded plates, sheets or strip)
								Plates, sheets, strip and foil, of nickel alloys (excl. expanded plates, sheets or strip)
								Tubes and pipes of non-alloy nickel
								Tubes and pipes of nickel alloys
								Tube or pipe fittings, of nickel
								Cloth, grill, netting and fencing, of nickel wire
								Articles of nickel, n.e.s.

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
7439921	Lead (Pb)	78....			X		7	Unwrought lead, refined
								Unwrought lead, containing by weight antimony as the principal other element
								Unwrought lead, containing by weight >= 0,02% of silver, for refining "bullion lead"
								Unwrought lead alloys (excl. lead containing by weight antimony as the principal other element, and lead containing by weight >= 0,02% of silver, for refining "bullion lead")
								Unwrought lead (excl. lead containing by weight antimony as the principal other element, and lead containing by weight >= 0,02% of silver, for refining "bullion lead", lead alloys and refined lead)
								Lead waste and scrap (excl. ashes and residues from lead production "heading No 2620", and ingots or other similar unwrought shapes, of remelted waste and scrap, of lead "heading No 7801" and waste an
								Lead bars, rods, profiles and wire, n.e.s.
								Lead strip and foil, of a thickness "excluding any backing" of <= 0,2 mm
								Lead plates and sheets; lead strip and foil, of a thickness "excluding any backing" of > 0,2 mm
								Lead powders and flakes (excl. grains of lead, and spangles of heading 8308)
								Lead tubes, pipes and tube or pipe fittings "for example, couplings, elbows, sleeves"
								Containers with an anti-radiation lead covering, for the transport or storage of radioactive materials "Euratom" (excl. containers specifically constructed or equipped for one or more types of transpo
								Articles of lead n.e.s.

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
7440666	Zinc (Zn)	79…			X		7	Unwrought zinc, not alloyed, containing by weight >= 99,99% of zinc Unwrought zinc, not alloyed, containing by weight >= 99,95% but < 99,99% of zinc Unwrought zinc, not alloyed, containing by weight >= 98,5% but < 99,95% of zinc Unwrought zinc, not alloyed, containing by weight >= 97,5% but < 98,95% of zinc Unwrought zinc alloys Zinc waste and scrap (excl. ash and residues from zinc production "heading 2620", ingots and other similar unwrought shapes, of remelted waste and scrap, of zinc "heading 7901" and waste and scrap of Zinc dust Zinc dust, powders and flakes (excl. grains of zinc, and spangles of heading 8308, and zinc dust) Zinc bars, rods, profiles and wire, n.e.s. Zinc plates, sheets, strip and foil Zinc tubes, pipes and tube or pipe fittings "for example, couplings, elbows, sleeves" Articles of zinc, n.e.s.
7440315	Tin (Sn)	80…			X		n/c	Unwrought tin, not alloyed Unwrought tin alloys Tin waste and scrap (excl. ash and residues from the manufacture of tin of heading 2620, and ingots and similar unwrought tin produced from melted tin waste and scrap of heading 8001) Tin bars, rods, profiles and wire, n.e.s. Tin plates, sheets and strip, of a thickness > 0,2 mm Tin foil of a thickness (excluding any backing) <= 0,2 mm Tin powders and flakes (excl. tin granules and spangles of heading 8308) Tin tubes, pipes and tube or pipe fittings "for example, couplings, elbows, sleeves" Articles of tin n.e.s.
7439987	Molybdenum (Mo)	8102…	X		X		n/c	Molybdenum powders Unwrought molybdenum, incl. bars and rods obtained simply by sintering Molybdenum waste and scrap (excl. ash and residues containing molybdenum) Molybdenum bars and rods (other than those obtained simply by sintering), profiles, plates, sheets, strip and foil, n.e.s. Molybdenum wire Articles of molybdenum, n.e.s.

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
7440484	Cobalt (Co)	8105....	X		X		n/c	Cobalt mattes and other intermediate products of cobalt metallurgy; unwrought cobalt; cobalt powders Cobalt waste and scrap (excl. ash and residues containing cobalt) Articles of cobalt, n.e.s.
7440439	Cadmium (Cd)	8107...	X		X		7	Unwrought cadmium; cadmium powders Cadmium waste and scrap (excl. ashes and residues containing cadmium) Articles of cadmium, n.e.s.
7440326	Titanium (Ti)	8108….	X		X		n/c	Unwrought titanium; titanium powders Titanium waste and scrap (excl. ash and residues containing titanium) Titanium tubes and pipes with attached fittings, suitable for gases or liquids, for civil aircraft Titanium bars, rods, profiles and wire, n.e.s. Titanium plates, sheets, strip and foil Titanium tubes and pipes (excl. those with attached fittings, suitable for gases or liquids, for civil aircraft) Articles of titanium, n.e.s
7440360	Antimony (Sb)	811000..	X		X		n/c	Unwrought antimony; antimony powders Antimony waste and scrap (excl. ash and residues containing antimony) Articles of antimony, n.e.s.
7440417	Beryllium (Be)	81121...	X		X		n/c	Unwrought beryllium; beryllium powders Beryllium waste and scrap (excl. ashes and residues containing beryllium) Articles of beryllium, n.e.s.
7440473	Cromium (Cr)	811220...			X		7	Chromium alloys containing > 10% by weight of nickel, unwrought, and powders, waste and scrap of these alloys (excl. ash and residues containing chromium or chromium alloys of this kind) Unwrought chromium; chromium powders (excl. chromium alloys containing > 10% by weight of nickel) Chromium waste and scrap (excl. ash and residues containing chromium and chromium alloys containing > 10% by weight of nickel) Articles of chromium, n.e.s.
7440622	Vanadium (V)	811240…	X	X	X		n/c	Unwrought vanadium; vanadium powders Vanadium waste and scrap (excl. ash and residues containing vanadium) Articles of vanadium, n.e.s.
7440280	Thallium (Tl)	81129990			X		n/c	Articles of gallium, indium and thallium, n.e.s.

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
104405	4-Nonylphenol	-		X			14	
319846	a-Hexachlorocyclohexane	-		X			n/c	
319857	b-Hexachlorocyclohexane	-		X		(X)	13	
319868	d-Hexachlorocyclohexane	-		X			n/c	
465736	Isodrin	-		X			n/c	
602017	2,3-Dinitrotoluene	-		X			18	
668348	Triphenyltin (cation)	-		X		(X)	13	
712481	Diphenylchloroarsene	-		X			12	
791286	Triphenylphospinoxide (TPPO)	-		X			n/c	
1335871	Hexachloronaphtalene	-		X			16	
3389717	1,2,3,4,7,7-Hexachloro-norbornadiene	-		X			16	
8012951	Mineral oil	-		X		X	17	
9036195	Octylphenolethoxylate	-		X			14	
10061026	trans-1,3-dichloropropene	-		X			n/c	
11138479	Perboric acid sodium salt	-		X			n/c	
13312588	2,4'-DDE	-		X		X	n/c	
14678058	5-Isoxazolamine	-		X			8	
25550145	Ethyltoluene	-		X			18	
25567673	Chlorodinitrobenzene	-		X			4	
25586430	Chloronaphthalene	-		X			16	
27193868	Dodecylphenol	-		X			14	
33855479	1,2,-N(4-bromophenyl)methyl-ethanediamine	-		X			8	
36643284	Tributyltin (cation)	-		X		(X)	13	
39368329	Bis(2-chloroisopropyl)-ether	-		X			9	
57966957	Cymoxanil	-		X			n/c	

CAS No.	Name	CN	Unique CN	No CN or CN = 0	Metal [C]	Pesticide [D]	Type of Chemical [E]	Description in Combined Nomenclature (CN) System
61789808	Dimethylbis(hydrogenated tallowalkyl)ammoniumchloride	-		X			11	
61790338	Amines, tallow alkyl	-		X			n/c	
65996921	Distillates (coal tar)	-		X			n/c	
65996932	Pitch, coal tar, high-temp	-		X			n/c	
67774747	Benzene; C10-13 -alkyl derivs.	-		X			n/c	
68515480	1,2-Benzenedicarboxylic acid, di-C6-10 branched alkyl esters, C9-rich	-		X			n/c	
68515491	1,2-Benzenedicarboxylic acid, di-C7-11-branched alkyl esters, C10-rich	-		X			n/c	
68783788	Dimethyl ditallowalkylammoniumchloride	-		X			11	
84852153	Phenol, 4-nonyl-, branched	-		X			n/c	
85535848	Chlorinated paraffins, short chained	-		X			1	
85535859	Alkanes, C14-17, chloro	-		X			n/c	
90193763	Phthalic acid	-		X			9	
1335859	Dinitro-2-methylphenol	-		X		(X)	13	

Notes on table

"Unique CN": this CN number is associated with only one substance

Rows in red = substances on list sharing CNs

Rows in black = Non-unique CN (other substances not on the list may share this CN)

"No CN or CN=0": These substances have not been allocated a CN number, implying they have not entered international trade in pure form, or else they have been allocated a CN number, but no imports or exports into/from Ireland have been recorded for 1995-7.

