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Concentrations of Industrial Organic Chemicals Measured in the Environment: The Influence of Physico-Chemical Properties, Tonnage and Use Pattern

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CONCENTRATIONS OF INDUSTRIAL ORGANIC CHEMICALS MEASURED IN THE ENVIRONMENT : THE INFLUENCE OF PHYSICO-CHEMICAL PROPERTIES. TONNAGE AND USE PATTERN

A. SUMMARY

Various regulatory schemes for the notification of chemicals require the notifier to supply information on possible adverse effects which a chemical may exert when it passes into the environment. To evaluate these effects an estimate of the concentration likely to occur in the environment is essential. In many cases this cannot be made except with the aid of models which oversimplify the complex problems involved. ECETOC therefore decided to see what useful generalisations on environmental concentrations could be made from an examination of actual measured values, and whether such generalisations could provide a more valid means of estimating environmental concentrations.

The approach adopted was to put chemicals into "environmental distribution categories" according to their route of entry and subsequent distribution in the environment, to seek chemicals, representative of each category, for which measured environmental concentrations were available and to look for relationships between categories, tonnage and concentration. The likelyhood that the distribution and concentration of a chemical could then be estimated by analogy from its category was examined.

The environmental distribution categories chosen were the 7 possible distributions of a chemical in one or more compartments, i.e. air (A), water (W), solids (S) (sediment and biota), air-water (AW), air-solids (AS), water-solids (WS) and air-water-solids (AWS). A chemical was allocated to its category by assuming that it was present in its entry compartment and in the compartment(s) in which it is distributed at equilibrium. This distribution was calculated using the Mackay Level I model from the molecular weight, water-solubility, octanol-water partition coefficient (P_{ow}) and vapour pressure.

The search for reference chemicals to fill these categories was carried out by the Water Research Centre, UK, who initially scanned the literature on 150 industrial organic compounds for data on the above physico-chemical properties and on concentrations found in the environment. Adequate data were found on 68 chemicals, covering all of the 7 environmental distribution categories.

There was some relationship between the measured environmental concentrations and the environmental distribution categories of the chemicals. Thus, chemicals in categories A and AW occurred at higher concentrations in air than did those in other categories, and the maximum concentrations in sediments and biota were highest for chemicals in categories S and AWS. There were significant correlations between concentrations in air with Henry's Constant, log P_{ow}, and tonnage. There were no correlations between those physical characters and concentrations in other media. With the possible exception of air these relationships were not strong enough to allow reliable quantitative predictions of concentration to be made from any one of the factors involved. In addition it has not yet been possible to determine the influence of degradation which is of major significance in predicting the environmental concentration of chemicals.

In general, the measured concentrations of a chemical in any one compartment covered a wide range (often several orders of magnitude); the rare exceptions were when only one or few values were recorded. With these 68 reference chemicals it was clear that away from points of discharge the concentration of non-ionic organic chemicals does not exceed :

15	μg/kg (15 ppb)	in air
30	μg/kg (30 ppb)	in water
10,000	μg/kg (10 ppm)	in sediment or biota

(with the exception of species which can biomagnify certain chemicals via the food chain).

The 68 reference chemicals covered a wide range of production tonnages, and assuming they are reasonably representative of industrial organic chemicals these figures can be taken, for the purposes of risk evaluation, as the maximum likely concentration of a chemical in the above compartments.

B. INTRODUCTION

Regulatory schemes for the notification of new chemicals, such as the European Communities' Council Directive amending for the sixth time Directive 67/548/EEC require provision of information on various aspects of the production, use, disposal, properties and possible adverse effects of a chemical on humans or the environment. To enable identification of environmental risks it is necessary to compare information on effects with the concentration of the chemical in relevant parts of the environment.

In the near field situation, close to the point of use, a useful estimate of the potential environmental concentration (PEC) may be obtained by using simple dispersion models. The far field situation, i.e. in all compartments of the environment well away from the initial point of use, is much more complicated and although there are a number of sophisticated models which attempt to predict PEC values, these suffer from a number of deficiencies. Firstly, as such models are extremely difficult to validate and, since many of the processes involved are not well understood, it is unlikely that the PEC values produced will always be reliable. Secondly, models of this type produce "average" values which cannot give any indication of the range of PEC's to be expected.

ECETOC therefore advanced the following hypothesis to assist in this far field situation, synthetic chemicals have been in use for greater than 100 years and there exists a large database relating to their concentrations in various environmental compartments. As a consequence these measured concentrations are likely to be more reliable than those derived from complex models. In theory the PEC of a "new" chemical might be estimated by analogy from the data on an already existing chemical with closely matching physico-chemical properties and similar use pattern, production tonnage and degradability. In practice it will often be difficult to find such a close analogue and thus a more general scheme was sought.

In such a scheme all existing chemicals would be devided into classes based on their physico-chemical properties, reference chemicals reflecting various use patterns, production tonnages and degradability would be selected and these would then be matched against the properties of a "new" chemical to provide PEC values by analogy.

To determine whether such a scheme was feasible ECETOC first sought to determine whether any relationships existed between measured environmental concentrations and the physico-chemical properties of the product concerned.

The terms of reference of the ECETOC Task Force examining this topic were :

a) To define the main categories of distribution patterns of industrial chemicals in the environment.
b) To define the properties of a chemical which determine into which category it falls.
c) To select a small number of industrial chemicals that are representative of each category on which environmental measurements have been made.
d) To collect data on actual environmental concentrations of the selected chemicals, produced from about 1975 onwards but including earlier data if they are adequate.
e) To assess how useful such data are for making broad generalisations relating actual concentration to tonnage.
f) To define what further work, if any, would be of value in relating actual environmental concentrations to quantities discharged or disposed and use patterns.

The Task Force set out to achieve these objectives by :

a) Defining a number of environmental distribution categories based on physico-chemical properties and where these chemicals enter the environment.

b) Selection of reference chemicals, for which measured concentrations are available and allocating them environmental distribution categories. The Mackay level I model was used to assist this allocation.

c) Gathering together published information on environmental concentrations for the reference chemicals and reviewing the data to see if there were any broad correlations with environmental distribution category, production and discharge tonnages or individual physico-chemical properties. It was not possible at this stage to incorporate one of the most important variables, namely degradation, into the analysis, and further work on this topic is recommended.

Much of the collection of data on environmental concentrations and physico-chemical properties and the Mackay level I calculations were carried out by the United Kingdom Water Research Centre.

C. ENVIRONMENTAL DISTRIBUTION CATEGORIES

A chemical discharged to one or more environmental compartments, i.e. air, water, soil, sediment or biota, may subsequently be transferred to others. The number of compartments is small and it is possible to derive a limited number of "categories of environmental distribution" characterised by the point(s) of entry into the environment and the compartment(s) occupied subsequently. To simplify the categorisation, the gas and air particulate phases were combined as "Air", the various water phases were considered as "Water" and the three solid phases (soil, sediments and biota) as "Solids". As seen from the Venn diagram in Fig. 1, when 3 compartments (air, water and solids) are considered, there are 7 possible categories of environmental distribution for a chemical. It may be found in a single compartment only air (A), water (W) or solids (S), or it may occur in two compartments simultaneously (A - W, W - S, A - S) or it may occur in all three (A - W - S).

A chemical can be assigned to its environmental distribution category as follows. If it is initially discharged, for example, to air (A), it will remain substantially in the air if this is its equilibrium compartment. Otherwise, it will begin to be transferred to those compartments which represent its equilibrium distribution, i.e. to water (W), or solids (S), or one of the combinations A-W, W-S, A-S or A-W-S. It is doubtful whether any chemical ever reaches a true equilibrium in the environment, and the environmental distribution category therefore includes its entry-compartment and the compartment(s) in which it would occur at equilibrium. The possible distribution categories are therefore as shown in the final column below :

Input Compartment	Equilibrium Compartment	Environmental Distribution Category
A	A	A
	W	A-W
	S	A-S
	A-W	A-W
	W-S	A-W-S
	A-S	A-S
	A-W-S	A-W-S

This reasoning can be extended to chemicals discharged to the remaining input compartments (W, S, A-W, A-S and AWS) to give the complete categorisation scheme shown in Table 1.

It is important to recognise that this categorisation is concerned with distribution compartments and not concentrations. The concentration of a chemical in a compartment will depend upon the tonnage discharged to the environment, its transfer between compartments and its stability, i.e. rate of degradation by processes such as biodegradation, hydrolysis, oxidation, phototransformation, etc. Unstable chemicals may never survive to reach their equilibrium compartment(s) in any significant quantity but may be found, for varying periods, in non-equilibrium compartments.

A somewhat more comprehensive categorisation scheme which took greater account of inter-compartmental transfer was considered (see Appendix 1) but it proved to be of no more value than the above scheme.

D. SELECTION OF REFERENCE CHEMICALS

Allocation of chemicals to their environmental distribution category required two pieces of information, the input and equilibrium compartments. The input compartment was defined by the pattern of use (Table 2). The equilibrium compartment is independent of point of entry, tonnage and degradability, and can be calculated using molecular weight, vapour pressure, and octanol-water partition coefficients. The Mackay Level I model (1979) was used for this purpose. Although more sophisticated Mackay models exist for predicting environmental concentrations it was considered that the Level I model, based solely on physico-chemical properties, was adequate to predict the environmental distribution at equilibrium.

The following types of chemicals could not be handled within the scheme, namely :

a) Ionised organic chemicals. The sorption of such chemicals by sediments and biota cannot be predicted from their partition coefficients.

b) Ionised inorganic chemicals. These may occur in air as particulates, in water as a solution or suspension, in sediments (by sorption or ion-exchange), or in biota via bioaccumulation. Their concentration in suspended particulate matter in air or water is not governed by partition coefficients, which are not measurable. Similarly, the distribution of water-soluble inorganic chemicals between water and sediment or biota is not governed by passive partitioning between the aqueous phase and organic matter or fatty tissue, and is thus not predictable from the partition coefficient. The equilibrium distribution of such materials cannot therefore be estimated. Within this category lie the inorganic compounds of heavy-metals.

c) Chemicals in the environment derived from sources other than industrial production and use (eg. synthesis via chemical reactions *in situ* or by living organisms).

It was considered desirable to include among the reference chemicals some which are environmentally widespread, such as agrochemicals and solvents, and some of which only a small proportion reaches the environment, e.g. chemical intermediates in factory effluent.

No attempt was made to collect degradability data (bio-degradability, photodegradability, oxidation, hydrolysis, etc.). Thus only non-ionised organic compounds on which the following information was available were considered suitable as reference chemicals:

- molecular weight,
- vapour pressure,
- solubility in water,
- octanol-water partition coefficient (P_{ow}),
- measured environmental concentrations in appropriate compartments,
- the input compartment.

Knowledge of world-wide production tonnage was also considered desirable so that any relationship between this and environmental concentration could be explored.

E. COLLECTION OF DATA ON PHYSICO-CHEMICAL PROPERTIES AND CONCENTRATIONS FOUND IN THE ENVIRONMENT FOR REFERENCE COMPOUNDS

During the past few decades increasing concern about the environment has led to the collection of a large amount of information on concentrations of substances occurring in the environment. Unfortunately the greater proportion of this is on a few compounds of particular scientific, medical and regulatory interest, e.g. some pesticides, chlorinated products, and heavy metals. There is a limited amount of data on a larger number of other chemicals but it is rare to find adequate data on the concentrations of these chemicals in all compartments of the environment in which it might occur.

1. Quality of Data

Many problems arise when attempting to draw valid general conclusions from environmental concentration data. The factors which effect the reliability and applicability of such measurements are discussed below; these were taken into account when the environmental concentration data were collected and evaluated (see section E.2, below).

1.1 Location of sampling. Environmental concentrations have been measured at various stages of the distribution of a chemical within the environment; data in general relate to three locations :

i) Close to a point of discharge from a production, use or disposal site e.g. factory air, factory gaseous and aqueous effluent, sewage-sludge and sewage-treatment waters and domestic discharges.

ii) After significant distribution has occured following initial discharge (dilution in a river/sea; partial or complete transfer to another compartment; etc.) but before equilibrium has occurred, e.g. locations nearto, or not-too-remote from, centres of population and industry : air over or near towns and over coastal or near-coastal regions ; rain water, groundwater, river/lake/coastal waters and drinking water ; top soil, river/sea sediments and biota.

iii) Sites remote from any source of input, e.g. locations comprising the non-coastal oceans, the Arctic, the Antarctic and certain desert regions.

A chemical will usually be at its highest concentration close to the point of discharge where its dilution and transfer to other compartments will only just have begun. Its concentration can often be estimated accurately from information on manufacture, use and disposal, or can be directly measured. It is at the point of discharge that the emission can be, and often is, controlled; once a chemical has begun to move away from the point of discharge, further action to reduce environmental concentrations is usually impracticable and much of the regulatory concern relates to possible concentrations and effects at type ii) and to some extent, type iii) locations.

1.2 Adequacy of measurements. The sensitivity, accuracy, precision and reliability of analytical methods for detecting and measuring small amounts of chemicals in the environment have increased very rapidly in recent years. When searching for data on environmental concentrations a suitable cut-off date should be imposed to eliminate much data of indeterminate value. Such a cut-off date means data will be more relevant to modern industrial practices.

Ideally, reports of environmental concentrations should include information on the adequacy of sampling and storage methods, the number of samples, any method used for concentrating the sample, the number of replicates and the recovery, reproducibility specificity, and limit of detection of the analytical method. Many analytical results are reported only as concentration ranges, sometimes covering orders of magnitude, with no indication of whether the highest and lowest values were outliers or part of a continuous spectrum.

1.3 Bias in Availability of Data. Selecting as reference chemicals those for which adequate data on environmental concentrations were available inevitably produced bias against :

i) degradable chemicals, which are less likely to be found in the environment than poorly degradable chemicals;

ii) chemicals sought but not found in the environment, since negative findings are infrequently reported;

iii) chemicals present in the environment for which an adequately-sensitive analytical method is not available.

When a chemical is reported as "not detected" all that can be inferred is that the chemical might be present at a concentration below the detection limit. Such information was of no value in the present exercise, since the true concentration could be slightly below or orders-of-magnitude below the limit of detection.

1.4 Concentrations in biota. P_{ow} (octanol-water partition coefficient) has been used as an index of accumulation in biota. Only organisms that take up organic chemicals directly from water into fatty tissues have been considered, even though birds and mammals may accumulate chemicals via the food chain, i.e. not directly from water. Concentrations in biota can be reported as concentrations in the whole-body or in specific organs or tissues, and on a dry-weight or wet-weight basis. It is often not clear from reports on which basis the concentrations are calculated, and this sometimes makes such information difficult to use and interpret.

2. Collection of Data

The task of scanning the voluminous literature and collecting data on physico-chemical properties and measured environmental concentrations was carried out for ECETOC by the Water Research Centre (WRC) Medmenham, UK. The data are reproduced in Appendices 2 and 3.

2.1 Criteria for collection and selection of environmental concentration data.

The WRC applied the following criteria and restrictions when collecting and selecting the data.

a) Ionic and naturally-occurring chemicals were omitted.

b) The validity of the concentration measurements was assessed from the the analytical and sampling methods used. In this WRC relied upon its own considerable experience. It was assumed that analytical measurements had been corrected for blanks.

c) Insofar as it was clear from the original papers, the sampling location was described in general terms such as "surface waters", "remote areas", or "urban area", or was identified more specifically, eg. "R. Rhine", "Mississipi Delta". Samples taken closer than 2 km to a discharge source were excluded.

d) Only environmental concentrations given in papers published since 1974 were accepted.

e) Concentrations in air and water were accepted even if fine particulate matter may have been present.

f) Data from remote marine waters were not included because the major current interest and concern is in fresh and coastal waters.

g) Data on birds and marine mammals were omitted because accumulation between water and fatty tissues in such species is not controlled solely by partitioning.

h) Only sediment-core data from surface samples of up to 10 cm deep were included. Samples from deeper sediments probably represent contamination which occurred too far in the past to be relevant to current discharges.

i) Little data was found for concentrations in soil with the exception of agrochemicals for which the soil is a point of discharge.

j) Data were omitted if the sampling location was unclear.

k) Compounds such as methyl chloride, chloroform and polycyclic aromatic hydrocarbons, which occur naturally or are formed by reaction of an industrial chemical in the environment, were not accepted as reference chemicals.

l) Since biota may contain high concentrations of certain accumulated materials of importance to human health and the environment, their environmental concentrations in sediment and biota were listed separately.

m) The following rules were applied in deriving average concentrations or the range within which the true averages must lie :

i) An average was calculated only if the values covered a range of less than 100-fold; otherwise, maximum and minimum values were given.

ii) If samples contained concentrations greater than the limits of detection, simple arithmetic averages (or arithmetic averages of the reported averages) were calculated.

iii) If some samples in a series were reported as "not detected" two averages were reported :

$$\text{- upper average} = \frac{\text{sum of reported concentrations}}{\text{no. of positive samples}}$$

$$\text{- lower average} = \frac{\text{sum of reported concentrations}}{\text{total no. of samples}}$$

iv) Where averages were reported from studies on different numbers of samples, a weighted average was calculated.

n) Several well-known compendia were used in the initial search for the physico-chemical properties. A more detailed search of the literature was then made to fill gaps and seek better-validated figures when the initially-selected values were suspect. Suspect values were identified by comparison with well-substantiated figures for analogous chemicals and from the experience of the WRC scientists.

2.2 Reliability of Environmental Concentration Data

The variable quality of the work reported in the literature made it necessary to check the reliability of the data on environmental concentrations. This was often difficult because insufficient detail was given in many papers. Consequently the WRC placed the data in 3 categories :

- Category 1 : data unlikely to be of use. Typically, data were put into this category when the analysis was intended only to be semi-quantitative, when the sample was highly likely to be contaminated or when GC analysis revealed a low signal-to-noise ratio.

- Category 2 : insufficient detail to classify in categories 1 or 3.

- Category 3 : data likely to be reliable, ie. sufficient detail was given to permit an evaluation.

The categorisations are given for each literature reference at the end of Appendix 3.

2.3 Criteria for the collection and selection of physico-chemical data

The physico-chemical data found by the WRC are reported in Appendix 2. The following points should be noted :

a) Vapour pressures were included irrespective of whether they had been measured at 20 or 25°C because there is little difference between the values in practice. Where values were available over a range of temperatures, that at 20°C was obtained by interpolation or extrapolation on the assumption that there was a linear relationship between the log (vapour pressure) and the (absolute temperature) $^{-1}$. This was not done if the temperature range included the chemical's melting point. A degree of judgement was used in selecting the most likely value when several different values were found.

b) The initial selection of water solubility and P_{ow} values was based on judgement and experience when several different figures were found. A regression of log P_{ow} against log (water solubility)$^{-1}$ was carried out on the initially-selected values to identify outliers. This gave the regression equation :

$$\log P_{ow} = 0.64 \log (WS)^{-1} + 1.24.$$

where P_{ow} = octanol-water partition coefficient,
WS = water solubility in mol/l.

The correlation coefficient, R was 0.96, and the percentage of fit 93%. The data is similar to that reported by other workers (Lyman et al, 1982).

No correction (see Miller et al, 1985) was applied to the values for solids because it was considered that the adjustment would have been too small to warrant the rejection of reasonable data.

For some of the chemicals only the water solubility or P_{ow} were available, in which case the missing value was calculated from the regression equation derived above.

2.4 Selection of reference chemicals

The WRC provided data on 150 chemicals, as shown in Appendix 2 (physico-chemical properties) and Appendix 3 (concentrations). The acceptable data were heavily biased in favour of N. American locations on which most information has been published. Data from only 50 of the chemicals were considered sufficiently complete for them to be used as reference chemicals. An additional 18 compounds were included following the process indicated in section 2.3.c above. Compounds for which the data were so calculated are given the reference (32) in Appendix 2. Given the reasonable accuracy of the regression equation and the insensitivity of the equilibrium distribution to wide variations in P_{ow} or WS (see section 2.5 below), the use of these calculated values was considered to be acceptable. The final list of 68 chemicals is given in Table 3.

2.5 Assessment of equilibrium compartments of reference chemicals

These were derived by using the Level I Mackay model described in Appendix 4. This model does not allow for chemical or biological reactions leading to the transformation of a chemical in the environment, or for time-dependent mixing. It simply calculates from the molecular weight, vapour pressure, water solubility and octanol-water partition coefficient, the theoretical equilibrium-partitioning of a chemical in a world containing assigned amounts of air, water, soil and biota. Previously determined relationships between P_{ow} and i) adsorption on soil and sediment, ii) absorption by biota, are then used to calculate the equilibrium distributions between air, water, and soil/sediment/suspended-matter -in-water (ie. "solids"). It is assumed that adsorption from water onto solids is determined by the organic-matter component of the solid phases (see Appendix 5).

For practical purposes, the Task Force followed Davids and Lange (1986) in defining the presence of a chemical in a compartment at equilibrium as being when the calculated mass in that compartment exceeded 10%. The resulting calculated equilibrium compartments are given in Tables 3 and 4.

Physico-chemical data quoted in the literature are sometimes not accurate. To determine how sensitive the calculated equilibrium distribution was to differences in the physico-chemical properties, a number of calculations were made using a range of values. The relationship between P_{ow} and water solubility (WS, in mol/l) was assumed to be as defined by the equation in Section 2.3.c, in which case water solubility and vapour pressure can be taken as independent variables. For this exercise a molecular weight of 200 was taken - the actual value makes little difference. The results of the sensitivity analyses are summarised in Fig.2 which shows that quite major differences in water solubility and vapour pressure make little difference to the final equilibrium compartment.

3. Data Development

3.1 Assessment of input compartment of reference chemicals (Table 2)

The environmental compartment through which each reference chemical is likely to enter the environment was assessed using informed judgement (Table 2).

3.2 Allocation of reference chemicals to environmental distribution categories (Table 4)

Consideration of the final equilibrium compartment and the likely input compartment lead to the categorisation of chemicals, as described in section C, into the categories shown in Table 4.

3.3 Measured environmental concentrations of reference chemicals (Table 5)

The WRC data (Appendix 3) are presented in the form of averages, maxima and ranges. They are summarised (Table 5) according to the following criteria :

a) All concentrations were expressed in μg/kg.

b) Concentrations in biota were converted, where necessary, to a dry-weight basis by multiplying wet-weight values by 5.

c) Concentration ranges quoted were the lowest and highest presented by the WRC. If the lowest figure was an average it appears in Table 5 with a "less than" sign. If the highest figure was an average it appears with a "greater than" sign.

d) The average concentrations consisted of the arithmetic mean of all the average concentrations presented by the WRC.

e) Where data had been reported as a range of averages, the maxima of the ranges were used to compute the overall average.

f) Only data in WRC validity classes 2 & 3 were used; data in class 1 were ignored.

The mean concentrations and concentration ranges in air, water, sediment and biota, derived using these criteria on the 68 reference chemicals are set out in Table 5. The data on concentrations in air, water, sediments and biota were plotted as bar charts (Figs. 3, 4, 5 and 6 respectively) for clarity and to assist in making comparisons. Possible correlations between these and production tonnage are dealt with in Appendix 6.

F. DISCUSSION OF FINDINGS

1. General

The major impact of any chemical is likely to be found at or near its point of use. The effects may also occur in the wider environment, e.g. although 1,4-dichlorobenzene exerts its major effect in water in the long term most of the compound is transfered to the atmosphere. Estimation of risk at point of use is a straight-forward procedure since the environmental concentration can be readily estimated. Assessment of risk away from the point of discharge is complicated by the difficulty in estimating potential environmental concentrations. The primary aim of this work was to seek generalisations which would enable estimates to be made of concentrations of non-ionised organic substances in the environment away from the point of use.

Establishment of the 7 environmental distribution categories (Table 1) and allocation of reference chemicals to them (Table 4) were carried out, in part, to ensure that chemicals with all types of distribution were represented in the recorded data. Without this any generalisations would have been weakened or unwarranted. In fact, all catagories were represented.

It had been hoped that clear relationships between the concentrations of chemicals found in the environment and their environmental distribution category would have been demonstrated. Had this been so any new chemical could be allocated to its category and its likely environmental concentration assessed by analogy. Although this expectation was not realised some useful generalisations became evident.

The collected data show that the concentration of a chemical in an environmental compartment varies, often by several orders of magnitude, from location to location. It is evident from the data that certain generalisations can be made for industrial organic chemicals thus, Figs. 4-6 show that the concentration of non-ionised organic chemicals at locations other than points of discharge does not normally exceed 15 μg/kg in air, 30 μg/kg (30 ppb) in water, and 10,000 μg/kg (10 ppm) in sediments or biota (with the possible exception of species which can biomagnify chemicals via the food chain). As can be seen from Table 2 these figures apply to industrial chemicals whose production and estimated release tonnages span a very wide range.

The data on sediments and biota relate to fewer chemicals than do those on air and water and it may be questioned whether 10,000 µg/kg represents a true likely maximum concentration. Figs. 5 (sediment) and 6 (biota), however, shows that eight of the nine chemicals whose concentration exceeds 1000 µg/kg have log P_{ow} values greater than 3.8, the exception being nitrobenzene (log p_{ow} = 2.15). Two of the eight chemicals (HCB, DDT) have log P_{ow} around 6.2. This suggests that even for chemicals of very high P_{ow} it is reasonable to assume that concentrations in sediments and biota away from discharge points are not likely to exceed 10,000 µg/kg. At present the measured concentrations in sediments and biota are of limited value for risk assessment since almost nothing is known about the relationship between these concentrations and adverse effects on man and other living organisms (see for example, ECETOC, 1985).

2. Relationships between concentrations and the environmental distribution categories

When the measured concentrations of the reference chemicals were examined in relation to their environmental distribution category (A, W, S, AW, AS, WS and AWS), as in Figs. 3-6, some trends were apparent :

a) Fig. 3 demonstrates that chemicals in categories A and AW occurred in concentrations of between 10^{-3} and $10^{+1.3}$ µg/kg in air, whereas those in the remaining categories were found at concentrations of below about 10^{-1} µg/kg.

b) Fig. 5 shows that maximum concentrations in sediments tend to be higher for chemicals in categories S and AWS. Nitrobenzene and aniline appear to be exceptions and as they are based on one study further confirmation is need. It should be noted that there are data on only 26 chemicals of which 12 are in categories S or AWS and 14 in the remainder; this means that the validity of this trend should be viewed with caution.

c) From the scant data available in Fig. 6 (on only 23 chemicals, of which 3 are represented by a single point) it appears that chemicals in categories A and AW generally have lower maximum concentrations in biota than do those in categories S, and AWS.

3. Quality of Reporting

Data in this report on the concentration in environmental compartments of reference chemicals represent but a fraction of that found in the literature. Much information had to be rejected because it was inadequate in one or more respects. It is recognised that many authors do not report data with risk evaluation in mind but the value of data would be greatly enhanced if as much detail as possible could be given about location, sampling and analytical procedures, etc. as discussed in section E.1. of this report.

4. Future Developments

In the present study no account was taken of the degradability of the reference chemicals. The concentrations used are those which would have occurred after degradation (photolysis in air, biodegradation or hydrolysis in water and sediments, metabolic conversion in biota) had taken place.

While incorporation of degradation rates into the assessment could have led to more reliable interpretation of the concentration data, the task of gathering and assessing the relevant information was beyond the capacity of the Task Force and it is doubted whether, in fact, enough of the data for the 68 reference chemicals exists. This should be considered in any extension of the work.

G. CONCLUSIONS

1. There is little data on environmental concentrations of most existing chemicals; what useful data exists has been collated in this report.

2. Non-ionised industrial organic chemicals can be divided into 7 environmental distribution categories based on their input compartment and equilibrium distribution (derived by calculation from the molecular weight, water solubility, vapour pressure and octanol-water partition coefficient).

3. Although chemicals may be placed in environmental distribution categories, as suggested by the remit, the observed environmental concentrations ranges overlap to such a large extent that the predictive value of the scheme is severely limited. No generalised basis could be derived and each new compound must be examined on a case by case basis.

4. Away from points of discharge, the concentrations of the non-ionised industrial chemicals examined span several orders of magnitude, but did not exceed 15 µg/kg in air, 30 µg/kg (30 ppb) in water, and 10,000 µg/kg (10 ppm) in sediments or biota.

5. For the purposes of risk assessment it can be assumed that the concentrations of non-ionised industrial organic chemicals will rarely exceed these maxima and will usually be considerably lower with the possible exception of species which biomagnify chemicals via the food chain.

6. Some correlations have been found that are worthy of further study, these primarily relate to concentrations in air with Henry's Constant, octanol-water partition coefficient and tonnage produced. The corresponding correlations to water, sediment and biota were very weak or non-existent.

7. There is a need to consider the production of guidelines for collecting and reporting data on environmental concentrations in a form which promotes the comparability of data and can be used for the purposes of risk evaluation.

8. The work of the Task Force might be developed further by seeking data on the degradability of the 68 reference chemicals so that the relationship between measured environmental concentrations, degradability and the other

parameters can be examined but in the opinion of the task force this is unlikely to provide a significant improvement.

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TABLE 1

Categories of Environmental Distribution

Input Compartment	Equilibrium Compartment	Environmental Distribution Category
A	A	A
	W or A-W	A-W
	S or A-S	A-S
	W-S or A-W-S	A-W-S
W	A or A-W	A-W
	W	W
	S or W-S	W-S
	A-S or A-W-S	A-W-S
S	A or A-S	A-S
	W or W-S	W-S
	S	S
	A-W or A-W-S	A-W-S
A-W	A, W or A-W	A-W
	S, W-S, A-S or A-W-S	A-W-S
W-S	A, A-W, A-S or A-W-S	A-W-S
	W, S or W-S	W-S
A-S	A, S or A-S	A-S
	W, WS, AW	A-W-S
A-W-S	Whatever the Equilibrium Compartment the expected distribution can only be A-W-S	A-W-S

A = air
W = water
S = solids

TABLE 2

Input Compartment of Reference Chemicals

Name	CAS.No.	Production (Kt/yr)	Est. Global Release	Use	Input Compartment
1) AGROCHEMICALS					
Alachlor	(15972-60-8)	41 (US 1980)	123	Herbicide	WS
Aldrin	(309-00-2)	2.5 (EC 1976)	7.5	Insecticide	S
Atrazine	(1912-24-9)	37 (US 1982)	111	Herbicide	WS
Chlorpyrifos	(2921-88-2)	3.3 (US 1982)	10	Insecticide	AS
p-p'-DDT	(50-29-3)	9.5 (EC 1981)	28.5	Insecticide	S
Dieldrin	(60-57-1)	1.0 (EC 1976)	3	Insecticide	S
Dimethoate	(60-51-5)	0.6 (US 1982)	1.8	Insecticide	S
Endrin	(72-20-8)	2 (EC 1976)	6	Insecticide	S
Heptachlor	(76-44-8)	2.7 (US 1971)	8.1	Insecticide	S
alpha-HCH	(319-84-6)	NA	NA	Insecticide	AWS
beta-HCH	(319-85-7)	NA	NA	Insecticide	AWS
gamma-HCH (Lindane)	(58-89-9)	4.7 (EC 1981)	14.1	Insecticide	AWS
Malathion	(121-75-5)	15.8 (US 1983)	47.4	Insecticide	S
Parathion (Methyl & Ethyl)	(56-38-2)	3.2 (US 1982)	9.6	Insecticide	S
2) PHTHALATE ESTER					
Di-N-Butylphthalate	(84-74-2)	230 (World 1973)	230	Plasticiser	AW
Diethylpthalate	(84-66-2)	7.7 (US 1982)	23.1	Solvent	W
Di(2-Ethylhexyl)Phthalate	(117-81-7)	136 (US 1984)	402	Plasticiser	AW
Di-Methylphthalate	(131-11-3)	2.2 (US 1982)	6.6	Solvent and Various	W
3) PHOSPHATE ESTER					
Tri-N-Butylphosphate	(126-73-8)	1 (US 1983)	3	Solvent; Plasticiser	W
Triphenylphosphate	(115-86-6)	14 (US 1983)	42	Solvent; Plasticiser	W
4) ETHER					
Dichloroisopropyl Ether	(63283-80-7)	15 (US 1975)	45	Solvent; Byproduct	AW
5) ALCOHOL					
Cyclohexanol	(108-93-0)	400 (EC 1985)	1200	Solvent; Intermediate (0.2%)	W
6) CHLOROBENZENE					
Chlorobenzene	(108-90-7)	75 (EC 1981)	6.6	Intermediate	W
1,2-Dichlorobenzene	(95-50-1)	2 (EC 1981)	?	Solvents; Intermediate (?)	AW
1,3-Dichlorobenzene	(541-73-1)	1 (EC 1981)	3	Byproduct	W
1,4-Dichlorobenzene	(106-46-7)	22 (EC 1981)	66	Deodorant	A
1,2,3-Trichlorobenzene	(87-61-6)	1 (EC 1981)	0.09	Intermediate	W
1,2,4-Trichlorobenzene	(120-82-1)	3 (EC 1981)	?	Intermediate (?); Solvent	W
1,3,5-Trichlorobenzene	(108-70-3)	1 (EC 1981)	0.09	Intermediate	W
1,2,3,4-Tetrachlorobenzene	(634-66-2)	N.A.	N.A.	Byproduct	W
1,2,3,5-Tetrachlorobenzene	(634-90-2)	N.A.	N.A.	Byproduct	W
1,2,4,5-Tetrachlorobenzene	(95-94-3)	1.7 (US 1983)	0.15	Intermediate	W
Pentachlorobenzene	(608-93-5)	N.A.	N.A.	Intermediate	W
Hexachlorobenzene	(118-74-1)	30 (EC 1981)	?	Byproduct; Intermediate (?)	W

Table 2 Input Compartment of Reference Chemicals (cont.)

