Institute for Environment and Health

A screening method for ranking chemicals by their fate and behaviour in the environment and potential toxic effects in humans following non-occupational exposure

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1 Introduction and Purposes of Prioritisation Scheme

A large number of chemicals are released intentionally or unintentionally into the environment each year. These include thousands of substances that are currently listed worldwide and several hundred new substances added annually (Mücke *et al*., 1986). When these compounds are used, they can reach microorganisms, plants, animals and man either in their original state or in the form of reaction and degradation products via air, water, soil or foodstuffs. Hence environmental chemicals can occur in practically all environmental compartments and ecosystems. It is not feasible to conduct assessments of human exposure and possible associated health effects for all chemicals. Even if the necessary resources were available, reliable data for a quantitative evaluation are likely to be absent in most cases. This has led to the development of schemes for prioritising compounds likely to be of environmental significance. Such schemes can be used to direct future research efforts towards the prioritised compounds.

This study was commissioned by the Department of Health (DH) as part of a broader research activity that aims to identify key priority chemicals of concern to human health at routine levels of environmental exposure. The main pathways of human exposure are shown in Figure 1.1. A review of the principal prioritisation schemes used by different organisations to assess the significance of chemical release into the environment has been conducted by the MRC Institute for Environment and Health (IEH, 2003). This review showed that the approaches used by different organisations vary widely, depending on the initial reasons for which the schemes were developed. The basic information presented in the review was used to develop a simple screening method for ranking chemicals. The model used in this prioritisation scheme is outlined in Figure 1.2. The main purpose in developing the prioritisation scheme for DH was to develop a dedicated priority setting method capable of identifying chemicals in air, water, soil and foodstuffs that might pose a significant risk to human health following low level environmental exposure. The methodology was developed in order to identify compounds that required further assessment and those that had data gaps. More detailed risk assessments were conducted at a later stage on those compounds prioritised as being of high importance[a].

The screening methodology was developed for 'existing chemicals' as these are of greatest concern because data on their toxicity and/or fate and behaviour are often unknown[b]. The production of a priority list was designed to highlight compounds that required further regulatory measures to reduce exposure of the general population and for which an in-depth risk characterisation would be necessary to assist in the evaluation and implementation of activities for reducing environmental risks. This might include an assessment of the costs of such risks to human health and the costs of reduction measures. As the scheme also aimed to identify data gaps that might warrant further investigation, the application of default categories for chemicals with no data was also considered. The overall aim was to develop a screening methodology that is quick, clear and simple to use and that can easily be revised to take into account new information on compounds as and when it becomes available.

[a] Benzene (*IEH Report on Benzene in the Environment*, R12); 4,6-dichlorocresol, hexachloro-1,3-butadiene, tetrachlorobenzene, 2,4,6-trichlorophenol (reports to DH; available from MRC Institute for Environment and Health

[b] 'Existing Substances' are those that were placed in the European Union (EU) market before 1981. Prior to 1981 regulatory requirements were related to products intended for certain uses (e.g. veterinary medicines) and did not require assessment of the hazardous properties of any substance before they were released into the market. For substances placed on the market after 1981 (classified as 'New Substances') there is a legal requirement to conduct such assessments. Regulatory agencies require the collection of extensive documentation for safety before a chemical, for example, can be used in foods or commercial products.

This report describes how physicochemical properties and toxicological data were incorporated into a screening model to assess the potential fate and transfer of chemicals between different environmental compartments and to predict the potential human exposure to toxic chemicals through the inhalation of contaminated air and the ingestion of water and food. It must be stressed, however, that the method devised is a simple screening process and that a more detailed assessment is necessary to determine the potential transfer through the foodchain of a chemical and the full extent of any adverse health effects. Sections 2 and 4 present the physicochemical properties, toxicological data and algorithms used to screen the compounds. Section 3 summarises the groups of chemicals that were included in the screening process. The results of the prioritisation scheme and comments on their limitations and constraints are presented in Section 5.

Figure 1.1 Schematic representation of the main exposure routes for humans

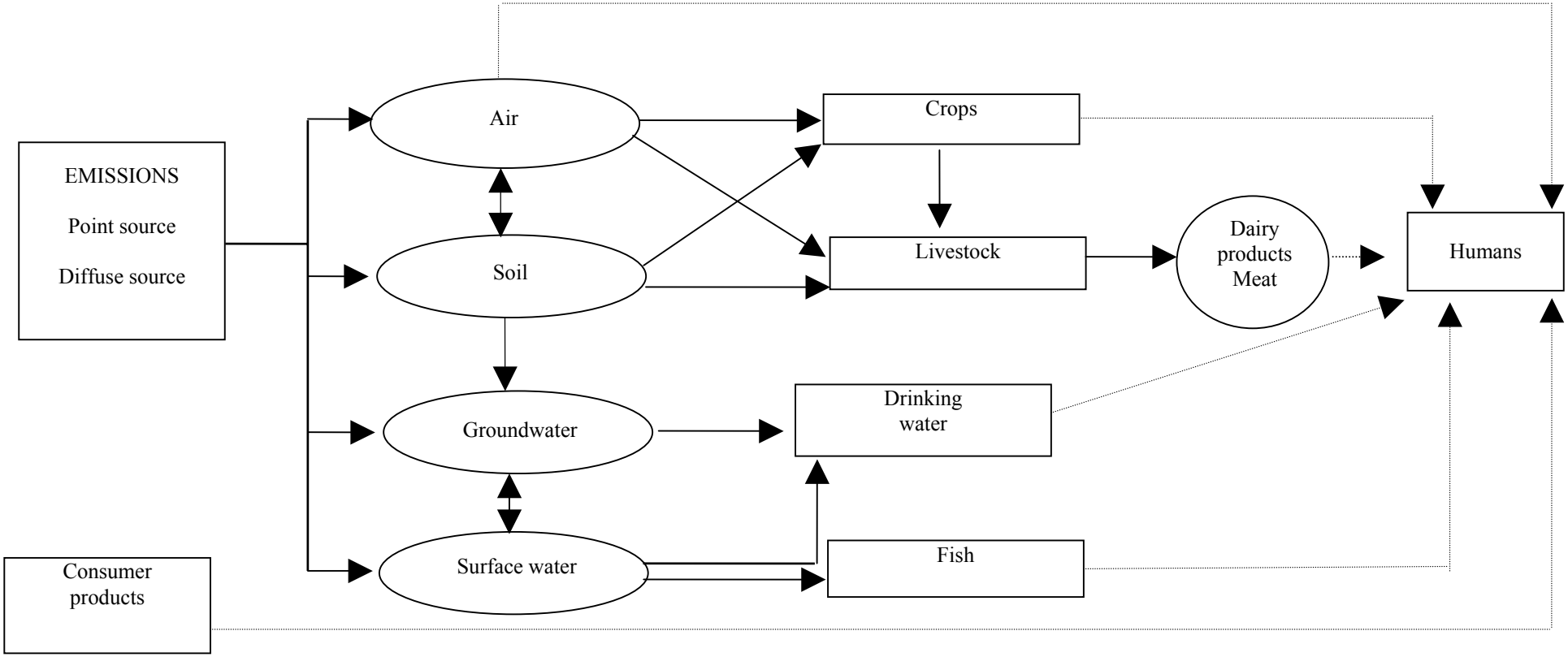
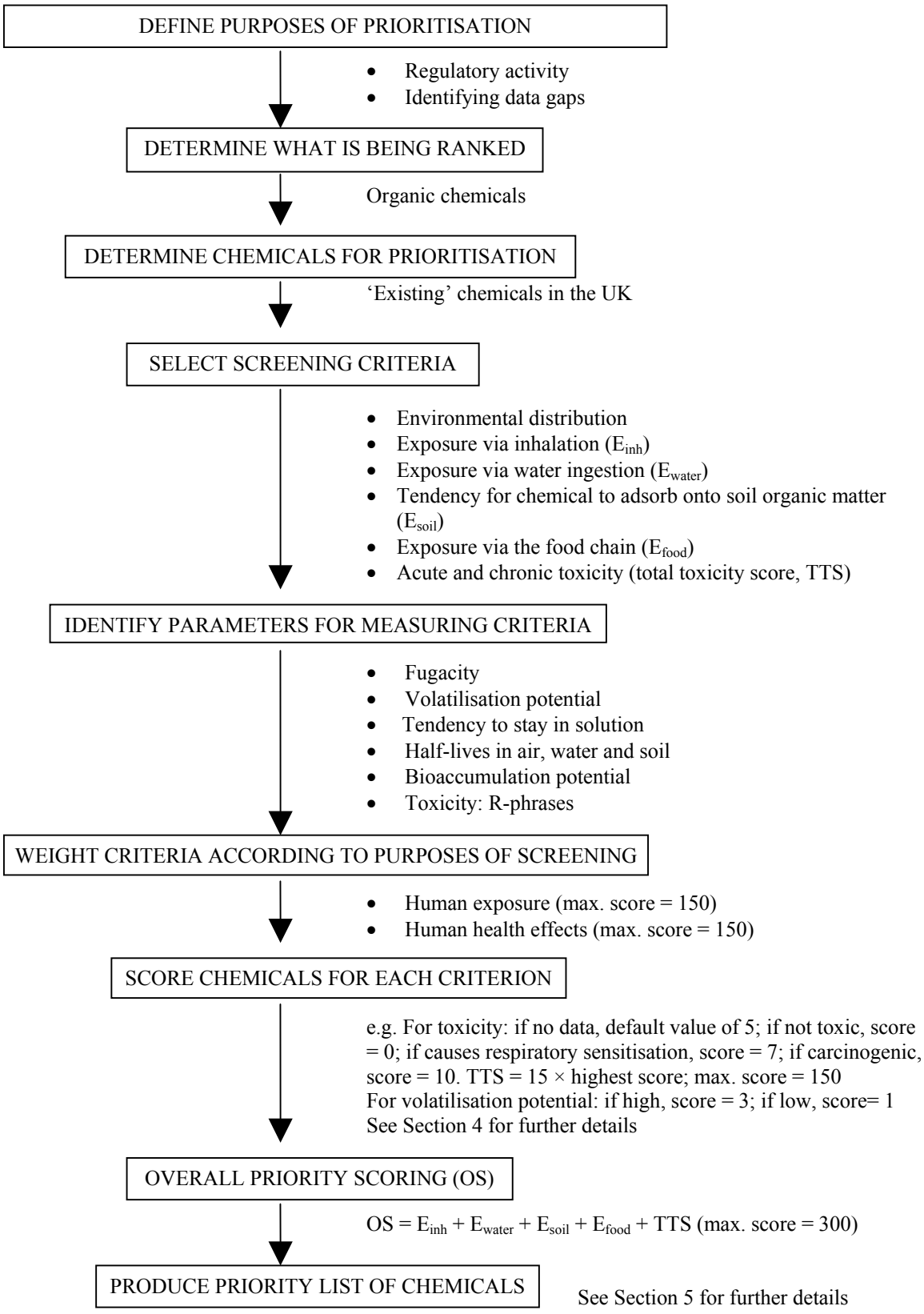


Figure 1.2 Model used in the prioritisation scheme (for further details see text)



2 Parameters Used in Screening

The partitioning of a chemical between different environmental compartments is determined by physicochemical properties such as the chemical's water solubility, vapour pressure and soil/sediment sorption/desorption. These properties are often used for predicting the fate and behaviour of compounds in the environment. In addition, prioritisation schemes commonly include a screening tier in which chemicals are ranked by their human health effects in relation to exposure to the chemical. This may include quantitative assessment of acute oral and inhalation toxicity, developmental, reproductive and neurotoxicity, semi-quantitative assessment of carcinogenicity and qualitative assessments of other effects such as mutagenicity and respiratory and skin sensitisation. The parameters that were been used to predict the behaviour and toxic effects of chemicals in this screening model are defined below.