[C] As classified by Fraunhofer and other sources
[D] Listed by Department of Agriculture marked with X
[D] Also listed by OSPAR (code 13) marked with (X)

[E] Codes for types of chemicals (as classified by OSPAR):

1	Alkanes
2	Alkenes
3	Anilines
4	Benzenes
5	Hormones
6	Inorganic Compounds
7	Metallic Compounds
8	Organic Nitrogen Compounds
9	Organic Oxygen Compounds
10	Organic Phosphorus Compounds
11	Organic Compounds
12	Organometallic Compounds
13	Pesticides
14	Phenols
15	Polycyclic Aromatic Compounds
16	PAH's
17	Products
18	Toluenes and Xylenes
N/c	Not Classified

Appendix IV: Reported uses of substances ranked 1-40

REPORTED USES OF SUBSTANCES RANKED 1-40

Rank 1: Acetonitrile
Acetonitrile is used as a solvent in hydrocarbon extraction processes, speciality solvent, chemical intermediate, separation of fatty acids from vegetable oils, pharmaceuticals and a laboratory chemical solvent: dilution, extraction, liquid chromatography.

Rank 2: Bis(tributyltin) oxide
Bis(tributyltin) oxide is used as a fungicide and molluscicide. It is used as a preservative in industrial applications and for manufacture of other pesticides. Bis(tributyltin) oxide is also used as an antifouling agent for ships, for the prevention of slimes in industrial recirculating water systems, for combating freshwater snails, as a wood and textile preservative and as a disinfectant.

Rank 3: Tetrabutyltin
Not enough information on use patterns can be found in literature.

Rank 4: Cresyldiphenyl phosphate
Cresyldiphenyl phosphate is used as a plasticizer, extreme-pressure lubricant, hydraulic fluid, petrol additive, food packaging and flame retardant.

Rank 5: Nonylphenol
Nonylphenol may be used as an ingredient of paints, adhesives, industrial detergents and pesticides. It may also be used in admixture with diisobutyl phthalate for marking fuel oil for taxation purposes.

Rank 6: 4-(1,1,3,3 tetramethylbutyl) phenol
Paint, lacquer and varnish industry, adhesive and binding agents, vulcanising agents.

Rank 7: Anthracene
Used in the manufacture of anthraquinone, alizarin dyes, insecticides and wood preservatives.

Rank 8: Isodecanol
Used as an antifoaming agent in textile processes.

Rank 9: 2,4 Dinitrotoluene
2,4 Dinitrotoluene is used primarily as an intermediate in the production of flexible polyurethane foams used in the bedding and furniture industry. 2,4 Dinitrotoluene is also used in the production of munitions and explosives, for which 2,4 Dinitrotoluene is a gelatinizing and waterproofing agent. It is also used as an intermediate in the manufacture of dyes, and as a purified form, in smokeless gunpowders.

Rank 10: Chloroacetic acid
Thioglycolic acid, cellulose ethers, mainly carboxymethylcellulose (CMC), 2,4-D esters and salts, surfactants, cyanoacetic acid, phenoxyacetic acid, glycine and chloroacetic acid esters.

Rank 11: Diphenyl carbonate
Diphenyl carbonate is used solely as an intermediate. It is important for the synthesis of lower-mass aliphatic monoisocyanates, which starts with the corresponding ureas or allophanates, and for the preparation of aliphatic and aromatic polycarbonates by means of transesterification.

Rank 12: 1-chloro-3-nitrobenzene
Reduction of 3-chloronitrobenzene to 3-chloroaniline (Orange GC base) is its primary outlet, with minor uses in other fields. Crude 3-chloronitrobenzene can be used for exhaustive chlorination to give pentachloronitrobenzene.

Rank 13: Di 'isononyl' phthalate
The substance is used as a plasticizer (vinyl swimming pools, plasticized vinyl seats and clothing) but also for several non-plasticizer products such as perfumes and cosmetics. Di 'isononyl' phthalate is also used as an organic intermediate.

Rank 14: Aniline
This compound is used in the manufacture of rubber chemicals, agriculture chemicals and dyestuffs and in the production of MDI (p,p-methylene diphenyl diisocyanate) group isocyanates used in polyurethane. It is the parent substance for many dyes and drugs. This compound is used in rubber accelerators, antioxidants, photographic chemicals, explosives, petroleum refining, diphenylamine, phenolics, herbicides and fungicides. It is used in marking inks, tetryl, optical whitening agents, resins, varnishes, perfumes, shoe polishes and many organic chemicals. Aniline is commonly used in laboratories.

Rank 15: Dimethyl sulphate
Dimethyl sulfate is used as a methylating agent in the manufacture of many organic chemicals. It is also used in the manufacture of dyes and perfumes, for the separation of mineral oils, and for the analysis of auto fluids.

Rank 16: Butylphenol
p-t-Butylphenol is used in the manufacture of oil-soluble phenolic resins made from pt-butylphenol and formaldehyde. These resins are used as binders in the manufacture of varnishes. It is also used as an oil-soluble antioxidant in motor-oil, in synthetic lubricants, in pourpoint depressors and in emulsion breakers for petroleum oils and some plastics. Other uses are as intermediate for antioxidants and as plasticiser for cellulose acetate.

Rank 17: 4-tert-butyltoluene
Not enough information on use patterns can be found in literature.

Rank 18: N,N-Diphenylamine
N,N-Diphenylamine is mainly used in synthesis of rubber chemicals (as an accelerator and antioxidant), dyestuff, antioxidants, pharmaceuticals, pesticides and explosives. It is also used as stabiliser in nitrocellulose and vinylacetate and as larvicide for veterinary use.

Rank 19: 1-chloro-2,4-dinitrobenzene
Industrially, the most important derivatives of 1-chloro-2,4-dinitrobenzene are obtained by nucleophilic reactions in aqueous media at moderate temperature. Ammonia gives 2,4-dinitroaniline, alkali gives 2,4-dinitrophenol and methanolic sodium hydroxide gives 2,4-dinitroanisole. Refluxing with hydrazine in ethanol yields 2,4-dinitrophenylhydrazine, a reagent used for the characterisation of carbonyl compounds. Reaction with ammonium thiocyanide in aqueous medium at 80ºC gives dinitrophenyl-rhodante, which was used as an insecticide. Reaction with substituted anilines gives 2,4-dinitrophenylamine derivatives that are used as yellow disperse dyes (nitro and nitroso dyes). Reaction with pyridine gives the reactive (2,4-dinitrophenyl) pyridinium chloride, an intermediate in the preparation of pentamethine dyes. Nitrochlorobenzenes, especially dinitrochlorobenzene, have traditionally been used to produce sulphur dyes; for example CI Sulphur Black I is obtained from 2,4-dinitrochlorobenzene by prolonged refluxing with sodium polysulphide liquor.

Rank 20: Xylene, mixed isomers/Rank 36: o-Xylene
Xylene is a constituent of gasoline and this results in a wide distribution of very large amounts. The isomer mixture is used as a solvent for alkyl resins, coatings and lacquers. The single isomers are seperated from this mixture. o-xylene is mainly (95% globally) used for the synthesis of phthalic acid anhydride. For p-xylene, (66% globally) is consumed for synthesis of dimethylterephthalate and 33% globally for terephthalic acid. m-xylene is used for synthesis of isophthalic acid and m-toluic acid. All three isomers are intermediates for vitamins, dyes, pharmaceutical, pesticides, flavouring agents and other fine chemicals. Xylene has many industrial uses, most notably as a solvent for numerous materials and as a fuel additive. Among the businesses that make use of aromatic hydrocarbons are the rubber and insecticide industries, chemical and pharmaceutical manufacturers, and explosive manufacturers.

Rank 21: Bis(2-ethylhexyl) phthalate (DEHP)
This chemical is used in vacuum pumps. It is also used as a plasticizer for polyvinyl chloride, especially in the manufacture of medical devices and dielectric fluid. It is also used as an acaricide for use in orchards, an inert ingredient in pesticides, a detector for leaks in respirators, testing of air filtration systems and component in cosmetic products.