Name	CAS.No.	Production (Kt/yr)	Est. Global Release	Use	Input Compartment
7) AROMATIC AMINES					
Aniline	(62-53-3)	364 (EC 1983)	32.7	Intermediate	W
2-Chloroaniline	(95-51-2)	1.9 (EC 1983)	0.17	Intermediate	W
4-Chloroaniline	(106-47-8)	1.8 (EC 1983)	0.16	Intermediate	W
3,4-Dichloroaniline	(95-76-1)	13.6 (EC 1983)	1.2	Intermediate	W
2-Methylaniline	(95-53-4)	N.A.	N.A.	Intermediate	W
N,N-Dimethylaniline	(121-69-7)	8 (EC 1983)	0.72	Intermediate	W
N-Methylaniline	(100-61-8)	N.A.	N.A.	Intermediate	W
4-Nitroaniline	(100-01-6)	5.9 (EC 1983)	0.55	Intermediate	W
8) CHLOROALKANES					
Tetrachloromethane	(56-23-5)	844 (World 1983)	24	Intermediate	A
Trichlorofluoromethane	(75-69-4)	291 (World 1983)	9	Blowing agent; aerosols	A
1,1-Dichloroethane	(75-34-3)	400 (World 1983)	12	Intermediate	AW
1,2-Dichloroethane	(107-06-2)	19225 (World 1983)	?	Intermdediate (?); Petrol additive	AW
1,2-Dibromoethane	(106-93-4)	90 (World 1983)	90	Petrol additive; Fumisant	A
1,1,1-Trichloroethane	(71-55-5)	537 (World 1983)	537	Cleaning solvents	AW
1,1,2,2-Tetrachloroethane	(79-34-5)	15 (World 1983)	?	Intermediate (?); Byproduct	A
1,2-Dichloropropane	(78-87-5)	100 (World 1983)	3	Intermediate	AW
1,1,2-Trichloroethane	(79-00-5)	80 (World 1983)	2.4	Intermediate	AW
9) CHLOROALKENES					
1,2-Dichloroethane	(540-59-0)	N.A.	N.A.	Intermdediate	AW
Trichloroethene	(79-01-6)	326 (World 1984)	326	Solvent	AW
Tetrachloroethene	(127-18-4)	553 (World 1984)	?	Solvent; Intermediate (?)	AW
Hexachlorobutadiene	(87-68-3)	20 (World 1984)	20	Byproduct	W
10) PHENOLS					
Phenol	(108-95-2)	1534 (EC 1984)	?	Intermediate (?); Disinfectant	W
4-Methylphenol	(106-44-5)	9.7 (EC 1983)	?	Intermediate (?); Disinfectant	W
Pentachlorophenol	(87-86-5)	9 (EC 1983)	27	Blacide; Disinfectant	WS
11) AROMATIC NITRO COMPOUND					
Nitrobenzene	(98-95-3)	500 (EC 1985)	46.5	Intermdediate (99.9%); Solvent	W
12) AROMATIC HYDROCARBONS					
Benzene	(71-43-2)	5000 (EC 1985)	11000	Intermediate (25%); Byproduct	AW
Toluene	(108-88-3)	2200 (EC 1985)	1800	Intermediate (75%)	W
Ethylbenzene	(100-41-4)	3200 (EC 1985)	?	Intermediate (?); Petrol additive	W
n-Xylene	(108-38-3)	40 (EC 1985)	3.6	Intermediate	W
p-Xylene	(106-42-3)	1200 (EC 1985)	100	Intermediate	W
o-Xylene	(95-47-6)	530 (EC 1985)	63	Intermediate (99.9%); Solvent	W
1,2,3,4-Tetramethylbenzene	(488-23-3)	<60 (EC 1985)	?	Solvent; Plasticiser; Intermediates (?)	W
Styrene	(100-42-5)	7000 (World 1977)	210	Manomer for plastic production	AW
13) MISCELLANEOUS					
Isophorone	(78-59-1)	40 (EC 1984)	?	Solvent; Intermediate (?)	AS
2-Chlorotoluene	(95-49-8)	N.A.	N.A.	Intermediate (?); Solvent	W

* The global release rate was estimated by assuming that world production was equivalent to 3x either US or EC production. A 3% input was assumed for those chemicals used as intermediates whilst 100% input was assumed for all other use patterns.

TABLE 3

Selection of Reference Chemicals and Assessment of Equilibirum Compartment

Name	MW	VAP.P (Pa)	SOL. (g/m^3)	H $(Pa/m^3/mol)$	Log P	MACKAY LEVEL I DISTRIBUTION			EQUILIBRIUM COMPARTMENT
						Air	Water	Solid	
1) AGROCHEMICALS									
Alachlor	270	0.0029	240	0.0033	3.2	0.09	79.63	20.29	WS
Aldrin	365	0.01	0.013	280	6.23	27.07	0.20	72.65	AS
Atrazine	216	0.00004	30	0.00029	2.68	0.01	93.15	6.84	W
Chlorpyrifos	350	0.0025	2	0.44	4.6	2.08	13.78	84.14	WS
p-p'-DDT	355	0.000025	0.0033	2.7	6.19	0.4	0.42	99.18	S
Dieldrin	381	0.000024	0.1	0.091	5.48	0.07	2.11	97.82	S
Dimethoate	229	0.0011	25000	0.000010	1.78	0	99.08	0.91	W
Endrin	381	0.000027	0.1	0.10	5.63	0.05	1.5	98.44	S
Heptachlor	373	0.04	0.03	500	5.44	79.9	0.46	19.64	AS
alpha-HCH	291	0.002	36	0.016	3.8	0.28	50.67	49.05	WS
beta-HCH	291	0.000029	36	0.00023	3.8	0.00	50.81	49.19	WS
gamma-HCH (Lindane)	291	0.0012	10	0.035	3.85	0.58	47.66	51.76	WS
Malathion	330	0.0053	150	0.012	2.9	0.36	88.82	10.82	WS
Parathion (Methyl & Ethyl)	291	0.00063	24	0.0076	3.8	0.13	50.75	49.13	WS
2) PHTHALATE ESTERS									
Di-N-Butylphthalate	278	0.0047	11.2	0.12	4.79	0.38	9.52	90.1	S
Diethylphthalate	222	0.22	1100	0.044	2.24	1.5	95.94	2.55	W
Di(2-Ethylhexyl)Phthalate	391	0.00086	0.34	0.99	5.11	1.62	4.74	93.65	S
Di-Methylphthalate	194	0.22	4000	0.011	1.5	0.37	99.15	0.48	W
3) PHOSPHATE ESTER									
Tri-N-Butylphosphate	266	0.23	280	0.22	4	2.9	38.32	58.79	WS
4) ETHER									
Dichloroisopropyl	171	110	1700	11	2.5	78.49	20.51	0.99	AW
5) ALCOHOL									
Cyclohexanol	100	130	36000	0.36	1.2	11.08	88.71	0.21	AW
6) CHLOROBENZENES									
Chlorobenzene	113	1600	290	620	2.98	99.45	0.48	0.07	A
1,2-Dichlorobenzene	147	200	92	320	3.38	98.77	0.9	0.33	A
1,3-Dichlorobenzene	147	300	69	640	3.48	99.36	0.44	0.21	A
1,4-Dichlorobenzene	147	80	31	380	3.37	98.98	0.75	0.27	A
1,2,3-Trichlorobenzene	182	28	12	420	4.1	97.99	0.69	1.32	A
1,2,4-Trichlorobenzene	182	61	48	240	4.1	96.6	1.16	2.24	A
1,3,5-Trichlorobenzene	182	32	4.1	1400	4.1	99.4	0.2	0.39	A
1,2,3,4-Tetrachlorobenzene	216	5.2	12	94	4.55	83.16	2.61	14.22	AS
1,2,3,5-Tetrachlorobenzene	216	9.8	5.3	400	4.65	94.62	0.69	4.7	A
1,2,4,5-Tetrachlorobenzene	216	0.72	2.4	65	4.51	79.32	3.47	17.21	AS
Pentachlorobenzene	250	0.22	0.83	66	5.19	48.1	2.1	49.81	AS
Hexachlorobenzene	285	0.0012	0.0045	76	6.18	10.11	0.39	89.5	AS

Table 3 Selection of Reference Chemicals and Assessment of Equilibrium Compartment (cont.)

Name	MW	VAP.P (Pa)	SOL. (g/m³)	H (Pa/m³/mol)	Log P	MACKAY LEVEL I DISTRIBUTION			EQUILIBRIUM COMPARTMENT
						Air	Water	Solid	
7) AROMATIC AMINES									
Aniline	93	40	34000	0.11	0.95	3.64	96.23	0.13	W
2-Chloroaniline	128	24	9500	0.32	1.9	9.95	88.27	1.00	AW
4-Chloroaniline	128	2	13000	0.020	1.8	0.67	93.30	0.95	W
3,4-Dichloroaniline	162	1.3	92	2.3	3.35	37.07	46.04	16.09	AWS
2-Methylaniline	107	13	15000	0.093	1.3	3.1	96.61	0.29	W
N,N-Dimethylaniline	121	67	1200	6.8	2.5	69.02	29.55	1.43	AW
N-Methylaniline	107	40	16000	0.27	1.7	8.41	90.89	0.7	W
4-Nitroalinine	138	0.2	800	0.035	2.66	1.1	92.42	6.49	W
8) CHLOROALKANES									
Tetrachloromethane	153	12000	1200	1530	2.7	99.8	0.19	0.02	A
Trichlorofluoromethane	137	89000	1100	11000	2.4	99.97	0.03	0.00	A
1,1-Dichloroethane	99	31000	5500	560	1.99	99.48	0.52	0.0	A
1,2-Dichloroethane	99	8100	800	1000	2.82	99.97	0.03	0.0	A
1,2-Dibromoethane	188	1500	4.3	66000	4.3	99.90	0.0	0.02	A
1,1,1-Trichloroethane	133	13000	130	13000	2.95	99.98	0.02	0.0	A
1,1,2,2-Tetrachloroethane	168	670	2900	39	2.45	92.75	6.95	0.3	A
1,2-Dichloropropane	113	6700	2700	280	2.34	98.95	1.02	0.02	A
1,1,2-Trichloroethane	133	2500	4500	74	2.13	96.16	3.76	0.00	A
9) CHLOROALKENES									
1,2-Dichloroethene	97	27000	800	3300	2.55	99.91	0.09	0.0	A
Trichloroethene	131	9870	1400	920	2.53	99.67	0.31	0.02	A
Tetrachloroethene	166	2100	480	730	3.30	99.45	0.4	0.15	A
Hexachlorobutadine	261	0.84	2	110	4.8	78.02	2.06	19.93	AS
10) PHENOLS									
Phenol	94	27	82000	0.031	1.5	1.05	98.47	0.48	W
4-Methylphenol	108	14.4	1800	0.86	2.2	22.58	75.58	1.84	AW
Pentachlorophenol	266	0.015	14	0.29	5.01	0.58	5.95	93.47	S
11) AROMATIC NITRO COMPOUND									
Nitrobenzene	123	20	1900	1.3	2.15	30.49	68.04	1.47	AW
12) AROMATIC HYDROCARBONS									
Benzene	78	10000	1800	430	2.13	99.34	0.65	0.02	A
Toluene	92	2900	580	460	2.65	99.34	0.62	0.04	A
Ethylbenzene	106	930	190	520	3.13	99.35	0.54	0.11	A
m-Xylene	106	800	160	530	3.2	99.33	0.54	0.13	A
p-Xylene	106	870	210	440	3.18	99.18	0.67	0.15	A
o-Xylene	106	670	220	320	3.13	98.92	0.89	0.19	A
1,2,3,4-Tetramethylbenzene	134	30	9.1	440	3.98	98.41	0.64	0.95	A
Styrene	104	670	300	230	2.95	98.6	1.23	0.17	A
13) MISCELLANEOUS									
Isophorone	138	49	1400	4.8	1.67	65.92	33.83	0.25	AW
2-Chlorotoluene	127	350	57	780	3.42	99.48	0.37	0.15	A

TABLE 4

Environmental Distribution Categories of Reference Chemicals

Name	CAS No.	Input	Compartment Equilibrium	Compartment Category
1,4-Dichlorobenzene	(106-46-7)	A	A	A
Tetrachloromethane	(56-23-5)	A	A	
Trichlorofluoromethane	(75-69-4)	A	A	
1,2-Dibromoethane	(106-93-4)	A	A	
1,1,2,2-Tetrachloroethane	(79-34-5)	A	A	
Diethylphthalate	(84-66-2)	W	W	W
Di-Methylphthalate	(131-11-3)	W	W	
Aniline	(62-53-3)	W	W	
4-Chloroaniline	(106-47-8)	W	W	
2-Methylaniline	(95-53-4)	W	W	
N-Methylaniline	(100-61-8)	W	W	
4-Nitroaniline	(100-01-6)	W	W	
Phenol	(108-95-2)	W	W	
p-p'-DDT	(50-29-3)	S	S	S
Dieldrin	(60-57-1)	S	S	
Endrin	(72-20-8)	S	S	
Dichloroisopropyl Ether	(63283-80-7)	AW	AW	AW
Cyclohexanol	(108-93-0)	W	AW	
Chlorobenzene	(108-90-7)	W	A	
1,2-Dichlorobenzene	(95-50-1)	AW	A	
1,3-Dichlorobenzene	(541-73-1)	W	A	
1,2,3-Trichlorobenzene	(87-61-6)	W	A	
1,2,4-Trichlorobenzene	(120-82-1)	W	A	
1,3,5-Trichlorobenzene	(108-70-3)	W	A	
1,2,3,5-Tetrachlorobenzene	(634-90-2)	W	A	
2-Chloroaniline	(95-51-2)	W	AW	
N,N-Dimethylaniline	(121-69-7)	W	AW	
1,1-Dichloroethane	(75-34-3)	AW	A	
1,2-Dichloroethane	(107-06-2)	AW	A	
1,1,1-Trichloroethane	(71-55-6)	AW	A	
1,2-Dichloropropane	(78-87-5)	AW	A	
1,1,2-Trichloroethane	(79-00-5)	AW	A	
1,2-Dichloroethene	(540-59-0)	AW	A	
Trichloroethene	(79-01-6)	AW	A	
Tetrachloroethene	(127-18-4)	AW	A	

Table 4 Environmental Distribution Categories of Reference Chemicals (cont.)

Name	CAS No.	Input	Compartment Equilibrium	Compartment Category
4-Methylphenol	(106-44-5)	W	AW	
Nitrobenzene	(98-95-3)	W	AW	
Benzene	(71-43-2)	AW	A	
Toluene	(108-88-3)	W	A	
Ethylbenzene	(100-41-4)	W	A	
m-Xylene	(108-38-3)	W	A	
p-Xylene	(106-42-3)	W	A	
o-Xylene	(95-47-6)	W	A	
1,2,3,4-Tetramethylbenzene	(488-23-3)	W	A	
Styrene	(100-42-5)	AW	A	
2-Chlorotoluene	(95-49-8)	W	A	
Alachlor	(15972-60-8)	WS	WS	WS
Atrazine	(1912-24-9)	WS	W	
Dimethoate	(60-51-5)	S	W	
Malathion	(121-75-5)	S	WS	
Parathion (Methyl & Ethyl)	(56-38-2)	S	WS	
Tri-N-Butylphosphate	(126-73-8)	W	WS	
Pentachlorophenol	(87-86-5)	WS	S	
Aldrin	(309-00-2)	S	AS	AS
Heptachlor	(76-44-8)	S	AS	
Chlorpyrifos	(2921-88-2)	AS	WS	AWS
alpha-HCH	(319-84-6)	AWS	WS	
beta-HCH	(319-85-7)	AWS	WS	
gamma-HCH (Lindane)	(58-89-9)	AWS	WS	
Di-N-Butylphthalate	(84-74-2)	AW	S	
Di(2-ethylhexyl)phthalate	(117-81-7)	AW	S	
1,2,3,4-Tetrachlororobenzene	(634-66-2)	W	AS	
1,2,4,5-Tetrachlorobenzene	(95-94-3)	W	AS	
Pentachlorobenzene	(608-93-5)	W	AS	
Hexachlorobenzene	(118-74-1)	W	AS	
3,4-Dichloroaniline	(95-76-1)	W	AWS	
Hexachlorobutadine	(87-68-3)	W	AS	
Isophorone	(78-59-1)	AS	AW	

TABLE 5

Summary of Environmental Concentration Data
(All data are presented in μg/kg)

Name	Air	Water	Sediment	Biota
Category A				
1,4-DICHLOROBENZENE (106-46-7)	N.A.	0.84 (0.004 - 2.92)	30.8 (5 - 94.0)	13.3 (<5 - >20)
TETRACHLOROMETHANE (56-23-5)	0.182 (<0.025 - 0.37)	2.0	N.A.	N.A.
TRICHLOROFLUOROMETHAME (75-69-4)	0.58 (0.1 - 3.8)	N.A.	N.A.	N.A.
1,2-DIBROMOETHANE (106-93-4)	0.0258 (0.002 - 0.368)	N.A.	N.A.	N.A.
1,1,2,2-TETRACHLOROETHANE (79-34-5)	0.369 (<0.0018 - 9.75)	N.A.	N.A.	N.A.
Category W				
DIETHYLPHTHALATE (84-66-2)	N.A.	N.A.	18.5 (<5 - >32)	N.A.
DI-METHYLPHTHALATE (131-11-3)	N.A.	0.3	N.A.	N.A.
ANILINE (62-53-3)	N.A.	6.16 (<0.03 - >28)	500 (<350 - >500)	N.A.
4-CHLOROANILINE (106-47-8)	N.A.	0.15 (<0.02 - >0.22)	N.A.	N.A.
2-METHYLANILINE (95-53-4)	N.A.	6.93 (<0.03 - >20)	72 (<30 - >72)	N.A.
N-METHYLANILINE (100-61-8)	N.A.	N.A.	12	N.A.
4-NITROANILINE (100-01-6)	N.A.	3.8	N.A.	N.A.
PHENOL (108-95-2)	N.A.	15.0 (0.03 - 30.0)	N.A.	N.A.
Category S				
DDT (All isomers)	0.0000201 (<0.000002 - 0.00045)	0.0026 (0.0000013 - 07)	20.51 (0.77 - 100)	144.8 (3 - 53100)
DIELDRIN (60-57-1)	0.00002 (<0.000002 - 0.00031)	0.006 (<0.00003 - 0.61)	166.7 (<0.003 - 5300)	144 (<0.5 - 5010)
ENDRIN (72-20-8)	0.000034 (<0.000034 - 0.000252)	N.A. (0.04 (Max))	N.A. (2.9 (Max))	0.03 (<0.03 - 2000)
Category AW				
DICHLOROISOPROPYL ETHER (63283-80-7)	N.A.	1.45 (<0.1 - 10.1)	N.A.	N.A.
CYCLOHEXANOL (108-93-0)	N.A.	10.0	N.A.	N.A.
CHLOROBENZENE (108-90-7)	0.62 (0.005 - 2.8)	1.7 (0.1 - 5.3)	5.5 (1.0 - 11.0)	0.8 (0.3 - 1.0)
1,2-DICHLOROBENZENE (95-50-1)	0.0127 (0.001 - 0.236)	2.7 (0.002 - 8.9)	N.A.	N.A.
1,3-DICHLOROBENZENE (541-73-1)	0.007 (0.001 - 0.055)	0.51 (<0.011 - >1.01)	20.5 (<2.0 - >74.0)	5.0 (<1.5 - >12.5)

Table 5 Summary of Environmental Concentration Data (cont.)

Name	Air	Water	Sediment	Biota
Catagory AW				
1,2,3-TRICHLOROBENZENE (87-61-6)	N.A.	0.27 (0.001 - 0.8)	1.98 (<0.2 - 7.0)	1.25 (>0.5 - >3.0)
1,2,4-TRICHLOROBENZENE (120-82-1)	0.005 (0.001 - 0.040)	0.2582 (<0.0002 - >1.0)	26 (<1.0 - >94.01)	7.0 (<2.5 - >17.5)
1,3,5-TRICHLOROBENZENE (108-70-3)	N.A.	0.133 (<0.0001 - 0.4)	15.5 (<0.2 - >60.0)	6.25 (<0.5 - >20.0)
1,2,3,5-TETRACHLOROBENZENE (634-90-2)	N.A.	0.0014 (<0.0014 - >0.0014)	1.7 (<0.1 - 6.0)	1.375 (<0.5 - >3.75)
2-CHLOROANILINE (95-51-2)	N.A.	0.396 (<0.03 - >0.54)	98 (<30 - >98)	N.A.
N,N-DIETHYLANILINE (91-66-7)	N.A.	0.43 (<0.28 - >0.43)	N.A.	N.A.
N,N-DIMETHYLANILINE (121-69-7)	N.A.	0.56 (<0.07 - >1.18)	N.A.	N.A.
1,1-DICHLOROETHANE (75-34-3)	0.041 (0.003 - 0.147)	N.A.	N.A.	N.A.
1,2-DICHLOROETHANE (107-06-2)	0.338 (<0.015 - 7.3)	3.3 (<0.06 - 10.0)	N.A.	N.A.
1,1,1-TRICHLOROETHANE (71-55-6)	0.517 (<0.055 - 5.15)	N.A. (1.0(Max.))	N.A.	N.A.
1,2-DICHLOROPROPANE (78-87-5)	0.039 (0.004 - 0.253)	1.37 (<0.68 - 1.37)	N.A.	N.A.
1,1,2-TRICHLOROETHANE (79-00-5)	0.0168 (0.004 - 0.129)	0.61 (<0.03 - >1.55)	N.A.	N.A.
1,2-DICHLOROETHENE (540-59-0)	0.004 (0.004 - 0.605)	0.1	N.A.	N.A.
TRICHLOROETHENE (79-01-6)	0.196 (0.005 - 3.07)	0.75 (0.06 - 1.0)	N.A.	280
TETRACHLOROETHENE (127-18-4)	0.054 (<0.016 - 7.60)	2.9 (0.3 - 10.0)	N.A.	N.A.
4-METHYLPHENOL (106-44-5)	N.A.	0.03 (<0.03 - >0.03)	N.A.	N.A.
NITROBENZENE (98-95-3)	2.32 (<0.07 - 6.5)	2.3 (0.07 - 30.0)	1900 (<610 - >1900)	N.A.
BENZENE (71-43-2)	0.58 (<0.1 - >0.58)	0.3 (<0.02 - >0.8)	N.A.	N.A.
TOLUENE (108-88-3)	15.4 (<2.9 - >15.4)	1.2 (<0.8 - >1.9)	N.A.	N.A.
ETHYLBENZENE (100-41-4)	2.3 (<0.7 - >2.3)	0.14 (<0.12 - >0.14)	N.A.	N.A.
m-XYLENE (108-38-3)	4.95 (<1.24 - >4.95)	N.A.	N.A.	N.A.
p-XYLENE (106-42-3)	2.12 (<0.35 - >2.12)	N.A.	N.A.	N.A.
o-XYLENE (95-47-6)	2.47 (<0.7 - >2.47)	N.A.	N.A.	N.A.
1,2,3,4-TETRAMETHYLBENZENE (488-23-3)	0.020 (<0.013 - >0.020)	N.A.	N.A.	N.A.
STYRENE (100-42-5)	1.21 (<0.07 - >1.21)	N.A.	N.A.	N.A.
2-CHLOROTOLUENE (95-49-8)	<0.005 (<0.005 - >0.111)	2.267 (<0.6 - >5.3)	N.A.	N.A.

Table 5 Summary of Environmental Concentration Data (cont.)

Name	Air	Water	Sediment	Biota
Category WS				
ALACHLOR (15972-60-8)	N.A.	0.089 (<0.089 - >0.089)	N.A.	N.A.
ATRAZINE (1912-24-9)	N.A.	0.58 (0.223 - 7.66)	N.A. (11.9 (Max.))	N.A.
DIMETHOATE (60-51-5)	0.0025 (<0.000008 - 0.015)	N.A.	N.A.	N.A.
MALATHION (121-75-5)	N.A. (0.00317 - 0.184)	N.A. (0.18(Max.))	N.A.	N.A.
PARATHION (METHYL & ETHYL) (56-38-2)	0.0024 (<0.0003 - 0.1344)	N.A.	N.A.	N.A.
TRI-N-BUTYLPHOSPHATE (126-73-8)	N.A.	0.33 (<0.22 - >0.4)	N.A.	N.A.
TRIPHENYLPHOSPHATE (115-86-6)	N.A.	0.4 (0.08 - 0.4)	N.A.	N.A.
PENTACHLOROPHENOL (87-86-5)	0.0032 (0.0002 - 0.0065)	0.074 (0.00085 - 0.2)	0.43 (0.18 - 0.83)	20.56 (<19.75 - >22.0)
Category AS				
ALDRIN (309-00-2)	.00003 (<0.00003 - >0.00003)	0.06 (<0.06 - >0.06)	N.A.	14.2 (11.1 - 17.2)
HEPTACHLOR (76-44-8)	0.000311	0.005 (<0.005 - >0.005)	N.A.	N.A. (5850 (Max.))
Category AWS				
CHLORPYRIFOS (2921-88-2)	0.0018 (0.0002 - 0.084)	N.A.	N.A.	N.A.
alpha-HCH (319-84-6)	0.00065 (0.000008 - 0.129)	0.025 (0.00026 - 0.05)	0.53 (0.06 - 1.8)	6.3 (1.85 - 1500)
beta-HCH (319-85-7)	N.A.	N.A.	0.45 (<0.2 - >0.7)	39.3 (<37.7 - >41.3)
gamma-HCH (LINDANE) (58-89-9)	0.00000807 (<0.000002 - 0.00286)	0.025 (0.00007 - 0.05)	N.A. (0.003)	12.8 (<0.03 - 1400)
BUTYLBENZYLPHTHALATE (85-68-7)	N.A.	121.2 (0.12 - 483)	N.A.	N.A.
DI-N-BUTYLPHTHALATE (84-74-2)	0.0095 (<0.0002 - 0.060)	0.485 (<0.08 - 1.1)	52.75 (5.5 - 160)	250.25 (0.5 - 500)
DI(2-ETHYLHEXYL)PHTHALATE (117-81-7)	N.A. (0.03 - 100)	0.62 (0.005 - 2.5)	677 (4.3 - 2500)	195 (4.5 - 290)
1,2,3,4-TETRACHLORBENZENE (634-66-2)	N.A.	0.0114 (<0.00005 - 0.034)	8.75 (<0.3 - 33.0)	10.125 (<1.5 - >26.5)
1,2,4,5-TETRACHLOROBENZENE (95-94-3)	N.A.	0.0061 (<0.0001 - >0.012)	13.6 (<0.3 - >52.0)	6.25 (<1.5 - >17.5)
PENTACHLOROBENZENE (608-93-5)	0.0000165 (<0.000008 - >0.000025)	0.00208 (<0.00004 - 0.006)	8.53 (<0.1 - >32.0)	19.125 (<3.0 - >60.0)
HEXACHLOROBENZENE (118-74-1)	0.0000733 (<0.00005 - 0.0004)	0.335 (<0.00024 - >2.2)	27.9 (<0.011 - 120)	209.9 (<1.75 - 3500)
3,4-DICHLOROANILINE (95-76-1)	N.A.	0.346 (<0.02 - >0.42)	110 (<50 - >110)	N.A.
HEXACHLOROBUTADIENE (87-68-3)	0.00475 (0.001 - 0.154)	1.48 (<0.25 - 4.4)	210 (<210 - >210)	2348 (<200 - >4100)
ISOPHORONE (78-59-1)	0.3	N.A. (<0.05 - >0.3)	N.A.	N.A.

Figure 1

ENVIRONMENTAL DISTRIBUTION CATEGORIES

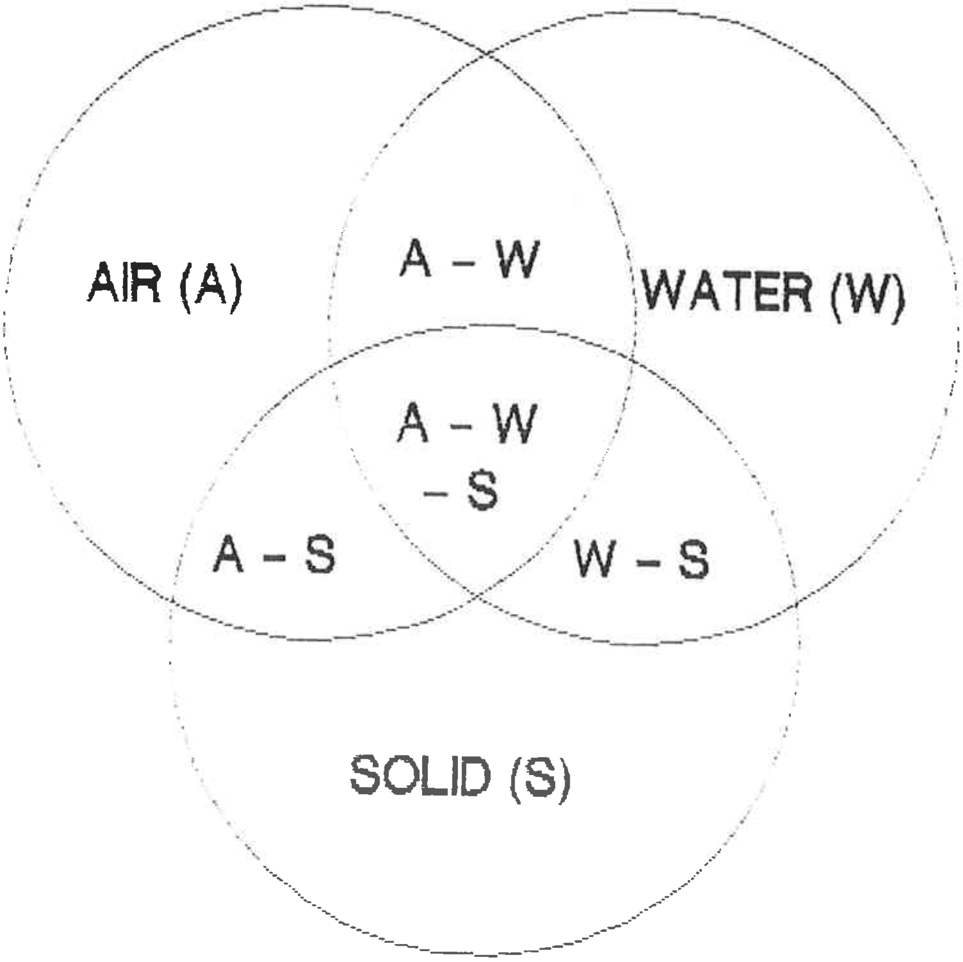


Figure 2

ENVIRONMENTAL MASS DISTRIBUTION IN UNIT WORLD RELATED TO WATER-SOLUBILITY AND VAPOUR PRESSURE

Log Vapour Pressure (Pascals)

4	A	A	A	A	A	A	A	A	A	AW	AW
3	A	A	A	A	A	A	A	A	AW	AW	W
2	A	A	A	A	A	A	A	AW	AW	W	W
1	A	A	A	A	A	A	AW	AW	W	W	W
0	A	A	A	A	AS	AWS	AWS	W	W	W	W
-1	A	A	AS	AS	AWS	AWS	WS	W	W	W	W
-2	AS	AS	AS	AS	WS	WS	WS	W	W	W	W
-3	AS	S	S	S	WS	WS	WS	W	W	W	W
-4	S	S	S	S	WS	WS	WS	W	W	W	W

Log Water Solubility (mol/l at 298°K)

