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Regional and Global Cycling of Persistent Organic Pollutants (POPs):

An Assessment and a Feasibility Study in a Nordic Perspective

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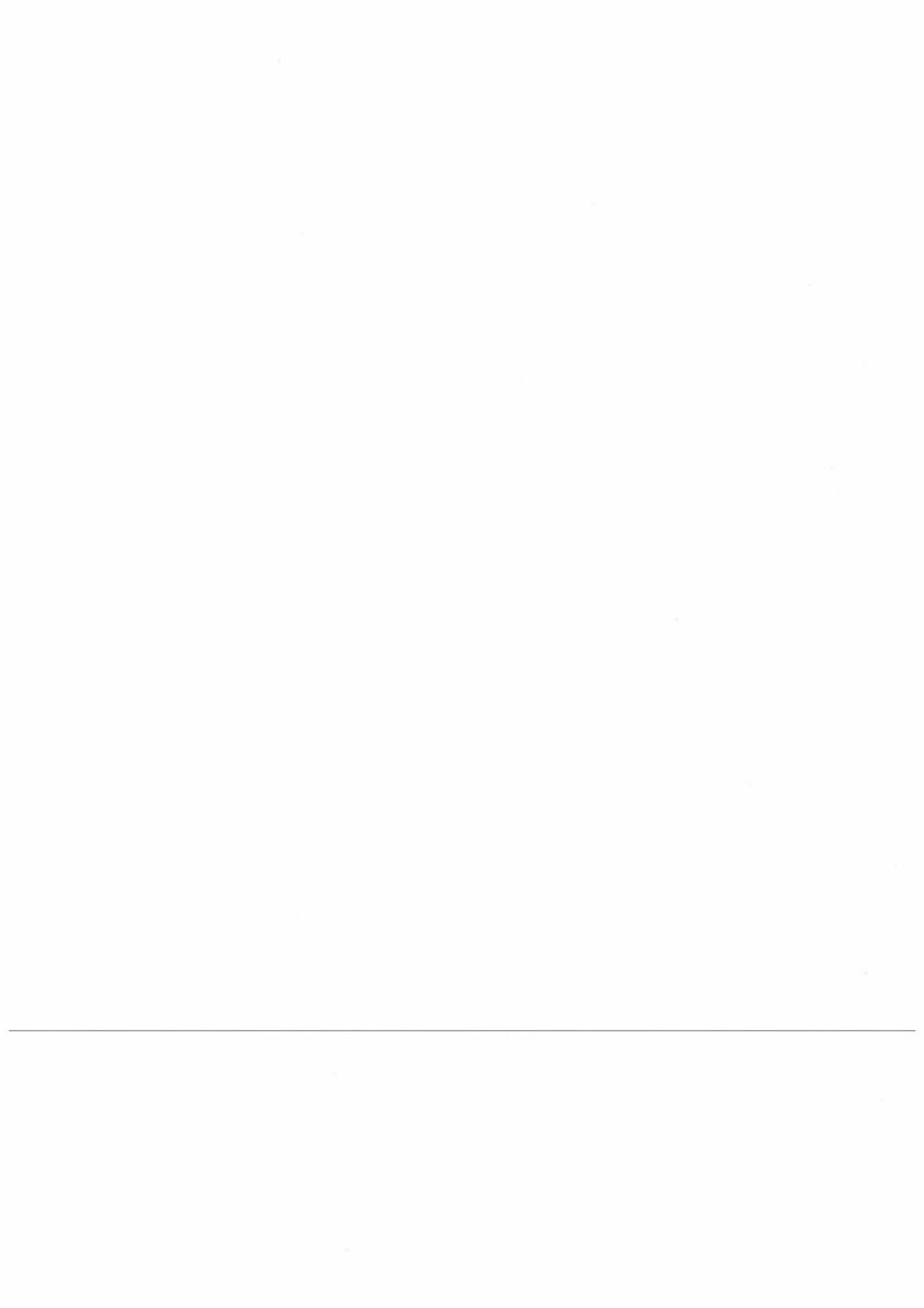# Regional and Global Cycling of Persistent Organic Pollutants (POPs):

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Contents

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1. Introduction

During the last decade several studies have been carried out aiming at the improvement of our knowledge on the behavior of persistent organic pollutants (POPs) in the environment. Evidence has been found that many of these compounds create serious problems due to their toxicity, persistance, and bio-accumulation in various environmental compartments (e.g. Pacyna et al., 1993). Examples of POPs that behave in this way are many polychlorinated pesticides (e.g. lindane, dieldrin, DDT, toxaphene, chlordanes), industrial compounds (e.g. polychlorinated biphenyls-PCBs), and some degradation, industrial, and combustion by-products (e.g. polycyclic aromatic hydrocarbons-PAHs, polychlorinated dibenzo-p-dioxins - PCDDs, polychlorinated dibenzofurans - PCDFs, and hexachlorobenzene).