Rank 22: 4-chloro-o-cresol
4-chloro-o-cresol is used in the manufacture of herbicides (MCPA).

Rank 23: 2-chlorophenol/Rank 25: 4-chlorophenol
Chlorophenols are used as agricultural chemicals, pharmaceutical biocides and dyes. The preparation of agricultural chemicals consumes 80-90% of chlorophenol production. Chlorophenols are commonly used as herbicides, insecticides and fungicides in the agricultural sector. Pharmaceuticals derived from chlorophenols include clofibrate, ethyl 2-(4-chlorophenoxy)-2-methyl propionate (ICI) which is used in the treatment of high sterum cholestrol and Mervan and Aldofene, an anti-inflammatory and analgesic drug (Continental Pharma). Biocides that are based on chlorophenols include the molluscicide Bayluscide (Bayer) and the bactericide Santophen or Chlorophen (Monsanto). Chlorophenols are also used in the synthesis of anthraquinone dyes. Quinizann, 1-4-dihydroxy-9,10-anthracenedione is the most important example.

Rank 24: Benzyl chloride
Benzyl chloride is used in the manufacture of dyes, synthetic tannins, perfumery, pharmaceuticals, manufacture of photographic developer, gasoline gum inhibitors, penicillin precursors, quaternary ammonium compounds and intermediates benzyl compounds,.

Rank 26: 2-chloroanthraquinone
Not enough information on use patterns can be found in literature.

Rank 27: 1,3-Dinitrobenzene
1,3-Dinitrobenzene is used in organic synthesis and is commonly used as an intermediate for azo dyes.

Rank 28: Di 'isodecyl' phthalate
Di 'isodecyl' phthalate is used as a plasticizer for a wide variety of polymers.

Rank 29: 2-Methylphenol
This compound is used as a disinfectant, solvent, resins, metal cleaner, food antioxidant, ore flotation, textile scouring agent, organic intermediate, surfactant, cresylic acid constituent, additives to lubricating oil and insecticide. It is also used in the manufacturing of perfumes, dyes, plastics, herbicides, tricresyl phosphate, salicylaldehyde and coumarin.

Rank 30: Trichloroacetic acid
Trichloroacetic acid is used as an intermediate in pesticide manufacture and in the production of sodium trichloroacetate (a reagent for albumin detection), in organic synthesis, in medicine and pharmaceuticals and herbicide

Rank 31: 1,2,4-Trichlorobenzene
Trichlorobenzene is used as a textile dye carrier, solvent and heat transfer medium. The substance is used for the synthesis of pesticides and in lubricants and dielectric media.

Rank 32: 4,4-Methylenedianiline
This compound is used as a curing agent for epoxy resins and urethane elastomers, as an intermediate in the preparation of polyurethanes and Spandex fibers, in the determination of tungsten and sulfates and in the preparation of azo dyes. It is also used as a corrosion inhibitor, cross-linking agent for epoxy resins, in the preparation of isocyanates and polyisocyanates, in the rubber industry, as a curative for neoprene, as an anti-frosting agent (anti-oxidant) in footwear and raw material in preparation of poly(amide-imide) resins (used in magnet wire enamels).

Rank 33: Piperazine
Piperazine, in the form of the hexahydrate or of salts, is used in the treatment of intestinal worms in human and veterinary medicine. Furthermore, the piperazine ring is a constituent of a large number of other drugs. The production of polyamides from piperazine and alphatic dicarboxylic acids has long been known; but has remained unimportant. The polymers so formed have a heat resistance superior to that of conventional polyamides but stabilisers must be added.

Rank 34: 2,2, Bis(4-hydroxyphenyl) propane
Some polyester resins incorporate 2,2, Bis(4-hydroxyphenyl) propane in their structure for improved properties. 2,2, Bis(4-hydroxyphenyl) propane is also used to prepare epoxy resins, modify phenolic resins, polycarbonates, aromatic polyesters and polysulfones.

Rank 35: Acrylaldehyde
This compound is used as a lacrimogenic warning agent in methyl chloride refrigerant, as a component of military poison gases, as a synthetic reagent in the manufacture of methionine, glycerol and glutaraldehyde; as an aquatic herbicide and as an algaecide for water treatment. It is also used as an intermediate for polyurethane and polyester resins, in pharmaceuticals, as a herbicide, as a biocide, in the manufacture of colloidal forms of metals, in making plastics and perfumes, to modify food starch, in the manufacture of 1,3,6-hexanetriol, as a fungicide and bactericide, as a liquid fuel, as an antimicrobial agent and as a slimicide in paper manufacture. It is an intermediate for acrylic acid and its esters and is used in the manufacture of 2-hydroxyadipaldehyde, quinoline, pentaerythritol, cycloaliphatic epoxy resins, oil-well additives and water treatment formulae.

Rank 37: 2,4-Dichlorophenol
Organic synthesis, pesticides, insecticides, manufacture of 2,4,-D, wood preservatives, antiseptics and seed disinfectants.

Rank 38: Epichlorohydrin
This compound is used in the manufacture of epoxy resins, glycerol and various other intermediates. It is a solvent for natural and synthetic resins, gums, cellulose esters and ethers, paints, varnishes, nail enamels and lacquers, and cements for celluloid. It is used in surface-active agents, pharmaceuticals, insecticides, agricultural chemicals, textile chemicals, coatings, adhesives, ion-exchange resins, plasticizers, glycidyl esters, ethymyl-ethylenic alcohol and fatty acid derivatives. It is a stabilizer in chlorine-containing materials and an intermediate in the preparation of condensates with polyfunctional substances.

Rank 39: Nitrobenzene
Manufacture of aniline, benzidine, quinoline, azobenzene, pyroxylin compounds; soaps, shoe and metal polishes; Solvent for cellulose ester; modifying esterification of cellulose acetate, for refining lubricating oils.

Rank 40: 1,4-Dichlorobenzene
This compound is used as a moth repellant, general insecticide, pesticide, fumigant, germicide, miticide, space odorant, air deodorant, chemical intermediate for dyes and organic chemicals, mildew control agent, disintegrating paste for molding concrete and stoneware, lubricant and disinfectant. It is used in the manufacture of 2,5-dichloroaniline, pharmaceutical manufacture, agriculture (to fumigate soil), manufacture of polyphenylene sulfide resins (used for surface coatings and molding resins) and organic synthesis.

Appendix V: Comparison of rankings and scores, using variations on the original system.

APPENDIX V: COMPARISON OF RANKINGS AND SCORES, USING VARIATIONS ON THE ORIGINAL SYSTEM

Using the original data, the following five tables present information on the rankings achieved by altering the assumptions from the original proposal.

Tables 1 & 2: Comparison of original ranking (using import/export data and emission factor = 1) with 1000t usage at different emission factors.

The original ranking used the import/export data from the CN system with all the deficiencies of shared CN numbers etc. In addition, a worst case emission factor of 1 was assumed. These tables present the ranks of the substances at a standardised 1000t usage figure, eliminating any confusion introduced by the CN system. In addition, these calculations have been conducted for emission factors of 1, 0.1 and 0.01. A number of substnaces become "rankable" at 1000t, since previously their exports exceeded imports.

Table 1 presents the absolute values of the ranking.

Table 2 shows the changes from the original for the different emission factors at 1000t.

Table 3 & 4: Comparison of original ranking (using import/export data and emission factor = 0 1) at different emission factors.

These tables show the effect of different emission factors on the ranking, all using the original import/export data from the CN system.

Table 3 presents the absolute values of the ranking.

Table 4 shows the changes from the original for the different emission factors.

Table 5: Ranking of substances at 1000t and an emission factor = 0 1

This presents the information already provided in Tables 1 & 2, but in rank order, solely at 1000t usage and an emission factor = 0 1.

Table 6: List of substances identified by Irish Chemical Suppliers Association, with scores. Substances are ordered by score using an emission factor of 1 and the CN derived import/export data for usage.

Examination of ranking is a confusing approach. If one substance is re-ranked, others will automatically be re-ranked, since the first substance has changed its position. This Table 6 examines the list of substances identified by the Irish Chemical Suppliers Association. Scoring is used as the indicator for the variations arising from using CN or a standard 1000t usage, and for different emission factors.