A = amount in air >10%
W = amount in water >10%
S = amount in solid >10%

Figure 3

MEASURED CONCENTRATION OF REFERENCE CHEMICALS IN AIR

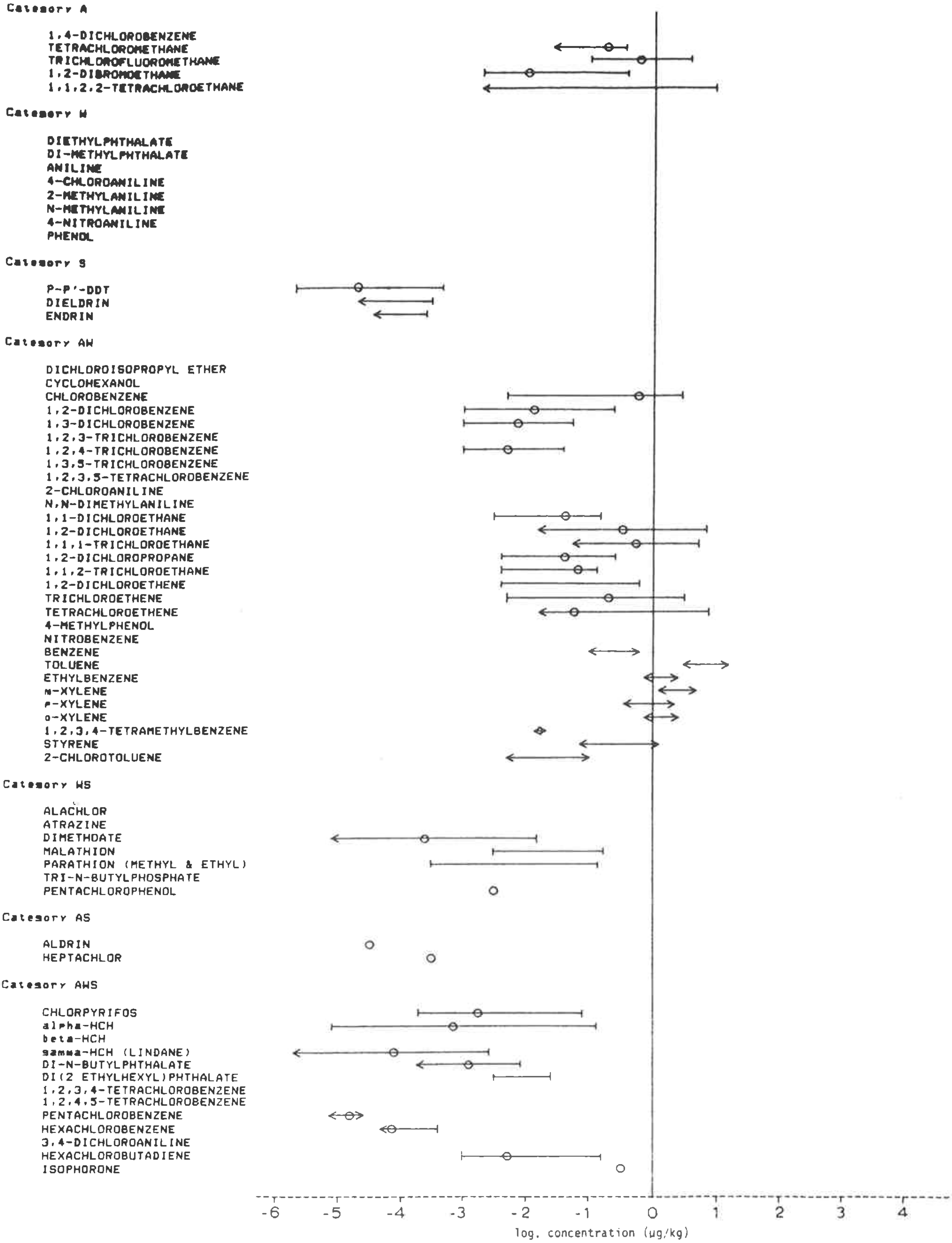


Figure 4

MEASURED CONCENTRATION OF REFERENCE CHEMICALS IN WATER

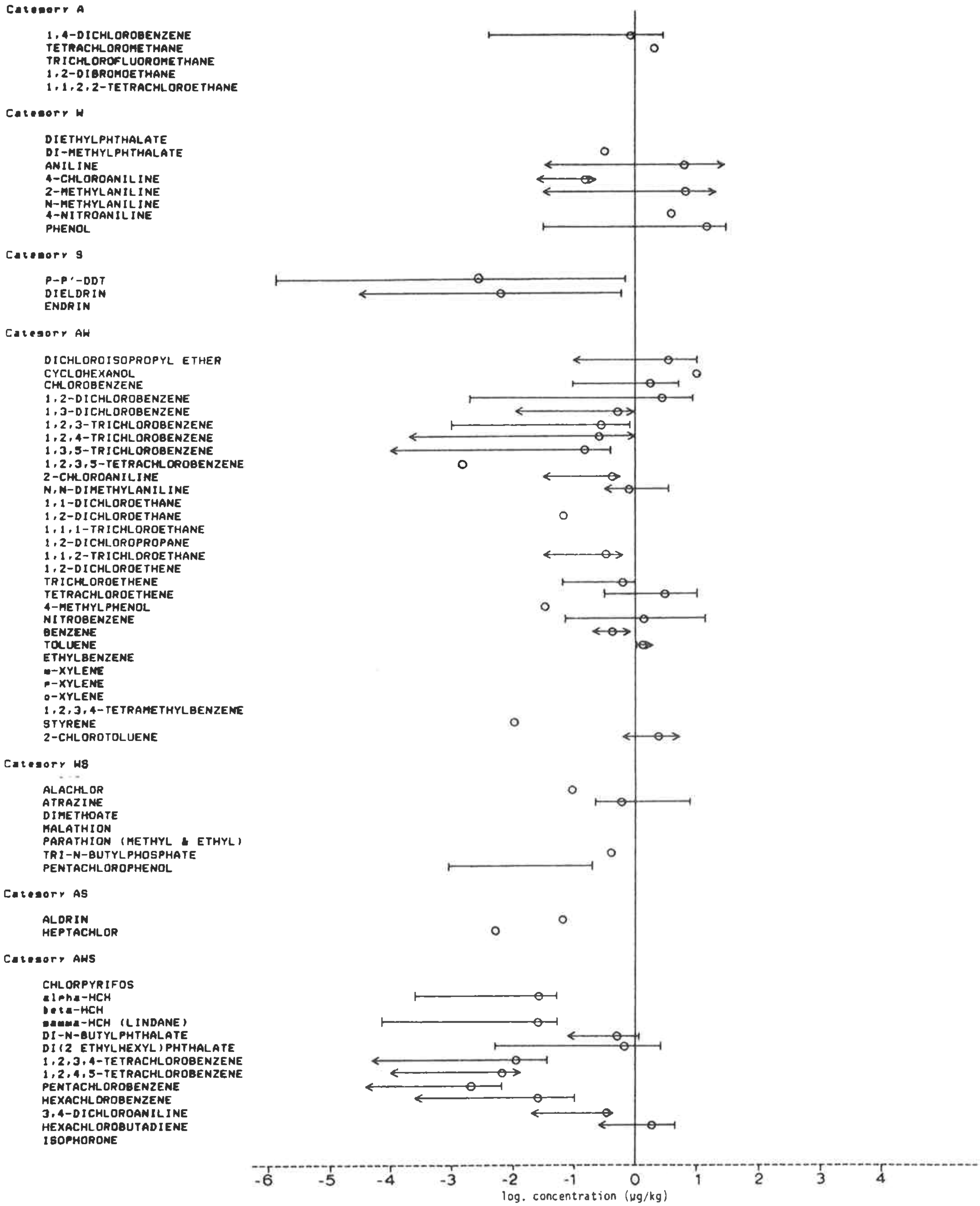


Figure 5

MEASURED CONCENTRATION OF REFERENCE CHEMICALS IN SEDIMENT

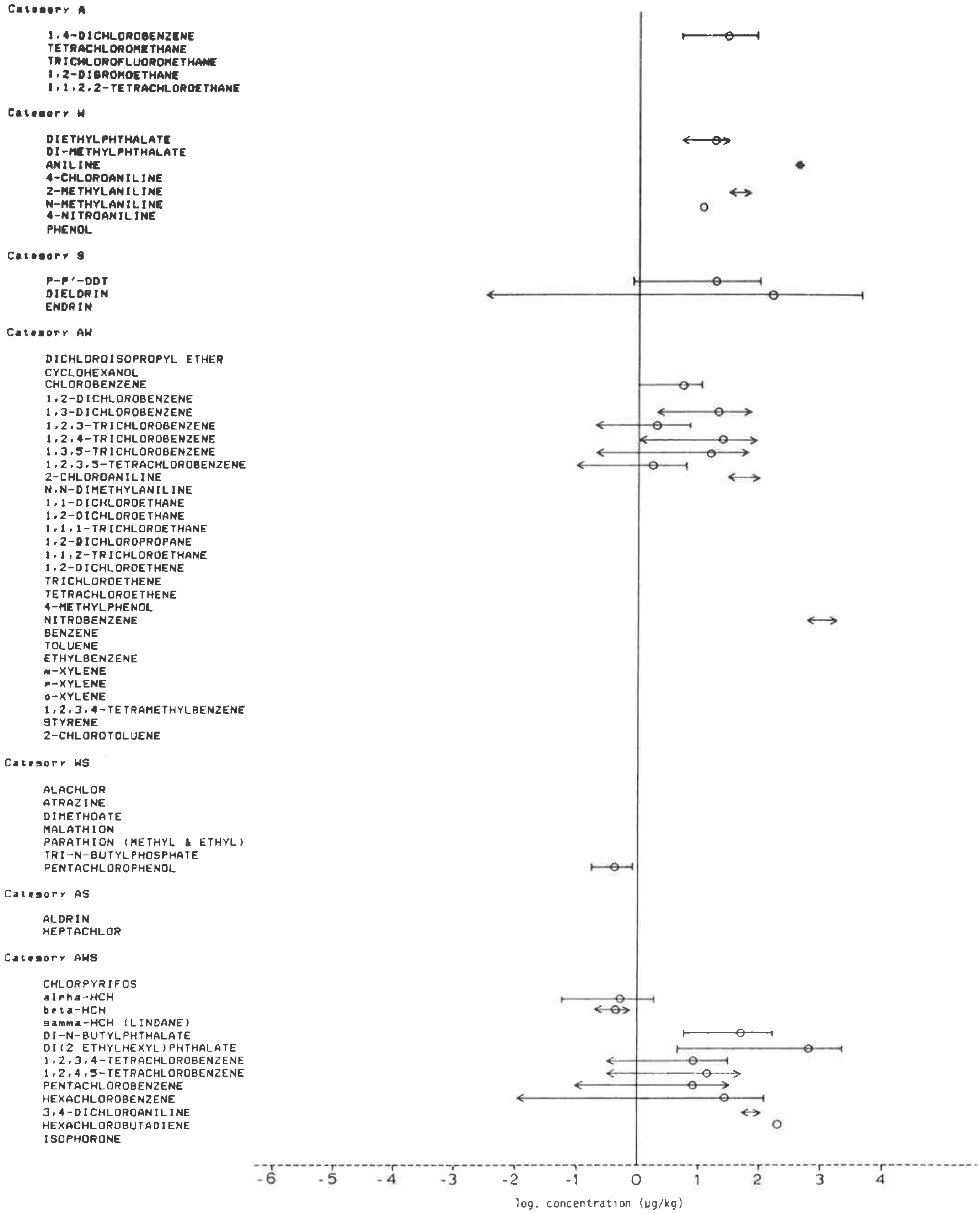
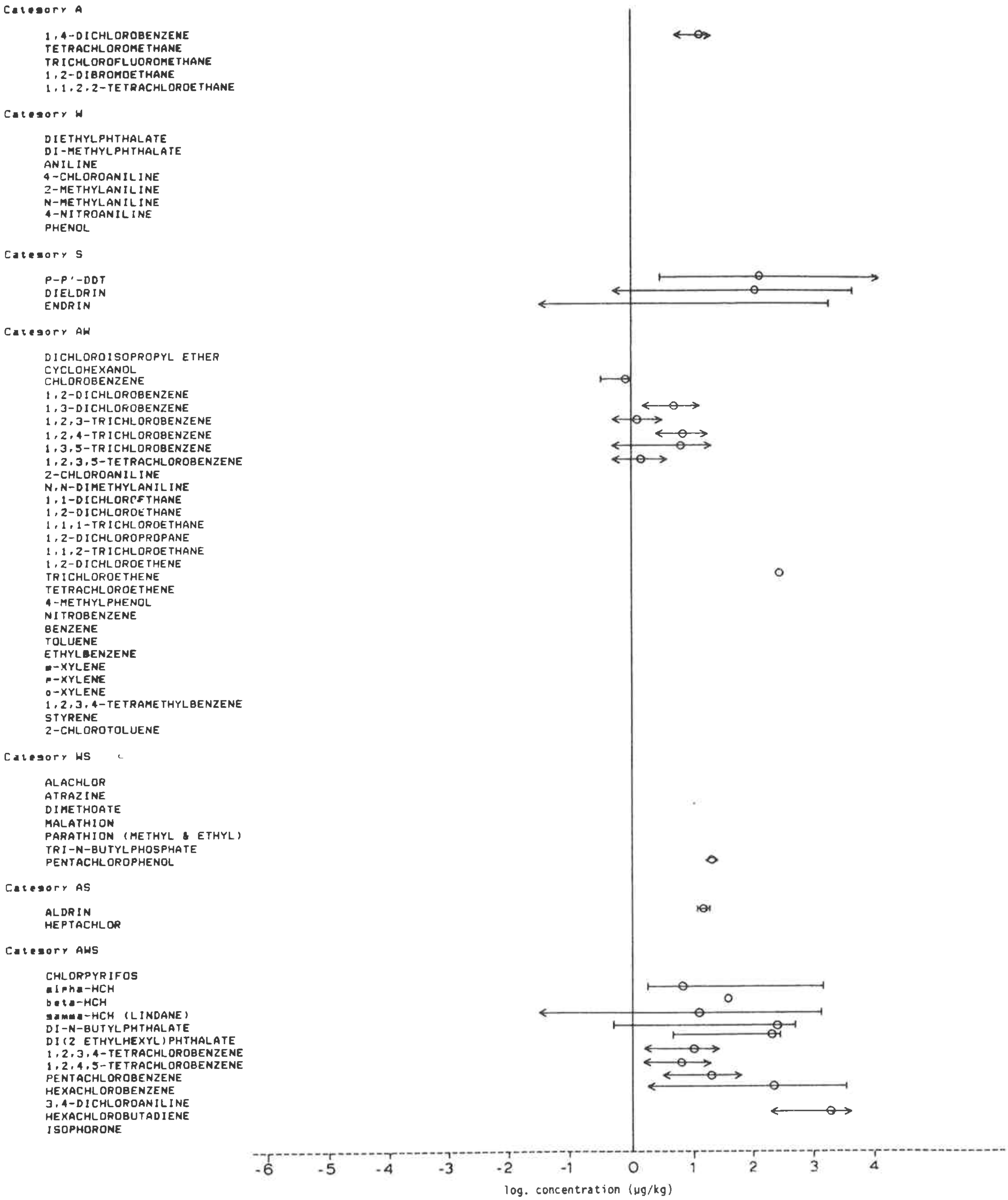


Figure 6

MEASURED CONCENTRATION OF REFERENCE CHEMICALS IN BIOTA



APPENDICES

APPENDIX 1

Environmental Distribution Categories

A. Environmental Distribution Categories

The seven environmental distribution categories distinguish between chemicals only on the basis of the compartment or compartments in which they ultimately appear after entry into the environment. In this scheme a chemical which enters the air compartment and is then transferred to water is placed in the same category (AW) as a substance which enters the water compartment and transfers to air.

A more complex categorisation scheme was also considered. In this the transfer process was taken into account as well as the ultimate environmental distribution, as follows.

B. Environmental Transfer Categories

There are 7 compartments or combinations of compartments by which chemicals can enter the environment, i.e. A, W, S, AW, AS, WS and AWS. Unless the entry compartment is the equilibrium compartment, a chemical will additionally be found in one or more of the remaining 6 compartments or combination of compartments. By combining the 7 possible entry compartments with the 7 possible transfer compartments, 49 expected distributions can be deduced as in Table A1.1. This was an unmanageably large number. Therefore duplicate distributions within each input compartment (in brackets in the final column of Table A1) were eliminated as being of minor significance leaving 19 "environmental transfer categories".

It was hoped that the environmental transfer categories would enable a more refined and informative study of concentrations to be made than would the use of the, simpler, environmental distribution categories. However, when the reference chemicals were allocated to their respective transfer categories and the data on concentration were examined in the light of the categories, no further useful information or correlations resulted.

TABLE A1.1.

Theoretically Possible Distribution Patterns derived from Environmental Transfer of Organic Chemicals

(A = air W = water S = solids)

Input Compartment	Equilibrium Compartment	Expected Distribution	Category
A	A	A	1
	W	A-W	2
	S	A-S	3
	A-W	(A-W)	4
	W-S	A-W-S	5
	A-S	(A-S)	6
	A-W-S	(A-W-S)	7
W	A	A-W	8
	W	W	9
	S	W-S	10
	A-W	(A-W)	11
	W-S	(W-S)	12
	A-S	A-W-S	13
	A-W-S	(A-W-S)	14
S	A	A-S	15
	W	W-S	16
	S	S	17
	A-W	A-W-S	18
	W-S	(W-S)	19
	A-S	(A-S)	20
	A-W-S	(A-W-S)	21
A-W	A	A-W	22
	W	(A-W)	23
	S	A-W-S	24
	A-W	(A-W)	25
	W-S	(A-W-S)	26
	A-S	(A-W-S)	27
	A-W-S	(A-W-S)	28
W-S	A	A-W-S	29
	W	W-S	30
	S	(W-S)	31
	A-W	(A-W-S)	32
	W-S	(W-S)	33
	A-S	(A-W-S)	34
	A-W-S	(A-W-S)	35
A-S	A	A-S	36
	W	A-W-S	37
	S	(A-S)	38
	A-W	(A-W-S)	39
	W-S	(A-W-S)	40
	A-S	(A-S)	41
	A-W-S	(A-W-S)	42
A-W-S	A	A-W-S	43
	W	(A-W-S)	44
	S	(A-W-S)	45
	A-W	(A-W-S)	46
	W-S	(A-W-S)	47
	A-S	(A-W-S)	48
	A-W-S	(A-W-S)	49

Duplicate expected distributions for any one input compartment are shown in brackets.

TABLE A1.2.

Environmental Distribution Categories

(A = Air W = Water S = Solids)

Input Compartment	Equilibrium Compartment	Environmental Distribution Category	Category
A	A	A	1
	W or A-W	A-W	2
	S or A-S	A-S	3
	W-S or A-W-S	A-W-S	4
W	A or A-W	A-W	5
	W	W	6
	S or W-S	W-S	7
	A-S or A-W-S	A-W-S	8
S	A or A-S	A-S	9
	W or W-S	W-S	10
	S	S	11
	A-W or A-W-S	A-W-S	12
A-W	A, W or A-W	A-W	13
	S, W-S, A-S or A-W-S	A-W-S	14
W-S	A, A-W, A-S or A-W-S	A-W-S	15
	W, S or W-S	W-S	16
A-S	A, S or A-S	A-S	17
	W, WS, AW	A-W-S	18
A-W-S	Whatever the Equilibrium Compartment the expected distribution can only be A-W-S	A-W-S	19

Appendix 2 : WRC Table of Physico-Chemical Properties and Equilibrium Distributions of All Chemicals Searched (Literature refs. in brackets)

AGROCHEMICALS

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Alachlor	270	2.9x10^{-3} (3)	240 (3)	3.22 (32)	0.09	79.63	20.29
Aldrin	365	1.0x10^{-2} (6)	0.013 (4)	6.23 (32)	27.07	0.28	72.65
Atrazine	216	4.0x10^{-5} (5)	30 (20)	2.68 (21)	0.01	93.15	6.84
Chlordane	410		0.056 (4)				
Chlorpyrifos	350	2.5x10^{-3} (2)	2.0 (2)	4.6 (2)	2.08	13.78	84.14
Cyanazine	241	2.7x10^{-7} (3)	171 (3)	2.2 (16)			
p-p'-DDT	355	2.5x10^{-5} (19)	3.3x10^{-3} (19)	6.19 (19)	0.40	0.42	99.18
* DDT							
Diazinon	304		41 (17)	3.14 (8)			
Dimethoate	229	1.1x10^{-3} (5)	25 000 (4)	1.78 (32)	0.00	99.08	0.91
Dieldrin	381	2.4x10^{-5} (19)	0.1 (19)	5.48 (19)	0.07	2.11	97.82
Endosulfan							
Endrin	381	2.7x10^{-5} (3)	0.1 (3)	5.63 (32)	0.05	1.50	98.44
Heptachlor	373	4.0x10^{-2} (6)	0.03 (4)	5.44 (8)	79.90	0.46	19.64
Heptachlor epoxide				5.40 (8)			
*-BCH	291	2.0x10^{-3} (18)	36 (32)	3.8 (16)	0.28	50.67	49.05
*-BCH	291	2.9x10^{-5} (18)	36 (32)	3.8 (16)	0.00	50.81	49.19
*-BCH (Lindane)	291	1.2x10^{-3} (22)	10 (22)	3.85 (21)	0.58	47.66	51.76
Malathion	330	5.3x10^{-3} (6)	150 (4)	2.9 (16)	0.36	88.82	10.82
Metribuzin	214		1200 (4)				
Parathion (methyl & ethyl)	291	6.3x10^{-4} (5)	24 (4)	3.8 (16)	0.13	50.75	49.13
Simazine	202	8.0x10^{-7} (3)	5 (3)	2.2 (16)			

PHTHALATE AND TEREPHTHALATE ESTERS

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Butylbenzylphthalate	312	1.1X10^{-3} (19)	2.9 (19)	4.78 (19)	0.42	9.72	89.86
Di-n-Butylphthalate	278	4.7X10^{-3} (23)	11.2 (13)	4.79 (13)	0.38	9.52	90.1
Di-i-Butylphthalate	278			4.11 (23)			
Di-s-Butylphthalate							
Di-i-Decylphthalate							
Diethylphthalate	222	0.22 (13)	1100 (13)	2.24 (13)	1.50	95.94	2.55
Di(2 Ethylhexyl)phthalate	391	8.6x10^{-4} (13)	0.34 (13)	5.11 (24)	1.62	4.74	93.65
Di-methylphthalate	194	0.22 (13)	4000 (13)	1.5 (13)	0.37	99.15	0.48
Diphenylphthalate							
Terephthalic acid							
Dimethyl terephthalate							

Appendix 2 WRC Table of Physico-Chemical Properties and Equilibrium Distributions of All Chemicals Searched (Literature refs. in brackets)(cont.)

PHOSPHATE ESTERS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Tri(2-butoxyethyl)phosphate							
Tri-n-Butylphosphate	266	0.23 (30)	280 (10)	4.00 (10)	2.90	38.32	58.79
Tri-i-Butylphosphate							
Tri-t-Butylphosphate							
Tri-(2-chloroethyl)phosphate							
Triethylphosphate							
Triphenylphosphate	326	9.3x10^{-4} (11)	1.9 (10)	4.6 (10)	0.77	13.96	85.28

ETHERS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Dibenzyl ether							
Dichloroisopropyl ether	171	110 (19)	1700 (19)	2.50 (32)	78.49	20.51	0.99
Bisdichloropropylether							
Tetrachloroisopropylether							
Tetrahydrofuran (THF)	72	1.7x10^{4} (19)					

ALCOHOLS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
2-Ethylhexanol	130	6.7 (19)	1000 (19)	2.9 (19)	21.16	70.27	8.56
Cyclohexanol	100	130 (7)	3.6x10^{4} (19)	1.2 (19)	11.08	88.71	0.21
1-phenylethanol	122	21 (7)					

Appendix 2 WRC Table of Physico-Chemical Properties and Equilibrium Distributions of All Chemicals Searched (Literature refs. in brackets) (cont.)

CHLOROBENZENES

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Chlorobenzene	113	1600 (25)	290 (1)	2.98 (1)	99.45	0.48	0.07
Σ Dichlorobenzenes							
1,2-Dichlorobenzene	147	200 (18)	92 (1)	3.38 (1)	98.77	0.90	0.33
1,3-Dichlorobenzene	147	300 (25)	69 (19)	3.48 (1)	99.36	0.44	0.21
1,4-Dichlorobenzene	147	80 (19)	31 (26)	3.37 (1)	98.98	0.75	0.27
Σ Trichlorobenzenes							
1,2,3-Trichlorobenzene	182	28 (25)	12 (26)	4.1 (25)	97.99	0.69	1.32
1,2,4-Trichlorobenzene	182	61 (25)	46 (26)	4.1 (25)	96.60	1.16	2.24
1,3,5-Trichlorobenzene	182	32 (25)	4.1 (26)	4.1 (25)	99.40	0.20	0.39
Σ Tetrachlorobenzenes							
1,2,3,4-Tetrachlorobenzene	216	5.2 (25)	12 (26)	4.55 (26)	83.16	2.61	14.22
1,2,3,5-Tetrachlorobenzene	216	9.8 (25)	5.3 (26)	4.65 (26)	94.62	0.69	4.70
1,2,4,5-Tetrachlorobenzene	216	0.72 (25)	2.4 (26)	4.51 (26)	79.32	3.47	17.21
Pentachlorobenzene	250	0.22 (25)	0.83 (26)	5.19 (21)	48.10	2.10	49.81
Hexachlorobenzene	285	$1.2x10^{-3}$ (19)	$4.5x10^{-3}$ (26)	6.18 (19)	10.11	0.39	89.50

AROMATIC AMINES

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Aniline	93	40 (30)	$3.4x10^{4}$ (19)	0.95 (30)	3.64	96.23	0.13
Chloroaniline							
2-Chloroaniline	128	24 (7)	9500 (32)	1-9 (19)	9.95	88.97	1.08
3-Chloroaniline							
4-Chloroaniline	128	2 (19)	$1.3x10^{4}$ (32)	1.8 (19)	0.67	93.38	0.95
2,4-Dichloroaniline							
3,4-Dichloroaniline	162	1.3 (12)	92 (12)	3.35 (32)	37.07	46.84	16.09
2,5-Dichloroaniline							
2,6-Dichloroaniline							
3,5-Dichloroaniline							
2,3 & 2,5-Dichloroaniline							
2-Methoxyaniline							
4-Methoxyaniline							
2-Methylaniline	107	13 (19)	$1.5x10^{4}$ (19)	1.3 (19)	3.10	96.61	0.29
4-Methylaniline	107		7400 (19)	1.4 (19)			
Σ Dimethylaniline							
N,N-Diethylaniline	149	18 (7)	1400 (6)	2.52 (32)	38.67	58.37	2.96
N,N-Dimethylaniline	121	67 (19)	1200 (32)	2.5 (19)	69.02	29.55	1.43
N-Ethylaniline							
N-Methylaniline	107	40 (19)	16 000 (32)	1.7 (19)	8.41	90.89	0.70
Σ Nitroanilines							
2-Nitroaniline	138		1300 (19)	1.6 (19)			
3-Nitroaniline	138		890 (19)	1.4 (19)			
4-Nitroaniline	138	0.2 (19)	800 (19)	2.66 (32)	1.10	92.42	6.49

Appendix 2 WRC Table of Physico-Chemical Properties and Equilibrium Distributions of All Chemicals Searched (Literature refs. in brackets) (cont.)

CHLOROALKANES

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Tetrachloromethane	153	$1.2x10^4$ (19)	1200 (19)	2.7 (8)	99.80	0.19	0.02
Trichlorofluoromethane	137	$8.9x10^4$ (2)	1100 (2)	2.4 (2)	99.97	0.03	0.00
1,1-Dichloroethane	99	$3.1x10^4$ (19)	5500 (19)	1.99 (32)	99.48	0.52	0.00
1,2-Dichloroethane	99	8100 (19)	800 (27)	2.82 (27)	99.97	0.03	0.00
1,2-Dibromoethane	188	1500 (19)	4.3 (19)	4.30 (32)	99.98	0.00	0.02
1,1,1-Trichloroethane	133	$1.3x10^4$ (19)	130 (27)	2.95 (27)	99.98	0.02	0.00
1,1,2-Trichloroethane	133	2500 (19)	4500 (19)	2.13 (32)	96.16	3.76	0.08
Trichloroethane							
1,1,1,2-Tetrachloroethane	168						
1,1,2,2-Tetrachloroethane	168	670 (19)	2900 (19)	2.45 (27)	92.75	6.95	0.30
1,2-Dichloropropane	113	6700 (19)	2700 (19)	2.24 (32)	98.95	1.02	0.02
$C_{10}-C_{20}$ Chlorinated paraffins							
$C_{20}-C_{30}$ Chlorinated paraffins							

CHLOROALKENES

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
1,1-dichloroethene	97	$7.9x10^4$ (19)					
1,2-dichloroethene	97	$2.7x10^4$ (19)	800 (19)	2.55 (32)	99.91	0.09	0.00
Trichloroethene	131	9870 (30)	1400 (1)	2.53 (1)	99.67	0.31	0.02
Tetrachloroethene	166	2100 (28)	480 (27)	3.38 (28)	99.45	0.40	0.15
Hexachlorobutadiene	261	0.84 (19)	2.0 (19)	4.8 (8)	78.02	2.06	19.93

PHENOLS

Chemical	Physico-chemical parameters				Equilibrium Mass %		
	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Phenol	94	27 (19)	$8.2x10^4$ (19)	1.5 (8)	1.05	98.47	0.48
Σ Dichlorophenols							
Σ Trichlorophenols							
Σ Tetrachlorophenols							
Pentachlorophenol	266	0.015 (19)	14 (19)	5.01 (19)	0.58	5.95	93.47
t-Butylphenol	150		650 (15)	3.3 (19)			
Nonylphenol							
Propoxyphenol							
Σ Cresols							
2-methylphenol							
3-methylphenol							
4-methylphenol	108	14.4 (33)	1800 (33)	2.2 (33)	22.58	75.58	1.84

Appendix 2 : WRC Table of Physico-Chemical Properties and Equilibrium Distributions of All Chemicals Searched (Literature refs. in brackets) (cont.)

AROMATIC NITRO COMPOUNDS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Nitrobenzene	123	20 (19)	1900 (19)	2.15 (26)	30.49	68.04	1.47
o & p Nitrotoluene							
2-Nitrotoluene							
4-Nitrotoluene							
2-Nitroanisole							
4-Nitroanisole	153		70 (19)	20 (19)			
Σ Chloro nitro benzenes							

AROMATIC HYDROCARBONS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Benzene	78	1.0x10^4 (19)	1800 (19)	2.13 (19)	99.34	0.65	0.02
Toluene	92	2900 (19)	580 (1)	2.65 (1)	99.34	0.62	0.04
Ethylbenzene	106	930 (19)	190 (19)	3.13 (1)	99.35	0.54	0.11
Σ Xylenes							
m-xylene	106	800 (1)	160 (19)	3.2 (1)	99.33	0.54	0.13
p-xylene	106	870 (19)	210 (26)	3.18 (1)	99.18	0.67	0.15
o-xylene	106	670 (19)	220 (19)	3.13 (1)	98.92	0.89	0.19
styrene	104	670 (19)	300 (19)	2.95 (31)	98.60	1.23	0.17
2-Methyl Ethylbenzene	120		74 (1)	3.53 (1)			
Σ Trimethylbenzenes							
1,3,5-Trimethylbenzenes	120		0.81 (29)	3.42 (29)			
1,2,3,4-Tetramethylbenzene	134	30 (7)	9.1 (32)	3.98 (1)	98.41	0.64	0.95

MISCELLANEOUS

	Physico-chemical parameters				Equilibrium Mass %		
Chemical	Molecular weight	Vapour pressure (Pa)	Solubility (gm^{-3})	log Kow	Air	Water	Solid
Acetophenone	120	45 (7)					
3,4-Dichloroacetophenone							
N-Butylbenzenesulphonamide							
Di(2-Ethylhexyl)adipate							
Isophorone	138	49 (7)	1400 (9)	1.67 (9)	65.92	33.83	0.25
Methylbutanoate							
Methylmaleate							
Methylmethacrylate							
2-Chlorotoluene	127	350 (7)	57 (32)	3.42 (19)	99.48	0.37	0.15
PCB (1242 &/or 1254)							
PCB (1242)							
PCB (1254)							
PCB (1260)							
Σ PCB							

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Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated)