2.1 Physicochemical properties used to assess exposure

Standard physicochemical and persistence data were entered into a spreadsheet. The information was obtained from the published literature, mainly from Howard (1989, 1990, 1991, 1993), Howard *et al.* (1991) and Mackay *et al.* (1991, 1992, 1993, 1995). These authors have compiled lists of data from a large number of sources and have summarised much of the data available in the literature. They also used equations extrapolated from the available data to determine appropriate formulae which could be used to estimate missing data. Some of these equations were used in the prioritisation scheme described here to calculate physicochemical properties for chemicals with no data. Data were collected as reported ranges and the estimated mean or median value was used in the screening process. Information was also collected from various chemical databases and manuals, mainly the International Union Chemical Information Database (IUCLID)[a], the Nordic Council of Ministers Environmental Hazard Classification scheme (Pedersen *et al*., 1995) and the Pesticides Manual (Tomlin, 1994). The physicochemical properties that were used to assess exposure end-points are summarised in Table 2.1 and are described below.

Table 2.1 Physicochemical parameters used to assess exposure end-points

Physicochemical property	Units
Molecular weight, MW	g/mol
Water solubility, S	g/m^3 or mg/l at 25°C
Vapour pressure, Vp	Pa (N/m^2) at 25°C
Octanol–water partition coefficient, K_{ow}	Unitless
Organic carbon–water partition coefficient, K_{oc}	Unitless
Henry's Law Constant, H_c or H_c'	Pa m^3/mol or dimensionless
Bioconcentration factor in fish (BCF_{fish})	Unitless
Half-lives in soil ($T_{1/2\ soil}$), water ($T_{1/2\ water}$) and air ($T_{1/2\ air}$)	Hours, days or years

2.1.1 Molecular weight

Molecular weight (MW) expressed as the number of grams per mole of a substance as specified by its chemical formula was used.

[a] See http://ecb.jrc.it

2.1.2 Water solubility

Water solubility (S) describes the amount of a chemical that can dissolve freely in a known quantity of water, that is it refers to the concentration of a chemical dissolved in water when the water is both in contact and at equilibrium with the pure chemical.

2.1.3 Vapour pressure

Vapour pressure (Vp) is the partial pressure of a chemical in the gaseous phase at equilibrium with the pure liquid or solid chemical.

2.1.4 Octanol–water partition coefficient

A partition coefficient is the ratio of the concentration of a chemical in two different phases under equilibrium conditions. The octanol–water partition coefficient (K_{ow}) is the ratio of a chemical's concentration in octanol ($C_7H_{15}CH_2OH$) to that in water of a two-phase octanol/water experimental system at equilibrium, which represents the distribution tendency of an organic chemical between the organic and aqueous phases. K_{ow} values can vary over several orders of magnitude so they are therefore generally expressed as a logarithmic value (i.e. log K_{ow}). This parameter is extensively used to estimate the environmental fate of organic compounds because it approximates to the lipid–water partition coefficient, providing an indication of the tendency of a compound to partition between water and body fat or between water and organic matter.

In general, substances with low K_{ow} values tend to be smaller and more polar (hydrophilic) molecules, which dissolve more readily in water and thus have a low tendency to adsorb to soil. Larger and less polar (hydrophobic) molecules have higher K_{ow} values and tend to associate more readily with less polar phases such as lipids, waxes, body fat and soil organic matter. K_{ow} is also related to lipophilicity, water solubility, soil/sediment adsorption and aquatic bioconcentration factors (BCF) and is therefore a useful parameter for estimating organic carbon–water partition coefficients (K_{oc}) and BCFs (see Sections 2.1.5 and 2.1.7 below). A chemical with a low K_{ow} value is considered hydrophilic and tends to have a low fat solubility, high water solubility, low soil/sediment adsorption coefficient and a low BCF and vice versa for chemicals with high K_{ow} values.

2.1.5 Organic carbon–water partition coefficient

A large number of chemicals are hydrophobic and therefore have limited solubility in water but tend to dissolve easily in fats, non-polar organic solvents and bind to organic carbon in soil. From the numerous properties that affect sorption of chemicals to soil, such as organic carbon content, particle size, clay mineral composition, pH, the organic carbon content of soil is the most important. Thus the estimation of the organic carbon–water partition coefficient (K_{oc}) provides an estimate of the tendency of a compound to adsorb and become tightly bound to the humic material in soil. It is defined as the ratio between the concentration of a compound on organic carbon and the concentration in water.

K_{oc} can be estimated from K_{ow} as this parameter provides a direct estimate of hydrophobicity of a compound and provides a good indication of the likelihood of leaching through soil or adsorbing onto soil organic carbon. For compounds that have no measured or reported K_{oc} values, K_{oc} has been estimated by using the following formula: $K_{oc} = 0.41\ K_{ow}$ (Mackay *et al.*, 1991).

In general, compounds with higher K_{oc} values tend to adsorb onto organic carbon while those with smaller K_{oc} values are more readily leached. As with K_{ow}, K_{oc} values can vary over orders of magnitude, so they are therefore often expressed as a logarithmic value.

2.1.6 Henry's Law constant

Henry's Law describes the partitioning of a compound between a solution and the air above it. The Henry's Law constant (H_c) is a partition coefficient defined by the ratio of a chemical's concentration

in air to its concentration in water at equilibrium. Therefore H_c is used to describe the tendency for chemicals to move from the aqueous phase to the gas phase. This includes the tendency of a chemical to volatilise from soil, water and plant surfaces into the atmosphere.

H_c can be expressed with or without units. In its dimensionless form (H_c') the same units of concentration are used for both the air and water phases (e.g. mg/dm^3 of air or mg/l of water). The dimensional form can be estimated as follows:

$$\mathbf{H_c} = \quad Vp/S \text{ (atm m}^3\text{/mol)} \qquad (1)$$

where Vp is the vapour pressure of the compound in atmospheres and solubility is the aqueous solubility in mol/m^3. H_c can also be expressed in terms of Pa m^3/mol where 1 Pa = 9.872×10^{-6} atm

Where H_c data have not been measured experimentally, they can be estimated by dividing the Vp of the chemical by its S. Therefore, where no measured values were available, calculated Henry's constants were used in this screening method.

The dimensionless form can be converted to the dimensional form as follows:

$$\mathbf{H_c} = \quad H_c' \, RT \qquad (2)$$

where R = universal gas constant (i.e. 8.2×10^{-5} atm m^3/mol K) and T = absolute temperature in degrees Kelvin (i.e. 298 K)

High H_c values generally indicate a greater tendency of a compound to volatilise, while compounds with lower H_c tend to stay in solution.

2.1.7 Bioconcentration factors

The bioconcentration factor (BCF) indicates the tendency of a compound to partition between different environmental compartments and is defined as the ratio between the concentration of a chemical in biota and the concentration in water at equilibrium. BCFs can also be calculated by the ratio of the first order uptake and elimination rate constants, where equilibrium conditions are not a requirement. While bioaccumulation may occur in both aquatic and terrestrial organisms, most of the data available in the literature relate to the former. As a consequence only BCFs in aquatic organisms, mainly fish (BCF_{fish}), were considered in this scheme. However, it should be noted that bioaccumulation in terrestrial species does not correlate well with bioconcentration in aquatic species because it is not as dependent on chemical lipid solubility. Rather it depends more on the rate of metabolism, excretion and other mechanisms. Data were collected for BCFs measured directly, where available.

Bioaccumulation can also be estimated as a function of the physicochemical properties of a chemical. For example, K_{ow} is commonly used as an estimate of fat solubility and, in turn, to estimate BCF. The estimation of the BCF from K_{ow} appears to be relatively accurate, although values may vary depending on the test system used. Also, where metabolic processes are significant, estimated BCFs are less reliable.

When there were no measured BCF_{fish} data reported in the literature, the following equation was used in this screening process:

$$BCF_{fish} = \quad a \, K_{ow} \qquad (3)$$

where BCF_{fish} is the bioconcentration factor of fish (kg wet fish/litre water) and *a* represents the lipid fraction of the fish, which is generally in the range of 0.02–0.20

The most widely used relationship is that of Mackay (1982) where:

$$BCF_{fish} = \quad 0.048 \, K_{ow} \qquad (4)$$

This equation is based on experimental data for several different classes of chemicals with a log K_{ow} ranging from approximately 1 to 6. When the log K_{ow} is greater than 6, the measured BCF data tend to decrease with increasing log K_{ow}. This change in the relationship towards non-linearity has been attributed to biotransformation, reduced membrane permeation kinetics and/or reduced biotic lipid solubility for large molecules, though uncertainty inherent from the experimental tests (e.g. caused by the difficulties of reaching equilibrium or by reduced bioavailability due to chemical sorption to organic matter in the aqueous phase) may also contribute towards non-linearity (European Commission, 1996). In order to account for this plateau relationship between BCF_{fish} and K_{ow} the following parabolic equation (European Commission, 1996) developed by Connell and Hawker (1988) was used to estimate BCFs where $6 < \log K_{ow} < 10$:

$$\log BCF_{fish} = (-0.2(\log K_{ow})^2) + (2.74 \log K_{ow}) - 4.72 \quad (5)$$

In conclusion, BCFs for substances with log $K_{ow} > 6$ should be treated with caution owing to the large experimental uncertainties, and compounds that have log K_{ow} values >10 should only be considered in a qualitative rather than quantitative manner.

It should be noted that the use of K_{ow} alone as an estimation of bioconcentration is limited to un-ionised organic chemicals. Chemicals that dissociate 50% or more bioconcentrate significantly less than predicted by K_{ow} based on estimation methods and therefore, when evaluating an ionised chemical, consideration should be given to the dissociation constant. However, a conservative approach is best at this stage of the screening process.