Table 1: Comparison of original ranking (using import/export data and emission factor=1) with 1000t usage at different emission factors – absolute ranking

CAS NO	Name	ORIGINAL	1000 TONNE RANKING		
			1	0.1	0.01
1746016	TCDD, PCDD, PCDF	1	4	9	45
56359	Bis-(tributyltin) oxide	2	6	5	8
1461252	Tetrabutyltin	3	9	20	59
117840	n-dioctylphthalate	4	21	35	65
25154523	Nonylphenol	5	19	14	18
26444495	Cresyldiphenylphosphate	6	3	6	14
140669	4-(1,1,3,3-tetramethylbutyl)phenol	7	15	15	28
92875	4,4'-Diaminobiphenyl	8	1	1	1
120127	Anthracene	9	14	16	30
108430	3-Chlorophenol	10	5	3	2
25339177	Isodecanol	11	23	21	22
121142	2,4-Dinitrotoluene	12	24	13	10
126727	Tris(2,3-bromo-1-propyl)phosphate	13	10	18	50
79118	Chloroacetic acid	14	8	7	5
102090	Diphenyl carbonate	15	40	36	24
121733	1-Chloro-3-nitrobenzene	16	29	25	15
28553120	Di-'isononyl'phthalate	17	45	52	71
56553	Benzo-a-anthracene	18	11	22	60
62533	Aniline	19	30	24	13
50328	Benzo-a-pyrene	20	13	27	62
77781	Dimethyl sulphate	21	55	50	35
98544	Butylphenol	22	42	48	44
98511	4-tert.-butyltoluene	23	31	32	37
122394	N,N-Diphenylamine	24	25	17	17
97007	1-Chloro-2,4-dinitrobenzene	25	44	37	23
85018	Phenanthrene	26	20	34	64
101815	Diphenylmethane	27	35	40	41
1330207	Xylene, mixed isomers	28	57	62	77
117817	Bis (2-ethylhexyl) phthalate (DEHP)	29	92	96	106
1570645	4-Chloro-o-cresol	30	17	12	19
95578	2-Chlorophenol	31	37	28	20
100447	Benzyl chloride	32	41	41	32
106489	4-Chlorophenol	33	39	31	21
131099	2-Chloroanthraquinone	34	79	83	76
83329	Acenaphthene	35	48	51	53
99650	1,3-Dinitrobenzene	36	63	54	38
26761400	Di-'isodecyl'phthalate	37	65	98	117
95487	2-Methylphenol	38	34	26	16
76039	Trichloroacetic acid	39	52	45	26
108952	Phenol	40	38	38	33
120821	1,2,4-Trichlorobenzene	41	36	42	43
101779	4,4'-Methylenedianiline	42	28	23	12
110850	Piperazine	43	88	75	49
80057	2,2-Bis-(4-hydroxyphenyl)-propane	44	69	59	40
206440	Fluoroanthene	45	49	57	74
107028	Acrylaldehyde	46	53	60	75
544105	1-Chlorohexane	47	2	2	4
120832	2,4-Dichlorophenol	48	51	49	34
106898	Epichlorohydrin	49	54	47	27
98953	Nitrobenzene	50	84	68	47
108703	1,3,5-Trichlorobenzene	51	32	44	68
106467	1,4-Dichlorobenzene	52	64	67	73
88733	2-Chloronitrobenzene	53	86	71	48
98464	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	54	80	70	51
1817476	4-Nitrocumol	55	71	78	85
95476	o-Xylene	56	78	82	88
98873	a,a-Dichlorotoluene	57	76	65	55
79414	Methacrylic acid	58	61	58	46
75092	Dichloromethane	59	99	99	99

Table 1: Comparison of original ranking (using import/export data and emission factor=1) with 1000t usage at different emission factors – absolute ranking, contd

CAS NO	Name	ORIGINAL	1000 TONNE RANKING		
			1	0.1	0.01
111659	Octane	60	47	53	72
108054	Vinyl acetate	61	91	91	92
71432	Benzene	62	93	94	91
90131	1-Chloronaphthalene	63	81	79	63
87616	1,2,3-Trichlorobenzene	64	58	63	78
84742	Phthalic acid dibutylester (DBP)	65	75	90	114
111875	Octan-1-ol	66	43	39	25
95498	2-Chlorotoluene	67	62	69	79
103117	2-Ethylhexyl acrylate	68	67	64	67
115968	Tris(2-chloroethyl)phosphate	69	83	72	54
126738	Tributyl phosphate	70	82	76	61
59507	Chlorocresol	71	85	81	66
79016	Trichloroethene	72	100	101	95
541731	1,3-Dichlorobenzene	73	95	93	84
109660	Pentane	74	89	88	90
67721	Hexachloroethane	75	33	30	31
115866	Phosphoric acid triphenyl-ester	76	22	33	58
109897	Diethylamine	77	94	85	69
78875	1,2-Dichloropropane	78	97	95	80
106478	4-Chloroaniline	79	7	4	3
67663	Trichloromethane	80	105	105	96
71556	1,1,1-Trichloroethane	81	101	102	98
95512	2-Chloroaniline	82	16	10	7
76017	Pentachloroethane	83	59	61	52
106434	4-Chlorotoluene	84	103	103	100
108429	3-Chloroaniline	85	27	19	11
104767	2-Ethyl-1-hexanol	86	60	56	42
100425	Styrol	87	74	84	111
79005	1,1,2-Trichloroethane	88	96	89	70
95761	3,4-Dichloroaniline	89	18	11	9
112345	2-(2-butoxyethoxy)ethanol	90	109	109	104
80626	Methyl methacrylate	91	110	110	105
111159	2-Ethoxyethyl acetate	92	108	108	97
79209	Methyl acetate	93	111	112	109
75456	Chlorodifluoromethane	94	112	113	108
75343	1,1-Dichloroethane	95	106	106	101
75252	Tribromomethane	96	77	66	56
90040	o-Anisidine	97	50	46	29
75014	Vinyl chloride	98	104	104	102
108883	Toluene	99	113	111	93
540590	1,2-Dichloroethene	100	102	100	89
1634044	Tert.-butyl methyl ether	101	114	115	112
126998	Chloroprene	102	107	107	103
127184	Tetrachloroethene	103	115	114	110
106423	p-Xylene	104	72	80	86
101848	Diphenyl ether	105	73	86	113
141979	Ethyl acetoacetate	106	116	116	115
107051	Allychloride	107	98	97	94
75354	1,1-Dichloroethylene	108	90	87	87
75058	Acetonitrile	109	118	118	118
100414	Ethylbenzene	110	70	77	83
76131	1,1,2-Trichlorotrifluoroethane	-	66	73	81
95501	1,2-Dichlorobenzene	-	56	55	57
14861177	2,4-Dichlorophenoxy-4-aniline	-	26	29	39
79061	Acrylamide	-	46	43	36
108907	Chlorobenzene	-	87	92	107
110827	Cyclohexane	-	68	74	82
534521	DNOC	-	12	8	6
100970	Methenamine	-	117	117	116

Table 2: Comparison of original ranking (using import/export data and emission factor=1) with 1000t usage at different emission factors – relative ranking