3.1 Agrochemicals - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
ALACHLOR 15972-60-8							
W	USA, Iowa	R Des Moines	0.089	-	-	-	81-5
ALDRIN 309-00-2							
A	NL, various	-	0.03 ppt	-	-	-	85-1
W	NL, Lobith	R Rhine	0.06	-	-	-	80-2
B	Turkey, E Coast Med	Fish	11.1 (dry)	-	5-species	-	80-4
	Various, Mediterranean	fish	17.2 (dry)	-	-	-	80-4
ATRAZINE 1912-24-9							
W	USA, Iowa	R Des Moines	0.223	-	-	-	81-5
	Canada, S W Ontario	Billman Creek	0.85-0.94	-	-	-	79-2
	USA, various	S waters	-	7.66	6.8%	-	85-5
S	USA, various	S waters	-	11.9	0.7%	-	85-5
CHLORDANE 12789-03-6							
A	Pacific, Enewetak Atoll	Remote	0.01 ppt	-	-	-	81-2
	American Samoa, Samoa	Remote	0.0008 ppt	-	-	-	85-2
	Peru, Peruvian coast	Remote	0.0008 ppt	-	-	-	85-2
	New Zealand	Remote	0.002 ppt	-	-	-	85-2
	USA, 10 locations	Various	0.04-0.3 ppt	6.13 ppt	14/123	-	85-5
W	USA, Texas	Est. Nueces	0.18 ppt	-	-	-	83-2
	USA, various	S waters	-	0.23	1.1%	-	85-5
S	USA, various	S waters	-	2964	15.3%	-	85-5
	USA, Texas	Est. Nueces	0.77 ppt (dry)	-	-	-	83-2
	USA (Maine), Portland	Estuarine	1.8 (dry)	-	8/8	-	83-3
	USA (Fl), R Apalachicola	Bottom load	6900 (dry)	-	-	1700-10 000	84-1
B	Finland. South Lakes	Fish (Pike)	20.0 (wet)	-	1-species	-	83-4
	Finland, North Lakes	Fish (Pike)	16.0 (wet)	-	1-species	-	83-4
	Finland, Coast	Fish (Pike)	14.0 (wet)	-	1-species	-	83-4
	USA (Maine), Portland Coast	Shellfish	3.1	-	2-species	-	83-3
	USA (Fl), R Apalachicola	Shellfish (Clams)	21.0 (dry)	-	1-species	16-68	84-1
	Mexico, Gulf Coast	Shellfish (Oysters)	0.03-0.1	-	1-species	-	79-3
	USA, various (76-81)	Fish	-	2530 (wet)	(NPMP-87%)	-	85-4
CHLORPYRIFOS 2921-88-2							
A	USA	10 locations	0.2-1.8 ppt	84.0 ppt	14/123	-	85-5
CYANAZINE 21725-46-2							
W	USA, Iowa	R Des Moines	0.091	-	-	-	81-5
	Canada, S W Ontario	Billman Creek	11.5	-	2	-	79-2
CYPRAZINE 22936-86-3							
W	Canada, S W Ontario	Billman Creek	273.0	-	1	-	79-2
o-p'DDD 53-19-0							
A	NL, various	-	0.014 ppt	0.1 ppt	-	-	85-1
B	Austria, Alpine lakes	Fish	6.0 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	0.2 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	2.0 (lipid)	-	several	-	80-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
p-p'-DDD 72-54-8							
A	NL, various	-	0.006 ppt	0.04 ppt	-	-	85-1
S	Turkey, E Coast Med	Marine	9.2 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	7.0 (dry)	-	-	-	80-4
B	USA, various (1976-1981)	Fish	-	3430.0 (wet)	many (NPMP)	98%	85-4
	Turkey, E Coast Med	Fish	30.7 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	293.0 (dry)	-	-	-	80-4
	Austria, Alpine lakes	Fish	79.0 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	0.6 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	10.0 (lipid)	-	several	-	80-5
Σ DDD							
W	NL, Lobith	R Rhine	0.004	-	-	-	80-2
S	USA, Florida	R Apalachicola	2300 (dry)	-	-	100-12000	84-1
B	USA (Fl), R Apalachicola	Shellfish (Clam)	8.0 (dry)	-	1-species	2.8-44.0	84-1
o,p'-DDE 3424-82-6							
A	NL, various	-	0.021 ppt	0.12 ppt	-	-	85-1
W	USA, various	S Waters	-	0.54	0.3%	-	85-5
S	USA, various	S Waters	-	1.3	0.5%	-	85-5
B	Austria, Alpine lakes	Fish	15.0 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	0.6 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	6.0 (lipid)	-	several	-	80-5
p,p'-DDE 72-55-9							
A	NL, various	-	0.014 ppt	0.076 ppt	-	-	85-1
	New Zealand	Remote	0.002 ppt	-	-	-	85-2
	N Atlantic	Remote Mar	0.005 ppt	-	-	-	81-2
	Gulf of Mexico	Remote Mar	0.07 ppt	-	-	-	81-2
	USA, Texas (Coll. St.)	Urban	0.29 ppt	-	-	-	81-2
	USA, Florida (Pigeon Key)	-	0.03 ppt	-	-	-	81-2
	Gulf of Mexico	Remote Mar	0.04 ppt	-	-	0.008-0.15 ppt	80-1
	Pacific, Enewetak Atoll	Remote	0.0025 ppt	-	-	0.002-0.004 ppt	81-2
W	NL, Lobith	R Rhine	0.003	-	-	-	80-2
	USA, 3 stations	R Des Moines	<0.001	-	-	-	81-5
	USA, various	S Waters	-	0.55	0.7%	-	85-5
S	USA, 3 stations	R Des Moines	0.0057	-	-	-	81-5
	Turkey, E Coast Med	Marine	1.9 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	2.7 (dry)	-	-	-	80-4
	USA, N W Florida	R Apalachicola	2500 (dry)	-	-	1500-4000	84-1
	USA, various,	S Waters	-	163-0	22.7%	-	85-5
B	Turkey, E Coast Med	Fish	56.4 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	296.0 (dry)	-	-	-	80-4
	USA, various	Fish	-	6760 (wet)	(many NPMP-100%)	-	85-4
	USA (Fl), R Apalachicola	Shellfish (Clams)	18.0 (dry)	-	1-species	9.1-46.0	84-1
	Gulf of Mexico	Fish	16.5 (wet)	-	1-species	-	74-1
	Grand Bahamas	Fish	2.12 (wet)	-	1-species	-	74-1
	Austria, Alpine lakes	Fish	477.0 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	5.2 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	44.0 (lipid)	-	several	-	80-5
o,p'-DDT 789-02-6							
W	NL, Lobith	R Rhine	0.003	-	-	-	80-2
	USA, Various	S waters	-	0.42	0.1%	-	85-5
S	USA, various	S waters	-	7.2	2.9%	-	85-5
B	Austria, Alpine lakes	Fish	10.0 (lipid)	-	several	-	80-5
	Antarctic, Ocean	Fish	1.0 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	1.0 (lipid)	-	several	-	80-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL	CONCENTRATIONS			
			Average	Max	Samples	Range	Ref.
p,p'-DDT 50-29-3							
A	NL, various	-	0.048 ppt	0.45 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.01	-	-	-	80-2
	USA, various	S waters	-	0.7	0.5%	-	85-5
S	USA, various	S Waters	-	110.6	13.2%	-	85-5
B	Gulf of Mexico	Fish	12.19 (wet)	-	1-species	-	74-1
	Grand Bahamas	Fish	1.15 (wet)	-	2 species	-	74-1
	NL, Coast (various)	Shellfish (Mussel)	4.0 (wet)	-	1-species (2/14)	-	79-5
	USA, various (76-81)	Fish	-	2690 (wet)	many (NPMP) 79%	-	85-4
	Turkey, E Coast Med	Fish	40.0 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	370.0 (dry)	-	-	-	80-4
	Austria, Alpine lakes	Fish	59.0 (lipid)	-	several	-	80-5
	Antarctic, Ocean	Fish	3.9 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	10.0 (lipid)	-	several	-	80-5
Σ DDT							
A	Gulf of Mexico	Remote	0.03 ppt	-	-	0.008-0.07 ppt	80-1
	USA, Gulf of Mexico	Remote & Coastal	0.034 ppt	-	8	-	78-1
	N Atlantic	Remote	0.005 ppt	-	5	-	78-1
	American Samoa Islands	Remote	0.002 ppt	-	-	-	85-2
	Peru, Coast	Remote	0.002 ppt	-	-	-	85-2
W	USA, Gulf of Mexico	Remote & Coastal	0.03 ppt	-	17	-	78-1
	N Atlantic	-	ND	-	0/10	-	78-1
	USA	Mississipi Delta	0.0017	-	14	-	78-1
	USA, Texas	Est Nueces	0.0013	-	-	-	83-2
S	Turkey, E Coast Med	Marine	16.1 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	13.0 (dry)	-	-	-	80-4
	USA, Maine (Portland)	Estuarine	8.0 (dry)	-	-	-	83-3
	USA, Texas	Est Nueces	1.5 (dry)	-	-	-	83-2
	USA, Florida	R Apalachicola	<100.0 (dry)	-	-	<100-7800	84-1
	USA, Gulf of Mexico	Remote & Coastal	0.77	-	12	-	78-1
	USA, Mississipi Delta	-	4.2	-	22	-	78-1
B	Gulf of Mexico	Fish	27.75 (wet)	-	1-species	-	74-1
	Grand Bahamas	Fish	3.2 (wet)	-	2-species	-	74-1
	Gulf of Mexico	Fish/Shellfish	11.4	-	20	-	78-1
	Mexico, 6 coast stations	Shellfish (Oysters)	9.7-14.5 (wet)	-	1-species	-	79-3
	Turkey, E Coast Med	Fish	82.0 (wet)	-	4-species (82)	-	80-4
	Turkey, E Coast Med	Shellfish	19.5 (wet)	-	2-species (67)	-	80-4
	USA, R Des Moines	Fish	62.0 (wet)	-	7-species	-	81-5
	USA, Maine (Portland)	Shellfish	6.2	-	2-species	-	83-3
	USA (Fl), R. Apalachicola	Shellfish (Clams)	3.0 (dry)	-	1-species	0.1-16.0	84-1
	Finland, South Lakes	Fish (Pike)	35.0 (wet)	-	1-species	-	83-4
	Finland, North Lakes	Fish (Pike)	42.0 (wet)	-	1-species	-	83-4
	Finland, Coast	Fish (Pike)	64.0 (wet)	-	1-species	-	83-4
	USA, various (76-81)	Fish	-	10620.0 (wet)	many (NPMP) 100%	-	85-4
	Austria, Alpine Lakes	Fish	646.0 (lipid)	-	several	-	80-5
	Antarctic, Ocean	Fish	11.5 (lipid)	-	-	-	80-5
	Peru, S Pacific	Fish	73.0 (lipid)	-	several	-	80-5
DIAZINON 333-41-5							
A	USA, 10 locations	-	0.85-1.76 ppt	19.32 ppt	59/123	-	85-5
W	USA, various	S Water	-	2.38	1.2%	-	85-5
S	USA, various	S Water	-	7.1	0.5%	-	85-5
DIMETHOATE 60-51-5							
A	USA, 10 locations	-	0.008-0.25 ppt	15.12 ppt	4/123	-	85-5
DIELDRIN 60-57-1							
A	Pacific, Enewetak Atoll	Remote	0.008 ppt	-	-	0.005-0.015 ppt	81-2
	USA, Texas (Coll.St.)	Urban	0.059 ppt	-	-	-	81-2
	Bermuda, Island	Remote	0.017 ppt	-	-	-	76-1

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
	American Samoa Island	Remote	0.002 ppt	-	-	-	85-2
	Peru, Coast	Remote	0.003 ppt	-	-	-	85-2
	New Zealand	Remote	0.002 ppt	-	-	-	85-2
	NL, various	-	0.061 ppt	0.31 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.003	-	-	-	80-2
	USA, Iowa	R Des Moines	0.003-0.014	-	-	-	81-5 & 8
	USA, Texas	Est Nueces	0.03 ppt	-	-	-	83-2
	USA, various	S waters	-	0.61	2.4%	-	85-5
S	USA, Iowa	R Des Moines	0.003-0.004	-	-	-	81-7
	USA, Texas	Est Nueces	0.14 (dry)	-	-	-	83-2
	USA, Florida	R Apalachicola	500.0 (dry)	-	-	300-1700	84-1
	USA, various	S waters	-	5300	21.7%	-	85-5
B	USA (Fl), R Apalachicola	Shellfish (Clams)	2.0 (dry)	-	1-species	0.5-2.9	84-1
	USA (Io), R Des Moines	Fish	67.0 (wet)	-	7-species	-	81-5
	NL, Coast (various)	Shellfish (Mussel)	4.0-10.0 (wet)	-	1-species (6/14)	-	79-5
	Mexico, Coast	Shellfish (Oyster)	0.6-0.91 (wet)	-	1-species	-	79-3
	USA, various (76-81)	Fish	-	5010 (wet)	many (NPMP) 83%	-	85-4
α-ENDOSULFAN 115-29-7							
A	NL, various	-	0.14 ppt	0.95 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.003	-	-	-	80-2
B	D, Wadden Sea	Shellfish	0.42 (wet)	-	4-species	-	79-4
	D, Wadden Sea	Fish (Sole)	1.3 (wet)	-	1-species	-	79-4
β-ENDOSULFAN 33213-65-9							
W	NL, Lobith	R Rhine	0.002	-	-	-	80-2
B	USA, Mexico coast	Shellfish (Oyster)	0.06-0.15 (wet)	-	1-species	-	79-3
ENDRIN 72-20-8							
A	NL, various	-	0.034 ppt	0.252 ppt	-	-	85-1
W	USA, various	S waters	-	0.04	0.1%	-	85-5
S	USA, various	S waters	-	2.9	1.3%	-	85-5
B	NL, Coast (various)	Shellfish (Mussel)	3.0-7.0 (wet)	-	1-species (5/14)	-	79-5
	USA, various (76-81)	Fish	-	400.0 (wet)	NPMP (34%)	-	85-4
	Mexico, Gulf coast	Fish (Oysters)	0-0.03	-	1-species	-	79-3
HEPTACHLOR 76-44-8							
A	NL, various	-	0.311 ppt	0.160 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.005	-	-	-	80-2
B	USA, various (76-81)	Fish	-	1170.0 (wet)	(NPMP-49%)	-	85-4
HEPTACHLOR EPOXIDE 1024-57-3							
A	NL, various	-	0.027 ppt	0.3 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.003	-	-	-	80-2
S	USA, Florida	R Apalachicola	<100.0 (dry)	-	-	<100-600	84-1
B	USA (Fl), R Apalachicola	Shellfish (Clam)	0.3 (dry)	-	1-species	0.1-0.6	84-1
	USA (Io) R Des Moines	Fish	8.0 (wet)	-	7-species	-	81-5 & 8
	Austria, Alpine lakes	Fish	5.0 (lipid)	-	several	-	80-5
	Antarctic, Ocean	Fish	0.02 (lipid)	-	several	-	80-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
α-HEXACHLOROCYCLOHEXANE 319-84-6							
A	Pacific, Enewetak Atoll	Remote	0.210 ppt	-	-	0.065-0.48 ppt	81-2
	Amer. Samoa islands	Remote	0.025 ppt	-	-	-	85-2
	Peru coast	Remote	0.008 ppt	-	-	-	85-2
	New Zealand	Remote	0.021 ppt	-	-	-	85-2
	NL, various	-	0.210 ppt	1.0 ppt	-	-	85-1
	USA, 10 locations	-	1.42-3.4 ppt	129.4 ppt	52/123	-	85-5
W	NL, Lobith	R Rhine	0.05	-	-	-	80-2
	USA, Texas	Est. Nueces	0.26 ppt	-	-	-	83-2
S	USA, Portland Maine	Estuarine	0.14 (dry)	-	-	-	83-3
	USA, Texas	Est. Nueces	0.06 (dry)	-	-	-	83-2
	Turkey, E Coast Med.	Marine	1.80 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	0.10 (dry)	-	-	-	80-4
B	Turkey, E Coast Med.	Fish	7.8 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	16.0 (dry	-	-	-	80-4
	USA, Portland Maine	Shellfish	0.37	-	2 species	-	83-3
	D, Wadden Sea	Shellfish	1.95 (dry)	-	4 species	-	79-4
	D, Wadden Sea	Fish (Sole)	4.1 (wet)	-	1 species	-	79-4
	USA, various (76-81)	Fish	-	300.0 (wet)	(NPMP 66%)	-	85-4
	Austria, Alpine lakes	Fish	40.2 (lipid)	-	various	-	80-5
	Ocean, Antarctic	Fish	0.1 (lipid)	-	various	-	80-5
	Peru, S. Pacific	Fish	7.4 (lipid)	-	various	-	80-5
β-HEXACHLOROCYCLOHEXANE 319-85-7							
S	Turkey, E Coast Med	Marine	0.2 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	0.7 (dry)	-	-	-	80-4
B	Turkey, E Coast Med	Fish	37.7 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	41.3 (dry)	-	-	-	80-4
	Austria, Alpine lakes	Fish	4.1 (lipid)	-	various	-	80-5
	Ocean, Antarctic	Fish	0.1 (lipid)	-	various	-	80-5
	Peru, S. Pacific	Fish	1.5 (lipid)	-	various	-	80-5
γ-HEXACHLOROCYCLOHEXANE (LINDANE) 58-89-9							
A	Pacific, Enewetak Atoll	Remote	0.013 ppt	-	-	0.005-0.018 ppt	81-2
	American Samoa Islands	Remote	0.002 ppt	-	-	-	85-2
	New Zealand	Remote	0.008 ppt	-	-	-	85-2
	NL, various	-	0.30 ppt	2.86 ppt	-	-	85-1
W	NL, Lobith	R Rhine	0.05	-	-	-	80-2
	USA, Texas	Est. Nueces	0.07 ppt	-	-	-	83-2
S	USA, Texas	Est. Nueces	0.03 (dry)	-	-	-	83-2
	NL Coast (various)	Shellfish (mussel)	0-5.0 (wet)	-	1 species (1/4)	-	79-5
	USA, various (76-81)	Fish	-	280.0 (wet)	(NPMP-18%)	-	85-4
	D, Wadden Sea	Shellfish	2.2 (wet)	-	4 species	-	79-4
	D, Wadden Sea	Fish (Sole)	3.1 (wet)	-	1 species	-	79-4
	Austria, Alpine lakes	Fish	17.2 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	0.1 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	1.5 (lipid)	-	several	-	80-5
MALATHION 121-75-5							
A	USA, 10 locations	-	3.17-6.3 ppt	184.8 ppt	62/123	-	85-5
W	USA, various	S waters	-	0.18	0.3%	-	85-5
S	USA, various	S waters	-	ND	-	-	85-5
METRIBUZIN 21087-64-9							
W	Canada, S W Ontario	Billman Creek	4.38-4.97	-	15/17	-	79-2
PARATHION (METHYL & ETHYL) 56-38-2							
A	USA, 10 locations	-	0.3-2.4 ppt	134.4 ppt	15/123	-	85-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

			ENVIRONMENTAL		CONCENTRATIONS		
	Location	Description	Average	Max	Samples	Range	Ref.
SIMAZINE 122-34-9							
W	Canada, S W Ontario	Hillman Creek	0.05-0.13	-	-	-	79-2
	USA, various	S waters	-	1.13	0.4%	-	85-5
S	USA, various	S waters	-	0.1	0.2%	-	85-5
TOXAPHENE 8001-35-2							
W	USA, various	S waters	-	1.65	0.01%	-	85-5
S	USA, various	S waters	-	814.5	1.8%	-	85-5
B	USA, various (76-81)	Fish	-	21000.0 (wet)	(NPMP-69%)	-	85-4
	USA (Fl), R Apalachicola	Shellfish (clam)	10.0 (dry)	-	1 species	10-300	84-1

3.2 Phthalate and terephthalate esters - environmental concentrations

			ENVIRONMENTAL		CONCENTRATIONS		
	Location	Description	Average	Max	Samples	Range	Ref.
BUTYL BENZYL PHTHALATE 85-68-7							
W	USA (Mi)	R Saginaw	0.43	-	7/7	-	80-3
	USA (Mo), 3 rivers,	R Maramec/Missouri/Mississipi	0.78-1.05	-	20/27	-	80-3
	USA (Il), Waukegan	S waters	0.12-0.24	-	5/10	-	80-3
	USA, Pa/NJ	R Delaware	-	-	16/16	0.3-1.0	78-5
	USA (Mi)	R Saginaw	483.0	-	6/6	-	80-3
DI-N-BUTYLPHTHALATE 84-74-2							
A	B, Antwerp	Urban	40.0 ppt	-	-	20-60 ppt	77-1
	Bolivia, various	Remote	20.0 ppt	-	-	20-30 ppt	77-1
	USA, New York	Urban	4.0 ppt	-	-	0.1-9.0 ppt	78-2
	USA,Gulf of Mexico	Remote & Coastal	0.2 ppt	-	8	-	78-1
	N Pacific	Remote	0.7 ppt	-	-	0.3-1.5 ppt	81-1
	USA, Gulf of Mexico	-	1.1 ppt	-	-	0.3-3.1 ppt	80-1
	N Atlantic	-	0.8 ppt	-	5	-	78-1
W	USA, Texas	Est. Nueces	0.13	-	-	-	83-2
	USA, Gulf of Mexico	Remote & Coastal	0.08	-	17	-	78-1
	USA	Mississipi Delta	0.10	-	14	-	78-1
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL/D border	R Rhine	1.1	-	-	-	78-4
	NL, Maassluis/Lobith	R Rhine	0.2-0.5	1.0	3/6	-	79-6
	USA, Pa/NJ	R Delaware	-	-	16/16	0.1-0.6	78-5
S	USA, Portland Maine	Estuarine	160.0 (dry)	-	-	-	83-3
	USA, Texas	Est Nueces	20.0 (dry)	-	-	-	83-2
	USA (Tx), St Luis Pass	-	60.0 (dry)	-	-	-	81-4
	USA, Chesapeake Bay	-	58.0 (dry)	-	-	-	82-3
	USA, Gulf of Mexico	Remote & Coastal	5.5	-	12	-	78-1
	USA	Mississsipi Delta	13.0	-	22	-	78-1
B	USA, Portland Maine	Shellfish	100.0	-	2 species	-	83-3
	USA, Gulf of Mexico	Fish/shellfish	0.1	-	20	-	78-1
DI-I-BUTYLPHTHALATE 84-69-5							
A	B, Antwewrp	Urban	31.0 ppt	-	-	20-42 ppt	77-1
	Bolivia	Remote	8.0 ppt	-	-	7-8 ppt	77-1
W	NL, Lobith	R Rhine	0-0.1	0.1	1/6	-	79-6
S	USA, Chesapeake Bay	-	5.8 (dry)	-	-	-	82-3

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
DI-S-BUTYLPHTHALATE							
A	B, Antwerp	Urban	4.0 ppt	-	-	-	77-1
	Bolivia	Remote	0.3 ppt	-	-	-	77-1
DI-I-DECYLPHTHALATE 26761-40-0							
W	Japan, Pacific coast	Remote & Indust.	0.52-0.94	-	206/375	-	79-7
S	Japan, Pacific coast	Remote & Indust.	40-80	-	162/370	-	79-7
B	Japan, Pacific coast	Fish	50-130	-	123/332	-	79-7
DIETHYL PHTHALATE 84-66-2							
A	B, Antwerp	Urban	3.7 ppt	-	-	1.8-4.9 ppt	77-1
	Bolivia	Remote	0.5 ppt	-	-	0.4-0.7 ppt	77-1
W	NL, Lobith	R Rhine	0.15-1.0	1.0	1/6	-	79-6
S	USA, Texas (St Luis Pass)	-	5.0 (dry)	-	-	-	81-4
	USA, Chesapeake Bay	-	32.0 (dry)	-	-	-	82-3
DI-(2-ETHYLHEXYL)PHTHALATE 117-81-7							
A	B, Antwerp	Urban	60.0 ppt	-	-	20.0-100 ppt	77-1
	Bolivia	Remote	16.0 ppt	-	-	15.0-17.0 ppt	77-1
	USA, New York	Urban	12 ppt	-	-	4-24.0 ppt	78-2
	USA, Gulf of Mexico	Remote & Coastal	0.4 ppt	-	8	-	78-1
	N Atlantic	Remote Mar.	2.4 ppt	-	5	-	78-1
	Gulf of Mexico	Remote Mar.	0.9 ppt	-	-	0.4-1.6 ppt	80-1
	N Pacific	Remote Mar.	1.2 ppt	-	-	0.3-2.2 ppt	81-2
W	USA, Pa/NJ	R Delaware	-	-	16/16	0.06-5.0	78-5
	USA, Texas	Est Nueces	0.35	-	-	-	83-2
	USA, Gulf of Mexico	Marine	0.1	-	17	-	78-1
	USA	Delta Mississipi	0.07	-	14	-	78-1
	N Atlantic	Marine	0.005	-	10	-	78-1
	NL/D border	R Rhine	2.5	-	-	-	78-4
	Japan, Pacific coast	Remote & Indust.	0.32-0.68	-	176/375	-	79-7
S	USA, Portland Maine	Estuarine	1500.0	-	-	-	83-3
	USA, Texas	Est Nueces	2500.0 (dry)	-	-	-	83-2
	USA (Tx), St Luis Pass	-	94.0 (dry)	-	-	-	81-4
	USA, Chesapeake Bay	-	96.0 (dry)	-	-	-	82-3
	USA, Gulf of Mexico	Remote & Coastal	4.3	-	12	-	78-1
	USA	Delta Mississipi	69.0	-	22	-	78-1
	Japan, Pacific Coast	Remote & Indust.	290-480	-	226/370	-	79-7
B	USA, Portland Maine	Shellfish	290.0	-	2 species	-	83-3
	USA, Gulf of Mexico	Fish/Shellfish	4.5	-	20	-	78-1
	Japan, Pacific coast	Remote & Indust.	80-290	-	93/332	-	79-7
DIMETHYLPHTHALATE 131-11-3							
W	NL, Lobith	R Rhine	0.3	-	-	-	80-2
DIPHENYLPHTHALATE 84-62-8							
S	USA, Chesapeake Bay	-	9.5 (dry)	-	2 cores (0-10 cm)	-	82-3
TEREPHTHALIC ACID 100-21-0							
W	Japan, Pacific coast	Remote & Indust.	0.04-0.7	-	6/100	-	79-7
DIMETHYL TEREPHTHALATE 120-61-6							
W	USA, Pa/NJ	R Delaware	0.01-0.06	-	1/5	-	78-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

3.3 Phosphate esters - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
TRI-(2-BUTOXYETHYL)PHOSPHATE 78-51-3							
W	USA, Pa/NJ	R Delaware	-	-	16/16	0.3-3.0	78-5
TRI-N-BUTYLPHOSPHATE 126-73-8							
W	D/NL border	R Rhine	0.4	-	-	-	78-4
	NL, Maassluis/Lobith	R Rhine	0.22-0.26	0.3	5/6	-	79-6
TRI-I-BUTYLPHOSPHATE 126-71-6							
W	NL, Maassluis/Lobith	R Rhine	0.22-0.65	1.0	2/6	-	79-6
TRI-T-BUTYLPHOSPHATE							
W	USA, Pa/NJ	R Delaware	-	-	14/16	0.06-2.0	78-5
TRI-(2-CHLOROETHYL)PHOSPHATE 115-96-8							
W	D/NL, border	R Rhine	0.2	-	-	-	78-4
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL, Maassluis-Lobith	R Rhine	0.4-0.6	1.0	4/6	-	79-6
TRI-ETHYLPHOSPHATE 78-40-0							
W	D/NL border	R Rhine	0.01	-	-	-	78-4
	NL, Maassluis/Lobith	R Rhine	0.3-0.36	0.3	5/6	-	79-6
TRI-PHENYLPHOSPHATE 115-86-6							
W	USA, Pa/NJ	R Delaware	-	-	13/16	0.08-0.4	78-5

3.4 Ethers - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
DIBENZYL ETHER 103-50-4							
W	NL, Lobith/Maassluis	R Rhine	0.01-0.03	0.03	2/6	-	79-6
DICHLOROISOPROPYLETHER 63283-80-7							
W	NL, Lobith/Maassluis	R Rhine	0.83-1.0	1.0	5/6	-	79-6 &
	NL, Brakel	R Waal	2.6	10.1	4/4	-	76-4
	NL, Berg	R Maas	0.1-0.3	1.3	3/4	-	76-4
BIS(2-CHLOROPROPYL)ETHER 54460-96-7							
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	D/NL border	R Rhine	0.2	-	-	-	78-4
	NL, Lobith/Maassluis	R Rhine	0.77	1.0	6/6	-	79-6
TETRACHLOROISOPROPYLETHER							
W	NL, Brakel	R Waal	0.75	3.0	4/4	-	76-4
	NL, Berg	R Maas	0.3-0.45	1.2	3/4	-	76-4

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
TETRAHYDROFURAN 109-99-9							
W	NL, Lobith/Maassluis	R Rhine	1.0-3.0	3.0	2/6	-	79-6

3.5 Alcohols - environmental concentrations

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
2-ETHYLHEXANOL 104-76-7							
W	USA, Pa/NJ	R Delaware	0.8-4.0	-	2/5	3.0-5.0	78-5
CYCLOHEXANOL 108-93-0							
W	NL	R Rhine	10.0	-	-	-	84-3
I-PHENYL ETHANOL 98-85-1							
W	NL, Lobith/Maassluis	R Rhine	0.02-0.1	0.1	1.6	-	79-6

3.6 Chlorobenzenes - environmental concentrations

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
CHLOROBENZENE 108-90-7							
A	USA, Los Angeles (Ca)	-	0.2	-	-	.05-0.5	81-1
	USA, Phoenix (Az)	-	0.2	-	-	.05-0.5	81-1
	USA, Oakland (Ca)	-	0.1	-	-	.05-0.3	81-1
	USA, Houston (Tx)	-	0.31	-	-	.009-2.8	83-1
	USA, St. Louis (Mo)	-	0.24	-	-	.005-1.17	83-1
	USA, Denver (Co)	-	0.29	-	-	.033-1.12	83-1
	NL, various	-	16.2-27.0 ppt	197-675 ppt	-	-	85-1
W	CZ, Basle	R Rhine	0.9	-	-	-	78-3
	D, Cologne	R Rhine	0.6	-	-	-	78-3
	D, Duisburg	R Rhine	5.3	-	-	-	78-3
	NL, Lobith	R Rhine	0.1	-	-	-	80-2
	USA, Pa-NJ	R Delaware	0.44-7.0	-	1/16	-	78-5
	NL, Lobith/Maassluis	R Rhine	0.57-0.68	1.0	5/6	-	79-6
Σ DICHLOROBENZENES							
A	NL, various	-	6.0-12.0 ppt	66-244 ppt	-	-	85-1
W	USA, Pa-NJ	R Delaware	0.08-0.4	-	1/16	-	78-5
	NL, Brakel	R Waal	4.08	12.5	4/4	-	76-4
	NL, Berg	R Maas	0.13-0.2	0.9	3/4	-	76-4
1,2-DICHLOROBENZENE 95-50-1							
A	USA, Los Angeles (Ca)	-	13.0 ppt	-	-	2-50 ppt	81-1
	USA, Phoenix (Az)	-	23.0 ppt	-	-	1-236 ppt	81-1
	USA, Oakland (Ca)	-	4.0 ppt	-	-	1-33 ppt	81-1
	USA, Houston (Tx)	-	7.0 ppt	-	-	1-67 ppt	83-1

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
	USA, St Louis (Mo)	-	6.0 ppt	-	-	1-95 ppt	83-1
	USA, Denver (Co)	-	26.0 ppt	-	-	2-227 ppt	83-1
	USA, Riverdale (Ca)	-	10.0 ppt	-		3-76 ppt	83-1
W	NL, Lobith	R Rhine	2.0	-	-	-	80-2
	NL, Lobith/Maassluis	R Rhine	2.67	3.0	6/6	-	79-6
	NL	R Rhine/Maas	8.9	-	-	-	73-1
	USA	L Ontario	0.005	-	-	0.002-0.007	82-2
	USA	R Niagara	0.026	-	-	-	82-2
S	USA	L Superior	1.0	-	-	-	82-2
	USA	L Huron	8.0	-	-	-	82-2
	USA	L Erie	2.0	-	-	-	82-2
	USA	L Ontario	11.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.3	-	1 species	-	82-2
	USA, L Huron	Fish (Trout)	1.0	-	1 species	-	82-2
	USA, L Erie	Fish (Trout)	1.0	-	1 species	-	82-2
	USA, L Ontario	Fish (Trout)	1.0	-	1 species	-	82-2
1,3-DICHLOROBENZENE 541-73-1							
A	USA, Los Angeles (Ca)	-	0.008	-	-	0.001-0.025	81-1
	USA, Phoenix (Az)	-	0.009	-	-	0.001-0.028	81-1
	USA, Oakland (Ca)	-	0.007	-	-	0.003-0.015	81-1
	USA, Houston (Tx)	-	0.007	-	-	0.001-0.047	83-1
	USA, St Louis (Mo)	-	0.004	-	-	0.001-0.055	83-1
	USA, Denver (Co)	-	0.008	-	-	0.001-0.036	83-1
	USA, Riverside (Ca)	-	0.006	-	-	0.001-0.021	83-1
W	USA	R Niagara	0.011	-	-	-	82-2
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL, Lobith/Maassluis	R Rhine	0.2	0.3	6/6	-	79-6
S	USA, L Superior	-	2.0	-	-	-	82-2
	USA, L Huron	-	2.0	-	-	-	82-2
	USA, L Erie	-	4.0	-	-	-	82-2
	USA, L Ontario	-	74.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.6	-	1 species	-	82-2
	USA, L Huron	Fish (Trout)	0.6	-	1 species	-	82-2
	USA, L Erie	Fish (Trout)	0.3	-	1 species	-	82-2
	USA, L Ontario	Fish (Trout)	2.5	-	1 species	-	82-2
1,4-DICHLOROBENZENE 106-46-7							
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL, Lobith/Maassluis	R Rhine	0.88	1.0	6/6	-	79-6
	NL	R Rhine/Maas	2.92	-	-	-	73-1
	Japan, Pacific coast	Remote & Indust	0.02-1.0	-	2/95	-	79-7
	USA	R Niagara	0.041	-	-	-	82-2
	USA	L Ontario	0.045	-	-	-	82-2
	USA	L Huron	0.004	-	-	-	82-2
S	Japan, Pacific coast	Remote & Indust	0-30	-	1/95	-	79-7
	USA, L Superior	-	5.0	-	-	-	82-2
	USA, L Huron	-	16.0	-	-	-	82-2
	USA, L Erie	-	9.0	-	-	-	82-2
	USA, L Ontario	-	94.0	-	-	-	82-2
B	USA, L Huron	Fish (Trout)	1.0	-	-	-	82-2
	USA, L Erie	Fish (Trout)	4.0	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	3.0	-	-	-	82-2
Σ TRICHLOROBENZENES							
A	NL, various	-	1.7-3.4 ppt	6.8-230 ppt	-	-	85-1
W	NL, Lobith/Maassluis	R Rhine	0.12	0.3	6.6	-	79-6
	USA, Pa-NJ	R Delaware	-	-	3/16	0.5-1.0	78-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
1,2,3-TRICHLOROBENZENE 87-61-6							
W	NL, Lobith	R Rhine	0.8	-	-	-	80-2
	USA	R Niagara	0.014	-	-	-	82-2
	USA	L Ontario	0.001	-	-	-	82-2
S	USA, L Superior	-	0.2	-	-	-	82-2
	USA, L Huron	-	0.3	-	-	-	82-2
	USA, L Erie	-	0.4	-	-	-	82-2
	USA, L Ontario	-	7.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.1	-	-	-	82-2
	USA, L Huron	Fish (Trout)	0.2	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.1	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	0.6	-	-	-	82-2
1,2,4-TRICHLOROBENZENE 120-82-1							
A	USA, Los Angeles (Ca)	-	0.007	-	-	0.002-0.034	81-1
	USA, Phoenix (Az)	-	0.003	-	-	0.001-0.010	81-1
	USA, Oakland (Ca)	-	0.003	-	-	0.001-0.015	81-1
	USA, Houston (Tx)	-	0.002	-	-	0.001-0.013	83-1
	USA, St. Louis (Mo)	-	0.001	-	-	0.001-0.004	83-1
	USA, Denver (Co)	-	0.006	-	-	0.001-0.035	83-1
	USA, Riverside (Ca)	-	0.010	-	-	0.002-0.040	83-1
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	USA	R Niagara	0.032	-	-	-	82-2
	USA	L Ontario	0.0006	-	-	-	82-2
	USA	L Huron	0.0002	-	-	-	82-2
S	USA, L Superior	-	1.0	-	-	-	82-2
	USA, L Huron	-	6.0	-	-	-	82-2
	USA, L Erie	-	3.0	-	-	-	82-2
	USA, L Ontario	-	94-0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.6	-	-	-	82-2
	USA, L Huron	Fish (Trout)	1.0	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.5	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	3.5	-	-	-	82-2
1,3,5-TRICHLOROBENZENE 108-70-3							
W	NL, Lobith	R Rhine	0.4	-	-	-	80-2
	USA	R Niagara	0.004	-	-	-	82-2
	USA	L Ontario	0.0001	-	-	-	82-2
S	USA, L Superior	-	0.2	-	-	-	82-2
	USA, L Huron	-	0.7	-	-	-	82-2
	USA, L Erie	-	1.0	-	-	-	82-2
	USA, L Ontario	-	60.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.6	-	-	-	82-2
	USA, L Huron	Fish (Trout)	0.3	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.1	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	4.0	-	-	-	82-2
Σ TETRACHLOROBENZENE							
W	NL, Lobith/Maassluis	R Rhine	0-0.03	0.03	1.6	-	79-6
1,2,3,4-TETRACHLOROBENZENE 634-66-2							
W	USA	R Niagara	0.034	-	-	-	82-2
	USA	L Ontario	0.1 ppt	-	-	-	82-2
	USA	L Huron	0.05 ppt	-	-	-	82-2
S	USA, L Superior	-	0.3	-	-	-	82-2
	USA, L Huron	-	1.0	-	-	-	82-2
	USA, L Erie	-	0.7	-	-	-	82-2
	USA, L Ontario	-	33.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.5	-	-	-	82-2
	USA, L Huron	Fish (Trout)	2.0	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.3	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	5.3	-	-	-	82-2