2.1.8 Half-lives

Most organic compounds degrade in the environment. The loss of a chemical from a system is extremely complex and depends on both the intrinsic properties of the chemical and the nature of the surrounding environment. Factors such as the microbial population, soil organic matter, sunlight intensity and environmental factors such as temperature and pH affect the chemical's half-life. The rate of loss of a compound from a system can be described by the first order rate constant or half-life ($T_{1/2}$), which refers to the time taken for half the compound to disappear from the relevant medium (e.g. $T_{1/2\ air}$, $T_{1/2\ water}$ or $T_{1/2\ soil}$). Half-lives will be determined by various processes operating simultaneously, including biotic and abiotic degradation, volatilisation and leaching. It should be noted that primary biodegradation can sometimes result in the formation of a contaminant that is more toxic and/or more persistent than the parent compound and, unless these metabolites have been incorporated into the initial spreadsheet, they cannot be accounted for by this screening method. Because so many factors can affect a chemical's $T_{1/2,}$ it can be misleading to document a single $T_{1/2}$ value. Ranges of data reported in the literature have therefore been incorporated into the spreadsheets. However, for the purposes of screening, the estimated median values of the reported ranges were taken as representative of $T_{1/2}$.

2.2 Toxicity data used to assess health effects

In screening processes, human health effects are quantified on the basis of predefined toxicological end-points. A number of prioritisation schemes developed in the UK and Europe have used 'Risk' phrases (R-phrases) to rank environmental chemicals for human health effects. R-phrases are phrases used to classify and label commercial substances according to the possible hazard(s) to humans resulting from their general use. R-phrase definitions cover the health effects known to be associated with exposure following ingestion, skin contact and inhalation in humans. Guidance information on how to use R-phrases is provided under the Chemicals (Hazard Information and Packaging for Supply) (CHIP) Regulations 1997 (see HSC, 1997 for further details). The Health and Safety Executive (HSE), the European Union Risk Ranking Method (EURAM) and the Ministry of Agriculture Fisheries and Food (MAFF) have all successfully used R-phrases in prioritisation schemes (Shillaker, 1992; Wearne *et al.,* 1996; Hansen *et al*., 1999).

R-phrases cover a wide range of effects, including carcinogenicity, mutagenicity, reproductive toxicity, teratogenicity, irritancy, sensitisation and repeat exposure toxicity, for a large number of new and existing chemicals. They are therefore suitable for prioritisation schemes which prioritise chemicals on the basis of their mammalian toxicity because R-phrase information is available for a large number of chemicals from a number of chemical databases and directories, such as IUCLID[a], pesticides manuals (e.g. Tomlin, 1994) and the European Union (EU) Official Journal (e.g. Commission of the European Communities, 1993). The disadvantage of using R-phrases is that they are designed for the purposes of classifying and labelling commercial substances, to inform potential users of the substances about the possible adverse health effects that can be incurred by the use of these commercial products. Consequently, there are no R-phrases for chemicals that are not produced commercially, that are produced unintentionally or that have been banned. Also, when dealing with existing substances, the potential variability in the quality of data used to support an R-phrase needs to be noted. However, because R-phrases provide a rapid and relatively easy method of obtaining information on the health effects of chemicals (because the expert assessment of the available toxicological data on a chemical has already been done), they were used in this screening method as a surrogate for the hazard potential of substances. The relevant R-phrases and their toxicological end-points are summarised in Table 2.2.

Table 2.2 R-phrase classifications based on health effects in humans (from HSC, 1997)

Toxicity end-point		R-Phrase
Acute effects	Harmful, toxic and very toxic by inhalation	R20, R23, R26
	Harmful, toxic and very toxic in contact with the skin	R21, R24, R27
	Harmful, toxic and very toxic if swallowed	R22, R25, R28
Corrosive potential	Causes severe burns	R35
	Causes burns	R34
Irritancy	Irritating to skin	R38
	Risk of serious damage to eyes	R41
	Irritating to eyes	R36
	Irritating to respiratory system	R37
Sensitisation	May cause sensitisation by inhalation	R42
	May cause sensitisation by skin contact	R43
Carcinogenicity	May cause cancer in humans	R45
	May cause cancer in humans (inhalation)	R49
	Possible risk of irreversible effects	R40[a]
Mutagenicity	May cause heritable genetic damage	R46
	May cause irreversible effects	R40[a]
Reproductive toxicity	May impair fertility	R60
	Possible risk of impaired fertility	R62
	May cause harm to unborn child	R61
	Possible risk of harm to the unborn child	R63
	May cause harm to breast-fed babies	R64
Other health effects	Danger of cumulative effects on health	R33
	Danger of serious damage to health from prolonged exposure	R48

[a] R40 has been redefined as 'Limited evidence of a carcinogenic effect'; see http://www.hse.gov.uk/chip/phrases.htm [accessed 10/03/04]

[a] See http://ecb.jrc.it

3 Compounds Selected for Screening

3.1 Selection of chemicals to be screened

The first stage in the development of the prioritisation scheme was to determine which of the many thousands of chemicals in the environment should be selected and incorporated into the screening process. As the scheme aimed to prioritise 'existing' chemicals, substances that were subject to legislation, regulation or guidance or that had recently been reported as being of environmental concern were identified and incorporated into a spreadsheet. In total, a pool of nearly 600 chemicals or groups of chemicals were added to the spreadsheet; with the methodology in place, additional chemicals can be added to the list as necessary. The different legislation, regulations or guidance documents from which the individual chemicals or groups of compounds were obtained are shown in Table 3.1; where applicable, the country or organisation of origin of the legislation, regulation or guidance document is also provided in this table. The groups of chemicals that were identified through the process are presented in Table 3.2.

In addition, further information was obtained through a postal questionnaire survey of Environmental Health Officers (EHOs) and Directors of Public Health (DsPH) in Great Britain on compounds and groups of compounds that were perceived to be of greatest concern to EHOs, DsPH and to the general public (as perceived by the EHOs and DsPH who filled in the questionnaires)[a]. The objective of the survey was to identify specific compounds (and risk issues) that cause concern to the general population and to those active in the field of environmental health during the course of their professional activities. Chemicals perceived as being of greatest concern and for which there was uncertainty regarding the level of concern are summarised in Tables 3.3 and 3.4, respectively[b]. Public and professional perceptions of chemical risks were taken into consideration when selecting the final list of compounds that required more detailed risk characterisation.

[a] The questionnaire aimed to identify areas of concern from a public and professional perspective. Results from this survey did not provide a direct measure of public concern but rather indicated likely concerns as assessed by professionals in the field

[b] For further details on this survey refer to the following report: IEH (1997) *Postal Survey Results: An Assessment of the Level of Concern About Various Environment and Health Issues From a Public and Professional Perspective* (Report to DH), available from MRC Institute for Environment and Health

Table 3.1 Legislation, regulation and guidance documents used to identify chemicals for inclusion in prioritisation scheme

Title of Legislation, Regulation, Guidance or Document[a]	Country or Organisation of Origin	Reference[b]
Air Quality Guidelines	World Health Organization	WHO (2000) *Air Quality Guidelines for Europe*, 2nd Edition, Copenhagen, World Health Organization Regional Office for Europe http://www.who.int/peh/air/Airqualitygd.htm
IPCS Environmental Health Criteria	World Health Organization	http://www.inchem.org/pages/ehc.html
Environmental Hazard Assessments	UK Department of the Environment	http://www.defra.gov.uk/environment/chemicals/strategy/contents.htm
Cancer classification	International Agency for Research on Cancer	http://www.iarc.fr/
Contaminants of Food	UK Ministry of Agriculture, Fisheries and Food	http://archive.food.gov.uk/maff/archive/food/foodch.htm
Freshwater/Aquatic Life	Canada	http://www.ec.gc.ca/water/en/manage/poll/e_poll.htm
Drinking Water	Canada	http://www.ec.gc.ca/water/en/manage/poll/e_poll.htm
Groundwater Reference, Assessment, Treatment Values	Netherlands	Ministry of Housing, Spatial Planning and the Environment (1999) *Environmental Quality Standards in the Netherlands*, The Netherlands, Kluwer http://arch.rivm.nl/environmentaldata/E_Environmental_quality/E4_groundwater_quality/index.html
Surface Water Target and Limit Values	Netherlands	http://arch.rivm.nl/environmentaldata/E_Environmental_quality/E2_Surface_water_quality/index.html
Surface Water Dissolved Limit Value	Netherlands	http://arch.rivm.nl/environmentaldata/E_Environmental_quality/E2_Surface_water_quality/index.html
Groundwater Target Value	Netherlands	http://arch.rivm.nl/environmentaldata/E_Environmental_quality/E4_groundwater_quality/index.html
The Surface Waters (Dangerous Substances) (Classification) Regs 1989	EU	http://europa.eu.int/scadplus/leg/en/s15005.htm
75/440 Surface Water (Class.) Regs 1989 Category A1, A2, A3	EU	http://europa.eu.int/scadplus/leg/en/s15005.htm
EEC 80/778 Quality of Water for Human Consumption, Guide Level, MAC	EU	http://europa.eu.int/scadplus/leg/en/s15005.htm
US EPA Priority List (note: no values)	US EPA	http://www.atsdr.cdc.gov/clist.html
EC Black List (note: no values)	EU	OJ L129/28 18/05/96 http://europa.eu.int/comm/environment/water/water-dangersub/76_464.htm
UK Red List (note: no values)	UK	http://www.sustainable-development.gov.uk/sdig/improving/partf/gguide2/gg2annc.htm#e
EU Risk Assessment List (note: no values)	EU	http://ecb.jrc.it/existing-chemicals/

Title of Legislation, Regulation, Guidance or Document[a]	Country or Organisation of Origin	Reference[b]
Numerical emissions limits applicable to scheduled processes	UK	http://www.defra.gov.uk/environment/chemicals/ukpolicy.htm
80/779 Air Quality Standards - Limit Values	EU	http://www.defra.gov.uk/environment/ppc/ippcguide/28.htm
Federal Air Quality Guidelines	USA	http://www.epa.gov/ttn/atw/188polls.html
Air Quality Data	UK Department of the Environment	Bertorelli V, Derwent R (1995) *Air Quality A to Z: A Directory of Air Quality Data for the United Kingdom in the 1990s*, DoE & The Met Office, Bracknell
RCEP 19th Report - Typical Normal ranges in soil	UK Royal Commission on Environmental Pollution	http://www.rcep.org.uk/reports2.html#19
Typical uncontaminated, slight contaminated, contaminated, heavy contaminated, and unusually heavy contaminated values	Society of Chemical Industry	http://www.soci.org/SCI/index.jsp
Sludge: Use in Agriculture regulations (soil and soil under grass)	UK Department of the Environment	http://www.defra.gov.uk/environment/consult/sewagesludge/index.htm
Trigger, threshold and action concentrations for soil contaminants	Interdepartmental Committee on the Redevelopment of Contaminated Land	http://www.environment-agency.gov.uk/subjects/landquality/?lang=_e
Limit, target, reference, assessment, and treatment values for soil	Netherlands	http://arch.rivm.nl/environmentaldata/E_Environmental_quality/E3_Soil_quality/index.html