CAS NO	Name	ORIGINAL	1000 TONNE RANKING		
			1	0.1	0.01
1746016	TCDD, PCDD, PCDF	1	-3	-8	-44
56359	Bis-(tributyltin) oxide	2	-4	-3	-6
1461252	Tetrabutyltin	3	-6	-17	-56
117840	n-dioctylphthalate	4	-17	-31	-61
25154523	Nonylphenol	5	-14	-9	-13
26444495	Cresyldiphenylphosphate	6	3	0	-8
140669	4-(1,1,3,3-tetramethylbutyl)phenol	7	-8	-8	-21
92875	4,4'-Diaminobiphenyl	8	7	7	7
120127	Anthracene	9	-5	-7	-21
108430	3-Chlorophenol	10	5	7	8
25339177	Isodecanol	11	-12	-10	-11
121142	2,4-Dinitrotoluene	12	-12	-1	2
126727	Tris(2,3-bromo-1-propyl)phosphate	13	3	-5	-37
79118	Chloroacetic acid	14	6	7	9
102090	Diphenyl carbonate	15	-25	-21	-9
121733	1-Chloro-3-nitrobenzene	16	-13	-9	1
28553120	Di-'isononyl'phthalate	17	-28	-35	-54
56553	Benzo-a-anthracene	18	7	-4	-42
62533	Aniline	19	-11	-5	6
50328	Benzo-a-pyrene	20	7	-7	-42
77781	Dimethyl sulphate	21	-34	-29	-14
98544	Butylphenol	22	-20	-26	-22
98511	4-tert.-butyltoluene	23	-8	-9	-14
122394	N,N-Diphenylamine	24	-1	7	7
97007	1-Chloro-2,4-dinitrobenzene	25	-19	-12	2
85018	Phenanthrene	26	6	-8	-38
101815	Diphenylmethane	27	-8	-13	-14
1330207	Xylene, mixed isomers	28	-29	-34	-49
117817	Bis (2-ethylhexyl) phthalate (DEHP)	29	-63	-67	-77
1570645	4-Chloro-o-cresol	30	13	18	11
95578	2-Chlorophenol	31	-6	3	11
100447	Benzyl chloride	32	-9	-9	0
106489	4-Chlorophenol	33	-6	2	12
131099	2-Chloroanthraquinone	34	-45	-49	-42
83329	Acenaphthene	35	-13	-16	-18
99650	1,3-Dinitrobenzene	36	-27	-18	-2
26761400	Di-'isodecyl'phthalate	37	-28	-61	-80
95487	2-Methylphenol	38	4	12	22
76039	Trichloroacetic acid	39	-13	-6	13
108952	Phenol	40	2	2	7
120821	1,2,4-Trichlorobenzene	41	5	-1	-2
101779	4,4'-Methylenedianiline	42	14	19	30
110850	Piperazine	43	-45	-32	-6
80057	2,2-Bis-(4-hydroxyphenyl)-propane	44	-25	-15	4
206440	Fluoroanthene	45	-4	-12	-29
107028	Acrylaldehyde	46	-7	-14	-29
544105	1-Chlorohexane	47	45	45	43
120832	2,4-Dichlorophenol	48	-3	-1	14
106898	Epichlorohydrin	49	-5	2	22
98953	Nitrobenzene	50	-34	-18	3
108703	1,3,5-Trichlorobenzene	51	19	7	-17
106467	1,4-Dichlorobenzene	52	-12	-15	-21
88733	2-Chloronitrobenzene	53	-33	-18	5
98464	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	54	-26	-16	3
1817476	4-Nitrocumol	55	-16	-23	-30
95476	o-Xylene	56	-22	-26	-32
98873	a,a-Dichlorotoluene	57	-19	-8	2
79414	Methacrylic acid	58	-3	0	12
75092	Dichloromethane	59	-40	-40	-40

Table 2 contd: Comparison of original ranking (using import/export data and emission factor=1) with 1000t usage at different emission factors – relative ranking

CAS NO	Name	ORIGINAL	1000 TONNE RANKING		
			1	0.1	0.01
111659	Octane	60	13	7	-12
108054	Vinyl acetate	61	-30	-30	-31
71432	Benzene	62	-31	-32	-29
90131	1-Chloronaphthalene	63	-18	-16	0
87616	1,2,3-Trichlorobenzene	64	6	1	-14
84742	Phthalic acid dibutylester (DBP)	65	-10	-25	-49
111875	Octan-1-ol	66	23	27	41
95498	2-Chlorotoluene	67	5	-2	-12
103117	2-Ethylhexyl acrylate	68	1	4	1
115968	Tris(2-chloroethyl)phosphate	69	-14	-3	15
126738	Tributyl phosphate	70	-12	-6	9
59507	Chlorocresol	71	-14	-10	5
79016	Trichloroethene	72	-28	-29	-23
541731	1,3-Dichlorobenzene	73	-22	-20	-11
109660	Pentane	74	-15	-14	-16
67721	Hexachloroethane	75	42	45	44
115866	Phosphoric acid triphenyl-ester	76	54	43	18
109897	Diethylamine	77	-17	-8	8
78875	1,2-Dichloropropane	78	-19	-17	-2
106478	4-Chloroaniline	79	72	75	76
67663	Trichloromethane	80	-25	-25	-16
71556	1,1,1-Trichloroethane	81	-20	-21	-17
95512	2-Chloroaniline	82	66	72	75
76017	Pentachloroethane	83	24	22	31
106434	4-Chlorotoluene	84	-19	-19	-16
108429	3-Chloroaniline	85	58	66	74
104767	2-Ethyl-1-hexanol	86	26	30	44
100425	Styrol	87	13	3	-24
79005	1,1,2-Trichloroethane	88	-8	-1	18
95761	3,4-Dichloroaniline	89	71	78	80
112345	2-(2-butoxyethoxy)ethanol	90	-19	-19	-14
80626	Methyl methacrylate	91	-19	-19	-14
111159	2-Ethoxyethyl acetate	92	-16	-16	-5
79209	Methyl acetate	93	-18	-19	-16
75456	Chlorodifluoromethane	94	-18	-19	-14
75343	1,1-Dichloroethane	95	-11	-11	-6
75252	Tribromomethane	96	19	30	40
90040	o-Anisidine	97	47	51	68
75014	Vinyl chloride	98	-6	-6	-4
108883	Toluene	99	-14	-12	6
540590	1,2-Dichloroethene	100	-2	0	11
1634044	Tert.-butyl methyl ether	101	-13	-14	-11
126998	Chloroprene	102	-5	-5	-1
127184	Tetrachloroethene	103	-12	-11	-7
106423	p-Xylene	104	32	24	18
101848	Diphenyl ether	105	32	19	-8
141979	Ethyl acetoacetate	106	-10	-10	-9
107051	Allychloride	107	9	10	13
75354	1,1-Dichloroethylene	108	18	21	21
75058	Acetonitrile	109	-9	-9	-9
100414	Ethylbenzene	110	40	33	27
76131	1,1,2-Trichlorotrifluoroethane	-	P.U.	P.U.	P.U.
95501	1,2-Dichlorobenzene	-	P.U.	P.U.	P.U.
14861177	2,4-Dichlorophenoxy-4-aniline	-	P.U.	P.U.	P.U.
79061	Acrylamide	-	P.U.	P.U.	P.U.
108907	Chlorobenzene	-	P.U.	P.U.	P.U.
110827	Cyclohexane	-	P.U.	P.U.	P.U.
534521	DNOC	-	P.U.	P.U.	P.U.
100970	Methenamine	-	P.U.	P.U.	P.U.

P.U. = previously unranked

Table 3: Comparison of original ranking (using import/export data and emission factor=1) at different emission factors – absolute ranking

CAS NO	Name	Emission factor		
		ORIGINAL	0.1	0.01
1746016	TCDD, PCDD, PCDF	1	2	4
56359	Bis-(tributyltin) oxide	2	1	1
1461252	Tetrabutyltin	3	4	5
117840	n-dioctylphthalate	4	3	3
25154523	Nonylphenol	5	5	2
26444495	Cresyldiphenylphosphate	6	8	53
140669	4-(1,1,3,3-tetramethylbutyl)phenol	7	6	9
92875	4,4'-Diaminobiphenyl	8	18	80
120127	Anthracene	9	11	22
108430	3-Chlorophenol	10	12	23
25339177	Isodecanol	11	10	11
121142	2,4-Dinitrotoluene	12	9	7
126727	Tris(2,3-bromo-1-propyl)phosphate	13	31	89
79118	Chloroacetic acid	14	13	16
102090	Diphenyl carbonate	15	7	6
121733	1-Chloro-3-nitrobenzene	16	14	10
28553120	Di-'isononyl'phthalate	17	19	38
56553	Benzo-a-anthracene	18	49	99
62533	Aniline	19	16	14
50328	Benzo-a-pyrene	20	51	97
77781	Dimethyl sulphate	21	15	8
98544	Butylphenol	22	20	28
98511	4-tert.-butyltoluene	23	28	56
122394	N,N-Diphenylamine	24	22	32
97007	1-Chloro-2,4-dinitrobenzene	25	17	12
85018	Phenanthrene	26	54	92
101815	Diphenylmethane	27	35	63
1330207	Xylene, mixed isomers	28	25	40
117817	Bis (2-ethylhexyl) phthalate (DEHP)	29	21	17
1570645	4-Chloro-o-cresol	30	44	75
95578	2-Chlorophenol	31	26	27
100447	Benzyl chloride	32	34	41
106489	4-Chlorophenol	33	32	29
131099	2-Chloroanthraquinone	34	27	24
83329	Acenaphthene	35	42	64
99650	1,3-Dinitrobenzene	36	23	15
26761400	Di-'isodecyl'phthalate	37	69	93
95487	2-Methylphenol	38	36	42
76039	Trichloroacetic acid	39	29	21
108952	Phenol	40	45	65
120821	1,2,4-Trichlorobenzene	41	56	81
101779	4,4'-Methylenedianiline	42	43	55
110850	Piperazine	43	24	13
80057	2,2-Bis-(4-hydroxyphenyl)-propane	44	30	18
206440	Fluoroanthene	45	61	82
107028	Acrylaldehyde	46	60	79
544105	1-Chlorohexane	47	102	109
120832	2,4-Dichlorophenol	48	40	45
106898	Epichlorohydrin	49	39	39
98953	Nitrobenzene	50	33	19
108703	1,3,5-Trichlorobenzene	51	88	102
106467	1,4-Dichlorobenzene	52	47	68
88733	2-Chloronitrobenzene	53	37	20
98464	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	54	38	26
1817476	4-Nitrocumol	55	59	71
95476	o-Xylene	56	55	67
98873	a,a-Dichlorotoluene	57	46	46
79414	Methacrylic acid	58	52	58
75092	Dichloromethane	59	41	25