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
1,2,3,5-TETRACHLOROBENZENE 634-90-2							
W	USA	R Niagara	0.0014	-	-	-	82-2
S	USA, L Superior	-	0.1	-	-	-	82-2
	USA, L Huron	-	0.4	-	-	-	82-2
	USA, L Erie	-	0.3	-	-	-	82-2
	USA, L Ontario	-	6.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.1	-	-	-	82-2
	USA, L Huron	Fish (Trout)	0.2	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.05	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	0.75	-	-	-	82-2
1,2,4,5-TETRACHLOROBENZENE 95-94-3							
W	USA	R Niagara	0.012	-	-	-	82-2
	USA	L Ontario	0.1 ppt	-	-	-	82-2
S	USA, L Superior	-	0.3	-	-	-	82-2
	USA, L Huron	-	1.0	-	-	-	82-2
	USA, L Erie	-	1.0	-	-	-	82-2
	USA, L Ontario	-	52.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.3	-	-	-	82-2
	USA, L Huron	Fish (Trout)	1.0	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.2	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	3.5	-	-	-	82-2
PENTACHLOROBENZENE 608-93-5							
A	Enewetak Atoll (Pacific)	Remote	0.025 ppt	-	-	-	85-2
	American Samoa Islands	Remote	0.008 ppt	-	-	-	85-2
	Peru coast, various	Remote	0.020 ppt	-	-	-	85-2
	New Zealand	Remote	0.013 ppt	-	-	-	85-2
W	USA	R Niagara	6.0 ppt	-	-	-	82-2
	USA	L Ontario	0.2 ppt	-	-	-	82-2
	USA	L Huron	0.04 ppt	-	-	-	82-2
S	USA, L Superior	-	0.1	-	-	-	82-2
	USA, L Huron	-	1.0	-	-	-	82-2
	USA, L Erie	-	1.0	-	-	-	82-2
	USA, L Ontario	-	32.0	-	-	-	82-2
B	USA, L Superior	Fish (Trout)	0.7	-	-	-	82-2
	USA, L Huron	Fish (Trout)	2.0	-	-	-	82-2
	USA, L Erie	Fish (Trout)	0.6	-	-	-	82-2
	USA, L Ontario	Fish (Trout)	12.0	-	-	-	82-2
HEXACHLOROBENZENE 118-74-1							
A	NL, various	-	0.08 ppt	0.4 ppt	-	-	85-1
	Enewetak Atoll, Pacific	Remote Mar	0.08 ppt	-	-	-	81-2
	N Atlantic	Remote Mar	0.13 ppt	-	-	-	81-2
	American Samoa Islands	Remote Mar	0.05 ppt	-	-	-	85-2
	Peru Coast	Remote Mar	0.05 ppt	-	-	-	85-2
	New Zealand	Remote Mar	0.05 ppt	-	-	-	85-2
W	NL, Lobith	R Rhine	0.1	-	-	-	80-2
	USA	R Niagara	5.0 ppt	-	-	-	82-2
	USA	L Ontario	0.6 ppt	-	-	-	82-2
	USA	L Huron	0.4 ppt	-	-	-	82-2
	USA	R Missisipi	2.2	-	-	-	76-2
	D/NL Border	R Rhine	0.04	-	-	-	78-4
	USA, Texas	Est Nueces	0.24 ppt	-	-	-	83-2
S	USA, L Superior	S water	0.2	-	-	-	82-2
	USA, L Huron	S water	2.0	-	-	-	82-2
	USA, L Erie	S water	3.0	-	-	-	82-2
	USA, L Ontario	S water	97.0	-	-	-	82-2
	USA,Portland (Maine)	Estuarine	0.14 (dry)	-	-	-	83-3
	USA, Texas	Est Nueces	0.11 (dry)	-	-	-	83-2
	USA, Texas	St Luis Pass	0.49 (dry)	-	-	-	81-4
	Japan, Pacific coast	Remote & Indust	10-120	-	36/399	-	79-7

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
B	USA, Portland (Maine)	Shellfish	0.35 (wet)	-	2 species	-	83-3
	USA (Tx) St Luis Pass	Shellfish	3.73 (wet)	-	3 species	-	81-4
	USA (Tx) St Luis Pass	Fish	0.57 (wet)	-	2 species	-	81-4
	USA, L Superior	Fish (Trout)	13.0	-	1 species	-	82-2
	USA, L Huron	Fish (Trout)	25.0	-	1 species	-	82-2
	USA, L Erie	Fish (Trout)	8.0	-	1 species	-	82-2
	USA, L Ontario	Fish (Trout)	94.0	-	1 species	-	82-2
	USA, R Mississipi	Fish	258.0	-	1 species	-	76-2
	Japan, Pacific Coast (various)	Fish	0-1.2	-	111/369	-	79-7
	NL, Coast (various	Shellfish (Mussel)	0-16.0 (wet)	-	1 species	-	79-5
	USA, various (76-81)	Fish	-	700.0 (wet)	(NPMP 30%) (5/14)	-	85-4
	Austria, Alpine lakes	Fish	65.0 (lipid)	-	several	-	80-5
	Ocean, Antarctic	Fish	7.5 (lipid)	-	several	-	80-5
	Peru, S Pacific	Fish	3.0 (lipid)	-	several	-	80-5

3.7 Aromatic amines - environmental concentrations

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
ANILINE 62-53-3							
W	NL, Lobith	R Rhine	0.03	-	-	-	80-2
	NL/D border	R Rhine	2.97	-	-	-	81-3
	NL	R Rhine (tribs)	2.3	-	-	-	81-3
	NL	R Meuse	0.7	-	-	-	81-3
	Japan, Pacific coast	Remote & Indust.	16.5-28.0	-	40/68	-	79-7
	NL, Lobith	R Rhine	2.97	-	-	-	81-11
S	Japan, Pacific coast	Remote & Indust.	350-500	-	48/68	-	79-7
Σ CHLOROANILINES							
W	NL, Lobith/Maassluis	R Rhine	0.53	1.0	6/6	-	79-6
2-CHLOROANILINE 95-51-2							
W	NL/D border	R Rhine	0.54	-	-	-	81-3
	NL	R Rhine (tribs)	0.45	-	-	-	81-3
	NL	R Meuse	0.10	-	-	-	81-3
	Japan, Pacific coast	Remote & Indust.	0.03-0.35	-	12/120	-	79-7
	NL, Lobith	R Rhine	0.54	-	-	-	81-11
S	Japan, Pacific coast	Remote & Indust.	30-98	-	29/113	-	79-7
3-CHLOROANILINE 108-42-9							
W	NL, Lobith	R Rhine	0.14	-	-	-	81-11
4-CHLOROANILINE 106-47-8							
W	NL/D border	R Rhine	0.22	-	-	-	81-3
	NL	R Rhine (tribs)	0.14	-	-	-	81-3
	NL	R Meuse	0.02	-	-	-	81-3
	NL, Lobith	R Rhine	0.22	-	-	-	81-11
2,4-DICHLOROANILINE 554-00-7							
W	NL, Lobith	R Rhine	0.02	-	-	-	81-11
3,4-DICHLOROANILINE 95-76-1							
W	NL/D border	R Rhine	0.39	-	-	-	81-3
	NL	R Rhine (tribs)	0.31	-	-	-	81-3

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
	NL	R Meuse	0.22	-	-	-	81-3
	Japan, Pacific coast	Remote & Indust.	0.02-0.42	-	4/68	-	79-7
	NL, Lobith	R Rhine	0.39	-	-	-	81-11
S	Japan, Pacific coast	Remote & Indust.	50-110	-	31/68	-	79-7
2,5-DICHLOROANILINE 95-82-9							
W	Japan, Pacific coast	Remote & Indust.	0.05-0.53	-	7/68	-	79-7
S	Japan, Pacific coast	Remote & Indust.	10-34	-	12/68	-	79-7
2,6-DICHLOROANILINE 608-31-1							
W	NL, Lobith	R Rhine	<0.05	-	-	-	81-11
3,5-DICHLOROANILINE 626-43-7							
W	NL, Lobith	R Rhine	0.02	-	-	-	81-11
2,3, & 2,5-DICHLOROANILINE							
W	NL, Lobith	R Rhine	0.04	-	-	-	81-11
2-METHOXYANILINE (o-ANISIDINE) 90-04-0							
W	Japan, Pacific coast	Remote & Indust.	0.07-0.8	-	6/68	-	79-7
	NL, Lobith/Maassluis	R Rhine	0.01-0.02	0.03	2/6	-	79-6
S	Japan, Pacific coast	Remote & Indust.	220-550	-	27/68	-	79-7
4-METHOXYANILINE (p-ANISIDINE) 104-94-9							
W	Japan, Pacific coast	Remote & Indust.	0.04-0.72	-	4/68	-	79-7
S	Japan, Pacific coast	Remote & Indust.	0-6.0	-	12/68	-	79-7
2-METHYLANILINE (o-TOLUIDINE) 95-53-4							
W	Japan, Pacific coast	Remote & Indust.	2.35-20.0	-	8/68	-	79-7
	NL, Brakel	R Waal	0.75	1.3	4/4	-	76-4
	NL, Lobith	R Rhine	0.03	-	-	-	81-11
S	Japan, Pacific coast	Remote & Indust.	30.0-72.0	-	27/68	-	79-7
4-METHYLANILINE (p-TOLUIDINE) 106-49-0							
W	Japan, Pacific coast	Remote & Indust.	0.03-0.18	-	11/68	-	79-7
	NL, Lobith	R Rhine	0.17	-	-	-	81-11
S	Japan, Pacific coast	Remote & Indust.	50-90	-	35/68	-	79-7
Σ DIMETHYLANILINE							
	WNL, Lobith/Maassluis	R Rhine	0.05-0.3	0.3	1/6	-	79-6
	NL, Lobith	R Rhine	0.3	-	-	-	80-2
N,N-DIETHYLANILINE 91-66-7							
W	NL, Lobith/Maassluis	R Rhine	0.28-0.43	1.0	5/6	-	79-6
N,N-DIMETHYLANILINE 121-69-7							
W	NL, Lobith/Maassluis	R Rhine	0.07-0.2	0.3	2/6	-	79-6
	NL, Brakel	R Waal	1.18	3.6	4/4	-	76-4
	NL, Lobith	R Rhine	0.3	-	-	-	80-2

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
N-ETHYLANILINE 103-69-5							
W	NL, Lobith/Maasluis	R Rhine	0.17-1.0	1.0	2/6	-	79-6
	NL, Lobith	R Rhine	0.3	-	-	-	80-2
N-METHYLANILINE 100-61-8							
S	Japan, Pacific coast	Remote & Indust.	0-12.0	-	11/68	-	79-7
Σ-NITROANILINES							
W	NL, Lobith/Maassluis	R Rhine	0.45-0.54	1.0	5/6	-	79-6
2-NITROANILINE 88-74-4							
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
3-NITROANILINE 99-09-2							
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
4-NITROANILINE 100-01-6							
W	NL,Lobith	R Rhine	3.8	-	-	-	80-2

3.8 Chloroalkanes - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
TETRACHLOROMETHANE 56-23-5							
A	NL, various	-	25-30 ppt	66-95 ppt	-	-	85-1
	USA, Seagirt (NJ)	Coastal	0.23	-	-	0.12-0.36	75-1
	USA, New York (NY)	Urban	0.27	-	-	0.16-0.37	75-1
	USA, Baltimore (Md)	Urban	0.12	-	-	0.06-0.16	75-1
	USA, New York State	Alpine	0.26	-	-	0.2-0.33	75-1
W	NL, Maassluis/Lobith	R Rhine	2.0	3.0	6/6	-	79-6
	NL, Lobith	R Rhine	2.0	-	-	-	80-2
TRICHLOROFLUOROMETHANE 75-69-4							
A	NL, various	-	0.84	-	-	-	85-1
	USA, Seagirt (NJ)	Coastal	0.25	-	-	0.12-0.55	75-1
	USA, New York (NY)	Urban	1.44	-	-	0.5-3.8	75-1
	USA, Baltimore (Md)	Urban	0.24	-	-	0.1-0.68	75-1
	USA, New York State	Alpine	0.13	-	-	0.1-0.18	75-1
1,1-DICHLOROETHANE 75-34-3							
A	USA. Houston (Tx)	-	.063	-	-	.009-.126	83-1
	USA, St Louis (Mo)	-	.060	-	-	.026-.105	83-1
	USA, Denver (Co)	-	.065	-	-	.011-.142	83-1
	USA, Riverside (Ca)	-	.066	-	-	.008-.147	83-1
	USA, Staten Is (NY)	-	.013	-	-	.003-.037	83-1
	USA, Pittsburgh (Pa)	-	.012	-	-	0.003-0.105	83-1
	USA, Chicago (Il)	-	.011	-	-	.005-.026	83-1

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
1,2-DICHLOROETHANE 107-06-2							
A	NL, various	-	15-90 ppt	450-2700 ppt	-	-	85-1
	USA, Los Angeles (Ca)	-	0.52	-	-	0.173-1.35	81-1
	USA, Phoenix (Az)	-	0.22	-	-	0.038-1.45	81-1
	USA, Oakland (Ca)	-	0.083	-	-	0.038-0.84	81-1
	USA. Houston (Tx)	-	1.51	-	-	0.05-7.3	82-1
	USA, St Louis (Mo)	-	0.124	-	-	0.045-0.6	82-1
	USA, Denver (Co)	-	0.24	-	-	0.05-2.09	82-1
	USA, Riverside (Ca)	-	0.36	-	-	0.06-2.5	82-1
	USA, Staten Is (NY)	-	0.26	-	-	0.05-4.3	82-1
	USA, Pittsburgh (Pa)	-	0.12	-	-	0.07-0.24	82-1
	USA, Chicago (Il)	-	0.19	-	-	0.02-2.82	82-1
W	NL, Maassluis/Lobith	R Rhine	6.0-7.6	10.0	5/6	3-10	79-6
	D	R Lippe	0.06	-	7	-	81-10
1,2-DIBROMOETHANE 106-93-4							
A	NL, various	-	2.4-4.8 ppt	12.8-32 ppt	-	-	85-1
	USA, Los Angeles (Ca)	-	0.033	-	-	0.005-0.12	81-1
	USA, Phoenix (Az)	-	0.040	-	-	0.002-0.2	81-1
	USA, Oakland (Ca)	-	0.016	-	-	0.002-0.085	83-1
	USA. Houston (Tx)	-	0.059	-	-	0.010-0.368	83-1
	USA, St Louis (Mo)	-	0.016	-	-	0.008-0.026	83-1
	USA, Denver (Co)	-	0.031	-	-	0.010-0.078	83-1
	USA, Riverside (Ca)	-	0.022	-	-	0.010-0.047	83-1
	USA, Staten Is (NY)	-	0.020	-	-	0.012-0.036	83-1
	USA, Pittsburgh (Pa)	-	0.016	-	-	0.006-0.059	83-1
	USA, Chicago (Il)	-	0.026	-	-	0.006-0.249	83-1
1,1,1-TRICHLOROETHANE 71-55-6							
A	NL, various	-	55.0-66.0 ppt	550-1650 ppt	-	-	85-1
	USA, Los Angeles (Ca)	-	1.028	-	-	0.224-5.14	81-1
	USA, Phoenix (Az)	-	0.823	-	-	0.198-2.81	81-1
	USA, Oakland (Ca)	-	0.291	-	-	0.143-0.97	81-1
	USA, Houston (Tx)	-	0.353	-	-	0.134-1.49	83-1
	USA, St Louis, (Mo)	-	0.235	-	-	0.132-0.896	83-1
	USA, Denver (Co)	-	0.713	-	-	0.171-2.7	83-1
	USA, Riverside (Ca)	-	0.747	-	-	0.205-1.35	83-1
	USA, Staten Is (NY)	-	0.468	-	-	0.221-1.43	83-1
	USA, Pittsburgh (Pa)	-	0.486	-	-	0.158-1.59	83-1
	USA, Chicago (Il)	-	0.476	-	-	0.241-0.51	83-1
W	NL, Maassluis	R Rhine	-	1.0	1	-	79-6
1,1,2-TRICHLOROETHANE 79-00-5							
A	USA, Los Angeles (Ca)	-	0.009	-	-	0.004-0.045	81-1
	USA, Phoenix (Az)	-	0.016	-	-	0 - 0.042	81-1
	USA, Oakland (Ca)	-	0.008	-	-	0.004-0.028	81-1
	USA, Houston (Tx)	-	0.032	-	-	0.005-0.129	83-1
	USA, St Louis, (Mo)	-	0.015	-	-	0.006-0.045	83-1
	USA, Denver (Co)	-	0.027	-	-	0.007-0.056	83-1
	USA, Riverside (Ca)	-	0.041	-	-	0.005-0.089	83-1
	USA, Staten Is (NY)	-	0.007	-	-	0.003-0.011	83-1
	USA, Pittsburgh (Pa)	-	0.006	-	-	0.003-0.011	83-1
	USA, Chicago (Il)	-	0.007	-	-	0.003-0.014	83-1
W	NL, Lobith	R Rhine	0.03	-	-	-	80-2
	NL, Maassluis/Lobith	R Rhine	0.52-1.55	3.0	2/6	-	79-6
	D	R Lippe	0.57	-	11	-	81-10
	D	R Weser	0.29	-	12	-	81-10
1,1,1,2-TETRACHLOROETHANE 630-20-6							
A	USA, Los Angeles (Ca)	-	0.004	-	-	0 - 0.012	81-1
	USA, Phoenix (Az)	-	0.008	-	-	0 - 0.016	81-1
	USA, Oakland (Ca)	-	0.004	-	-	0 - 0.008	81-1
	USA, Houston (Tx)	-	0.012	-	-	0.002-0.080	83-1
	USA, St Louis, (Mo)	-	0.006	-	-	0.004-0.018	83-1
	USA, Denver (Co)	-	0.010	-	-	0.005-0.089	83-1
	USA, Riverside (Ca)	-	0.009	-	-	0.004-0.018	83-1
	USA, Pittsburgh (Pa)	-	0.004	-	-	0.004-0.005	83-1
	USA, Chicago (Il)	-	0.006	-	-	0.002-0.035	83-1

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
1,1,2,2-TETRACHLOROETHANE 79-34-5							
A	NL, various	-	1.8-3.6 ppt	2.7-18.0 ppt	-	-	85-1
	USA, Los Angeles (Ca)	-	0.017	-	-	0.004-0.096	81-1
	USA, Phoenix (Az)	-	0.017	-	-	0-0.031	81-1
	USA, Oakland (Ca)	-	0.007	-	-	0.003-0.013	81-1
	USA, Houston (Tx)	-	0.011	-	-	0.002-0.077	83-1
	USA, St Louis, (Mo)	-	0.006	-	-	0.004-0.012	83-1
	USA, Denver (Co)	-	0.010	-	-	0.003-0.017	83-1
	USA, Riverside (Ca)	-	0.012	-	-	0.005-0.077	83-1
	USA, Pittsburgh (Pa)	-	0.004	-	-	0.003-0.004	83-1
	USA, Chicago (Il)	-	0.003	-	-	0.002-0.006	83-1
	USA, Seagirt (NJ)	-	0.32	-	-	0.1-0.88	75-1
	USA, New York (NY)	-	4.5	-	-	1.0-9.75	75-1
	USA, Baltimore (Md)	-	0.18	-	-	0.02-0.29	75-1
	USA, New York State	Alpine	0.07	-	-	0.02-0.19	75-1
W	NL, Maassluis/Lobith	R Rhine	0.13-0.2	0.3	416	-	79-6
1,2-DICHLOROPROPANE 78-87-5							
A	NL, various	-	16.2-37.8 ppt	405-810 ppt	-	-	85-1
	USA, Houston (Tx)	-	-	-	-	0.022-0.253	83-1
	USA, St Louis, (Mo)	-	0.053	-	-	0.022-0.088	83-1
	USA, Denver (Co)	-	0.048	-	-	0.020-0.099	83-1
	USA, Riverside (Ca)	-	0.057	-	-	0.011-0.088	83-1
	USA, Staten Is (NY)	-	0.026	-	-	0.010-0.079	83-1
	USA, Pittsburgh (Pa)	-	0.023	-	-	0.004-0.050	83-1
	USA, Chicago (Il)	-	0.029	-	-	0.010-0.040	83-1
W	NL, Maassluis/Lobith	R Rhine	0.68-1.37	3.0	316	-	79-6
C_{10}-C_{20} CHLORINATED PARAFFINS							
W	UK, various	Marine	0.6-1.0	-	11/18	-	80-6
	UK, various	Freshwaters	0.3-0.6	-	6/13	-	80-6
S	UK, various	Marine	40-200	-	4/18	-	80-6
	UK, various	Freshwater	1040-2700	-	3/8	-	80-6
C_{20}-C_{30} CHLORINATED PARAFFINS							
W	UK, various	Marine	0.3-1.2	-	5/18	-	80-6
	UK, various	Freshwaters	0.32-0.8	-	4/11	-	80-6
S	UK, various	Marine	56-300	-	3/18	-	80-6
	UK, various	Freshwaters	7.1-50-0	-	1/7	-	80-6

3.9 Chloroalkenes - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
1,1-DICHLOROETHENE 75-35-4							
A	NL, various	-	1.5-3.7 ppt	3.1-7.8 ppt	-	-	85-1
	USA, Los Angeles (Ca)	-	0.005	-	-	0.001-0.010	81-1
	USA, Phoenix (Az)	-	0.030	-	-	0 - 0.016	81-1
	USA, Oakland (Ca)	-	0.013	-	-	0.005-0.024	81-1
	USA, Houston (Tx)	-	0.025	-	-	0.004-0.136	83-1
	USA, St Louis, (Mo)	-	0.009	-	-	0.004-0.034	83-1
	USA, Denver (Co)	-	0.031	-	-	0.004-0.022	83-1
	USA, Riverside (Ca)	-	0.009	-	-	0.004-0.056	83-1
	USA, Chicago (Il)	-	0.022	-	-	0.003-0.068	83-1

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
1,2-DICHLOROETHENE 540-59-0							
A	USA, Houston (Tx)	-	0.071	-	-	0.021-0.429	83-1
	USA, St Louis, (Mo)	-	0.039	-	-	0.025-0.066	83-1
	USA, Denver (Co)	-	0.076	-	-	0.025-0.605	83-1
	USA, Riverside (Ca)	-	0.06	-	-	0.033-0.173	83-1
	USA, Staten Is (NY)	-	0.018	-	-	0.008-0.041	83-1
	USA, Pittsburgh (Pa)	-	0.013	-	-	0.004-0.025	83-1
	USA, Chicago (Il)	-	0.019	-	-	0.004-0.033	83-1
W	NL, Lobith/Maassluis	R Rhine	0-0.1	-	(2/6)	-	79-6
TRICHLOROETHENE 79-01-6							
A	USA, Los Angeles (Ca)	-	0.4	-	-	0.036-1.7	81-1
	USA, Phoenix (Az)	-	0.48	-	-	0.012-3.07	81-1
	USA, Oakland (Ca)	-	0.19	-	-	0.014-1.56	81-1
	USA, Houston (Tx)	-	0.14	-	-	0.005-0.98	82-1
	USA, St Louis, (Mo)	-	0.11	-	-	0.008-1.04	83-1
	USA, Denver (Co)	-	0.2	-	-	0.007-2.5	83-1
	USA, Riverside (Ca)	-	0.12	-	-	0.015-0.24	83-1
	USA, Staten Is (NY)	-	0.17	-	-	0.026-1.0	83-1
	USA, Pittsburgh (Pa)	-	0.096	-	-	0.013-0.42	83-1
	USA, Chicago (Il)	-	0.22	-	-	0.018-1.39	85-1
	NL	-	13.8-32.2 ppt	345-690 ppt	-	-	85-1
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	CZ, Basle	R Rhine	0.9	-	-	-	78-3
	D, Cologne	R Rhine	0.8	-	-	-	78-3
	D, Duisberg	R Rhine	0.6	-	-	-	78-3
	NL, Maassluis/Lobith	R Rhine	0.98	3.0	6/6	-	79-6
	D	R Lippe	0.06	-	9	-	81-10
	D	R Weser	0.34	-	11	-	81-10
B	Norway, various S waters	Fish	280.0 (lipid)	-	9 species	-	81-9
TETRACHLOROETHENE 127-18-4							
A	USA, Los Angeles (Ca)	-	1.48	-	-	0.17-2.07	81-1
	USA, Phoenix (Az)	-	1.00	-	-	0.13-3.70	81-1
	USA, Oakland (Ca)	-	0.31	-	-	0.05-1.45	81-1
	USA, Houston (Tx)	-	0.40	-	-	0.03-3.21	82-1
	USA, St Louis, (Mo)	-	0.33	-	-	0.07-7.60	82-1
	USA, Denver (Co)	-	0.40	-	-	0.09-1.13	82-1
	USA, Riverside (Ca)	-	0.68	-	-	0.17-1.63	82-1
	USA, Staten Is (NY)	-	0.29	-	-	0.08-1.03	82-1
	USA, Pittsburgh (Pa)	-	0.41	-	-	0.08-1.66	82-1
	USA, Chicago (Il)	-	0.59	-	-	0.09-1.79	82-1
	NL	-	16.2-63.0 ppt	95.4-1026 ppt	-	-	85-1
W	CZ, Basle	R Rhine	0.3	-	-	-	78-3
	D, Cologne	R Rhine	0.8	-	-	-	78-3
	D, Duisberg	R Rhine	1.5	-	-	-	78-3
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL, Maassluis/Lobith	R Rhine	2.3	10.0	6/6	-	79-6
	D	R Lippe	4.9	-	11	-	81-10
	Japan, Pacific coast	Remote & Indust.	1.71-9.5	-	71/395	-	79-7
B	Norway, various S waters	Fish	180.0 (lipid)	-	9 species	-	81-9
HEXACHLOROBUTADIENE 87-68-3							
A	USA, Houston (Tx)	-	0.01	-	-	0.001-0.154	82-1
	USA, St Louis, (Mo)	-	0.003	-	-	0.001-0.01	82-1
	USA, Denver (Co)	-	0.002	-	-	0 - 0.007	82-1
	USA, Riverside (Ca)	-	0.004	-	-	0.001-0.016	82-1
W	USA	R Mississipi	1.4	-	-	-	76-2
	CZ, Basle	R Rhine	4.4	-	-	-	78-3
	D, Cologne	R Rhine	0.4	-	-	-	78-3
	D, Duisburg	R Rhine	0.3	-	-	-	78-3
	NL, Lobith	R Rhine	2.0	-	-	-	80-2
	NL, Maassluis/Lobith	R Rhine	0.25-0.38	1.0	-	-	79-6
S	NL, Ketelmeer	Susp. solid & sed.	210.0 (wet)	-	-	-	76-3

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
B	NL, Ketelmeer	Fish	670.0 (wet)	-	7 species	-	76-3
	NL, Ketelmeer	Invertebrates	820.0 (wet)	-	several	-	76-3
	NL, Ijsselmeer	Fish	40.0 (wet)	-	5 species	-	76-3
	USA, R Mississipi	Fish	379.0	-	1 species	-	76-2
	USA (Wa), Puget Sound	Fish (liver)	380.0	-	1 species	-	84-2
	USA (Wa), Puget Sound	Fish (muscle)	59.0	-	1 species	-	84-2

3.10 Phenols - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
PHENOL 108-95-2							
W	UK	R Mole/R Thames	0.03	-	-	-	84-3
	UK, Oxfordshire	R Cherwell	30.0	-	-	-	84-3
	USA,Pa-NJ	R Delaware	1.2-3.0	-	2/5	-	78-5
Σ DICHLOROPHENOLS							
W	USA, Pa-NJ	R Delaware	0.06-0.3	-	1/5	-	78-5
	D, various	R Weser	0.001	-	-	-	78-6
	NL, Lobith/Maassluis	R Rhine	0.02-0.1	0.1	1/6	-	79-6
Σ TRICHLOROPHENOLS							
W	USA, Pa-NJ	R Delaware	0.4-2.0	-	1/5	-	78-5
	D, various	R Weser	0.005	-	-	-	78-6
	D, various	German Bight	0.01 ppt	-	-	-	78-6
Σ TETRACHLOROPHENOLS							
W	D, various	R Weser	0.021	-	-	-	78-6
	D, various	German Bight	0.07 ppt	-	-	-	78-6
PENTACHLOROPHENOL 87-86-5							
A	B, Antwerp	Urban	5.9 ppt	-	-	4.8-6.5 ppt	77-1
	Bolivia, various	Remote	0.5 ppt	-	-	0.2-0.8 ppt	77-1
W	USA, Texas	Est Nueces	0.022	-	-	-	83-2
	D, various	R Weser	0.2	-	-	-	78-6
	D, various	German Bight	0.85 ppt	-	-	-	78-6
S	USA, Texas	Est Nueces	0.29 (dry)	-	-	-	83-2
	USA, Texas	St Luis Pass	0.18 (dry)	-	-	-	81-4
	USA, Portland Maine	Estuarine	0.83 (dry)	-	-	-	83-3
	USA, Wisconsin	R Fox	-	-	-	220-280	79-1
B	USA (Tx), St Luis Pass	Shellfish	4.4 (wet)	-	3 species	-	81-4
	USA (Tx), St Luis Pass	Fish	3.95 (wet)	-	2 species	-	81-4
	USA (Maine), Portland	Shellfish	4.0	-	2 species	-	83-3
t BUTYLPHENOL							
W	NL, Lobith/Maassluis	R Rhine	0.32	1.0	6/6	-	79-6
NONYL PHENOL 25154-52-3							
W	USA, Pa-NJ	R Delaware	-	-	16/16	0.04-2.0	78-5

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
PROPOXYPHENOL							
W	NL, Lobith/Maassluis	R Rhine	0.17-0.52	1.0	2/6	-	79-6 & 80-
* **CRESOLS**							
W	USA, Pa-NJ	R. Delaware	0.4-2.0	-	1/5	-	78-5
2-METHYLPHENOL (o-CRESOL) 95-48-7							
W	UK	R Mole/R Thames	0.1	-	-	-	84-6
3-METHYLPHENOL (m-CRESOL) 108-39-4							
W	UK	R Mole/R Thames	0.03	-	-	-	84-6
4-METHYLPHENOL (p-CRESOL) 106-44-5							
W	UK	R Mole/R Thames	0.03	-	-	-	84-6

3.11 Aromatic nitro compounds - environmental

	Location	Description	ENVIRONMENTAL		CONCENTRATIONS		
			Average	Max	Samples	Range	Ref.
NITROBENZENE 98-95-3							
W	NL, Lobith	R Rhine	1.0	-	-	-	80-2
	NL, Lobith/Maassluis	R Rhine	6.5	30.0	6/6	-	79-6
	NL, Brakel	R Waal	1.7	13.8	4/4	-	76-4
	NL, Berg	R Maas	0.07-1.0	0.3	3/4	-	76-4
	Japan, Pacific coast	Remote & Indust.	0.54-1.4	-	27/70	-	79-7
S	Japan, Pacific coast	Remote & Indust.	610-1900	-	15/47	-	79-7
o & p NITROTOLUENE							
W	NL, Brakel	R Waal	4.5	18.1	4/4	-	76-4
	NL, Berg	R Maas	0.07-0.2	0.3	3/4	-	76-4
2-NITROTOLUENE 88-72-2							
W	Japan, Pacific coast	Remote & Indust.	0 - 0.08	-	3/70	-	79-7
	NL, Lobith	R Rhine	3.0	-	-	-	80-2
	NL, Maassluis/Lobith	R Rhine	5.0	10.0	6/6	-	79-6
S	Japan, Pacific coast	Remote & Indust.	50-140	-	16/49	-	79-7
4-NITROTOLUENE 99-99-0							
W	Japan, Pacific coast	Remote & Indust.	0 - 0.1	-	1/70	-	79-7
	NL, Maassluis/Lobith	R Rhine	2.5	10.0	6/6	-	79-6
S	Japan, Pacific coast	Remote & Indust.	10-38	-	12/60	-	79-7
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
2-NITROANISOLE 91-23-6							
W	Japan, Pacific coast	Remote & Indust.	0.03-0.69	-	3/70	-	79-7
	NL, Lobith/Maassluis	R Rhine	0.42	1.0	6/6	-	79-6
S	Japan, Pacific coast	Remote & Indust.	0 - 10	-	1/58	-	79-7

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC (in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
4-NITROANISOLE 100-17-4							
W	NL, Lobith/Maassluis	R Rhine	0.32-0.48	1.0	4/6	-	79-6
Σ CHLORONITROBENZENE							
W	NL, Brakel	R Waal	0.8	1.7	4/4	-	76-4
	NL, Berg	R Maas	0.03-0.1	0.2	3/4	-	76-4

3.12 Aromatic hydrocarbons - environmental concentrations

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
BENZENE 71-43-2							
A	NL, various	-	0.1-0.58	-	-	-	85-1
W	CZ, Basle	R Rhine	0.2	-	-	-	78-3
	D, Cologne	R Rhine	0.3	-	-	-	78-3
	D, Duisburg	R Rhine	0.8	-	-	-	78-3
	NL, Maassluis/Lobith	R Rhine	0.02-0.05	0.1	2/6	-	79-6
TOLUENE 108-88-3							
A	NL, various	-	2.9-15.4	-	-	-	85-1
W	CZ, Basle	R Rhine	0.8	-	-	-	78-3
	D, Cologne	R Rhine	0.7	-	-	-	78-3
	D, Duisburg	R Rhine	1.9	-	-	-	78-3
	NL, Maassluis, Lobith	R Rhine	1.4	3.0	6/6	-	79-6
ETHYLBENZENE 100-41-4							
A	NL, various	-	0.7-2.3	-	-	-	85-1
W	NL, Maassluis-Lobith	R Rhine	0.12-0.14	0.3	5/6	-	79-6
Σ-XYLENES							
W	NL, Maassluis/Lobith	R Rhine	0.53	1.0	6/6	-	79-6
m-XYLENE 108-38-3							
A	NL, various	-	1.24-4.95	-	-	-	85-1
p-XYLENE 106-42-3							
A	NL, various	-	0.35-2.12	-	-	-	85-1
o-XYLENE 95-47-6							
A	NL, various	-	0.7-2.47	-	-	-	85-1
STYRENE 100-42-5							
A	NL, various	-	0.07-1.21	-	-	-	85-1
W	NL, Maassluis/Lobith	R Rhine	0.07-0.13	0.3	3/6	-	79-6
	NL, Lobith	R Rhine	0.01	-	-	-	80-2

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC
(in ppb unless otherwise stated) (cont.)