[a]Accessed June 2003. Sites are given as an indication only; original data may no longer be available
[b]No values means that the legislation, regulation or document did not have any values or limits (e.g. air, soil or water quality standards or limit values) for individual compounds listed

Table 3.2 Main chemical groups included in prioritisation scheme

Compound group	Compound group
Non-halogenated monocyclic aromatics	Triaryl phosphate esters
Chloro-anilines	Haloethers
Nitrobenzenes	PCBs
Nitro- & chloro-cresols	Dioxins & furans
Chloro-, nitro- & other substituted phenols	Organochlorine pesticides
Other phenols	Organophosphorous pesticides
Phenoxyalkanoic acids	Carbamates
Phthalates & phthalate acid esters	Dithiocarbamates
Chloro- & nitro-toluenes	Aromatic chloramines
Alkyl & aromatic amines/imines	Chlorophenoxacetic acid herbicides
Organotin compounds	Halogenated aromatic nitrocompounds
Halogenated aliphatics	Triazines
Chloro-, bromo- & fluoro-methanes	Anilides
Chloroethanes	Carboximides
Chloroethenes	Alkylbenzenes & other alkyls
Chloro-propanes, propenes & propanols	Nonylphenol and nonylphenol polyethoxylates
Other halogenated aliphatics	Other organics
Carbonyls	Metals[a]
Aldehydes	Other inorganics[a]
Acids and their esters	

[a] Included in database but not prioritisation process

Table 3.3 Chemicals perceived to be of concern to EHOs, DsPH and the general public

Chemicals or groups of chemicals	Overall ranking for high levels of concern[a]			
	DsPH[b]	EHOs[b]	EHO public[c]	DsPH public[c]
Fine particulates	**1**	**1**	**1**	**3**
Ozone	**3**	**5**	**2**	**2**
Nitrogen oxides	**4**	**2**	**2**	**4**
Dioxins and PCBs	**2**	**6**	**3**	**1**
Hydrocarbons	**5**	**4**	**4**	**7**
Benzene	6	7	5	6
Lead	7	9	6	3
VOCs	9	3	7	10
PAHs	8	8	8	12
Pesticides	9	11	9	5
Environmental oestrogens	10	10	11	9
Synthetic hormones used in contraceptives	12	12	10	8
Phthalates	11	13	12	11
Alkylphenols (e.g. nonylphenol)	13	14	13	13

DsPH, Directors of Public Health; EHOs, Environmental Health Officers

[a] The ranking relates to the number of respondents who scored each chemical as one of high concern. In this context the chemical of greatest concern is indicated as having a rank of 1 and the chemical of least concern a rank of 14. Compounds in bold (i.e. fine particulates, ozone, nitrogen dioxide and dioxins and furans) are those generally perceived to be of greatest concern by both the public and professional perspectives

[b] Professional perspective

[c] Public perspective as perceived by the health professionals

Table 3.4 Chemicals for which the levels of concern to EHOs, DsPH and the general public was uncertain[a]

Chemicals or groups of chemicals	Overall ranking for high level of uncertainty[a]			
	DsPH[b]	EHOs[b]	EHOs public[c]	DsPH public[c]
Alkylphenols (e.g. nonylphenol)	**1**	**1**	**1**	**2**
Phthalates	**2**	**1**	**1**	**4**
Synthetic hormones used in contraceptives	**3**	**2**	**2**	**7**
PAHs	**2**	**4**	**4**	**3**
VOCs	2	6	5	1
Environmental oestrogens	4	3	3	5
Benzene	5	4	7	6
Hydrocarbons	6	6	7	7
Nitrogen oxides	7	5	7	8
Fine particulates	9	4	7	9
Ozone	10	5	8	8
Dioxins and PCBs	8	6	7	10
Lead	7	7	7	11
Pesticides	11	6	6	12

DsPH, Directors of Public Health; EHOs, Environmental Health Officers

[a] The ranking relates to the number of respondents who thought that there was a considerable uncertainty with regard to the level of concern for that chemical. In this context the chemical for which there is greatest uncertainty is indicated as having a rank of 1 and the chemical of least concern a rank of 12. Compounds in bold (i.e. nonyl alkylphenols, phthalates and synthetic hormones used in contraceptives) are those compounds generally considered to have the greatest level of uncertainty with regard to the level of concern by both the public and professional perspectives.

[b] Professional perspective

[c] Public perspective as perceived by the health professionals

3.2 Chemical classification according to the chemical's likely partitioning between media

There is no universal method for predicting the fate and behaviour of all chemicals in the environment, as models developed to predict the behaviour of a specific group of substances may not accurately predict the behaviour of other groups of compounds. However, it is possible to classify chemicals into broad groups which are likely to behave in a similar manner. Once compounds have been properly classified, physicochemical and degradation data can then be used to screen compounds within each group. For example, though the octanol–water partition coefficient (K_{ow}) is an appropriate indicator of the lipophilicity of many organic compounds, it is not a relevant indicator of hydrophobicity for substances such as organo-metals or surfactants (MacKay *et al*. 1996b). Similarly, solubilities or vapour pressures are not applicable to insoluble or involatile substances, respectively (Mackay *et al*., 1996b). This highlights the need for a system to classify substances to ensure that appropriate data and models are used. Mackay *et al.* (1996b) have proposed a classification scheme that uses the partitioning properties of the substances, as these are key parameters that control their fate and behaviour in different environmental compartments. Figure 3.1 shows graphically the various environmental media that play a key role in chemical partitioning; this figure shows that a compound may behave in one or more of the following ways:

- stay in the pure phase of the substance;
- partition to the atmospheric environment;
- partition to the water environment;
- partition to the solid phases by sorption to a surface or formation of a solid solution (i.e. solid inorganic or solid organic matter phases); or

- partition to the organic biological media by dissolution in lipids or waxes, association with proteins or other organic matter, dissolution in water or sorption to biological surfaces.

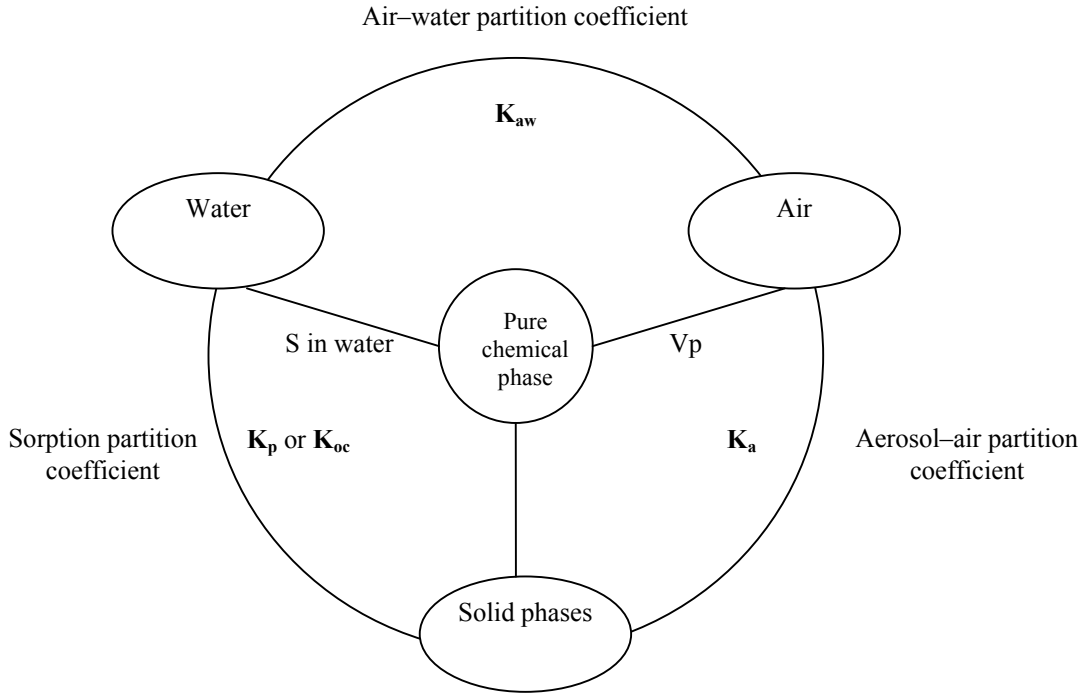
According to this scheme chemicals can be classified into five groups, summarised in Table 3.5: compounds may partition into all phases (i.e. water, air and solid phases; Type 1), or they may not appreciably partition into air or water or both air and water (Types 2, 3 and 4, respectively). Type 2 refers to highly involatile chemicals (i.e. Vp $<10^{-7}$ Pa); Type 3 refers to highly insoluble/hydrophobic compounds (i.e. S $<10^{-6}$ g/m^3); and Type 4 refers to chemicals that are both involatile and insoluble. Finally, a category was also assigned to chemicals that may exist as several species that are capable of interconversion (Type 5). In such cases the fate of the compound (and as a consequence the model used to describe its fate) becomes more complex (Mackay *et al.*, 1996b).

Type 4 substances are likely to be present in the environment as a pure phase, or possibly sorbed to surfaces and may be slightly lipophilic. Models that incorporate conventional partitioning expressions are unlikely to be useful for this type of chemical. Mackay *et al.* (1996b) have suggested that chemicals that fall into this category are those which have a vapour pressure of $<10^{-7}$ Pa and a solubility of $<10^{-6}$ g/m^3, although they emphasised that these criteria should only be viewed as a suggestion based on the authors' judgement concerning the current difficulties in measuring properties below these levels and the observed environmental behaviour of chemicals with properties in these ranges. Substances with lower vapour pressures appear to occur to a negligible extent in the gaseous phase, being primarily associated with aerosols. Those with lower solubilities are primarily in the sorbed rather than the dissolved form in water. These criteria have been used in this screening exercise to classify substances into the Type 4 category. For the purpose of this screening process, compounds which fall into this category are assumed to stay in the pure phase and therefore have not been addressed further.

A distinction must be made between organic and inorganic chemicals. For organic chemicals it is possible to use a set of physicochemical properties to predict the likely environmental fate of the compound. However, the environmental transport of inorganic compounds and metals is highly site specific and more difficult to predict. Factors such as soil type and pH, speciation of the metal, ion exchange capacity, availability of oxygen and valency state will greatly influence the way in which these compounds behave in the environment. Toxicity is also highly dependent on the speciation of the compound.