Table 3 contd: Comparison of original ranking (using import/export data and emission factor=1) at different emission factors – absolute ranking

CAS NO	Name	Emission factor		
		ORIGINAL	0.1	0.01
111659	Octane	60	87	95
108054	Vinyl acetate	61	53	57
71432	Benzene	62	48	49
90131	1-Chloronaphthalene	63	50	51
87616	1,2,3-Trichlorobenzene	64	84	87
84742	Phthalic acid dibutylester (DBP)	65	86	90
111875	Octan-1-ol	66	73	76
95498	2-Chlorotoluene	67	81	85
103117	2-Ethylhexyl acrylate	68	75	77
115968	Tris(2-chloroethyl)phosphate	69	58	48
126738	Tributyl phosphate	70	63	59
59507	Chlorocresol	71	68	66
79016	Trichloroethene	72	57	44
541731	1,3-Dichlorobenzene	73	67	61
109660	Pentane	74	79	74
67721	Hexachloroethane	75	97	100
115866	Phosphoric acid triphenyl-ester	76	106	108
109897	Diethylamine	77	74	62
78875	1,2-Dichloropropane	78	77	69
106478	4-Chloroaniline	79	103	105
67663	Trichloromethane	80	62	43
71556	1,1,1-Trichloroethane	81	72	54
95512	2-Chloroaniline	82	100	101
76017	Pentachloroethane	83	92	88
106434	4-Chlorotoluene	84	71	52
108429	3-Chloroaniline	85	96	94
104767	2-Ethyl-1-hexanol	86	89	83
100425	Styrol	87	99	98
79005	1,1,2-Trichloroethane	88	82	70
95761	3,4-Dichloroaniline	89	101	103
112345	2-(2-butoxyethoxy)ethanol	90	64	34
80626	Methyl methacrylate	91	65	35
111159	2-Ethoxyethyl acetate	92	76	47
79209	Methyl acetate	93	70	37
75456	Chlorodifluoromethane	94	66	30
75343	1,1-Dichloroethane	95	85	60
75252	Tribromomethane	96	94	86
90040	o-Anisidine	97	98	91
75014	Vinyl chloride	98	91	72
108883	Toluene	99	78	33
540590	1,2-Dichloroethene	100	93	73
1634044	Tert.-butyl methyl ether	101	80	36
126998	Chloroprene	102	95	78
127184	Tetrachloroethene	103	83	31
106423	p-Xylene	104	104	104
101848	Diphenyl ether	105	108	106
141979	Ethyl acetoacetate	106	90	50
107051	Allychloride	107	105	96
75354	1,1-Dichloroethylene	108	109	107
75058	Acetonitrile	109	107	84
100414	Ethylbenzene	110	110	110
76131	1,1,2-Trichlorotrifluoroethane	-		
95501	1,2-Dichlorobenzene	-		
14861177	2,4-Dichlorophenoxy-4-aniline	-		
79061	Acrylamide	-		
108907	Chlorobenzene	-		
110827	Cyclohexane	-		
534521	DNOC	-		
100970	Methenamine	-		

Table 4: Comparison of original ranking (using import/export data and emission factor=1) at different emission factors – relative ranking

CAS NO	Name	Emission factor		
		ORIGINAL	0.1	0.01
1746016	TCDD, PCDD, PCDF	1	-1	-3
56359	Bis-(tributyltin) oxide	2	1	1
1461252	Tetrabutyltin	3	-1	-2
117840	n-dioctylphthalate	4	1	1
25154523	Nonylphenol	5	0	3
26444495	Cresyldiphenylphosphate	6	-2	-47
140669	4-(1,1,3,3-tetramethylbutyl)phenol	7	1	-2
92875	4,4'-Diaminobiphenyl	8	-10	-72
120127	Anthracene	9	-2	-13
108430	3-Chlorophenol	10	-2	-13
25339177	Isodecanol	11	1	0
121142	2,4-Dinitrotoluene	12	3	5
126727	Tris(2,3-bromo-1-propyl)phosphate	13	-18	-76
79118	Chloroacetic acid	14	1	-2
102090	Diphenyl carbonate	15	8	9
121733	1-Chloro-3-nitrobenzene	16	2	6
28553120	Di-'isononyl'phthalate	17	-2	-21
56553	Benzo-a-anthracene	18	-31	-81
62533	Aniline	19	3	5
50328	Benzo-a-pyrene	20	-31	-77
77781	Dimethyl sulphate	21	6	13
98544	Butylphenol	22	2	-6
98511	4-tert.-butyltoluene	23	-5	-33
122394	N,N-Diphenylamine	24	2	-8
97007	1-Chloro-2,4-dinitrobenzene	25	8	13
85018	Phenanthrene	26	-28	-66
101815	Diphenylmethane	27	-8	-36
1330207	Xylene, mixed isomers	28	3	-12
117817	Bis (2-ethylhexyl) phthalate (DEHP)	29	8	12
1570645	4-Chloro-o-cresol	30	-14	-45
95578	2-Chlorophenol	31	5	4
100447	Benzyl chloride	32	-2	-9
106489	4-Chlorophenol	33	1	4
131099	2-Chloroanthraquinone	34	7	10
83329	Acenaphthene	35	-7	-29
99650	1,3-Dinitrobenzene	36	13	21
26761400	Di-'isodecyl'phthalate	37	-32	-56
95487	2-Methylphenol	38	2	-4
76039	Trichloroacetic acid	39	10	18
108952	Phenol	40	-5	-25
120821	1,2,4-Trichlorobenzene	41	-15	-40
101779	4,4'-Methylenedianiline	42	-1	-13
110850	Piperazine	43	19	30
80057	2,2-Bis-(4-hydroxyphenyl)-propane	44	14	26
206440	Fluoroanthene	45	-16	-37
107028	Acrylaldehyde	46	-14	-33
544105	1-Chlorohexane	47	-55	-62
120832	2,4-Dichlorophenol	48	8	3
106898	Epichlorohydrin	49	10	10
98953	Nitrobenzene	50	17	31
108703	1,3,5-Trichlorobenzene	51	-37	-51
106467	1,4-Dichlorobenzene	52	5	-16
88733	2-Chloronitrobenzene	53	16	33
98464	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	54	16	28
1817476	4-Nitrocumol	55	-4	-16
95476	o-Xylene	56	1	-11
98873	a,a-Dichlorotoluene	57	11	11
79414	Methacrylic acid	58	6	0
75092	Dichloromethane	59	18	34

Table 4 contd: Comparison of original ranking (using import/export data and emission factor=1) at different emission factors – relative ranking