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
2-METHYL ETHYLBENZENE 611-14-3							
A	NL, various	-	0.4-1.6	-	-	-	85-1
W	NL, Lobith	R Rhine	0.01	-	-	-	80-2
Σ **TRIMETHYLBENZENES**							
W	NL, Maassluis/Lobith	R Rhine	0.17-1.0	1.0	1/6	-	79-6
1,3,5-TRIMETHYLBENZENE 108-67-8							
A	NL, various	-	0.4-1.2	-	-	-	85-1
W	NL, Lobith	R Rhine	0.01	-	-	-	80-2
1,2,3,4-TETRAMETHYLBENZENE 488-23-3							
A	NL, various	-	13-20 ppt	-	-	-	85-1

3.13 Miscellaneous - environmental concentrations

			ENVIRONMENTAL CONCENTRATIONS				
	Location	Description	Average	Max	Samples	Range	Ref.
ACETOPHENONE 98-86-2							
W	NL, Lobith/Maassluis	R Rhine	0.28-0.43	1.0	4/6	-	79-6
3,4-DICHLOROACETOPHENONE 2642-63-9							
W	NL, Lobith/Maassluis	R Rhine	0 - 0.1	0.1	1/6	-	79-6
N-BUTYLBENZENESULFONAMIDE 3622-84-2							
W	D/NL, Border	R Rhine	0.07	-	-	-	78-4
	NL, Lobith	R Rhine	1.0	-	-	-	80-2
DI-(2-ETHYLHEXYL)ADIPATE (DEHA) 103-23-1							
W	USA, Pa-NJ	R Delaware	-	-	16/16	0.02-0.3	78-5
ISOPHORONE 78-59-1							
W	USA, Pa-NJ	R Delaware	trace	-	1/16	-	78-5
	NL, Lobith/Maassluis	R Rhine	0.05-0.3	0.3	1/6	-	79-6
METHYLBUTANOATE 623-42-7							
W	NL, Maassluis/Lobith	R Rhine	0.05-0.3	0.3	1/6	-	79-6
MALEIC ACID, METHYL ESTER 624-48-6							
W	NL, Lobith/Maassluis	R Rhine	0.17-1.0	1.0	1/6	-	79-6
METHYL METHACRYLATE 80-62-6							
W	NL, Maassluis/Lobith	R Rhine	0.05-0.15	0.3	2/6	-	79-6

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS Average	Max	Samples	Range	Ref.
2-CHLOROTOLUENE 95-49-8							
A	USA, Houston (Tx)	Urban	< 5.0 ppt	-	-	<5 - 58 ppt	83-1
	USA, St Louis, (Mo)	Urban	< 5.0 ppt	-	-	<5 - 25 ppt	83-1
	USA, Denver (Co)	Urban	< 5.0 ppt	-	-	<5 -111 ppt	83-1
	USA, Riverside (Ca)	Urban	< 5.0 ppt	-	-	<5 - 39 ppt	83-1
W	CZ, Basle	R Rhine	0.9	-	-	-	78-3
	D, Cologne	R Rhine	0.6	-	-	-	78-3
	D, Duisburg	R Rhine	5.3	-	-	-	78-3
PCB (1242 &/or 1254)							
A	American Samoa	Remote Marine	0.01 ppt	-	-	-	85-3
	Peru coast	Marine	0.01 ppt	-	-	-	85-3
	Barbados	Marine	0.06 ppt	-	-	-	85-3
	USA, Texas coast	Marine	0.06 ppt	-	-	-	85-3
	Canada, Newfoundland	Marine	0.08 ppt	-	-	-	85-3
	Antarctic	Remote	0.09 ppt	-	-	-	85-3
	Bermuda	Marine	0.07 ppt	-	-	-	85-3
	Pacific, Enewetak Atoll	Remote Marine	0.09 ppt	-	-	-	85-3
	Indian Ocean	Remote Marine	0.13 ppt	-	-	-	85-3
	Gulf of Mexico	Remote Marine	0.13 ppt	-	-	-	85-3
	Pacific	Remote Marine	0.29 ppt	-	-	-	85-3
	USA, Texas (Coll. St)	Rural/Suburban	0.24 ppt	-	-	-	85-3
	USA (Fl), Pigeon Key	Coastal	0.34 ppt	-	-	-	85-3
	SCN Inlet Est.	Coastal	0.37 ppt	-	-	-	85-3
	USA,Texas	Coast	0.44 ppt	-	-	-	85-3
	Canada, Ontario	Rural/Suburban	4.54 ppt	-	-	-	85-3
	Canada, Ontario	Rural/Suburban	0.16 ppt	-	-	-	85-3
	USA, L Mighigan	Rural/Suburban	0.73 ppt	-	-	-	85-3
	USA, L Superior	Rural/Suburban	1.00 ppt	-	-	-	85-3
	USA, Denver (Co)	Urban	1.89 ppt	-	-	-	85-3
	USA, Milwaukee	Urban	1.89 ppt	-	-	-	85-3
	USA, Houston (Tx)	Urban	2.52 ppt	-	-	-	85-3
	USA, Jacksonville	Urban	3.95 ppt	-	-	-	85-3
	USA, Columbia	Urban	3.95 ppt	-	-	-	85-3
	USA, Ontario	Urban	2.6 ppt	-	-	-	85-3
	USA, Mineapolis	Urban	5.96 ppt	-	-	-	85-3
	USA, Madison	Urban	6.30 ppt	-	-	-	85-3
	USA, Chicago	Urban	6.72 ppt	-	-	-	85-3
	USA, Gainesville	Urban	16.80 ppt	-	-	-	85-3
	USA, New Bedford	Urban	36.80 ppt	-	-	-	85-3
PCB (1242)53469-21-9							
A	Pacific, Enewetak Atoll	Remote Marine	0.45 ppt	-	-	-	81-2
PCB (1254) 11097-69-1							
B	USA, Mass.	Shellfish	150.0 (wet)	-	-	-	81-8
	Turkey, E Coast Med.	Fish	1645.0 (dry)	-	-	-	80-4
	Various, Mediterranean	Fish	3220.0 (dry)	-	-	-	80-4
	USA, various (76-81)	Fish	-	22050.0 (wet)	(NCMP-90%)	-	85-4
PCB (AROCHLOR 1260) 11096-82-5							
W	USA, Texas (8 Sts)	Est Nueces	4.7 ppt	-	-	-	83-2
S	USA, Texas (8 Sts)	Est Nueces	4.7 (dry)	-	-	-	83-2
	USA, Texas (8 Sts)	St Luis Pass	0.52 (dry)	-	-	-	81-4
	USA, Maine (Portland) (8 Sts)	Estuarine	120.0 (dry)	-	-	-	83-3
	Turkey, E coast Med.	Marine	208.6 (dry)	-	-	-	80-4
	Various, Mediterranean	Marine	180 (dry)	-	-	-	80-4
B	USA, Maine (Portland)	Shellfish	44.0	-	2 species	-	83-3
	Gulf of Mexico	Fish (Groupers)	42.9 (wet)	-	1 species	-	74-1
	Grand Bahamas	Fish (Groupers)	6.2 (wet)	-	2 species	-	74-1
	USA, various (76-81)	Fish	-	7600.0 (wet)	(NPMP 88%)	-	85-4

Appendix 3 : Environmental Concentrations of Chemicals Collated by the WRC

(in ppb unless otherwise stated) (cont.)

	Location	Description	ENVIRONMENTAL CONCENTRATIONS				
			Average	Max	Samples	Range	Ref.
Σ PCB							
A	NL, various	-	0.81 ppt	2.56 ppt	-	-	85-1
	USA, Gulf of Mexico	Remote Marine	0.29 ppt	-	-	0.11-0.66 ppt	80-1
	USA, Gulf of Mexico	Remote Marine	0.34 ppt	-	8	-	78-1
	N Atlantic	Remote Marine	0.39 ppt	-	5	-	78-1
W	USA, Gulf of Mexico	Remote & Coastal	0.001	-	17	-	78-1
	USA, Mississipi Delta	Coastal	0.002	-	14	-	78-1
	N Atlantic	Marine	0.16 ppt	-	10	-	78-1
	Japan, Pacific coast	Remote & Indust.	0.88-23.0	-	30/788	-	79-7
S	USA, Gulf of Mexico	Marine	1.09	-	12	-	78-1
	USA, Mississipi Delta	Estuarine	18.7	-	22	-	78-1
	USA, Florida	R Apalachicola	2100.0 (dry)	-	-	1000-7000	84-1
	Japan, Pacific coast	Remote & Indust.	1160-2000	-	762/1314	-	79-7
B	USA, Gulf of Mexico	Fish/Shellfish	29.6	-	20	-	78-1
	USA (Fl) R Apalachicola	Shellfish (clams)	21.0 (dry)	-	1 species	10-44	84-1
	Mexico, Gulf coast	Shellfish (Oyster)	54.9 (wet)	-	1 species	-	79-3
	D, Wadden Sea	Shellfish	45.0 (wet)	-	4 species	-	79-4
	D, Wadden Sea	Fish (Sole)	206.0 (wet)	-	1 species	-	79-4
	NL, various coastal	Shellfish (Mussel)	280.0 (wet)	-	1 species (14/14)	-	79-5
	Japan, Pacific coast	Fish	510-540	-	(280/294)	-	79-7
	USA, L Ontario	Fish	1160	-	10 species	-	84-2
	Finland, S Lakes	Fish (Pike)	135.0 (wet)	-	1 species	-	83-4
	Finland, N Lakes	Fish (Pike)	160.0 (wet)	-	1 species	-	83-4
	Finland, coast	Fish (Pike)	270.0 (wet)	-	1 species	-	83-4
	USA, various (76-81)	Fish	-	92700.0 (wet)	(NPMP-94%)	-	85-4
	USA, L Superior	Fish	610	-	3 species	100-3700	79-1
	USA, L Michigan	Fish	10200	-	3 species	2100-18900	79-1
	USA, L Buron	Fish	820	-	3 species	100-7000	79-1
	USA, L Erie	Fish	880	-	3 species	100-9300	79-1
	USA, L Ontario	Fish	2370	-	3 species	100-21100	79-1

References to Appendix 3

1985

85-1 Guicherit R. and Schulting F.L.(1985). The occurrence of organic chemicals in the atmosphere of the Netherlands. Sci. Tot. Environ., 43(3), 193-219.

Air samples analysed by direct injection GC-FID or by collection, using cryogenic preconcentration, tenax adsorption, glass fibre and polyurethane foam filters and analysis by GC-ECD, GC-MS and HPLC.

Study catagory 2.

85-2 Atlas E. and Giam C.S.(1985). American Chem. Society (Div. Environ. Cgem.) 190th National Meeting, Chicago Illinois, Sept.8-13, 25(2), 5-7.

Air sampled through filter, filter solvent extracted, GC-ECD and GC-MS.

Study category 3.

85-3 Giam C.S., Phifer C.B. and Atlas E.(1985). Remote air concentrations of anthropogenic organics as basis for clean air standards. American Chem. Society (Div. Environ. Chem) National Meeting, Chicago Illinois, Sept. 8-13, 25(2), 170-171. Preprint of Extended Abstracts, Am. Chem. Soc. Symp., Sept. 1985.

Air sampled through filter, filter solvent extracted, GC-ECD and GC-MS.

Study category 3.

85-4 Schmitt C.J., Zajicek J.L. and Ribick M.A.(1985). National pesticide monitoring programme : residues of organochlorine chemicals in freshwater fish, 1980-81. Arch. Environ. Contam. Toxicol., 14(2), 225-260.

315 composite samples of 3 to 5 fish, homogenised, solvent extracted in a column, Gel permeation chromatography and Florisil column cleanup, silica gel column fractionation, Capillary and Packed column GC-ECD.

Study category 3 (Part of National Pesticide Monitoring Programme).

85-5 Carey A.E., Kutz F.W.(1985). Trends in ambient concentrations of agrochemicals in humans and the environment of the United States. Environ. Monit. Assess., 5(2), 155-163.

From US Food and Drug Administration Pesticide Analytical Manual.

Study category 3 (Part of National Pesticide Monitoring Programme).

1984

84-1 Elder J.F., Mattraw H.C.(1984). Accumulation of trace elements, pesticides and polychlorinated biphenyls in sediments and the clam Corbicula Manilensis of the Apalachicola River, Florida. Arch. Environ. Contam. and Toxicol., 13, 453-469.

Nine 50 g samples of homogenised clam, seven 50 g samples of detritus and twelve composited sieved sediment samples.

Organochlorine insecticide and PCBs were determined by : solvent extraction, alumina and silica gel column cleanup, GC-ECD.

Organophosphorus insecticides were determined by : solvent extraction, alumina and silica gel column cleanup, GC-FPD.

Chlorinated phenoxy acid herbicides and their esters were determined by : solvent extraction of acidified slurry, hydrolysis, methylation, GC-ECD.

Study category 2.

84-2 Malins D.C., McCaln B.B., Brown D.W., Chan S.L., Myers M.S., Landahl J.T., Prohaska P.G., Friedman A.J., Rhodes L.D., Burrows D.G., Gronlund W.D., Hodgins H.O.(1984). Chemical pollutants in sediments and diseases of bottom-dwelling fish in Puget Sound, Washington. Environ. Sci. Technol., 18(9), 705-713.

Solvent extraction, column chromatography, GC-MS, GC-FID and GC-ECD.

Study category 2.

84-3 Commission of the European Communities (1984). An inventory of polluting substances which have been identified in various fresh waters, effluent discharges, aquatic animals and plants, and bottom sediments. 4th Edition, 4 Vols.

Compilation of data from many sources.

Study category 2.

1983

83-1 Singh H.B., Salas L.J., Stiles R., Shigeishi H. Measurements of hazardous organic chemicals in the ambient atmosphere. NTIS, PB83-156935. Final Report, Sept. 1978 to Oct. 1981.

Air samples from ten sites, cryogenic preconcentration on packed loop of metal tubing, GC-FID and GC-ECD.

Study category 3.

83-2 Ray L.E., Murray H.E. and Giam C.S.(1983). Analysis of water and sediment from the Nueces Estuary, Corpus Christi Bay (Texas) for selected organic pollutants. Chemosphere, 12 (7-8), 1039-1045.

50 g samples of sediment refluxed with solvent, resulting extract solvent extracted under basic and acidic conditions, basic extract was Florisil column cleaned up, acidic extract was methylated then cleaned up on alumina column. Pentachlorophenol was quantitated using packed column GC-ECD other compounds were quantitated using capillary GC-ECD and GC-FID.

Study category 2.

83-3 Ray L.E., Murray H.E. and Giam C.S.(1983). Organic pollutants in marine samples from Portland, Maine. Chemosphere, 12(7-8), 1031-1038.

Clams and neanthes homogenised, analysis as for 83-3.

Study category 2.

83-4 Pyssalo H., Wickstrom K., Litmanen R.(1983). A baseline study on the concentrations of chlordane-, PCB- and DDT-compounds in Finnish fish samples in the year 1982. Chemosphere, 12(6), 837-842.

113 fish were analysed as follows :
2 g of homogenised fish tissue ultrasonicated with solvent, resultant extract was partitioned in salt solution, aqueous layer solvent extracted, solvent fraction evaporated in vacuo, dissolved; cleaned up by silica gel chromatography, GC-MS quantitation.

Study category 1. Because extraction efficiencies not assessed properly (internal standard heptachlor which may have different extraction efficiency to DDT and PCBs) and the method is likely to cause large losses.

1982

82-1 Singh H.B., Salas L.J., Stiles R.E.(1982). Distribution of selected gaseous organic mutagens and suspect carcinogens in ambient air. Environ. Sci. Technol., 16(12), 872-880.

400 ml samples of air taken 5 times a day over 10 days, sample preconcentrated on cryogenically cooled packed metal tube, GC-ECD or GC-FID.

Study category 2.

82-2 Oliver B.G. and Nicol K.D.(1982). Chlorobenzenes in sediments, water and selected fish from Lakes Superior, Huron, Erie and Ontario. Environ. Sci. and Technol., 16(8), 532-536.

Sediment :
Cores taken sectioned into 1 cm layers except top 3 cm, 15 g Soxhlet extracted, Na_2SO_4 and Florisil column cleanup, GC-ECD.

Fish :
15 g of fish homogenate soxhlet extracted, Na_2SO_4-alumina-silica gel-Florisil column cleanup, H_2SO_4-silica gel column cleanup, GC-ECD.

Water :
1 gallon of water solvent extracted, Na_2SO_4-Florisil column cleanup, GC-ECD.

Study category 3.

82-3 Peterson J.C., Freeman D.H.(1982). Phthalate ester concentration variations in dated sediment cores from the Chesapeake Bay. Environ. Sci. and Technol., 16(8), 464-469.

Sediment cores sectioned into 10 cm layers, ultrasocinated with solvent, GC-MS.

Study category 3.

1981

81-1 Singh H.B., Salas L.J., Smith A.J., Shigeishi H.(1981). Measurements of some potentially hazardous organic chemicals : in urban environments. Atmospheric Environment, 15, 601-612.

Air samples preconcentrated on cryogenically cooled loop of packed metal tubing, GC-ECD and GC-FID.

Study category 2.

81-2 Atlas E., Giam C.S.(1981). Global transport of organic pollutants : ambient concentrations in the remote marine atmosphere. Science, 211(4478), 163-165.

1000-2000 m^3 of air sampled on filters for high molecular weight compounds, 75-150 m^3 of air sampled on Florisil for low molecular weight compounds, absorbents soxhlet extracted, Florisil column cleanup, GC-ECD.

Study category 3.

81-3 Wegman R.C.C., DeKorte G.A.L.(1981). Aromatic amines in surface waters of the Netherlands. Water Research, 15, 391-394.

1 Litre water samples solvent extracted, hydrolysed, stealm distilled, brominated, GC.

Study category 2.

81-4 Murray H.E., Ray L.E., Giam C.S.(1981). Analysis of marine sediment, water and biota for selected organic pollutants. Chemosphere, 10(11-12), 1327-1334.

Sediment :
Duplicate 50 g samples collected from 3 sites, solvent extracted, GC-ECD and HPLC-spectrofluorimetry.

Water :
Solvent extracted, GC-ECD and HPLC-spectrofluorimetry.

Biota:
Hexachlorobenzene and benzo(a)pyrene were determined by : solvent extracting tissue homogenate, silica gel column cleanup, GC-ECD and HPLC-spectrofluorimetry.

Pentachlorophenol was determined by solvent extracting tissue homogenate, solvent cleanup at pH>11, solvent extracted at pH<2, methylated, acid alumina column cleanup, GC-ECD.

Study category 2.

81-5 Leung S.Y.T, Bulkley R.V., Richard J.J.(1981). Influence of a new impoundment of pesticide concentrations in warm water fish, Saylorville Reservoir, Des Moines River, Iowa, 1977-78. Pest. Monit. Journal, 15(3), 117-122.

25-30 g of fish tissue solvent extracted in blender salt solution-solvent partition, Florisil cleanup, packed column GC-ECD.

Study category 2.

81-6 Bulkley R.V., Leung S.Y.T., Richard J.J.(1981). Organochlorine insecticide concentrations in fish of the Des Moines River, Iowa, 1977-78. Pest. Minot. Journal, 15(2), 86-89.

25-30 g of fish tissue solvent extracted in blender, salt solution-solvent partition, Florisil cleanup, packed column GC-ECD.

Study category 2.

81-7 Leung S.Y.T, Bulkley R.V., Richard J.J.(1981). Persistence of dieldrin in water and channel catfish from the Des Moines River, Iowa, 1971-73 and 1978. Pest. Monit. Journal, 15(2), 98-102.

Water:
1971 : filtered, particulates soxhlet extracted and Florisil column cleaned, water solvent extracted, packed column GC-ECD.

1978: XAD2 column extraction, packed column GC-ECD.

Fish :
20-65 g of tissue solvent extracted in blender, partitioned between salt solution and solvent, Florisil column cleanup, packed column GC-ECD.

Study category 2.

81-8 Hatch W.I., Allen D.W., Brady P.D., Davis A.C., Farrington J.W.(1981). Polychlorinated biphenyls in clams and oysters from New Bedford Harbour, Massachusetts, march 1978. Pest. Monit. J., 15(3), 123-127.

Clam and oyster homogenate solvent extracted, alumina and silica gel column cleanup, packed column GC-ECD.

Study category 2.

81-9 Ofstad E.B., Drangsholt H. and Carlberg G.E.(1981). Analysis of volatile halogenated organic compounds in fish. Sci. Tot. Environ., 20(3), 205-216.

5 g of fish tissue homogenate solvent extracted, sulphuric acid cleanup, capillary GC-ECD.

Study category 3.

81-10 Sonneborn M., Gerdes S., Schwabe R.(1981). Volatile halogenated hydrocarbons in river water, groundwater, drinking water and swimming pool water in the Federal Republic of Germany. In: Analysis of Organic Micropollutants in Water, proceedings of the 2nd European Symposium held in Killarney (Ireland), Nov. 17-19. Edited by A. Bjorseth and G. Angeletti, R. Reidel Publ. Co.

250 ml water samples, purge and trap, packed column GC-FID and GC-ECD.

Study category 2.

81-11 Wegman R.C.C. and DeKorte G.A.L.(1981). The gas-chromatographic determinationof aromatic amines after bromination in surface waters. Intern. J. Environ. Anal. Chem., 9, 1-6.

Solvent extraction, hydrolysis, steam distillation, bromination, capillary GC-ECD.

Study category 2.

1980

80-1 Giam C.S., Atlas E., Chan H.S. and Neff G.S.(1980). Phthalate esters, PCB and DDT residues in the Gulf of Mexico atmosphere. Atmos. Environ., 14, 65-69.

600 m^3 air sampled through filters, soxhlet extracted, Florisil column cleanup, GC-ECD.

Study category 2.

80-2 Zoeteman B.C.J., Harmsen K., Linders J.B.H.J.(1980). Persistent organic pollutants in river water and groundwater of the Netherlands. Chemosphere, 9, 231-249.

XAD column extraction and closed loop stripping, GC-MS.

Study category 2.

80-3 Gledhill W.E., Kaley R.G., Adams W.J., Hicks O., Michael P.R., Saeger V.W. and Le Blanc G.A.(1980). An environmental safety assessment of butylbenzyl phthalate. Environ. Sci. and Technol., 14(3), 301-305.

Water samples and 10 g sediment samples solvent extracted, packed column GC-FID, GC-ECD and GC-MS.

Study category 1 (Blanks not run and likely to have contamination as compound to be determined is a pthalate).

80-4 Basturk O., Dogan M., Salihoglu I. and Balkas T.I.(1980). DDT, DDE and PCB residues in fish, crustaceans and sediments from the eastern Mediterranean coast of Turkey. Mar. Poll. Bull., 11(7), 191-195.

Biota:
10 g of tissue homogenate soxhlet extracted, alumina column cleanup, silica column fractionation, packed column GC-ECD.

Sediment :
Solvent extracted, copper column cleanup, packed column GC-ECD.

Study category 2.

80-5 Ballschmiter K. and Zell M.(1980). Occurrence of organohalogens in pristine European and Antarctic aquatic environments. Intern. J. Environ. Anal. Chem., 8, 15-35.

10-25 g of spawn of fish liver solvent extracted in a column of soxhlet extracted, 2-10 g of sperm oil dissolved, alumina column cleanup, fractionation on Florisil, capillary GC-ECD.

Study category 2.

80-6 Campbell I. and McConnel G.(1980). Chlorinated paraffins and the environment. 1. Environmental Occurrence. Environ. Sci. and Technol., 14(10), 1209-1214.

Water samples :
100 ml of water solvent extracted, adsorption column chromatography cleanup, TLC separation and quantitation.

Sediment samples :
10 g of sediment soxhlet extracted, adsorption column chromatography cleanup, TLC separation and quantitation.

Biota samples :
10 g of tissue homogenate soxhlet extracted, liquid-liquid extraction as cleanup (to remove lipids), adsorption column chromatography celanup, TLC separation and quantitation.

Study category 2 (Method has a quoted precision of up to ±50% at lowest concentrations).

1979

79-1 Delfino J.J.(1979). Toxic substances in the Great Lakes. Environ. Sci. and Technol., 13(12), 1462-1468.

Study category 3. Pluar joint US, Canada project.

79-2 Roberts G.C., Sirons G.J., Frank R. and Collins H.E.(1979). Triazine residues in a watershed in south-western Ontario (1973-1975). J. Great Lake Res., 5(3-4), 246-255.

1 litre water taken from 4-5 litre composite sample, solvent extracted, cleanup, GC-TCD.

33 fish, solvent extracted in blender, chilled to remove fat, diluted with water, solvent extracted, GC-TCD.

Study category 2.

79-3 Rosales M.T.L., Botello A.V., Bravo H. and Mandelli E.F.(1979). PCBs and organochlorine insecticides in oysters from coastal logoons of the Gulf of Mexico, Mexico. Bull. Environ. Contam. and Toxicol., 21, 652-656.

100 oysters from 9 locations, homogenised, freeze dried, soxhlet extracted, Florisil cleanup, packed column GC.

Study category 1. Packed column GC peaks difficult to quantify, extraction efficiencies not assessed properly.

79-4 Goerke H., Eder G., Weber K. and Ernest W.(1979). Patterns of organochlorine residues in animals of different trophic levels from Weser Estuary. Mar Poll. Bull., 10(5), 127-132.

Five composite samples homogenised, solvent extracted alumina column cleanup, Florisil column fractionation, GC-ECD.

Study category 2.

79-5 Quirijns J.K., Van der Paauw C.G., Ten Noever De Brauw M.C. and De Vos R.H.(1979). Survey of the contamination of Dutch coastal waters by chlorinated hydrocarbons including the occurrence of methylthio pentachlorobenzene and di-methylthio tetrachlorobenzene. Sci. Tot. Environ., 13, 225-233.

25 mussels sampled at each of 14 sites, 10 g of tissue homogenate soxhlet extracted, alumina-silica column cleanup, packed column GC and GC-MS.

Study category 1 (Packed column GC not easy to quantify peaks).

79-6 Morra C.F.H., Linders J.B.B.J., den Boer A., Ruijgrok M., Zoeteman B.C.J.(1979). Organic chemicals measured during 1978 in the River Rhine in the Netherlands. R I D Meddeling 79-3.

3 composite samples of water, closed loop stripping and XAD4-XAD8 extraction , GC-MS.

Static headspace, GC-ECD for volatile chlorinated hydrocarbons.

Study category 2 but 1 for XAD results as results may be a factor of 3 out according to authors.

79-7 Kubota Y.(1979). Experience with the chemical substances control law in Japan. Ecotoxicol. and Envrion. Safety, 3, 256-268.

20 water samples, 10 sediments samples, 10 fish samples; analysis unknown.

Study category 2.

1978

78-1 Giam C.S., Chan H.S., Neff G.S., Atlas E.L.(1978). Phthalate ester plasticizers : a new class of marine pollutant. Science, 199(4327), 419-421.

Solvent extraction, Florisil column cleanup, GC-ECD.

Study category 2.

78-2 Bove J.L., Dalven P., Kukreja V.P.(1978). Airborne di-butyl and di-(2-ethylhexyl)-phthalate at three New York city air sampling stations. Intern. J. Environ. Anal. Chem., 5, 189-194.

Filter sampling, soxhlet extraction, GC-MS.

Study category 2.

78-3 Kühn W., Sontheimer H., Steiglitz L., Maier D. and Kurz R.(1978). Use of ozone and chlorine in water utilities in the Federal Republic of Germany. JAWWA, 70, 326-331.

3 water samples, Grob closed loop stripping, GC-MS.

Study category 2.

78-4 Poels C.L.M., Snoek O.I., Huizenga L.J.(1978). Toxic substances in the Rhine River. Ambio, VII (5-6), 218-225.

No details available.

Study category 2.

78-5 Sheldon L.S., Hites R.A.(1978). Organic compounds in the Delaware River. Environ. Sci. and Technol., 12(10), 1188-1194.

Eleven 3.5 litre water samples, solvent extracted under acidic and basic conditions, silica gel column fractionation, GC-MS.

Two 7 litre water samples vapour stripped, GC-MS.

Sediment samples soxhlet extracted, copper column cleanup, GC-MS.

Study category 1 (Analytical approach qualitative only semi-quantitative results).

78-6 Weber K., Ernst W.(1978). Levels and pattern of chlorophenols in water of the Weser Estuary and the German Bight. Chemosphere, 7(1), 873-879.

15 litre and 40 litre samples of water solvent extracted under acidic and alkaline conditions, acetylation, GC-MS.

Study category 3.

1977

77-1 Cautreels W., Van Cauwenberghe K., Guzman L.A.(1977). Comparison between the organic fraction of suspended matter at a background and an urban station. Sci. Tot. Environ., 8, 79-88.

6000 m^3 air sampled through each of 3 filters, soxhlet extracted, evaporated and redissolved under acidic conditions and basic conditionsn acidic fraction methylated, GC-MS.

Study category 1 (Extraction efficiencies not determined and method likely to cause large losses).

1976

76-1 Bidleman T.F., Rice C.P., Olney C.E.. In: Marine Pollutant Transfer. Edited by J.L. Windom and R.A. Duce. Lexington Books, Lexington Mass 1976, 323-351.

Study category 2.

76-2 Laska A.L., Bartell C.K. and Laseter J.L.(1976). Distribution of hexachlorobenzene and hexachlorobutadiene in water, soil and selected aquatic organisms along the lower Mississippi River, Louisiana. Bull. Environ. Contam. and Toxicol., 15(5), 535-542.

Twenty-six 350 ml samples of water solvent extracted, packed column GC-ECD.

Twenty-six 20 g levee soil and twenty-six mud samples solvent extracted, packed column GC-ECD.

Fish and aquatic invertebrates homogenised, solvent extracted, Florisil cleanup, packed column GC-ECD.

Study category 1 (Extraction efficiencies not determined).

76-3 Goldbach R.W., Van Genderen H., Leeuwangh P.(1976). Hexachlorobutadiene residues in aquatic fauna from surface water fed by the River Rhine. Sci. Tot. Environ., 6, 31-40.

50 fish plus detritus and worms analysed as follows :

low chlorine hydrocarbons determined by co-distillation of 5-10 g of homogenised tissues or detritus with solvent, packed column GC-ECD;

high chlorine hydrocarbons determined by solvent extracting 5-10 g homogenate, Florisil column cleanup, packed column GC-ECD;

500 ml water samples solvent extracted, packed column GC-ECD.

Study category 3.

76-4 Meijers A.P. and van der Leer R.C.(1976). The occurrence of organic micropollutents in the R. Rhine and R. Meus in 1974. Water Res., 10, 597-604.

Study category 2.

1975

75-1 Lillian D., Singh H.B., Appleby A., Lobban L., Arnts R., Gumpert R., Hague R., Toomey J., Kazazis J., Antell M., Hansen D., Scott B.(1975). Atmospheric fate of halogenated compounds. Environ. Sci. and Technol., 9(12), 1042-1048.

100 ml air samples, packed column GC-ECD and GD-FID.

Study category 2.

1974

74-1 Giam C.S., Richardson R.L., Taylor D. and Wong M.K.(1974). DDT, DDE and PCBS in the tissues of reef dwelling groupers (Serrindae) in the Gulf of Mexico and the Grand Bahamas. Bull. Environ. Contam. and Toxicol.,11(2), 189-192.

19 groupers (Serranidae) sampled and analysed using methods from the US Food and Drug Administration pesticide Analytical Manual.

Study category 2.

Appendix 4 : The Mackay Level I Fugacity Model for Calculating Equilibrium Distributions

Equilibrium calculations presented in this report were based on several publications by Mackay (Mackay 1979; Mackay and Paterson 1981, 1982) and others who use similar approaches (Neely, 1980; Friske et al, 1984).

The fugacity of a chemical in a given phase (compartment) provides a measure of its tendency to escape from that phase. In a system containing many phases, molecules tend to move from those of high fugacity to those of lower fugacity until the fugacity of the chemical in all phases is the same and equilibrium is attained. For a three-phase system comprising air (a), water (w), and solid (s) at equilibrium, the fugacity of the chemical (f_i) in each phase is the same, i.e.

$$f_a = f_w = f_s$$

The concentration (C_i) of the chemical can be written as the product of the fugacity and a factor called the fugacity capacity factor designated as Z_i by Mackay (this factor will be discussed later) :

$$C_i = f_i Z_i$$

For the purposes of the calculation each phase is assigned a volume (V), and if M is the total number of moles of the chemical originally added to the system :

$$M = C_a V_a + C_s V_s + C_w V_w$$

$$= f_a (V_a Z_a + V_s Z_s + V_w Z_w)$$

$$C_a = \frac{M Z_a}{(V_a Z_a + V_s Z_s + V_w Z_w)}$$

From this expression it can be seen that the concentration in one phase is determined by the properties of the chemical and the volumes of the other phases. On the other hand, the ratios are invariant as can easily be shown, e.g. :

$$\frac{C_a}{C_w} = \frac{Z_a}{Z_w}$$

The Z values have been documented by Mackay (1985) :

$Z_a = {}^{1}/_{RT}$, where R = gas constant and T = absolute temperature;

$Z_w = {}^{1}/_{H} = {}^{WS}/_{P}$, where H = Henry's constant derived from the water solubility WS and the vapour pressure P of the chemicals concerned;

$Z_s = {}^{K}/_{H}$, where K is the equilibrium partition coefficient of the chemical between the solid phase and water. Values of K are generally derived from the octanol-water partition coefficient: see Appendix 2.

The volume of each phase in the model has to be defined, and , in fact, the "unit world" volumes of Neely and Mackay (1982) were used :

Compartment	Volume (m^3)	Density (kg/m^3)
Air	6×10^9	1.19
Water	7×10^6	1000
Soil	4.5×10^4	1500
Sediment	2.1×10^4	1500
Suspended matter (in water)	35	1500
Biota	7	1000

The last four compartments are summed to give the "solid" compartment which soil and sediment clearly predominate.

A specimen calculation is given below :

ALACHLOR

Molecular wieght	270.0 g/mol	
Solubility in water	2.400E+02 G/m³	8.889E-01 mol/m³
Vapour pressure	2.900E-03 pa or	2.862E-08 atm or 2.175E-05 mm hg
Henry's Constant	3.2625E-03 pa m³/mol	
Octanol-water part. coeff.	1659.59	
Temperature	25.0 °C (298.2K)	
Level I fugacity (Pa) =	3.7111543E-08.	

Compartment	Volume (m³)	Fugacity Capacity Constant mol/m³.pa	Density kg/m³	Amount mol.	Mass Percent
1 air	6.0000E+09	4.0342E-04	1.19	8.984E-02	0.09
2 water	7.0000E+06	3.0651E+02	1000.00	7.963E+01	79.63
3 soil	4.5000E+04	6.2721E+03	1500.00	1.048E+01	10.48
4 sediment	2.1000E+04	1.2544E+04	1500.00	9.777E+00	9.78
5 susp. aquat. mat.	3.5000E+01	1.2544E+04	1500.00	1.630E-02	0.02
6 biota	7.0000E+00	2.4417E+04	1000.00	6.344E-03	0.01
TOTAL				1.000E+02	

The equilibrium distribution is given in the "mass percent" column, and for alachlor is almost wholly between water and solid (soil and sediment). The resulting mass equilibrium distributions of all chemicals selected in the WRC analysis are tabulated in Appendix 2.

Mackay has described four levels of his fugacity model, of increasing complexity. The Level I model used here enables the equilibrium distribution of a given quantity of a chemical between the various environmental compartments to be calculated. It is based on the assumption that mixing in a compartment is instantaneous, i.e. none can model the real world in which mixing takes time, and concentrations, in fact, can cover a wide range.