Few prioritisation schemes incorporate inorganic chemicals in screening procedures because of the difficulties of accounting for chemical speciation. The US EPA is the only method reported in the literature which has attempted to incorporate inorganics and metals into a prioritisation scheme (Davis *et al*., 1994; Swanson *et al.,* 1997). The general approach followed was to either (i) choose a surrogate compound considered to be the most representative form of that chemical, based on specific industrial production or industrial application data or (ii) where no single surrogate was obvious, expert judgement was used to select the inorganic salts produced in the greatest quantity. Furthermore, details are needed on industrial production and environmental emissions of the individual metal species. However, this method does not incorporate the speciation of the compound which has the most significant influence on metal toxicity and availability. As a consequence, the fate of metals following their release into the environment could not be completely accounted for by this screening method.

Figure 3.1 Schematic diagram showing environmental media that play a role in chemical partitioning



K_a, aerosol–air partition coefficient; K_{aw}, air–water partition coefficient; K_{oc}, organic carbon–water partition coefficient; K_p, partition coefficient to solid surfaces; S, solubility; Vp, vapour pressure
From Mackay *et al.* (1996b)

Table 3.5 Chemical categories

Chemical category	Partition between phases	Partition data required	Example of compound
Type 1	Chemical partitions to all phases	S (in water and fat or lipid), Vp, H_c, K_{ow}	Chlorobenzenes
Type 2	Chemical does not partition to air (i.e. Vp $<10^{-7}$ Pa)	Partition coefficient to solid surfaces and to organic carbon, S (in water and fat)	Lead, linear alkylbenzene sulphonates
Type 3	Chemical does not partition to water (i.e. S $<10^{-6}$ g/m^3)	Partition coefficient to solids from air or a pure phase	Long-chain hydrocarbons, silicones and polymers
Type 4	Chemical involatile and insoluble (i.e. Vp $<10^{-7}$ Pa and S $<10^{-6}$ g/m^3)	Sorption properties from a pure phase to various solids	Large molecular weight substances, polymers (e.g. polyethylene), many elemental metals and inorganic substances such as minerals
Type 5	Speciating chemicals	Partitioning data for all species	Mercury

H_c, Henry's Law constant; K_{ow}, octanol–water partition coefficient; S, solubility; Vp, vapour pressure
From Mackay *et al.* (1996b)

To obtain accurate information on specific toxic and physicochemical properties of metal ions these have to be individually evaluated. This involves extensive literature review to obtain experimental data and, where these are unavailable, data must be estimated using structure–activity relationships (SARs) by making a number of assumptions. The use of extensive literature searches and SARs is outside the scope of this screening exercise as the main aim here is to develop a rapid evaluation of information which is either readily available or easily estimated. Therefore, though information for a number of metals and inorganic chemicals (i.e. Type 5 chemicals) has been entered into the database, they could not be included in the prioritisation process.

4 Approach and Algorithms

The main purpose of this prioritisation scheme was to identify chemicals of concern to humans at low levels of exposure. This was done by screening a large number of compounds according to their likely behaviour in the environment and mammalian toxicity to produce a shortlist of chemicals. Each chemical was scored by using a set of criteria. An arbitrary score was assigned for a chemical for each of the criteria (e.g. bioaccumulative potential or carcinogenicity) on the basis of its comparative importance or priority. Scores for each of the criteria were then weighted according to the importance of each criterion and integrated using a specially formulated mathematical model to produce a final overall priority score by which chemicals could be ranked in order of increasing importance. Prioritisation is a process of elimination, so it was imperative that the criteria and scores chosen fitted with the objectives of the prioritisation scheme while ensuring that important chemicals did not receive an unduly low priority (e.g. by giving a low score for a comparatively important parameter).

The two most important parameters used to prioritise environmental chemicals relevant to human health are the degree of exposure to a chemical and its likely toxicity to humans. Chemicals reach environmental compartments indirectly (e.g. atmospheric deposition or leaching) or directly (chemical spills, industrial discharges or application of pesticides to agricultural land). Compounds will only be of concern to human health if humans are exposed to the chemical from air, soil, water or foodstuffs, following contact via the skin, ingestion or inhalation (see Figure 1.1 for likely routes of human exposure) at levels sufficiently high to cause adverse health effects. Various models have been developed to estimate the distribution and fate, and hence the exposure levels, of chemicals in various environmental media and compartments as a first step in identifying potentially hazardous chemicals. These models usually use physicochemical properties for chemicals to predict fate and behaviour in the environment.

Since this prioritisation scheme aimed to identify chemicals that are a potential risk to humans as a result of their presence in the environment by assessing their potential for human exposure and their potential to cause human health effects, the following criteria were used:

- environmental distribution;
- exposure via inhalation;
- exposure via water ingestion;
- exposure via soil;
- exposure via food ingestion; and
- acute and chronic toxicity.

The algorithms and scores assigned to each of these criteria are explained in the following subsections. See Section 2 for further details and definitions of the physicochemical properties used.

Many prioritisation schemes use production volume and pattern of use scores to assess potential human exposure (for review see IEH, 2003). However, these criteria represent an oversimplified approach to exposure assessment, as the scores do not take into consideration the extent to which these chemicals may enter the environment and/or the environmental matrix into which the chemicals are released (e.g. air, water, landfill site). Another limitation of using these parameters to prioritise chemicals is the lack of reliable production data for the UK in the published literature. Though production volumes and production capacity data are available for some chemicals from commercial reports, these sources of information are often out of date. Furthermore, data are generally only

available for high production volume chemicals. For these reasons, these were not used in this prioritisation scheme.

4.1 Environmental distribution

A pivotal aspect of exposure assessment is the use of fate and transport models to quantify the concentration of a chemical as it moves from a source through the environment to the target population. Several multi-media fate models have been developed to predict the distribution of a chemical in the environment. The majority of non-site-specific fate and transport models have been based on the concept of fugacity. Fugacity models work by converting chemical concentrations in the major environmental compartments to fugacity, a thermodynamic equilibrium criterion which has units of pressure (see Table 4.1). This method of calculation can be extended to a variety of environmental media and has the advantage of being easy to compile and manipulate. Fugacity models have been developed to reflect several levels of complexity. This can be incorporated into the model as a further refinement in the prediction of potential human exposure.

Simple fate models that have the ability to account for multi-media partitioning of a chemical in the environment (i.e. that can predict a chemical's likely fate and distribution in the environment, based on its physicochemical properties) are useful for assessing potential chemical sources that are most likely to affect humans. Multi-media criterion models such as that developed by Mackay (see for example Mackay *et al*., 1996a) are often used to evaluate the environmental fate of a variety of chemicals. The concept of fugacity has been widely used to model the concentrations of a substance in different environmental compartments (water, air, soil, sediment, suspended solids and fish). The model estimates the proportion of a compound likely to partition between these compartments, based on a standard release of the chemical into the environment. A sequence of Level I, II and III calculations can be made, which have increasing data requirements each resulting in increasing information about the chemical's partitioning, its susceptibility to transformation and transport and the environmental process and chemical characteristics that most significantly influence chemical fate (see Mackay *et al*., 1996a for further details).

For the purpose of this screening process only the Level I model was calculated. This requires the use of standard physicochemical data for each chemical and involves estimating the storage (fugacity) capacity (Z) of each compartment for a particular chemical. Z is dependent on the pressure, temperature, the medium in which the chemical is present and the properties of the substance. Fugacity (*f*) is regarded as the escaping tendency of a chemical from a phase. It has units of pressure and can be related to concentration. Table 4.1 shows the formulae needed to calculate the storage capacity and fugacity of a chemical in the environment. Table 4.2 summarises the assumptions made to calculate Z and *f*. The model assumes that 100 000 kg of a chemical is emitted to an area of 100 000 km^2 of land; this area is considered to be representative of an ecologically homogeneous area (which would cover approximately 40% of the size of the UK).

Partitioning is described by Z values (i.e. fugacity capacities) which express the affinity of a chemical for each environmental phase. When Z is zero or near zero, the chemical shows a negligible tendency to partition into that phase. Thus fugacity values give an indication of the likely media into which a chemical will tend to partition and an indication of relative concentrations in each medium (i.e. c_i, see Table 4.1). The relative amount of a chemical likely to partition to each medium will be used to weight the contribution of that medium towards potential human population exposure. The fraction of the chemical released which is predicted to reside in each phase at equilibrium is normalised to fall within the range 0–10; a value of zero indicates that the compound is unlikely to partition to that compartment, while a value of 10 shows that 100% of that chemical is likely to partition to that phase. The values obtained for the environmental compartments of interest (air, soil, water and fish) were used as described in Sections 4.2–4.5 to reflect the relative contribution of each phase towards exposure via air ($fraction_{air}$), water ($fraction_{water}$) soil ($fraction_{soil}$) and fish ($fraction_{fish}$).

Table 4.1 Calculation of the storage capacity and fugacity of a chemical in the environment

	Model
Storage/Fugacity Capacity (Z) (mol/(m^3 Pa)) indicates potential of an environmental compartment to retain a chemical and therefore its capacity for fugacity	$\mathbf{Z_{air}} = 1/RT$ $\mathbf{Z_{water}} = Z_{air}/K_{aw} = 1/H = S/V_p$ $\mathbf{Z_{soil}} = (Z_{water}\ \rho\ f_{oc}\ K_{oc})/1000$ $\mathbf{Z_{sediment}} = (Z_{water}\ \rho\ f_{oc}\ K_{oc})/1000$ $\mathbf{Z_{susp.solids}} = (Z_{water}\ \rho\ f_{oc}\ K_{oc})/1000$ $\mathbf{Z_{fish}} = (Z_{water}\ \rho\ L\ K_{ow})/1000$
Fugacity (*f*) (Pa) indicates the tendency of a chemical to escape from a specific compartment	$f = M/\sum V_i Z_i$
Concentration in each medium (c_i) (mol/m^3)[a]	$c_i = f Z_i$

From MacKay *et al.* (1996a)

ρ, density of phase (kg/m^3); c, concentration (mol/m^3); f, fugacity (Pa); f_{oc}, mass fraction organic carbon in phase; H, Henry's Law constant (Pa m^3/mol); i, specific environmental compartment (air/soil/water); K_{aw}, air–water partition coefficient; K_{oc}, organic carbon–water partition coefficient (m^3/kg); L, lipid content (fraction of total mass); M, amount of chemical introduced into the system (mol) — (a total of 100 000 kg is assumed to be released to the environment, hence M is equivalent to 10^8/MW of the compound); MW, molecular weight; R, gas constant (8.314 J/(mol K)); S, solubility (m^3/mol); T, temperature (K) assumed to be 298 K (or 25°C); V, volume of the environmental compartment (m^3); Vp, vapour pressure (Pa); Z, storage capacity (mol/(m^3 Pa))