Major emphasis in these studies has been placed on the following subjects:

- identification and quantification of POPs in environmental samples,
- sources of POPs responsible for their origin in the environment,
- major pathways of POPs through the environmental compartments studied on local, regional, and global scale,
- environmental and health effects and the degree of public health concern associated with POPs, and
- technical and other measures to reduce the levels of POPs in the environment.

Recently the results of the above mentioned studies have been reviewed in connection with the UN ECE Task Force on Persistent Organic Pollutants. The overall objective of this Task Force is to substantiate the information on emissions, long-range transport, distribution between media, and abatement of POPs, giving priority to dioxins, furans, and PCBs (UN ECE, 1994). The outcome of this work should form the basis for a possible protocol on emission reductions. Several documents have been prepared within the Task Force activities, including an overview of POPs in the environment (Han, 1994), an overview on priority setting for long-range transboundary air pollution by POPs (AEA, 1993a), controls on prioritised POPs (AEA, 1993b), and abatement strategies for POPs (FIUO, 1993).

The main results of the substantiation work by the Task Force were summarized by its Chairmen as follows (Lindau and Stone, 1994). Many POPs are anthropogenic in origin, heavily used and released to the environment in large quantities. They have long environmental half-lives, resulting in continued increases in the global inventory of POPs in the environment. Being often semi-volatile, POPs can be transported through ecosystems and travel distances on a local to global scale with the atmosphere as a primary transport medium. For

many POPs there is a systematic migration to cooler latitudes. Finally, a number of bioaccumulative POPs produce a broad range of immunilogical, reproductive, developmental, behavioral, and carcinogenic effects (Lindau and Stone, 1994). Similar conclusions have been reached in North America from studies in the Great Waters region, carried out for the U.S. Congress (Keeler et al., 1993; Baker et al., 1993; Swain et al., 1993).

Although work has been done in order to understand the fate, behavior, and effects of POPs, less information is available on environmental cycling (migration) of these compounds through various environmental media. The major reason for this deficiency in our knowledge is related to a lack of detailed information on emissions of POPs and the parameters affecting their migration through the environment under various meteorological, chemical and physical conditions.

2. The objectives of the project and its structure

Extended research on the fate, behavior, and environmental and health effects of POPs has been carried out in Scandinavia starting in the 1970's (e.g. Ambio, 1980). Recognizing this fact, as well as the need for better understanding of POP cycling in the environment, at least on a regional scale, the Nordic Council of Ministers (NMR) has established an assessment and feasibility study on the POP cycling. The overall goal of the study is to provide up-to-date information on the regional and possibly global cycling of POPs. Therefore, the study should contribute to international activities aiming at the reduction of the POP levels in the environment, particularly to the work of the UN ECE Task Force on POPs.

The following questions have been addressed:

- Where are the major regions of POPs application, production, and emissions into the environment?
- What are the levels of POPs in various environmental compartments and which are the major exchange processes involving air, soil, water, and biota?
- What is the status of the development of regional models evaluating environmental cycling of POPs?
- What are the major ecological and human health effects caused by POPs?

A group of 9 experts from Denmark, Finland, Norway, and Sweden was established to carry out the project (Annex 1). The experts have worked within 3 working groups on:

- releases and distribution of POPs,
- transport, modeling, fate, and behavior of POPs in the environment, and
- effects and risk assessment.

It was decided that the feasibility study reported here should concentrate on the information available in the Nordic countries. It was important to reassure that the information on the levels and distributions of POPs in various environmental compartments was obtained with the similar or at least comparable degree of

accuracy and detailness using similar sampling and analytical procedures. Larger coverage of the study area can be considered in future research.