CAS NO	Name	Emission factor		
		ORIGINAL	0.1	0.01
111659	Octane	60	-27	-35
108054	Vinyl acetate	61	8	4
71432	Benzene	62	14	13
90131	1-Chloronaphthalene	63	13	12
87616	1,2,3-Trichlorobenzene	64	-20	-23
84742	Phthalic acid dibutylester (DBP)	65	-21	-25
111875	Octan-1-ol	66	-7	-10
95498	2-Chlorotoluene	67	-14	-18
103117	2-Ethylhexyl acrylate	68	-7	-9
115968	Tris(2-chloroethyl)phosphate	69	11	21
126738	Tributyl phosphate	70	7	11
59507	Chlorocresol	71	3	5
79016	Trichloroethene	72	15	28
541731	1,3-Dichlorobenzene	73	6	12
109660	Pentane	74	-5	0
67721	Hexachloroethane	75	-22	-25
115866	Phosphoric acid triphenyl-ester	76	-30	-32
109897	Diethylamine	77	3	15
78875	1,2-Dichloropropane	78	1	9
106478	4-Chloroaniline	79	-24	-26
67663	Trichloromethane	80	18	37
71556	1,1,1-Trichloroethane	81	9	27
95512	2-Chloroaniline	82	-18	-19
76017	Pentachloroethane	83	-9	-5
106434	4-Chlorotoluene	84	13	32
108429	3-Chloroaniline	85	-11	-9
104767	2-Ethyl-1-hexanol	86	-3	3
100425	Styrol	87	-12	-11
79005	1,1,2-Trichloroethane	88	6	18
95761	3,4-Dichloroaniline	89	-12	-14
112345	2-(2-butoxyethoxy)ethanol	90	26	56
80626	Methyl methacrylate	91	26	56
111159	2-Ethoxyethyl acetate	92	16	45
79209	Methyl acetate	93	23	56
75456	Chlorodifluoromethane	94	28	64
75343	1,1-Dichloroethane	95	10	35
75252	Tribromomethane	96	2	10
90040	o-Anisidine	97	-1	6
75014	Vinyl chloride	98	7	26
108883	Toluene	99	21	66
540590	1,2-Dichloroethene	100	7	27
1634044	Tert.-butyl methyl ether	101	21	65
126998	Chloroprene	102	7	24
127184	Tetrachloroethene	103	20	72
106423	p-Xylene	104	0	0
101848	Diphenyl ether	105	-3	-1
141979	Ethyl acetoacetate	106	16	56
107051	Allychloride	107	2	11
75354	1,1-Dichloroethylene	108	-1	1
75058	Acetonitrile	109	2	25
100414	Ethylbenzene	110	0	0
76131	1,1,2-Trichlorotrifluoroethane	-	-	-
95501	1,2-Dichlorobenzene	-	-	-
14861177	2,4-Dichlorophenoxy-4-aniline	-	-	-
79061	Acrylamide	-	-	-
108907	Chlorobenzene	-	-	-
110827	Cyclohexane	-	-	-
534521	DNOC	-		
100970	Methenamine	-		

Table 5: ranking of substances at 1000t and an emission factor = 1

Rank	CAS NO	ID No.	Name	SCORE
1	92875	188	4,4'-Diaminobiphenyl	63.17
2	544105	54	1-Chlorohexane	49.33
3	26444495	333	Cresyldiphenylphosphate	41.86
4	1746016	319	TCDD, PCDD, PCDF	40.35
5	108430	123	3-Chlorophenol	40.11
6	56359	229	Bis-(tributyltin) oxide	39.62
7	106478	180	4-Chloroaniline	38.51
8	79118	148	Chloroacetic acid	32.46
9	1461252	236	Tetrabutyltin	31.73
10	126727	165	Tris(2,3-bromo-1-propyl)phosphate	31.64
11	56553	357	Benzo-a-anthracene	31.52
12	534521	129	DNOC	31.30
13	50328	37	Benzo-a-pyrene	29.70
14	120127	35	Anthracene	29.09
15	140669	117	4-(1,1,3,3-tetramethylbutyl)phenol	28.97
16	95512	178	2-Chloroaniline	28.68
17	1570645	127	4-Chloro-o-cresol	27.63
18	95761	179	3,4-Dichloroaniline	27.54
19	25154523	115	Nonylphenol	26.85
20	85018	39	Phenanthrene	26.27
21	117840	290	n-dioctylphthalate	26.09
22	115866	288	Phosphoric acid triphenyl-ester	25.55
23	25339177	107	Isodecanol	25.39
24	121142	94	2,4-Dinitrotoluene	25.33
25	122394	291	N,N-Diphenylamine	24.99
26	14861177	191	2,4-Dichlorophenoxy-4-aniline	24.78
27	108429	181	3-Chloroaniline	23.59
28	101779	189	4,4’-Methylenedianiline	23.23
29	121733	101	1-Chloro-3-nitrobenzene	23.13
30	62533	176	Aniline	23.00
31	98511	40	4-tert.-butyltoluene	22.95
32	108703	87	1,3,5-Trichlorobenzene	22.63
33	67721	48	Hexachloroethane	22.60
34	95487	279	2-Methylphenol	22.05
35	101815	41	Diphenylmethane	21.73
36	120821	88	1,2,4-Trichlorobenzene	21.07
37	95578	120	2-Chlorophenol	20.85
38	108952	114	Phenol	20.21
39	106489	122	4-Chlorophenol	19.96
40	102090	171	Diphenyl carbonate	19.48
41	100447	84	Benzyl chloride	19.03
42	98544	116	Butylphenol	18.95
43	111875	105	Octan-1-ol	18.75
44	97007	99	1-Chloro-2,4-dinitrobenzene	18.69
45	28553120	155	Di-’isononyl’phthalate	18.46
46	79061	198	Acrylamide	18.46
47	111659	24	Octane	18.25
48	83329	38	Acenaphthene	17.59
49	206440	295	Fluoroanthene	16.89
50	90040	190	o-Anisidine	16.60
51	120832	125	2,4-Dichlorophenol	16.48
52	76039	147	Trichloroacetic acid	16.46
53	107028	140	Acrylaldehyde	16.39
54	106898	137	Epichlorohydrin	16.07
55	77781	170	Dimethyl sulphate	15.48
56	95501	75	1,2-Dichlorobenzene	15.18
57	1330207	368	Xylene, mixed isomers	14.22
58	87616	79	1,2,3-Trichlorobenzene	14.13
59	76017	50	Pentachloroethane	13.50
60	104767	104	2-Ethyl-1-hexanol	13.39

Table 5 continued : Ranking of substances at 1000t and an emission factor = 1

Rank	CAS NO	ID No.	Name	SCORE
61	79414	152	Methacrylic acid	13.38
62	95498	81	2-Chlorotoluene	13.16
63	99650	283	1,3-Dinitrobenzene	13.00
64	106467	93	1,4-Dichlorobenzene	12.88
65	26761400	154	Di-'isodecyl'phthalate	12.83
66	76131	67	1,1,2-Trichlorotrifluoroethane	12.66
67	103117	151	2-Ethylhexyl acrylate	12.59
68	110827	365	Cyclohexane	12.58
69	80057	273	2,2-Bis-(4-hydroxyphenyl)-propane	12.16
70	100414	33	Ethylbenzene	12.11
71	1817476	96	4-Nitrocumol	11.98
72	106423	31	p-Xylene	11.91
73	101848	130	Diphenyl ether	11.90
74	100425	32	Styrol	11.56
75	84742	276	Phthalic acid dibutylester (DBP)	11.42
76	98873	83	a,a-Dichlorotoluene	11.17
77	75252	362	Tribromomethane	11.05
78	95476	28	o-Xylene	11.01
79	131099	141	2-Chloroanthraquinone	10.46
80	98464	100	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	10.20
81	90131	80	1-Chloronaphthalene	10.08
82	126738	292	Tributyl phosphate	10.01
83	115968	162	Tris(2-chloroethyl)phosphate	9.96
84	98953	92	Nitrobenzene	9.80
85	59507	358	Chlorocresol	9.77
86	88733	97	2-Chloronitrobenzene	9.73
87	108907	76	Chlorobenzene	9.57
88	110850	244	Piperazine	9.31
89	109660	23	Pentane	8.88
90	75354	58	1,1-Dichloroethylene	8.87
91	108054	143	Vinyl acetate	8.73
92	117817	289	Bis (2-ethylhexyl) phthalate (DEHP)	8.47
93	71432	366	Benzene	7.88
94	109897	174	Diethylamine	7.71
95	541731	89	1,3-Dichlorobenzene	7.41
96	79005	52	1,1,2-Trichloroethane	7.34
97	78875	46	1,2-Dichloropropane	6.99
98	107051	60	Allychloride	5.30
99	75092	43	Dichloromethane	4.80
100	79016	272	Trichloroethene	4.45
101	71556	47	1,1,1-Trichloroethane	3.91
102	540590	303	1,2-Dichloroethene	3.83
103	106434	85	4-Chlorotoluene	3.15
104	75014	56	Vinyl chloride	2.99
105	67663	359	Trichloromethane	2.79
106	75343	49	1,1-Dichloroethane	2.71
107	126998	61	Chloroprene	2.70
108	111159	144	2-Ethoxyethyl acetate	1.40
109	112345	133	2-(2-butoxyethoxy)ethanol	0.00
110	80626	153	Methyl methacrylate	0.00
111	79209	145	Methyl acetate	-0.60
112	75456	68	Chlorodifluoromethane	-0.96
113	108883	367	Toluene	-1.50
114	1634044	318	Tert.-butyl methyl ether	-3.89
115	127184	57	Tetrachloroethene	-4.02
116	141979	157	Ethyl acetoacetate	-5.75
117	100970	247	Methenamine	-8.24
118	75058	210	Acetonitrile	-14.20

Table 6: List of substances identified by ICSA, with scores. Substances are ordered by score using an emission factor of 1 and the CN derived import/export data for usage.