[a] By converting the concentration for each medium from mol/m^3 to g/m^3 and by assuming that (i) each environmental medium has the dimensions shown in Table 4.2 and that (ii) 100 000 tonnes of the chemical is emitted to the environment annually, it is possible to estimate the amount of the chemical that will partition to each compartment

Table 4.2 Compartment dimensions and properties for Level I fugacity calculations

Compartment	Air	Water	Soil	Sediment	Suspended sediment	Fish
Depth (m)	1000	20	0.1	0.01	-	-
Area (m^2)	10^{11}	10^{10}	9×10^{10}	10^{10}	-	-
Volume (m^3)	10^{14}	2×10^{11}	9×10^9	10^8	10^6	2×10^5
f_{oc}	-	-	0.02	0.04	0.2	-
Density (ρ) (kg/m^3)	1.2	1000	2400	2400	1500	1000
Lipid content	-	-	-	-	-	0.048

From Mackay *et al.* (1996a)

4.2 Exposure via inhalation

Human exposure via inhalation is likely to be most significant for volatile, persistent compounds. Exposure via inhalation has been estimated from the compound's volatility potential and half-life in air. Henry's Law constants were used to estimate a compound's volatilisation potential. In addition, the compound's half-life in air was used as a measure of the likely persistence of the compound in the atmospheric environment. Compounds with an H_c' value above 1×10^{-4} are generally considered to be susceptible to volatilisation while compounds with H_c' values below 1×10^{-4} are considered to have a low volatilisation potential (see Table 4.3). This partition coefficient has been derived from air–water exchanges; therefore, the volatilisation potential from other surfaces (such as soil) is likely to be overestimated (due to increased sorption to such surfaces). However, an Hc' value of 1×10^{-4} is considered a useful cut-off point for the initial screening of the compound's volatilisation potential. The criteria used to rank the persistence of chemicals in air are summarised in Table 4.4. According to this scheme, compounds are short lived in air if their half-lives are in the range of hours and compounds that are present in air for periods of greater than 40 days are considered highly persistent and therefore were given a higher score. The overall exposure via inhalation (E_{inh}) was estimated as follows:

Exposure via inhalation (E_{inh}) = Volatilisation potential l× $T_{1/2\ air}$ × $fraction_{air}$ (Max. score 150) (6)

This equation takes into account the amount of the compound estimated to partition to air (i.e. $fraction_{air}$) as estimated in Section 4.1. A maximum score of 150 will be obtained for E_{inh} for highly persistent and extremely volatile compounds.

Table 4.3 Potential for compounds to volatilise

Volatilisation potential	Ranking	Score
$H_c' > 1 \times 10^{-4}$	High	3
$H_c' = 1 \times 10^{-4}$	Medium	2
$H_c' < 1 \times 10^{-4}$	Low	1

Table 4.4 Persistence classification based on the half-life of compound in air and water

Median half-life	Ranking	Score
<0.042 days (1 hour)	Very short-lived (L)	1
0.042–0.42 days	Short lived (L)	2
0.42–4 days	Moderately short lived (M)	3
4–40 days	Moderately persistent (H)	4
>40 days	Highly persistent (H)	5

4.3 Exposure via water ingestion

Compounds that are highly soluble and persist for relatively long periods in water are more likely to leach down the soil profile to groundwater or to remain in solution, leading to contamination of the drinking water supply, thereby increasing the potential for human exposure via the ingestion of drinking water. A compound's tendency to stay in solution can be estimated from its solubility and adsorption potential onto surfaces (e.g. soil/sediment). The solubility of a compound has been estimated by using an H_c' cut-off value of 1×10^{-4} (see Section 4.2 above). This means that compounds that have a small H_c' value are more likely to stay in solution and are less likely to volatise relative to chemicals that have a larger H_c' value. Similarly, substances that have a high log K_{ow} value (>4) have a greater tendency to adsorb onto organic matter and soil particles and are therefore less likely to stay in solution. Compounds that have a low log K_{ow} value (<2.5) are less likely to sorb onto surfaces and consequently more likely to stay in solution. Table 4.5 summarises the scores given to specific compounds according to their tendency to stay in solution.

Table 4.5 Estimation of the tendency of a compound to stay in solution

			Tendency to stay in solution	Score
$H_c' > 1 \times 10^{-4}$	and	$K_{ow} > 4$	Low	1
$H_c' \geq 1 \times 10^{-4}$	and	$2.5 < K_{ow} < 4$	Medium or possible	2
$H_c' < 1 \times 10^{-4}$	or	$K_{ow} < 2.5$	High	3

The following equation was used to estimate the likely human exposure to compounds via the ingestion of water (E_{water}):

$$\text{Exposure via water ingestion } (E_{water}) = \text{Tendency to stay in solution} \times T_{1/2\ water} \times fraction_{water} \quad \text{(Max. score 150)} \quad (7)$$

This equation takes into account the amount of the compound estimated to partition to water (i.e. $fraction_{water}$) as estimated in Section 4.1. A maximum score of 150 will be obtained for E_{water} for highly persistent and soluble compounds.

4.4 Tendency for a chemical to adsorb onto soil organic matter

The octanol–water partition coefficient is a good indicator of a chemical's potential to adsorb onto soil particles and organic matter. Compounds which have log K_{ow} values greater than 4 are considered to have a high tendency to adsorb onto soil and organic matter while those with lower log K_{ow} values are more readily leached down the soil profile. As a consequence compounds that fall into the high adsorption potential category have been given a high score for the purposes of this screening (Table 4.6). The criteria used to classify the persistence of chemicals to determine the degradability of each compound were determined from the compound's half-lives in soil as shown in Table 4.7. As with Equations 6 and 7, the fraction estimated to partition to soil ($fraction_{soil}$) was incorporated into the equation to take into account the environmental distribution of the compound (see Section 4.1 for further details).

Soil adsorption potential (E_{soil}) = Adsorption potential l× $T_{1/2}$ soil × $fraction_{soil}$ (Max. score 150) (8)

Table 4.6 Potential for compounds to adsorb to soil organic matter

Adsorption potential	Ranking	Score
log K_{ow} > 4	High	3
2.5 < log K_{ow} < 4	Medium	2
log K_{ow} < 2.5	Low	1

Table 4.7 Persistence classification based on the half-life of a compound in soil

Median half-life	Ranking	Score
$T_{1/2}$ < 5 days	Very short-lived (L)	1
5 < $T_{1/2}$ < 15 days	Short lived (L)	2
15 < $T_{1/2}$ < 30 days	Moderately short lived (M)	3
30 < $T_{1/2}$ < 100 days	Moderately persistent (H)	4
$T_{1/2}$ > 100 days	Highly persistent (H)	5

4.5 Exposure via the food chain

Compounds that are readily taken up from soil and air by plants or ingested by animals and fish and chemicals that are highly lipophilic are more likely to bioaccumulate through the food chain thereby leading to an increased potential to bioaccumulate in humans. As mentioned in Section 2.1.7, bioconcentration factors and K_{ow} values are good parameters for predicting the bioaccumulation potential of chemicals. The bioconcentration factor in fish (BCF_{fish}) was used in this prioritisation scheme as a surrogate for human exposure via ingestion of foodstuffs. Where available, data determined experimentally were used, since measured values take into account the distribution, metabolism and excretion of the chemical. As mentioned in Section 2.1.7, BCFs may vary widely depending on the experimental methodology, fish species, etc. and therefore values are often reported as ranges. The median value of these ranges was used in this assessment as being a representative value. For many compounds BCF_{fish} has not been measured experimentally. In such cases this value was estimated from the median K_{ow} by assuming that there is a linear relationship between bioaccumulation of the compound in fish and K_{ow} by using Equations 4 and 5 of Section 2.1.7. Tables 4.8 and 4.9 present the BCF_{fish} and log K_{ow} ranges used to score each compound for bioaccumulation potential. The final bioaccumulation potential score was estimated from the average

of the scores given for BCF_{fish} and log K_{ow}. The algorithm used to estimate the overall score for exposure via the food chain was as follows:

Exposure via the foodchain (E_{food}) = 3×Bioaccumulation potential × $fraction_{fish}$ (Max. score 150) (9)

where bioaccumulation potential = the average score obtained from Tables 4.8 and 4.9

This equation takes into account the amount of the compound estimated to partition to fish (i.e. $fraction_{fish}$) as estimated in Section 4.1. The algorithm has been multiplied by a factor of three to ensure that equal weight is given to all the exposure criteria used in the screening process (i.e. E_{air}, E_{water}, E_{soil} and E_{food}). The maximum score for bioaccumulation potential from food (E_{food}) is therefore 150.

Table 4.8 BCF_{fish} as an estimate of bioaccumulation potential

BCF_{fish}	Bioaccumulation potential	Score
<10	Unlikely (L)	1
10–100	Low (L)	2
100–1000	Moderately low (M)	3
1000–10,000	Moderately high (M)	4
>10,000	High (H)	5

Table 4.9 Log K_{ow} as an estimate of bioaccumulation potential

Log K_{ow}	Bioaccumulation potential	Score
<2	Unlikely (L)	1
2–3	Low (L)	2
3–4	Moderately low (M)	3
4–5	Moderately high (M)	4
>5	High (H)	5

4.6 Toxicological estimation

The R-phrases presented in Table 2.2 were used to prioritise chemicals for carcinogenic, mutagenic and reproductive effects, allergenic sensitisation, irritation and corrosive, acute and sub-chronic effects. The numerical score used was adapted from the European Union risk ranking method (EURAM; Hansen *et al*., 1999) to determine the toxicological significance of compounds screened. The EURAM method was derived from a method discussed by international experts in an Informal Working Group on Priority Setting (van der Zandt & Leeuwen, 1992, cited in Hansen *et al.,* 1999). This method assigns a higher priority to carcinogenic, mutagenic and reproductive effects than to other systemic effects when scoring available toxicological evidence, but does not account for missing data. As one of the purposes of this prioritisation scheme was to highlight data gaps, a default value of 5 was used (Table 4.10). The scores assigned to chemicals for human toxicity range from 1 to 10, with the highest score obtained for a toxicological end-point being used as the overall toxicity score. To give equal weight to exposure and toxicity, the maximum value obtained was multiplied by 15 so that:

Total Toxicity Score (TTS) = 15 × highest score obtained from Table 4.10 (Max. score 150) (10)

Table 4.10 Toxicological end-points and toxicity score index used to assess potential human toxicity[a]