References to Appendix 4

- Friske R., Klopper W., Rippen G. and Gunther K.O.(1984). Ecotox. and Environ. Safety, 8, 352-362.
- Mackay D.(1979). Finding fugacity feasible. Environ. Sci. & Technol., 13, 1218-1223.
- Mackay D. and Paterson S.(1981). Calculating fugacity. Environ. Sci. & Technolo., 15, 1006-1014.
- Mackay D. and Paterson S.(1982). Fugacity revisited. Environ. Sci. & Technol., 16, 654A-660A.
- Neely W.B.(1980). Chemicals in the environment - distribution, transport, fate, analysis. Dekker, New York.

Appendix 5 : Derivation of Soil-Water and Soil-Sediment Partition Coefficient (K_{oc}) from P_{ow}.

Various equations have been proposed to express the relationship between K_{oc} and P_{ow}. That developed by Karickhoff (1981) and later used by Mackay et al (1985) was adopted by the WRC :

$$K_{oc} = 0.411\ P_{ow}$$

or

$$\log K_{oc} = -0.386 + \log P_{ow}$$

Although Karickhoff initially derived this from data on only 5 chemicals, it was later confirmed to be satisfactory on a further 47, and has given predicted values of K_{oc} close to those derived from laboratory and field studies. Di Toro (1985) derived a rather similar equation from 129 data points :

$$\log K_{oc} = 0.983 \log P_{ow} + 0.00028$$

in which the $\log K_{oc}$ - $\log P_{ow}$ gradient was also close to one. However, Briggs (1981) in an extensive study of the adsorption of 105 chemicals on soils derived an equation with a much lower gradient :

$$\log K_{oc} = 0.52 \log P_{ow} + 0.86$$

The derived values of $\log K_{oc}$ were lower than those resulting from the Karickhoff equation, as exemplified below :

Chemical	$\log K_{oc}$	
	Briggs 1981*	Karickhoff 1981
Monuron	1.70	2.00, 2.26
Diuron	2.21	2.60, 2.58
Monoliuron	1.84	2.30, 2.45
Parathion	3.02	3.68, 4.03
Naphthaline	2.62	2.94

* based on K_{oc} = 0.58 x organic matter content.

This discrepancy may be due to differences between the soils and sediments chosen, and to Brigg's choice of values of P_{ow} which are not in agreement with those used by the other workers. For example, he took the P_{ow} of dieldrin as 6.2, but the WRC consider that a value of 5.5 is more likely to be correct.

References to Appendix 5

- Briggs G.G.(1981). Theoretical and experimental relationships between soil adsorption, octanol-water coefficients, water solubilities, bioconcentration factors and the Parachor. J. Agric. Food Chem., 29, 1050-1059.
- Karickhoff S.W.(1981). Semi-empical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere, 10, 833-846.
- Mackay D., Paterson S., Cheung B. and Neely W.B.(1985). Evaluating the environmental behaviour of chemicals with a level III fugacity model. Chemosphere, 14, 335-374.
- DiToro D.M.(1985). A particle interaction model of reversible organic chemical sorption. Chemosphere, 14, 1503-1538.

Appendix 6 : Statistical Relationships between Measured Environmental Concentrations and Physico-chemical Constants or Tonnage

A relationship between tonnage produced and the measured environmental concentration has often been assumed and used by regulatory authorities for the purpose of risk assessment although many other features also determine environmental concentrations e.g. biodegradation, lyophilization and absorption. In view of the extensive data obtained from this study the Task Force decided to test certain relationships.

1. Relationships Assessed

It was decided to assess whether concentrations correlated with individual physico-chemical properties. Log P_{ow} was available from the WRC work (Table 3). The water solubility, vapour pressure and the Henry's Constant are also given in Table 3. The mean concentrations of the reference chemicals in air, water, sediments and biota are plotted against their Henry's Constant and P_{ow} in Figs. A6.1.-A6.8. The reference chemicals are listed in order of the increasing value of their Henry's Constant and P_{ow} in Table A6.1. Values of the correlation coefficients and "% fit", derived from linear regression analyses of the plots in Fig. A6.1.-A6.8. are given in Table A6.2.

Estimates of the annual production of each reference chemical are given in Tables 2 and A6.1. Accurate estimates of production are hard to obtain and this is reflected in the quality of the information gathered. Estimated global production, if not directly available, was taken to be 3 times either the US or EC production. Where substances are used as such it has been assumed that all of the material produced is eventually released to the environment. Where substances are intermediates, 3% of total production has been assumed to be released; there is support for this assumption in a National Academy of Sciences (1978) report on 8 halogenated methanes.

The production and release tonnages of each reference chemical were plotted against their mean concentrations in air, water, sediments and biota, on a log-log scale. The resulting plots are given in Figs. A6.9-A6.16 and the results of linear regression analyses of the plots are recorded as "correlation coefficients" and values of "% fit" in Table 6A.2.

2. Statistical Relationships Observed

2.1 Relationships between concentrations and Henry's Constants

Fig. A6.1 and Table A6.2 show that Henry Constant is only significantly correlated with the concentration of chemicals in air (P=0.001); such a correlation is to be expected.

2.2 Relationships between concentrations and octanol-water partition coefficients

Figs. A6.2 and A6.4, and Table A6.2 show a significant negative correlation between log P_{ow} and concentrations in air and water (P=0.001). In view of this it is surprising that there is no correlation between log P_{ow} and concentrations of chemicals in sediments and biota (figs. A6.6 and A6.8).

2.3 Relationships Between concentrations and tonnages produced or released.

Figures A6.9-A6.16 and Table A6.2 show that :

a) there were modest statistically significant correlations between :
   - concentrations in sediment and tonnage produced (P=0.5),
   - concentrations in biota and tonnage produced and released (P=0.05),
   - concentrations in air and production tonnage (P=0.001), and production relased (P=0.05).

b) there was no significant relationship between :
   - concentration in water and tonnage produced or released,
   - concentration in sediments and tonnage released.

TABLE A6.1

Reference Chemicals in Order of Increasing Global Release Henry's Constant and P_{OW}.

Estimated Global Relase (Kt/yr)		Henry's Constant (Pa m³/mol)		Octanol/Water Partition	(Log P)
1,2,3-Trichlorobenzene	0.09	Dimethoate	0.000010	Aniline	0.95
1,3,5-Trichlorobenzene	0.09	beta-HCH	0.00023	Cyclohexanol	1.2
1,2,4,5-Tetrachlorobenzene	0.15	Atrazine	0.00029	2-Methylaniline	1.3
4-Chloroaniline	0.16	Alachlor	0.0033	Di-Methylpthalate	1.5
2-Chloroaniline	0.17	Parathion (Methyl & Ethyl)	0.0076	Phenol	1.5
1,2-Dichloroethene	0.3	Di-Methylphthalate	0.011	Isophorone	1.67
1,1,2,2-Tetrachloroethane	0.45	Malathion	0.012	N-Methylaniline	1.7
4-Nitroaniline	0.55	alpha-HCH	0.016	Dimethoate	1.78
Hexachlorobutadiene	0.6	4-Chloroaniline	0.020	4-Chloroaniline	1.8
N-N-Dimethylaniline	0.72	Phenol	0.031	2-Chloroaniline	1.9
3,4-Dichloroaniline	1.2	4-Nitroaniline	0.035	1,1-Dichloroethane	1.99
4-Methylphenol	1.2	gamma-HCH (Lindane)	0.035	1,1,2-Trichloroethane	2.13
Dimethoate	1.8	Diethylpthalate	0.044	Benzene	2.13
1,1,2-Trichloroethane	2.4	Dieldrin	0.091	Nitrobenzene	2.15
1,3-Dichlorobenzene	3	2-Methylaniline	0.093	4-Methylphenol	2.2
Dieldrin	3	Endrin	0.10	Diethylphthalate	2.24
Tri-N-Butylphosphate	3	Aniline	0.11	1,2-Dichloropropane	2.34
1,2,4-Trichlorobenzene	3.3	Di-N-Butylphthalate	0.12	Trichlorofluoromethane	2.4
m-Xylene	3.6	Tri-N-Butylphosphate	0.22	1,1,2,2-Tetrachloroethane	2.45
Endrin	6	N-Methylaniline	0.27	Dichloroisopropyl Ether	2.5
Chlorobenzene	6.6	Pentachlorophenol	0.29	N-N-Dimethylaniline	2.5
Di-Methylphthalate	6.6	2-Chloroaniline	0.32	Trichloroethene	2.53
Aldrin	7.5	Cyclohexanol C	0.36	1,2-Dichloroethene	2.55
Heptachlor	8.1	Chlorpyrifos	0.44	Toluene	2.65
1,2-Dibromoethane	9	4-Methylphenol	0.86	4-Nitroaniline	2.66
Parathion (Methyl & Ethyl)	9.6	Di(2-Ethylhexyl)Phthalate	0.99	Atrazine	2.68
Chlorpyrifos	10	Nitrobenzene	1.3	Tetrachloromethane	2.7
1,1-Dichloroethane	12	3,4-Dichloroaniline	2.3	1,2-Dichloroethane	2.82
gamma-HCH (Lindane)	14.1	p-p'-DDT	2.7	Malathion	2.9
1,2-Dichloropropane	15	Isophorone	4.8	1,1,1-Trichloroethane	2.95
Diethylphthalate	23.1	N-N-Dimethylaniline	6.8	Styrene	2.95
Pentachlorophenol	27	Dichloroisopropyl Ether	11	Chlorobenzene	2.98
p-p'-DDT	28.5	1,1,2,2-Tetrachloroethane	39	Ethylbenzene	3.13
Aniline	32.7	1,2,4,5-Tetrachlorobenzene	65	o-Xylene	3.13

Table A6.1 Reference Chemicals in Order of Increasing Global Release Henry's Constant and P_{ow}. (cont.)

Estimated Global Relase	(Kt/yr)	Henry's Constant	(Pa m^3/mol)	Octanol/Water Partition	(Log P)
Dichloroisopropyl Ehter	45	Pentachlorobenzene	66	p-Xylene	3.18
Nitrobenzene	46.5	1,1,2-Trichloroethane	74	Alachlor	3.2
Malathion	47.4	Hexachlorobenzene	76	m-Xylene	3.2
o-Xylene	63	1,2,3,4-Tetrachlorobenzene	94	3,4-Dichloroaniline	3.35
1,4-Dichlorobenzene	66	Hexachlorobutadine	110	1,4-Dichlorobenzene	3.37
Hexachlorobenzne	80	Styrene	230	1,2-Dichlorobenzene	3.38
Tetrachloromethane	84	1,2,4-Trichlorobenzene	240	Tetrachloroethene	3.38
p-Xylene	100	1,2-Dichloropropane	280	2-Chlorotoluene	3.42
Atrazine	111	Aldrin	280	1,3-Dichlorobenzene	3.48
Alachlor	123	1,2-Dichlorobenzene	320	alpha-HCH	3.8
Phenol	180	o-Xylene	320	beta-HCH	3.8
Styrene	210	1,4-Dichlorobenzene	380	Parathion (Methyl & Ethyl)	3.8
Di-N-Butylphthalate	230	1,2,3,5-Tetrachlorobenzene	400	gamma-HCH (Lindane)	3.85
Trichlorofluoromethane	291	1,2,3-Trichlorobenzene	420	1,2,3,4-Tetramethylbenzene	3.98
Trichloroethene	326	Benzene	430	Tri-N-Butylphosphate	4
Di(2-Ethylhexyl)Phthalate	402	1,2,3,4-Tetramethylbenzene	440	1,2,3-Trichlorobenzene	4.1
Tetrachloroethene	470	p-Xylene	440	1,2,4-Trichlorobenzene	4.1
1,1,1-Trichloroethane	537	Toluene	460	1,3,5-Trichlorobenzene	4.1
1,2-Dichloroethane	547	Heptachlor	500	1,2-Dibromoethane	4.3
Ethylbenzene	600	Ethylbenzene	520	1,2,4,5-Tetrachlorobenzene	4.51
Cyclohexanol	1200	m-Xylene	530	1,2,3,4-Tetrachlorobenzene	4.55
Toluene	1800	1,1-Dichloroethane	560	Chlorpyrifos	4.6
Benzene	1100	Chlorobenzene	620	1,2,3,5-Tetrachlorobenzene	4.65
		1,3-Dichlorobenzene	640	Di-N-Butylphthalate	4.79
		Tetrachloroethene	730	Hexachlorobutadiene	4.8
		2-Chlorotoluene	780	Pentachlorophenol	5.01
		Trichloroethene	920	Di(2-Ethylhexyl)Phthalate	5.11
		1,2-Dichloroethane	1000	Pentachlorobenzene	5.19
		1,3,5-Trichlorobenzene	1400	Heptachlor	5.44
		Tetrachloromethane	1530	Dieldrin	5.48
		1,2-Dichloroethene	3300	Endrin	5.63
		Trichlorofluoromethane	11000	Hexachlorobenzene	6.18
		1,1,1-Trichloroethane	13000	p-p'-DDT	6.19
		1,2-Dibromoethane	66000	Aldrin	6.23

TABLE A6.2.

Results of Linear Regression Analysis of Mean Environmental Concentrations and Other Parameters

Compartment	Data Type	Degrees of Freedom	Log Transformed	
			Correlation	% Fit
Air	Production	36	0.75 ***	55.4
	Release	34	0.43 *	16.5
	Henry Constant	42	0.55 ***	28.8
	Log P_{ow}	42	-0.72 ***	51.6
Water	Production	38	0.32 *	8.2
	Release	37	0.26	4.3
	Henry Constant	47	-0.07	-1.6
	Log P_{ow}	47	-0.61 ***	35.5
Sediment	Production	17	0.50 *	20.9
	Release	17	0.27	1.8
	Henry Constant	27	0.01	-4.2
	Log P_{ow}	27	0.24	1.8
Biota	Production	16	0.51 *	21.0
	Release	15	0.59 *	29.0
	Henry Constant	24	-0.09	-3.9
	Log P_{ow}	24	0.16	-8.1

Correlations significant at the P=0.001 level are indicated by ***, and those significant at the P=0.05 level by *.

Figure A6.1

Plot of Mean Concentration of Reference Chemicals In Air Against Henry Constant

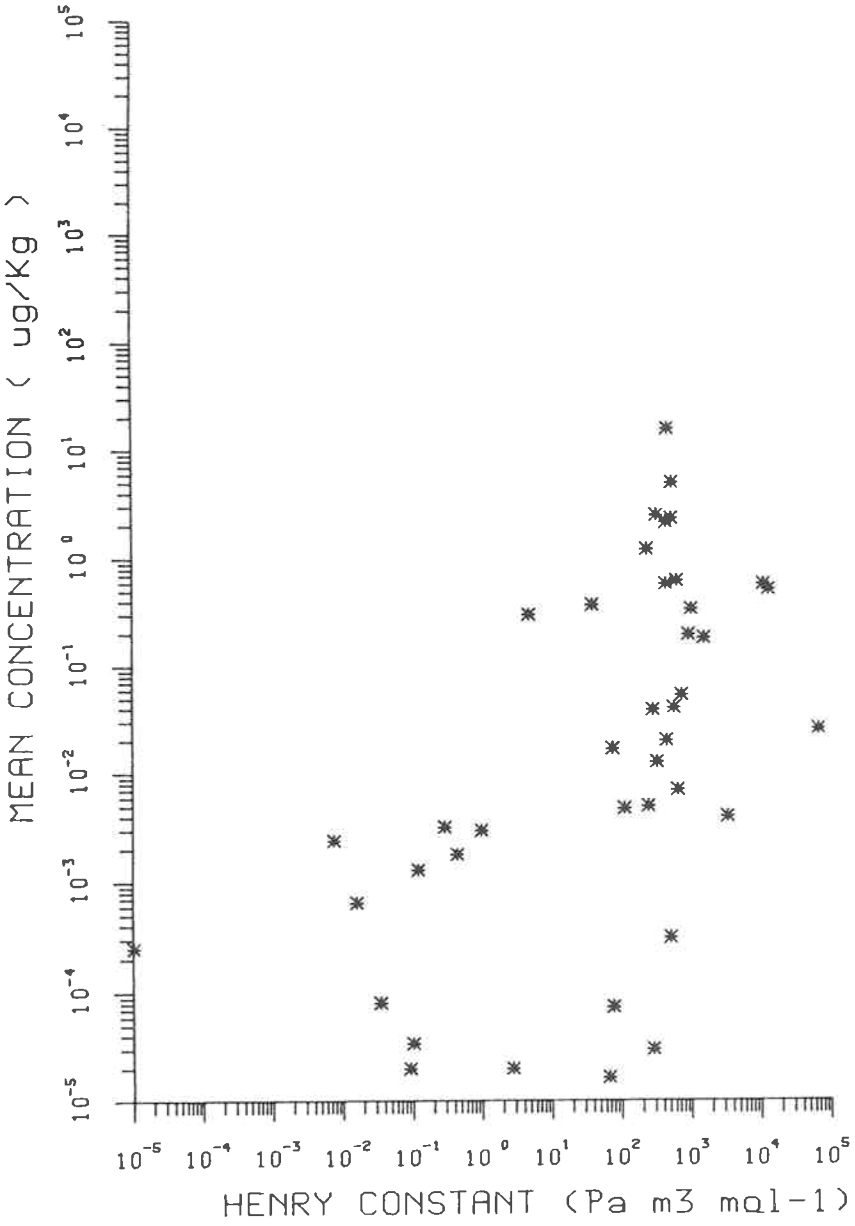


Figure A6.2

Plot of Mean Concentration of Reference Chemicals In Air Against Log P_{ow}.

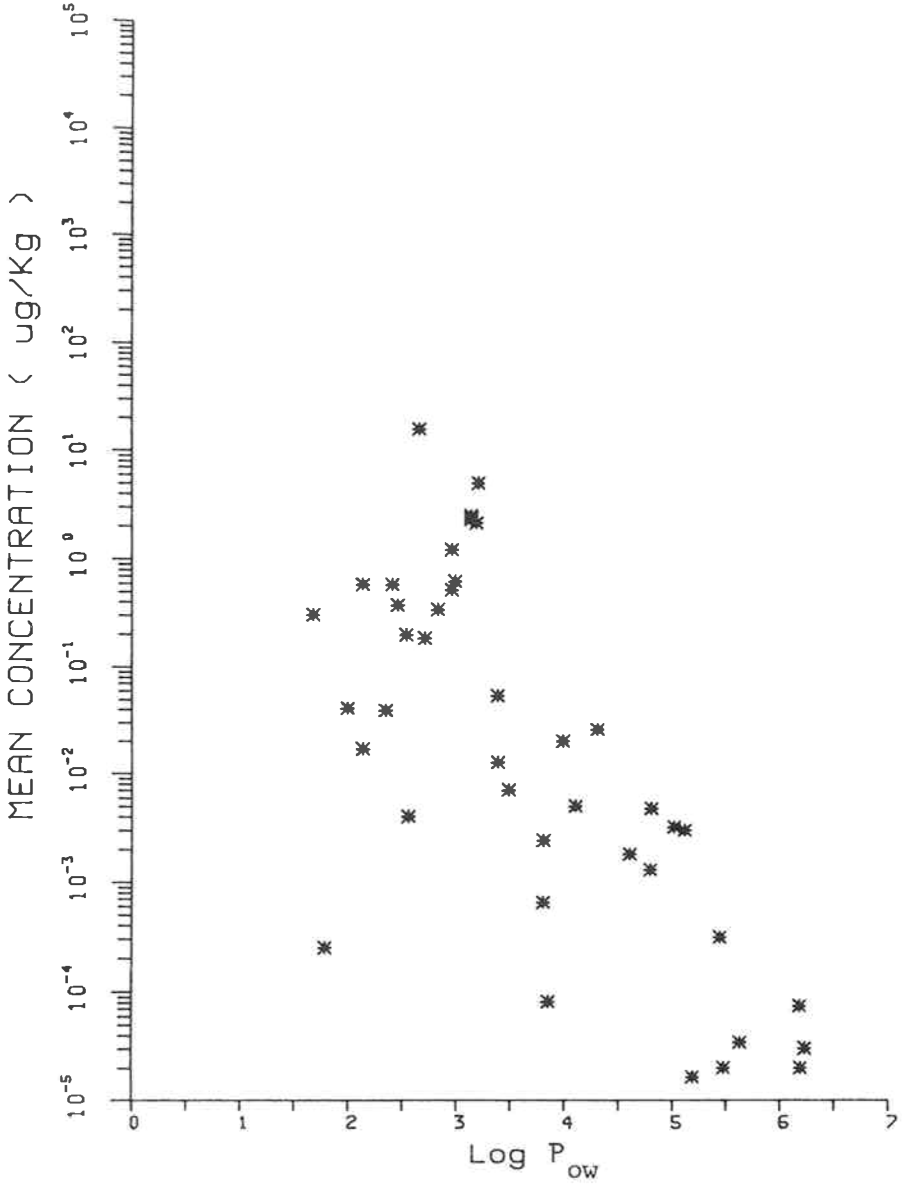


Figure A6.3

Plot of Mean Concentration of Reference Chemicals In Water Against Henry Constant

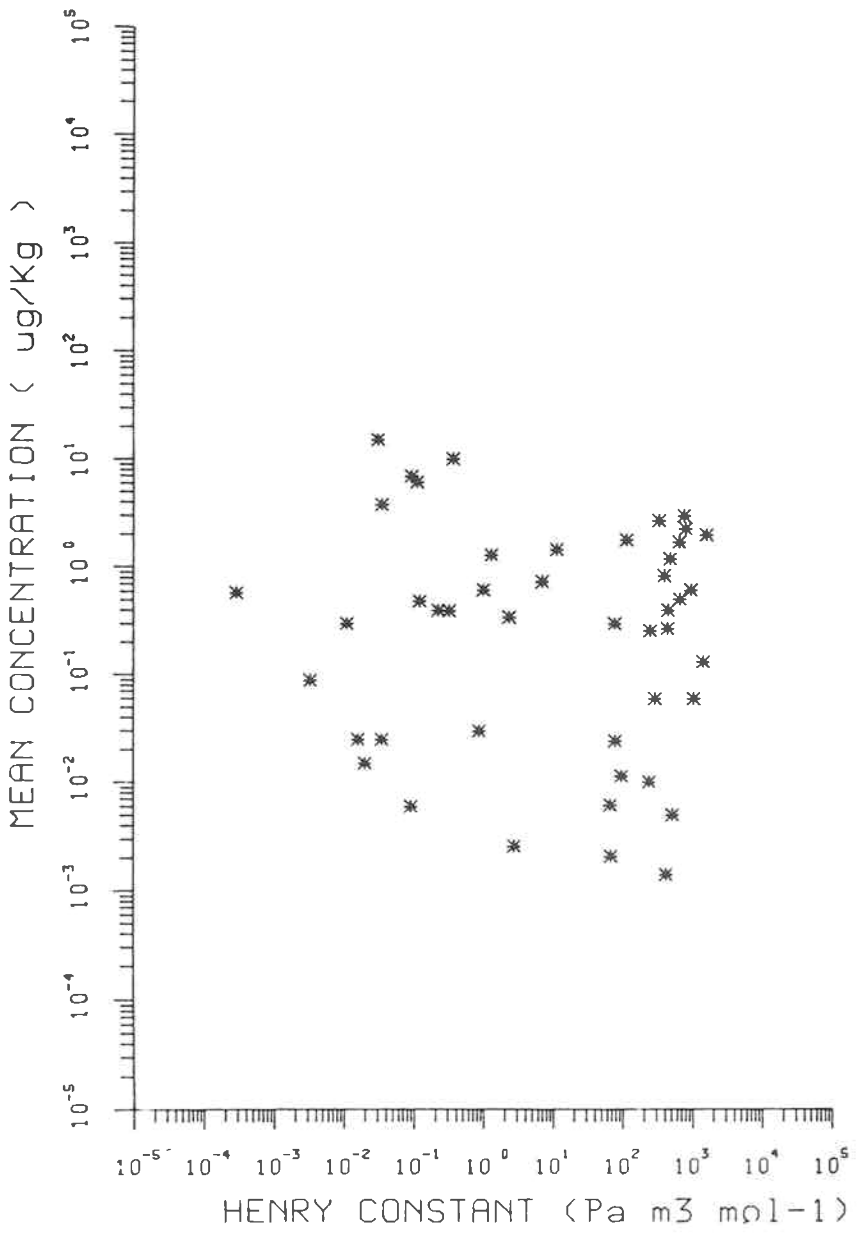


Figure A6.4

Plot of Mean Concentration of Reference Chemicals In Water Against P_{ow}.

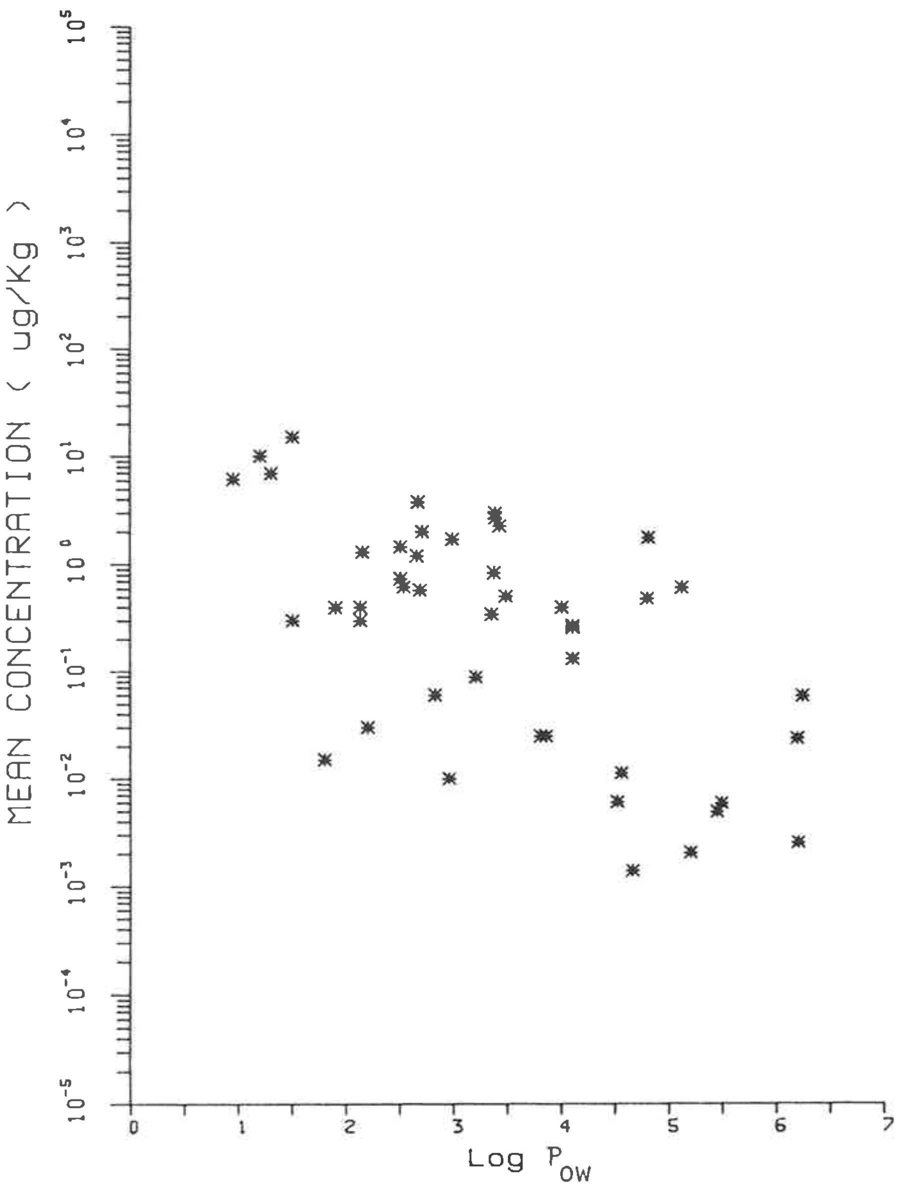


Figure A6.5

Plot of Mean Concentration of Reference Chemicals In Sediments Against Henry Constant

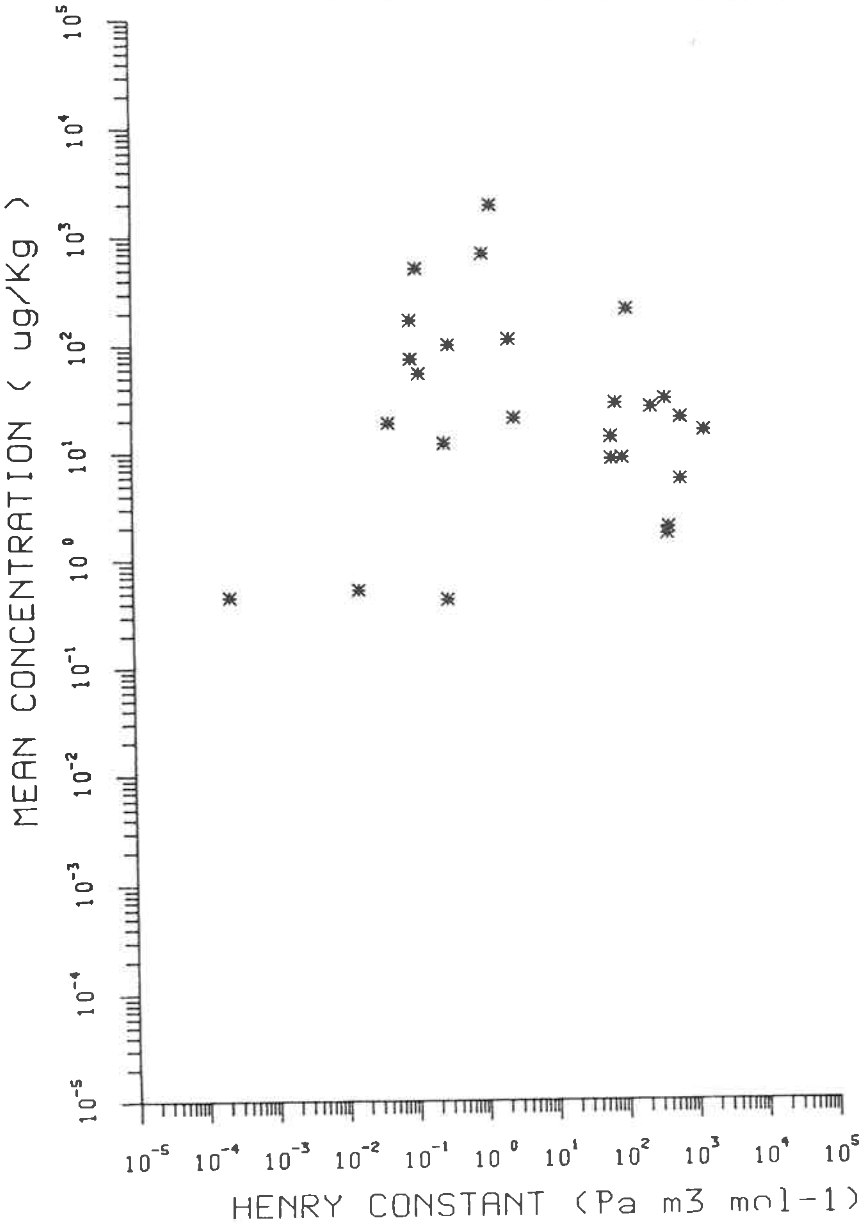


Figure A6.6

Plot of Mean Concentration of Reference Chemicals In Sediments Against Log P_{ow}.