			SCORE					
		Usage	CN			1000 tonne		
CAS NO	ID	Name	1 (Original)	0.1	0.01	1	0.1	0.01
1746016	319	TCDD, PCDD, PCDF	44.47	26.93	9.40	40.35	22.81	5.28
56359	229	Bis-(tributyltin) oxide	43.29	30.80	18.32	39.62	27.13	14.64
117840	290	n-dioctylphthalate	34.11	22.78	11.44	26.09	14.75	3.41
25154523	115	Nonylphenol	28.66	20.93	13.19	26.85	19.11	11.37
92875	188	4,4'-Diaminobiphenyl	23.40	8.60	-6.19	63.17	48.37	33.58
25339177	107	Isodecanol	20.18	12.63	5.08	25.39	17.84	10.29
79118	148	Chloroacetic acid	18.62	11.08	3.53	32.46	24.91	17.36
102090	171	Diphenyl carbonate	18.22	13.17	8.13	19.48	14.44	9.40
28553120	155	Di-'isononyl'phthalate	15.90	7.88	-0.14	18.46	10.44	2.41
62533	176	Aniline	14.76	9.39	4.03	23.00	17.63	12.27
77781	170	Dimethyl sulphate	14.45	10.38	6.30	15.48	11.40	7.33
122394	291	N,N-Diphenylamine	13.60	6.87	0.13	24.99	18.26	11.52
101815	41	Diphenylmethane	12.52	4.71	-3.10	21.73	13.92	6.10
1330207	368	Xylene, mixed isomers	12.17	5.99	-0.19	14.22	8.04	1.86
117817	289	Bis (2-ethylhexyl) phthalate (DEHP)	11.47	7.24	3.00	8.47	4.24	0.00
1570645	127	4-Chloro-o-cresol	11.13	2.97	-5.18	27.63	19.48	11.32
100447	84	Benzyl chloride	10.38	4.85	-0.69	19.03	13.50	7.96
106489	122	4-Chlorophenol	10.27	5.49	0.70	19.96	15.17	10.39
26761400	154	Di-'isodecyl'phthalate	9.69	-0.18	-10.04	12.83	2.97	-6.89
76039	147	Trichloroacetic acid	9.43	5.59	1.76	16.46	12.63	8.79
108952	114	Phenol	9.04	2.88	-3.27	20.21	14.06	7.90
101779	189	4,4'-Methylenedianiline	8.68	3.26	-2.16	23.23	17.82	12.40
110850	244	Piperazine	8.54	6.34	4.14	9.31	7.11	4.91
80057	273	2,2-Bis-(4-hydroxyphenyl)-propane	8.38	5.52	2.65	12.16	9.30	6.43
107028	140	Acrylaldehyde	8.08	0.96	-6.17	16.39	9.27	2.14
106898	137	Epichlorohydrin	7.42	3.63	-0.16	16.07	12.29	8.50
98953	92	Nitrobenzene	7.29	4.95	2.60	9.80	7.46	5.11
106467	93	1,4-Dichlorobenzene	7.18	1.87	-3.44	12.88	7.57	2.25
88733	97	2-Chloronitrobenzene	6.82	4.45	2.07	9.73	7.36	4.98
98464	100	alpha,alpha,alpha-Trifluoro-3-nitrotoluene	6.77	3.98	1.18	10.20	7.40	4.61
95476	28	o-Xylene	6.18	1.39	-3.39	11.01	6.23	1.44
79414	152	Methacrylic acid	5.64	1.57	-2.49	13.38	9.31	5.25
75092	43	Dichloromethane	5.63	3.47	1.32	4.80	2.64	0.48
111659	24	Octane	5.41	-2.52	-10.45	18.25	10.32	2.39
108054	143	Vinyl acetate	5.26	1.43	-2.41	8.73	4.89	1.06
71432	366	Benzene	5.20	1.80	-1.59	7.88	4.49	1.09
84742	276	Phthalic acid dibutylester (DBP)	4.38	-2.10	-8.59	11.42	4.93	-1.55

Table 6 continued: List of substances identified by ICSA, with scores. Substances are ordered by score using an emission factor of 1 and the CN derived import/export data for usage.

			SCORE					
		Usage	CN			1000 tonne		
CAS NO	ID	Name	1 (Original)	0.1	0.01	1	0.1	0.01
111875	105	Octan-1-ol	4.35	-0.46	-5.28	18.75	13.93	9.12
95498	81	2-Chlorotoluene	4.22	-1.50	-7.21	13.16	7.44	1.72
103117	151	2-Ethylhexyl acrylate	4.07	-0.67	-5.41	12.59	7.85	3.11
115968	162	Tris(2-chloroethyl)phosphate	3.92	1.19	-1.53	9.96	7.24	4.51
126738	292	Tributyl phosphate	3.27	0.23	-2.81	10.01	6.97	3.93
59507	358	Chlorocresol	3.17	-0.09	-3.35	9.77	6.51	3.25
79016	272	Trichloroethene	3.14	1.20	-0.73	4.45	2.52	0.58
109660	23	Pentane	2.63	-1.22	-5.08	8.88	5.02	1.16
67721	48	Hexachloroethane	2.34	-4.91	-12.17	22.60	15.34	8.09
115866	288	Phosphoric acid triphenyl-ester	1.86	-8.82	-19.50	25.55	14.87	4.19
109897	174	Diethylamine	1.77	-0.63	-3.03	7.71	5.31	2.91
78875	46	1,2-Dichloropropane	1.68	-0.99	-3.65	6.99	4.33	1.67
106478	180	4-Chloroaniline	1.61	-7.44	-16.48	38.51	29.46	20.42
67663	359	Trichloromethane	1.54	0.41	-0.71	2.79	1.67	0.55
71556	47	1,1,1-Trichloroethane	1.27	-0.43	-2.13	3.91	2.21	0.51
95512	178	2-Chloroaniline	1.11	-5.65	-12.40	28.68	21.93	15.17
108429	181	3-Chloroaniline	1.00	-4.54	-10.07	23.59	18.05	12.52
104767	104	2-Ethyl-1-hexanol	0.92	-2.80	-6.52	13.39	9.67	5.95
100425	32	Styrol	0.86	-5.28	-11.42	11.56	5.43	-0.71
79005	52	1,1,2-Trichloroethane	0.79	-1.55	-3.89	7.34	4.99	2.65
112345	133	2-(2-butoxyethoxy)ethanol	0.00	0.00	0.00	0.00	0.00	0.00
80626	153	Methyl methacrylate	0.00	0.00	0.00	0.00	0.00	0.00
111159	144	2-Ethoxyethyl acetate	-0.30	-0.73	-1.15	1.40	0.97	0.55
79209	145	Methyl acetate	-0.44	-0.29	-0.14	-0.60	-0.45	-0.30
75456	68	Chlorodifluoromethane	-0.46	-0.04	0.37	-0.96	-0.54	-0.13
75343	49	1,1-Dichloroethane	-0.51	-1.67	-2.82	2.71	1.56	0.40
75014	56	Vinyl chloride	-1.97	-3.27	-4.57	2.99	1.69	0.39
108883	367	Toluene	-2.24	-1.09	0.07	-1.50	-0.35	0.81
1634044	318	Tert.-butyl methyl ether	-2.60	-1.32	-0.03	-3.89	-2.60	-1.31
126998	61	Chloroprene	-3.30	-4.47	-5.64	2.70	1.52	0.35
127184	57	Tetrachloroethene	-3.34	-1.59	0.16	-4.02	-2.27	-0.53
106423	31	p-Xylene	-3.56	-8.74	-13.91	11.91	6.73	1.56
107051	60	Allychloride	-6.48	-8.78	-11.09	5.30	3.00	0.69
75058	210	Acetonitrile	-13.64	-10.13	-6.61	-14.20	-10.69	-7.17
76131	67	1,1,2-Trichlorotrifluoroethane	-	-	-	12.66	7.16	1.66
95501	75	1,2-Dichlorobenzene	-	-	-	15.18	9.72	4.26
108907	76	Chlorobenzene	-	-	-	9.57	4.78	0.00
100970	247	Methenamine	-	-	-	-8.24	-6.32	-4.40
110827	365	Cyclohexane	-	-	-	12.58	7.11	1.65