Toxicological evidence[a]	R-phrase[b]	Score
Human evidence or strong evidence in animals of carcinogenicity, heritable genetic damage or reproductive toxicity	R45, R46, R49, R60 or R61	10
Animal evidence of carcinogenicity, *in vivo* mutagenicity or reproductive toxicity, **or** human evidence of somatic cell genetic damage	R40, R62, R63 or R64	9
Positive in at least one *in vitro* test for mutagenicity **or** positive in an *in vivo* reproductive screening test **or** positive in Organisation for Economic Co-operation and Development (OECD) reproductive screening test		8
Evidence for respiratory sensitisation **or** oral toxicity at $\leq$5 mg/kg bw/day in a 90 day study	R42 or R48	7
Evidence for skin sensitisation **or** oral toxicity at $\leq$50 mg/kg bw/day in a 90 day study	R43 or R48	6
Evidence of cumulative effects **or** no data on mutagenicity or reproductive toxicity	R33	5[c]
No data on irritation to skin, eyes and respiratory system		5[c]
Negative in one *in vivo* test for mutagenicity but also positive in at least one *in vitro* test **or** negative in *in vivo* reproductive screening test **or** no data on repeat dose toxicity		4
Oral rat LD_{50} $\leq$25 mg/kg **or** negative only for teratogenicity	R28	3
Oral rat LD_{50} $\leq$200 mg/kg **or** corrosive to skin **or** causes severe damage to eyes **or** negative only for gene mutation or only for chromosomal aberrations *in vitro* **or** negative only for fertility	R25, R34, R35 or R41	2
Harmful by inhalation, skin contact or by ingestion (oral rat LD_{50} $\leq$2000 mg/kg)	R20, R21, R22	1

Adapted from Hansen *et al.* (1999) and Wearne *et al.* (1996). Based on a method discussed by international experts at an Informal Working Group on Priority Setting (van der Zandt & van Leeuwen, 1992, cited in Hansen *et al.,* 1999)

[a]The overall score is the highest score obtained for any aspect of toxicity

[b] See Table 2.2 for further details on R-phrases

[c] Default value

4.7 Overall priority scoring algorithm

To produce a reliable short list of priority chemicals, it is important that the final ranking takes into consideration both the toxicological effects and potential for human exposure. Therefore, once chemicals had been scored on the basis of specific types of health effect and exposure pathways, an overall score was generated that was used to produce the final priority list. The individual scores assigned to each chemical obtained from each of the individual criteria were added to produce an Overall Score as follows:

$$\text{Overall Score} = E_{inh} + E_{water} + E_{soil} + E_{food} + TTS \quad (\text{max. score} = 300) \qquad (11)$$

where maximum total exposure score (the sum of E_{inh}, $E_{water,}$ E_{soil} and E_{food} divided by four) for $E_{inh} + E_{water} + E_{soil} + E_{food}$ is 150 and the maximum score for TTS is also 150

Equal weights were given to each of the individual exposure criteria (E_{inh}, E_{water}, E_{soil} and E_{food}) because the purpose of this prioritisation scheme was not only to produce an overall priority score but also to determine the significance of different media to the overall exposure of humans. Thus a high E_{inh} (relative to E_{water}, E_{soil} and E_{food}) will indicate that inhalation is likely to be the dominant exposure route while a high E_{food} (relative to E_{inh}, E_{water} and E_{soil}) will indicate that humans are more likely to be exposed to the compound of interest via ingestion of foodstuffs. E_{soil} indicates the tendency for a chemical to adsorb onto soil organic matter. Therefore a high E_{soil} (relative to E_{air}, E_{water} and E_{food}) will indicate that the compound of concern is more likely to be present in this medium; in this situation exposure routes of concern may be, for example, via soil ingestion and/or soil contact (e.g. in the case of children who regularly visit playing fields). E_{soil} may also be significant exposure route in agricultural environments (e.g. soil — vegetable/root crop — human or soil grassland — cattle — human scenarios). In a similar manner, an equal weight of 150 was given to the sum of the exposure

criteria and toxicity criteria to give an Overall Score of 300. It should be noted that weights can be readily changed in this screening model if priorities change. For example, a higher or lower priority can be given to any of the individual exposure or toxicity criteria to obtain a 'new priority list' which is concerned with a specific exposure route or health effect (e.g. air, asthma).

5 Results of Prioritisation Scheme

The prioritisation method scheme described in Sections 1 to 4 was used to prioritise 600 compounds or groups of compounds[a]. The 100 compounds receiving the highest priority scores using this scheme are summarised in Table 5.1. Tables 5.2 and 5.3 present lists of compounds for which there was either insufficient information to assess human exposure (Table 5.2) or both exposure and toxicity (Table 5.3). Lack of information does not necessarily mean that this information was not known, but rather that it was not available in the published literature consulted for this prioritisation exercise.

It should be noted that although this method provides a numerical ranking of chemicals, the values are not representative of any quantitative measure of hazard or risk. Owing to the uncertainty and variability inherent in such a screening exercise, it was more appropriate to interpret the results in groups, that is to consider the top 30 or 50 chemicals rather than to make a direct comparison of the result for one chemical with another. Furthermore, not all compounds prioritised are necessarily of primary concern because some compounds may not be absorbed into the body and metabolism could not be included in the screening model. Some of the compounds given a high priority (e.g. PAHs and many chloroethanes and chloroethenes) are readily metabolised to toxic or non-toxic derivatives once they are ingested or inhaled. However only parent compounds were included in the screening. In deciding which chemicals were to be subject to a more detailed assessment, IEH, the Department of Health and DETR (now the Department for Environment, Food and Rural Affairs), considered the extent of use of the chemical, whether it was subject to a statutory approval process and whether an up-to-date, detailed assessment was already available.

Table 5.1 Summary of top 100 prioritised compounds

Chemical	CAS Number	Total Expos. Score	Total Tox. Score	Overall Score
Halogenated aliphatics				
1,2-Dichloroethane	107-06-2	149	150	299
PAHs				
Benzo(a)anthracene (benz(a)anthracene)	56-55-3	147	150	297
Benzo(b)fluoranthene (benzo(e)acephenanthrylene)	205-99-2	147	150	297
Halogenated aliphatics				
Pentachloroethane	76-01-7	146	150	296
PAHs				
Benzo(k)fluoranthene	207-08-9	146	150	296
Monocyclic aromatics				
Hexachlorobenzene	118-74-1	145	150	295
PAHs				
Benzo(a)pyrene (benzo[def]chrysene)	50-32-8	141	150	291
Halogenated aliphatics				
Methyl bromide	74-83-9	150	135	285
Chlorodibromomethane	124-48-1	150	135	285
Halogenated aliphatics				
Chloroform (Trichloromethane)	67-66-3	148	135	283
Organochlorine pesticides				
4,4' DDT (p,p'-Dichlorodiphenyltrichloroethane) (clofenotane)	50-29-3	146	135	281
Other organics				
Propylene oxide (methyloxirane)	75-56-9	130	150	280

[a] Details of the compounds included in this prioritisation exercise are available on request from the MRC Institute for Environment and Health

Chemical	CAS Number	Total Expos. Score	Total Tox. Score	Overall Score
Halogenated aliphatics				
2-Methoxyethanol	109-86-4	120	150	270
Vinyl chloride	75-01-4	120	150	270
Carbonyls				
Acrylamide	79-06-1	120	150	270
Phenols				
Pentachlorophenol	87-86-5	116	150	266
Halogenated aliphatics				
Methyl chloride	74-87-3	150	105	255
Tetrachloroethene (Tetrachloroethylene)	127-18-4	120	135	255
Carbon tetrachloride	56-23-5	150	105	255
Trichloroethene (Trichloroethylene)	79-01-6	120	135	255
Carbonyls				
Acrylonitrile	107-13-1	105	150	255
Phenols				
2,4,6 Trichlorophenol	88-06-2	118	135	253
Phenols				
2,4,5-Trichlorophenol	95-95-4	112	135	247
Monocylic aromatics				
4,6-Dichloro-o-cresol (2,4-Dichloro-6-methylphenol)	1570-65-6	107	135	242
Halogenated aliphatics				
Buta-1,3-diene (1,3-Butadiene)	106-99-0	90	150	240
Carbonyls				
Methyl methacrylate	80-62-6	150	90	240
Monocylic aromatics				
Benzene	71-43-2	89	150	239
PCBs				
PCB 14 (3,5-Dichlorobiphenyl)	34883-41-5	146	90	236
Phenols				
Dinoseb (4,6-Dinitro-2-sec-butylphenol)	88-85-7	85	150	235
Organochlorine pesticide				
Heptachlor epoxide	1024-57-3	97	135	232
Halogenated aliphatics				
1,1-Dichloroethene (Vinylidene Chloride, 1,1-Dichloroethylene)	75-35-4	90	135	225
1,2-Dichloroethene trans (trans-1,2-dichloroethylene)	156-60-5	150	75	225
Dichlorodifluoromethane	75-71-8	150	75	225
Trichlorofluoromethane	75-69-4	150	75	225
1,1,2-Trichlorotrifluoroethane	76-13-1	150	75	225
Carbonyls				
Vinyl acetate	108-05-4	150	75	225
Acrylic acid	79-10-7	150	75	225
Monocylic aromatics				
1,3,5-Trichlorobenzene	108-70-3	149	75	224
Halogenated aliphatics				
1,1-Dichloroethane	75-34-3	149	75	224
Hexachloro-1,3-butadiene (hexachlorobutadiene)	87-68-3	149	75	224
Methylene chloride (Dichloromethane)	75-09-2	89	135	224
Organochlorine pesticides				
Dieldrin	60-57-1	89	135	224
Monocyclic aromatics				
1,2,3,4-Tetrachlorobenzene	634-66-2	148	75	223
1,2,3,5-Tetrachlorobenzene	634-90-2	148	75	223