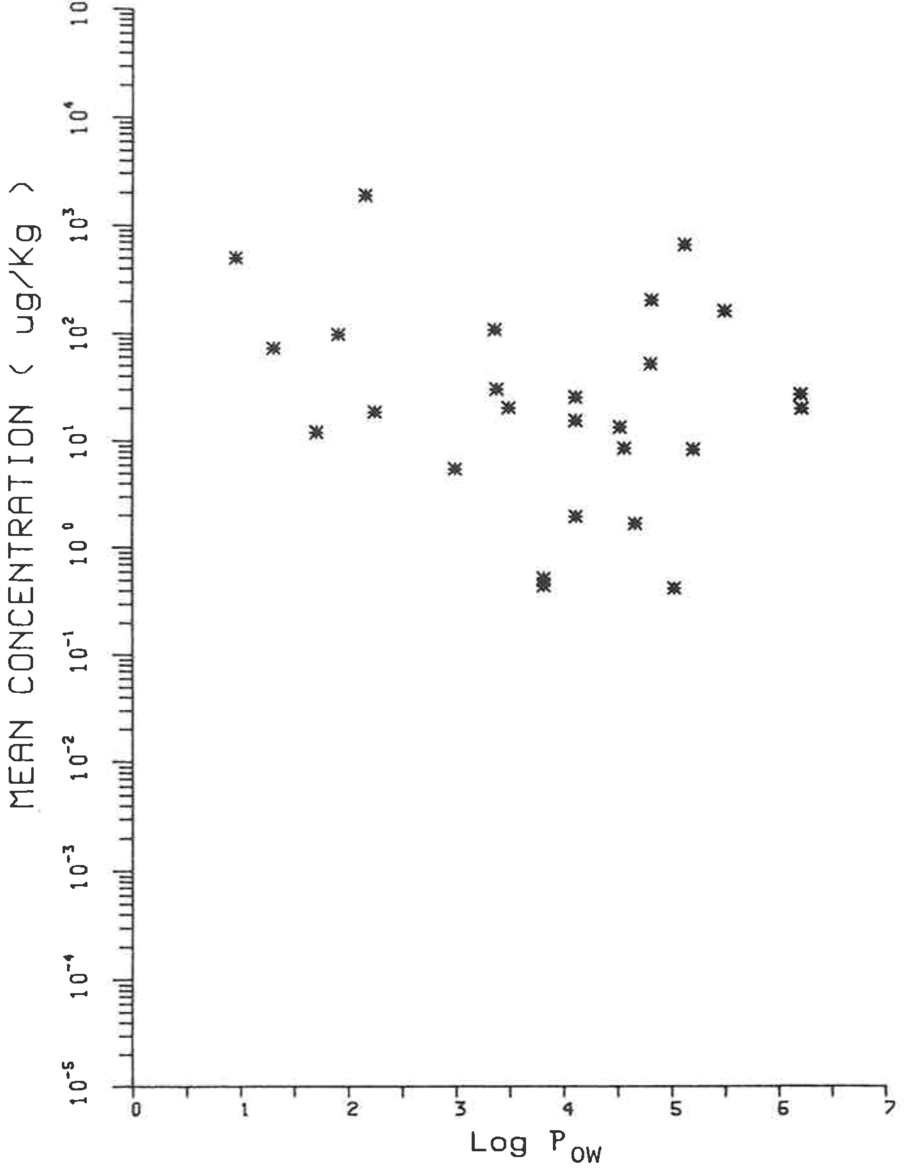


Figure A6.7

Plot of Mean Concentration of Reference Chemicals In Biota Against Henry Constants

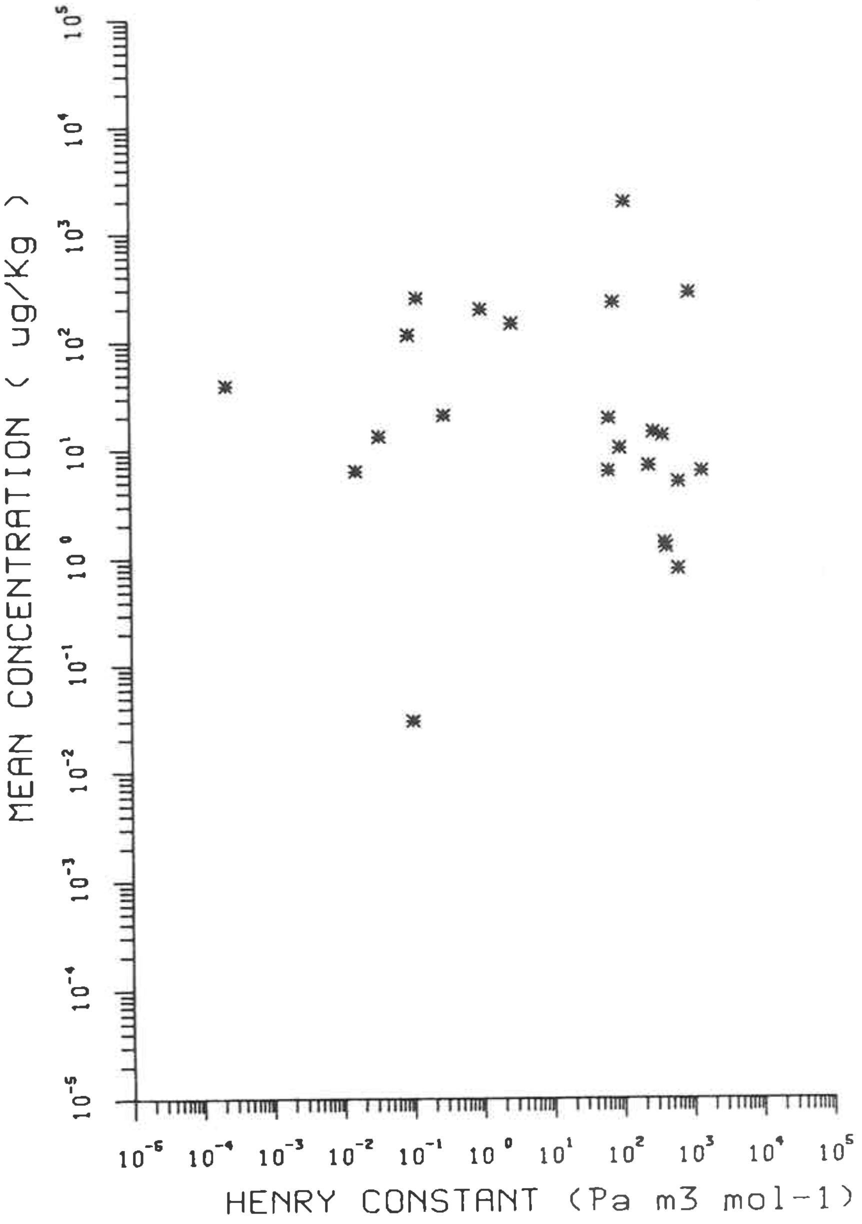


Figure A6.8

Plot of Mean Concentration of Reference Chemicals In Biota Against P_{ow}.

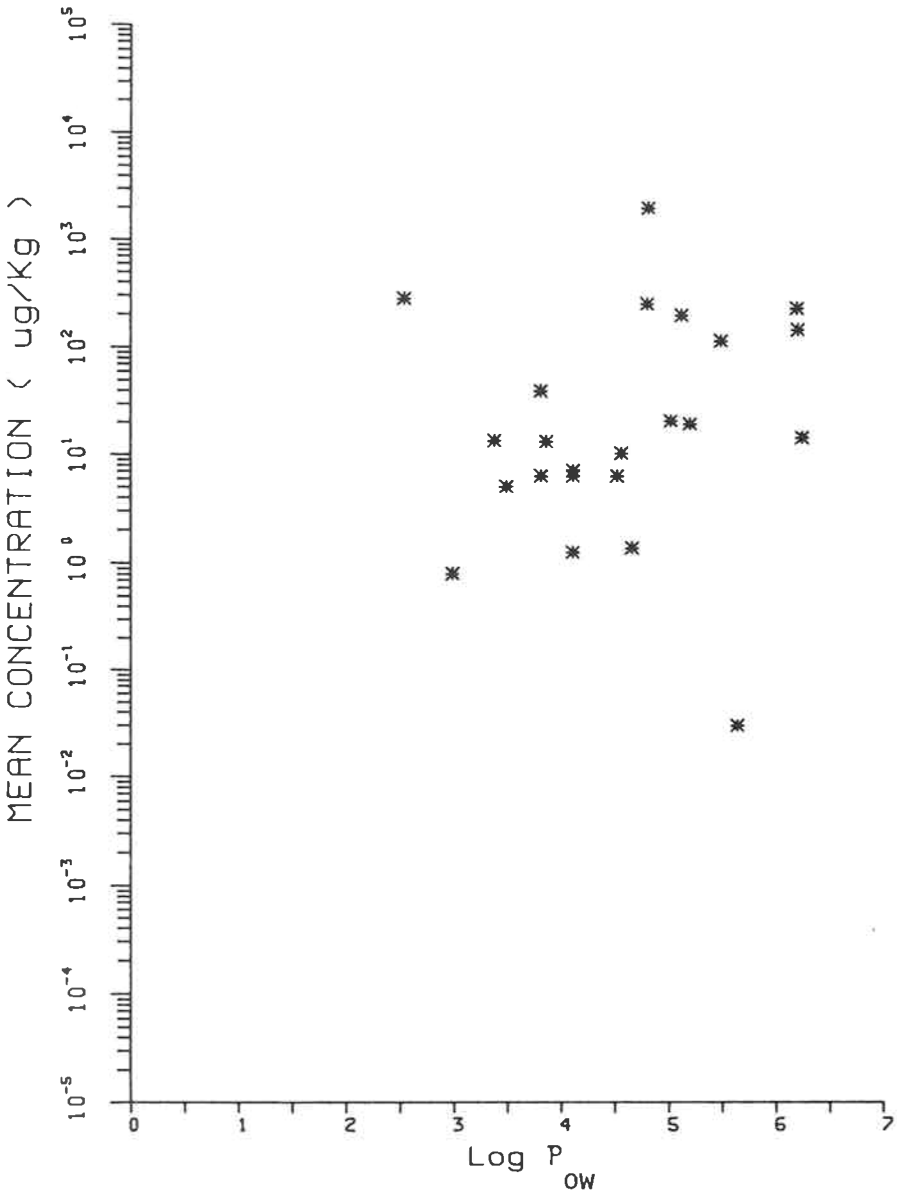


Figure A6.9

Plot of Mean Concentration of Reference Chemicals In Air Against Production Tonnage

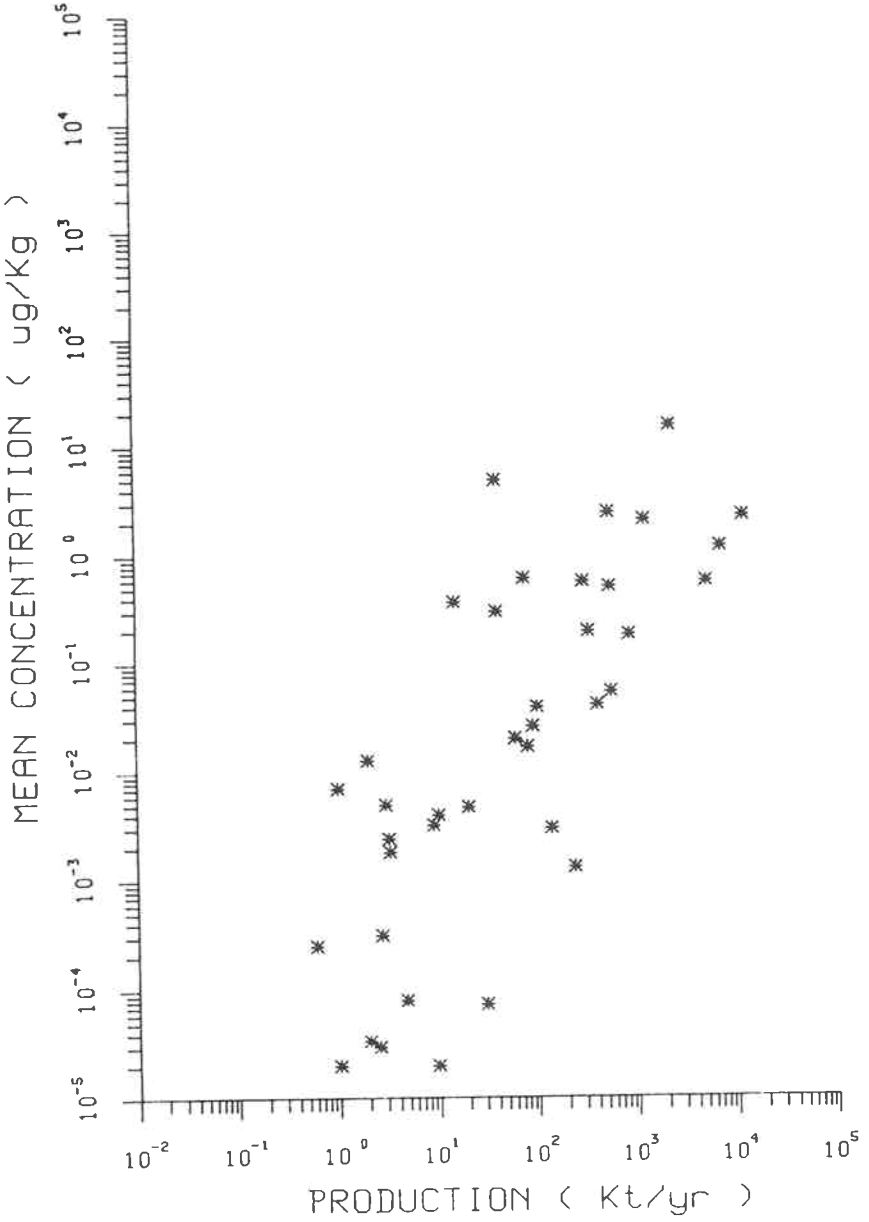


Figure A6.10

Plot of Mean Concentration of Reference Chemicals Chemicals in Air Against Tonnage Released

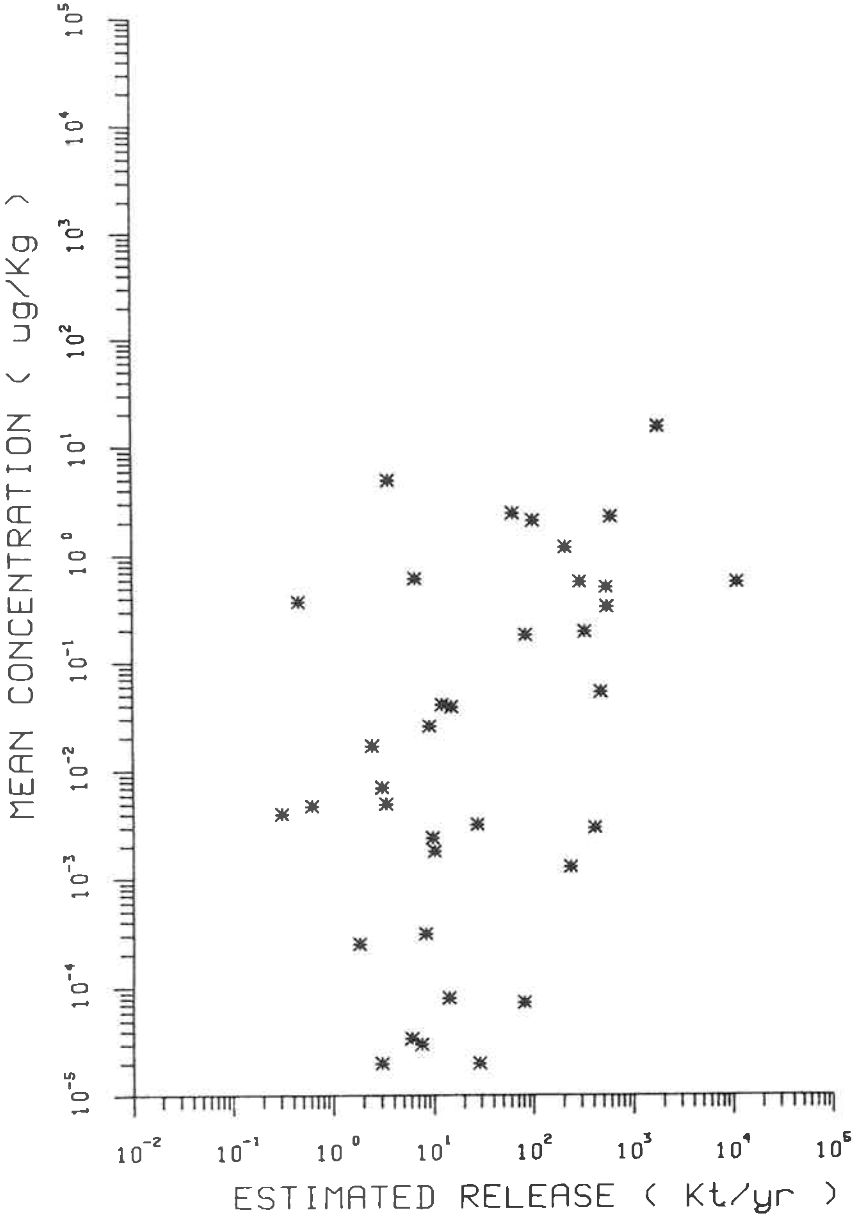


Figure A6.11

Plot of Mean Concentration of Reference Chemicals In Water Against Production Tonnage

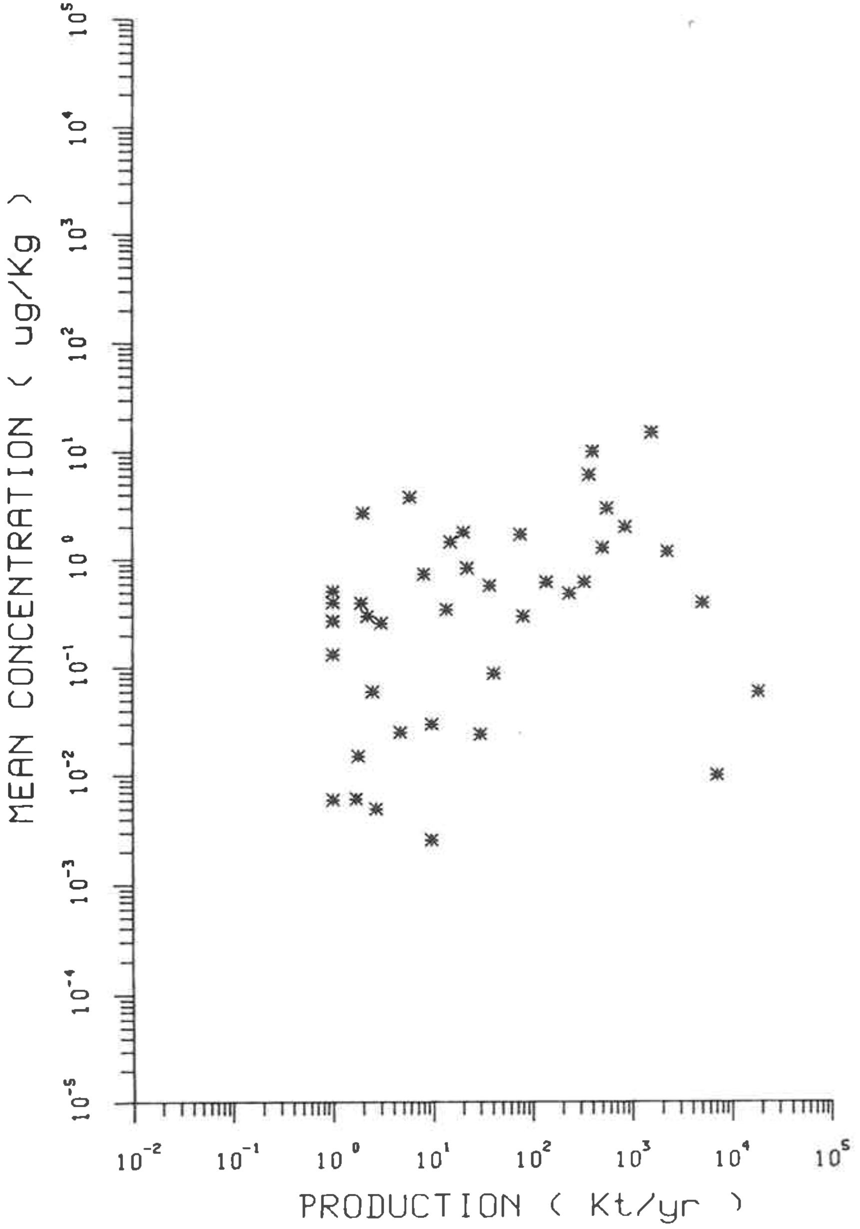


Figure A6.12

Plot of Mean Concentration of Reference Chemicals In Water Against Tonnage Released

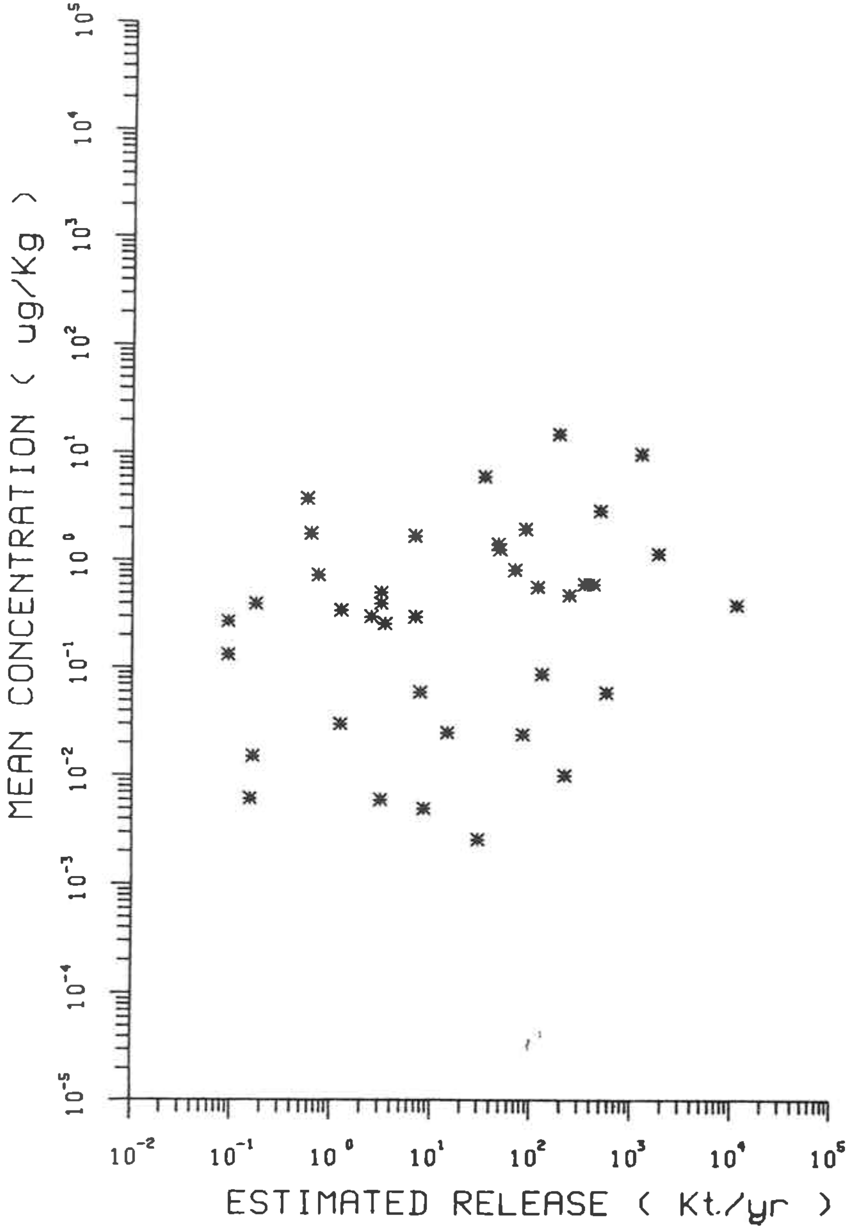


Figure A6.13

Plot of Mean Concentration of Reference Chemicals In Sediments Against Production Tonnage

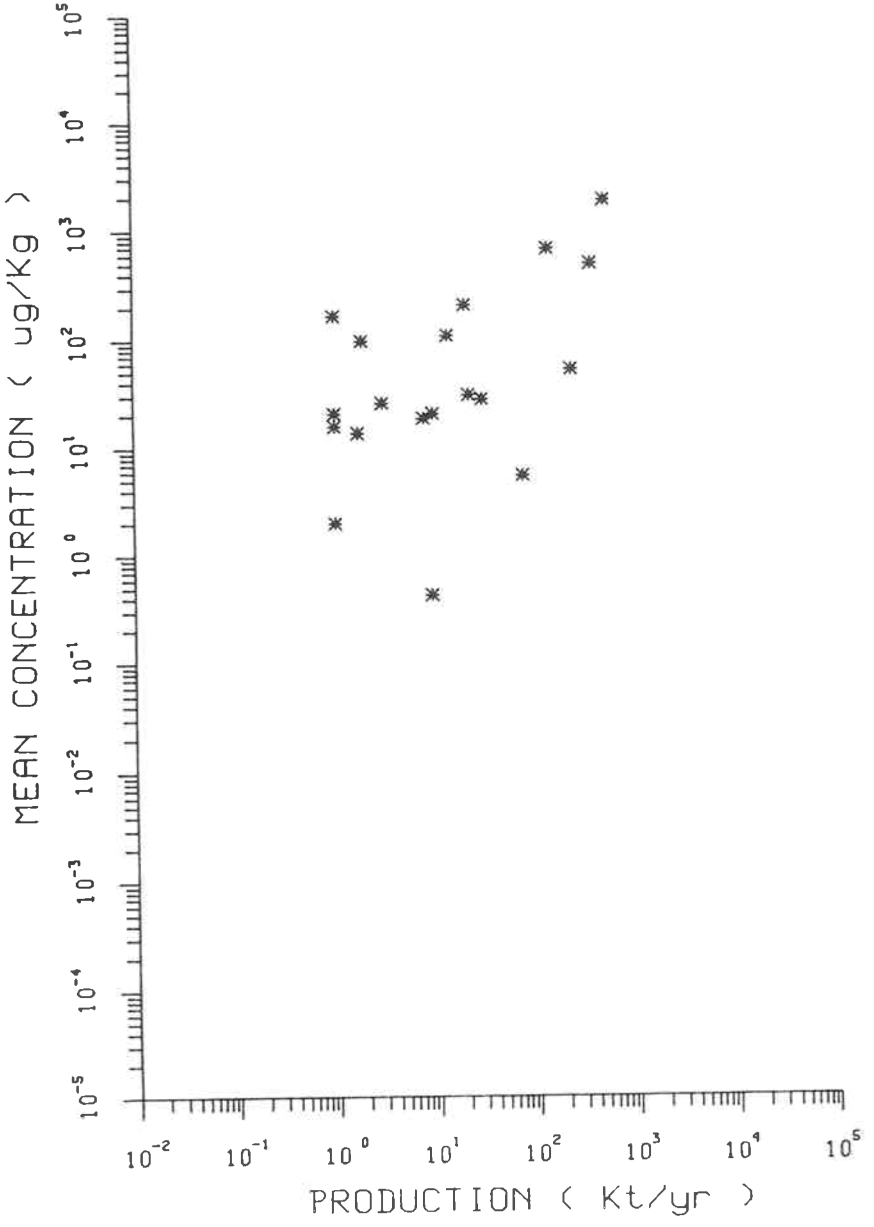
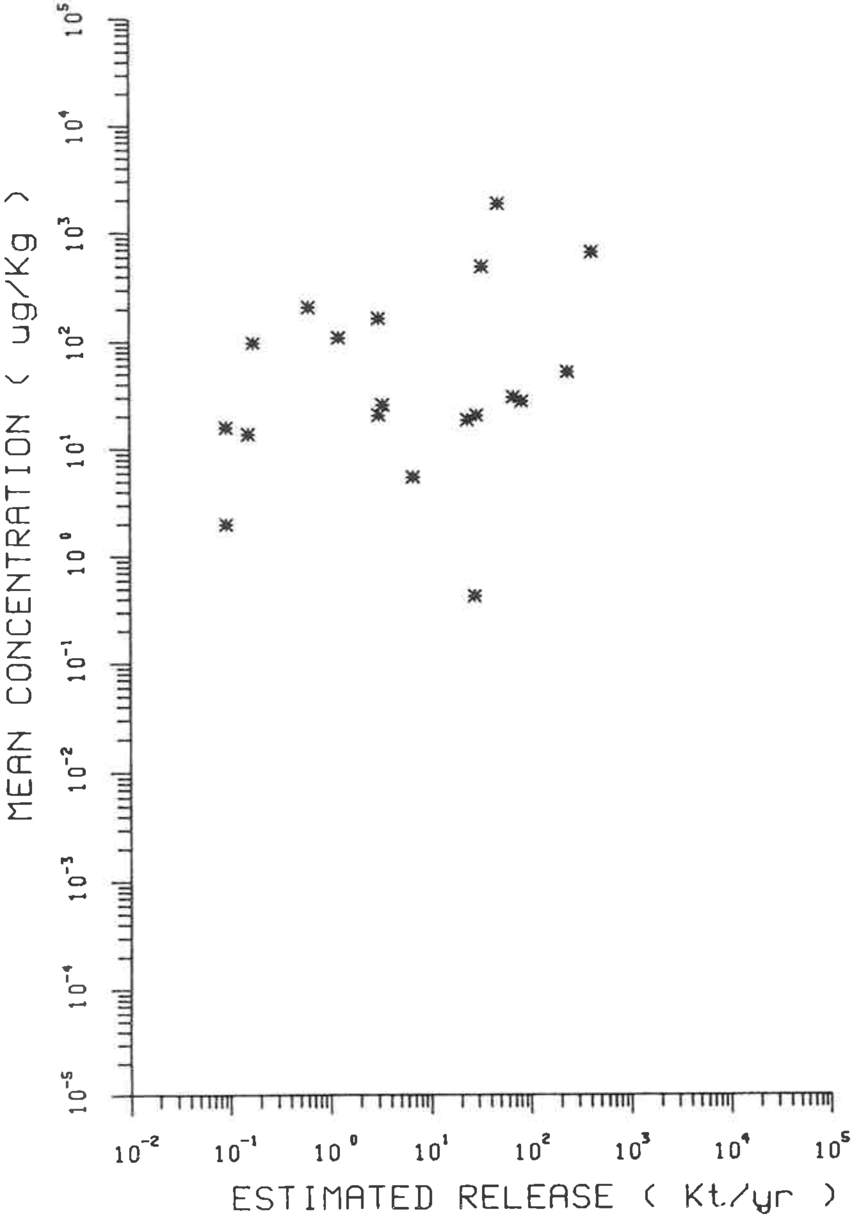
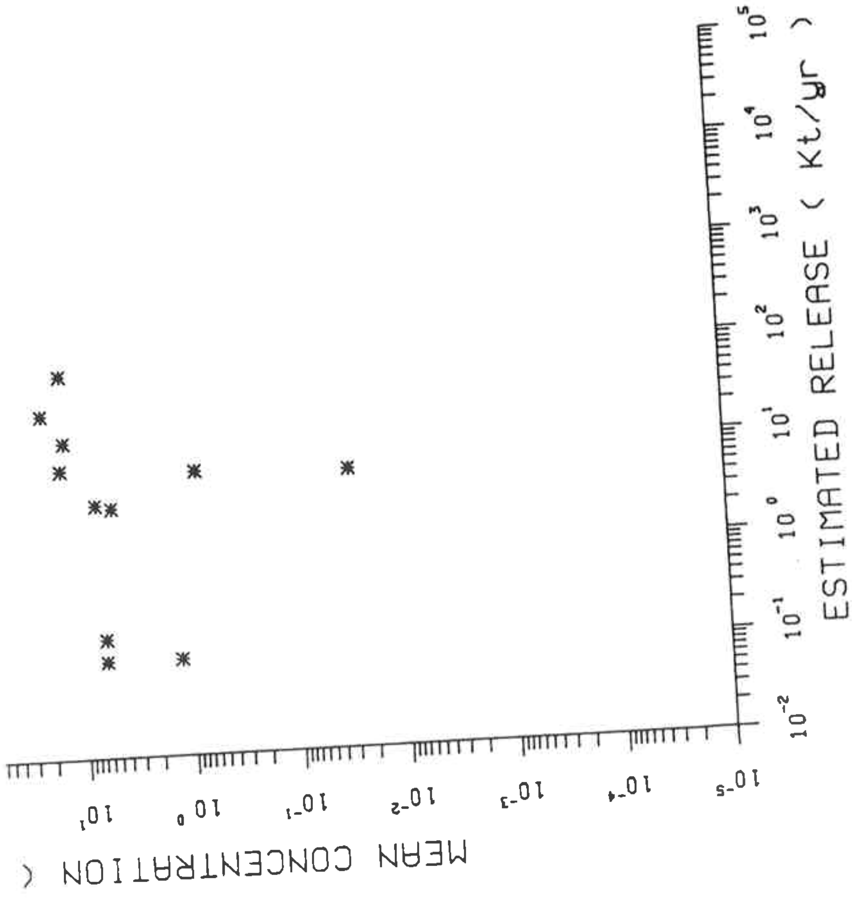
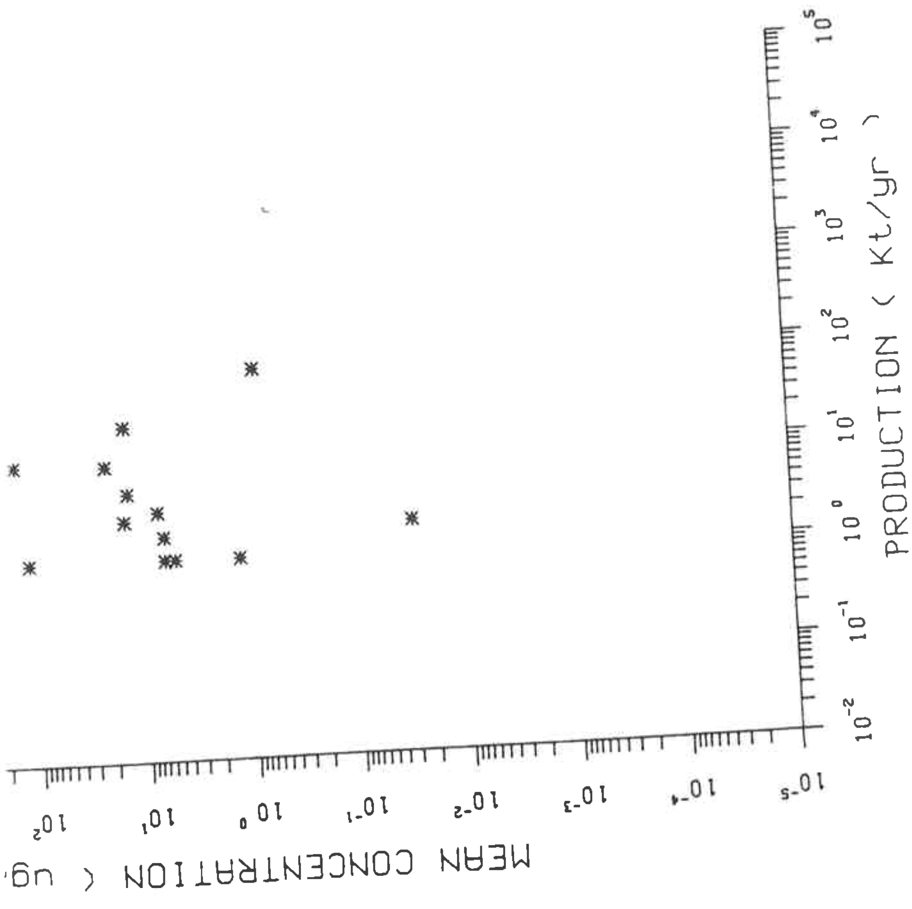


Figure A6.14

Plot of Mean Concentration of Reference Chemicals In Sediments Against Tonnage Released




ESTIMATED RELEASE (Kt/yr)
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
MEAN CONCENTRATION (
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}


PRODUCTION (Kt/yr)
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
MEAN CONCENTRATION (ug.
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

Appendix 7 : Members of Task Force

Dr. K. Beutel	Dow Chemical Europe (Horgen)
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Dr. S. Lambert	Rhône-Poulenc S.A. (Decines)
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Dr. H.W. Thamm	Henkel KGaA (Düsseldorf)
Dr. W.F. ten Berge	D S M (Geleen)
Dr. L. Turner	ECETOC
Dr. D.A. Stringer	ECETOC

Appendix 8 : Members of ECETOC Scientific Committee

Constituting the Peer Review Committee

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P.A. GILBERT, Head, Environmental Relations	UNILEVER (Port Sunlight)
U. KORALLUS, Medical Director	BAYER (Leverkusen)
C. LUNDBERG, Chief Toxicologist	NOBEL INDUSTRIES (Karlskoga)
R. MILLISCHER, Chief Toxicologist	ATOCHEM (Paris La Défense)
H.G. NOSLER, Head, Coord. Centre for Environmental Protection and Consumer Safety	HENKEL (Düsseldorf)
S. PAGLIALUNGA, Head of Industrial Toxicology	MONTEDISON (Novara)
C.L.M. POELS, Envir. Affairs Division	SHELL (den Haag)
W.F. TORDOIR, Head of Occupational Health and Toxicology Division	SHELL (den Haag)
H. VERSCHUUREN, Head, Department of Toxicology	DOW CHEMICAL (Horgen)