Chemical	CAS Number	Total Expos. Score	Total Tox. Score	Overall Score
Other organics				
Formaldehyde	50-00-0	88	135	223
Monocyclic aromatics				
1,2,4,5-Tetrachlorobenzene	95-94-3	147	75	222
Halogenated aliphatics				
Dichlorobromomethane (bromodichloromethane)	75-27-4	147	75	222
Haloethers				
Bis(2-chloroethyl) ether (2,2'-dichlorodiethylether)	111-44-4	147	75	222
PAHs				
Benzo(ghi)perylene	191-24-2	147	75	222
Coronene	191-07-1	147	75	222
Dibenzo(ah)anthracene (Dibenz[a,h]anthracene)	53-70-3	147	75	222
Indeno(123)pyrene (Indeno[1,2,3-cd]pyrene)	193-39-5	147	75	222
PCBs				
Nonachlorobiphenyl	53742-07-7	147	75	222
PCB 206 (2,2',3,3',4,4',5,5',6- nonachlorobiphenyl)	40186-72-9	147	75	222
Octachlorobiphenyl	55722-26-4	147	75	222
Heptachlorobiphenyl	28655-71-2	147	75	222
PCB 170 (2,2',3,3',4,4',5-heptachlorobiphenyl)	35065-30-6	147	75	222
PCB 180 (2,2',3,4,4',5,5'-heptachlorobiphenyl)	35065-29-3	147	75	222
Hexachlorobiphenyl	26601-64-9	147	75	222
PCB 138 (2,2',3,4,4',5'-hexachlorobiphenyl)	35065-28-2	147	75	222
PCB 153 (2,2',4,4',5,5'-hexachlorobiphenyl)	35065-27-1	147	75	222
Pentachlorobiphenyl	25429-29-2	147	75	222
PCB 99 (2,2',4,4',5-pentachlorobiphenyl)	38380-01-7	147	75	222
PCB 101 (2,2',4,5,5'-pentachlorobiphenyl)	37680-73-2	147	75	222
PCB 110 (2,3,3',4',6-pentachlorobiphenyl)	38380-03-9	147	75	222
PCB 40 (2,2',3,3'-tetrachlorobiphenyl)	38444-93-8	147	75	222
PCB 61 (2,3,4,5-tetrachlorobiphenyl)	33284-53-6	147	75	222
Dioxins and furans				
1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4	147	75	222
1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9	147	75	222
2,3,4,7,8-Pentachlorodibenzofuran	57117-31-4	147	75	222
2,3,7,8-Tetrachlorodibenzofuran	51207-31-9	147	75	222
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	35822-46-9	147	75	222
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227-28-6	147	75	222
1,2,3,4-Tetrachlorodibenzo-p-dioxin	30746-58-8	147	75	222
1,2,3,7-Tetrachlorodibenzo-p-dioxin	67028-18-6	147	75	222
1,2,4-Trichlorodibenzo-p-dioxin	39227-58-2	147	75	222
2,8-Dichlorodibenzo-p-dioxin	38964-22-6	147	75	222
1-Chlorodibenzo-p-dioxin	39227-53-7	147	75	222
PAHs				
Pyrene	129-00-0	146	75	221
Phenanthrene	85-01-8	146	75	221
PCBs				
PCB 44 (2,2',3,5'-tetrachlorobiphenyl)	41464-39-5	146	75	221
PCB 52 (2,2',5,5'-tetrachlorobiphenyl)	35693-99-3	146	75	221
PCB 66 (2,3',4,4'-tetrachlorobiphenyl)	32598-10-0	146	75	221
Trichlorobiphenyl	25323-68-6	146	75	221
PCB 18 (2,2',5-trichlorobiphenyl)	37680-65-2	146	75	221
Dioxins and furans				
Octachlorodibenzofuran	39001-02-0	146	75	221
1,2,3,4,7-Pentachlorodibenzo-p-dioxin	39227-61-7	146	75	221
2,3,7,8-Tetrachlorodibenzo-p-dioxin (2,3,7,8-tetrachlorodibenzo[b,e][1,4]dioxin)	1746-01-6	146	75	221

Chemical	CAS Number	Total Expos. Score	Total Tox. Score	Overall Score
Organochlorine pesticides				
Pentachloronitrobenzene (quintozene)	82-68-8	146	75	221
PAHs				
Chrysene	218-01-9	145	75	220
Fluoranthene	206-44-0	145	75	220
Dioxins and furans				
Octachlorodibenzo-p-dioxin	3268-87-9	145	75	220
Dioxins and furans				
1,3,6,8-tetrachlorodibenzo-p-dioxin	33423-92-6	144	75	219
PCBs				
PCB 8 (2,4'-dichlorobiphenyl)	34883-43-7	144	75	219
Tetrachlorobiphenyl	26914-33-0	144	75	219
Monocyclic aromatics				
Benzyl chloride (α-chlorotoluene)	100-44-7	129	90	219
Halogenated aliphatics				
1,2-Dibromomethane (Methylene dibromide)	74-95-3	143	75	218
PCBs				
PCB 28 (2,4,4'-trichlorobiphenyl)	7012-37-5	143	75	218
PAHs				
2-Methylnaphthalene	91-57-6	143	75	218
PCBs				
Dichlorobiphenyl	25512-42-9	142	75	217
Organochlorine pesticides				
4,4' DDE (p,p'-Dichlorodiphenyldichloroethylene) (2,2-bis(p-chlorophenyl)-1,1-dichloroethylene)	72-55-9	142	75	217
Carbamates				
Aldicarb	116-06-3	142	75	217

PAHs, polycyclic aromatic hydrocarbons, PCBs, polychlorinated byphenyls

Table 5.2. Groups of chemicals with missing exposure data

Groups of chemicals with insufficient exposure data	Total Tox. Score
Trichlorophenols (2,3,6- and 3,4,5-substituted)	135
Tri- and tetrachloromethane	135
Dichlorprop	135
Thiocarbamate pesticides	135
Simazine	135
4-Chloro-3-methylphenol	90
Ethylenediaminetetraacetic acid (EDTA)	90
4-methyl-*m*-phenylenediamine	90
Acrylaldehyde	90
Nitrilotriacetic acid (NTA)	90
2-Ethylhexyl acrylate	90
But-2-yne-1,4-diol	90
Methacrylic acid	90
Dicofol	90
Pyrazon	90
Metham-Sodium	90
Mecoprop	90
Trifluralin	90
Hydrazine	90

Table 5.3 Groups of chemicals with insufficient exposure and toxicity data

Groups of chemicals with insufficient exposure and toxicity data
Non-halogenated aromatic hydrocarbons: *o*-Ethyltoluene, p-Isopropyltoluene, Musk xylene, Anisoles, Isopropylanisoles, Butylated hydroxyanisole (BHA), Cyclohexanes (1,4-*trans*-dimethylcyclohexane, 1,2,3-trimethylcyclohexane)
Nitro and chloro anilines: 4-Chloro-2-nitroaniline, *p*-Nitroaniline
Chloronitrobenzenes
Nitro and chloro cresols: para-Chlorometacresol
Phenols: Dinitro-*o*-cresol (DNOC)
Diclorophenols - 2,3-, 2,5-, 3,4-, 3,5-dichlorophenols and 2-amino-4-chlorophenol
Other phenols: Thymol (5-methyl-2-(1-methylethyl)) phenol
Phenoxyalkanoic acids: 2-(2,4,5)-Trichlorophenoxypropionic acid
Phthalates: Di-propylphthalate, Di-(2-ethylhexyl)adipate, Diethylhexyl phthalate (DEHP)
Chloro and nitro toluenes: Benzylidine chloride (α,α-dichlorotoluene), 4 -Chloro-2-nitrotoluene Hexamethylenediamine, N-nitroso-dibutylamine, N-nitroso-morpholine, N-nitroso-di-piperidene, N-nitroso-pyrrol-idene, 2-chloro-*p*-toluidine, Indoles
Organotins
Chloro propanes, propenes and propanols: 2,3 -Dichloropropene, 1,2,3-Trichloro propene, 1,3-Dichloropropan-2-ol,
Other chlorinated aliphatics: 2-Chloro ethanol, Choral hydrate, Chlorinated paraffins, 2-Ethyl hexanol, 2-Butanone, Undecane, Pentadecane, Hexadecane, Terpenes, Limonene, 3-Carene, 4-Carene
Carbonyls: Isophorone, Edetic acid, 2-Methoxyethyl acetate, 2-(2-methoxyethoxy)ethanol, 2-(2-butoxyethoxy)ethanol, Ethyl acetoacetate
Acids and their ethers: Benzenacetic, Benzenepropanoic
Triaryl phosphate esters: Cresyldiphenyl phosphate, Tricresyl phosphate, Tryxylyl phosphate
Haloethers: Bis(2-chloromethyl) ether, Decabromodiphenylether (DeBDE), Octabromodiphenyl ether (OBDE), Hexabromodiphenyl ether (HxBDE), Pentabromodiphenyl ether (PeBDE), Tetrabromodiphenyl ether (TeBDE), Tribromodiphenyl ether (TrBDE), Bis(pentabromophenyl)ether
PAHs: 2,3,5-Trimethyl naphthalene, most halogenated naphthalenes, Alpha-naphthol
Dioxins and furans: 2-Methylfuran
PESTICIDES
Organochlorine pesticides: Endrin aldehyde, Beta-endosulfan, Endosulfan sulfate
Organophosphorous pesticides: Methamidophos, Mevinphos, Oxydemeton-methyl, Ethyl parathion, *cis*- and *trans*-Permethrin, Trichlorphon, Cypermethrin, Deltamethrin, Bifenthrin
Carbamates and dithiocarbamates: Oxamil, Carbaryl, Carbendazim, Maneb
Aromatic chloramines: Linuron, 3,3'-Dichlorobenzidine
Chlorophenoxacetic acid herbicides: (4-chloro-2-methylphenoxy)acetic acid (MCPA), (2,4-dichlorophenoxy)acetic acid (2,4-D), 2,4-D Butoxyethyl ester, 2,4-D Butyl ester, 2,4-D Dimethylamine
Other pesticides: Propachlor, Vinclozolin, Omethoate
OTHER COMPOUNDS
Most alkylbenzenes and other alkyls: e.g. Trialkyl amines, Alkylphenol polyethoxylates
Nonylphenols: 4-Octylphenol, 4-Nonylphenol
Other organics: 1-amino-2-methylanthraquinone, *o*-ansidine, Cyclophosphamide, 4-Dimethyl aminoazobenzene, Formamide, Melphalan, Phenacetin, Phenazopyridine hydrochloride, Reserpine, Cupferron, Michler's ketone, Musk ketone, Thioacetamide, Thiourea, 1,4-Butanediol dimethansulphonate, 1-(2-Chloroethyl)-3-cyclohexyl-1-nitrosourea (CCNU), 1-(2-Chloroethyl)-3-(4-methylcyclohexyl)-1-nitrosourea (Methyl-CCNU), 5-Methoxypsoralen, Allethrins, Azathioprine, Bis(chloroethyl)nitrosourea (BCNU, Carmustine), Chlorambucil, Chlordecone, Cisplatin, Cyhalothrin, Ethyl oestradiol, Diethylstilboestrol, Dimethylcarbomoyl chloride, Erionite, Fenvalerate (pyridin), Isobenzan, Kelevan, N,N-bis(2-chloroethyl)-2-naphthylamine (Chlornaphazine), N-ethyl-N-nitrosourea, Paraquat, Phosphine, Procarbazine hydrochloride, Pyrrolizidine alkaloids, Tecnazene, Terphenyls, Tetradifon, Tetramethrin, Treosulphan

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