The experts agreed that the project should focus on those POPs which are considered as priority compounds in various international programs, particularly in the UN ECE Task Force on POPs, and on compounds for which relevant and reliable information can be obtained. Therefore, four groups of priority compounds have been identified for this study:

- PCBs, selecting the IUPAC (ICES) congeners: CB-28, CB-52, CB-101, CB-118, CB-138, CB-153, and CB-180,

- PAHs, selecting anthracene, benzo(b)fluoranthene, benzo(a)pyrene, fluoranthene, phenanthrene, pyrene,

- dioxins and furans selecting all 2,3,7,8-chlorine substituted isomers: 2378-TCDD, 12378-PCDD, 123478-HxCDD, 123678-HxCDD, 123789-HxCDD, 1234678-HpCDD, 12346789-OCDD, 2378-TCDF, 12378-PCDF, 23478-PCDF, 123478-HxCDF, 123678-HxCDF, 234678-HxCDF, 1235789-HxCDF, 1234789-HpCDF, 1234678-HpCDF, and 12346789-OCDF, and

- polychlorinated pesticides selecting HCHs, DDTs, DDE, chlordane, toxaphene, and HCB.

3. Releases and distribution of POPs

A collection of data on concentrations of the selected POPs air, atmospheric deposition, vegetation, sediments, sea water, and mussels in the Nordic countries has been carried out within the project (Annex 2). The purpose of this collection was twofold. First, it was desirable to obtain as much reliable information as possible in order to investigate the level of environment contamination by POPs in the Nordic countries. Second, the collected data are needed for the verification of cycling model estimates.

Large differences in concentrations, reaching a few orders of magnitude are observed for PCBs, particularly in the air samples. A similar conclusion was reached by Jansson et al. (1993). They have compared monitoring data for HCHs, PCBs, and PCDDs and PCDFs in air and deposition samples collected in selected UN ECE countries. The differences can be related to the distance of the sampling site from the emission site. The PCB concentrations in air, measured in the Nordic countries are several times lower than those measured in other parts of Europe (e.g. Jansson et al., 1993) and a factor of about 2 lower than in the Great Lakes area in North America (Swain et al., 1993).

The PCB pattern in the air over the Baltic Sea has been studied during different wind directions indicating the possible origin of these pollutants in the Nordic countries. The pattern shown in Fig.1 relates to the pollution transport with air masses arriving to Gotland from the south-westerly direction while the pattern in Fig. 2 relates to the pollution transport to the sites in the north of Sweden and

Gotland from the North. As expected, higher concentrations of various PCB congeners were measured during the transport from the south-westerly direction.

The results from analysis of PCDDs and PCDFs indicate that air samples from Scandinavia are dominated by highly chlorinated species, particularly octachlorodibenzo-p-dioxin (OCDD). The same observation was made by Jansson et al. (1993). They speculated that the major source of this compound is probably pentachlorophenol products. OCDD is present as a contaminant in these products and can also be formed during incineration of wastes, particularly pentachlorophenol impregnated wood. More research is clearly needed to validate the above mentioned sources.

Air concentrations of other POPs in Annex 2 are of the same order of magnitude as the concentrations measured in the Great Lakes region (Swain et al., 1993).

Data on deposition levels of POPs in the Nordic countries also revealed interesting features. An enrichment of the highly chlorinated congeners of PCBs can be observed in the deposition samples in relation to the air samples. The OCDD congener dominating the pattern of PCDDs in the air samples is not dominant in the pattern of PCDDs in the deposition samples (see also Jansson et al., 1993).

Information on the deposition of POPs is still being collected, particularly on the POP concentrations in precipitation. This new material can be included in future studies. The same applies also to data from measurements carried out in other compartments of the environment.

The concentrations of POPs in pine needles in Norway, Sweden and Denmark are quite comparable during the period from 1984 to 1986. Data from other regions are scarce and, therefore, a comparson is difficult.

The PCB concentrations in sediments measured in Ølensfjord in Norway and in Skagerrak are in the lower range of the concentrations measured in the Lake Superior and the Lake Michigan (Swain et al., 1993). Information on POPs other than PCBs, measured outside the Nordic countries is rather limited.

The concentrations of HCHs in the Baltic Sea, Skagerrak, and Kattegat waters are quite even indicating downward trend due to their reduced use in the neighbouring areas. A clear downward trend is also observed for DDT in the Baltic Sea starting in the 1970's (e.g. Carlberg, 1990).

Information on the POP concentrations in fish, seals, and birds in the Nordic countries is still being collected. A review of data from Finland is already enclosed in Annex 2. A summary of data on POP concentrations in mussels in the Nordic countries is also enclosed. Rather large differences can be noted for the PCB concentrations in the region.

Limited information is available on the releases of studied POPs in the Nordic countries. In general, most of the polychlorinated pesticides and PCBs are prohibited to be produced or imported to the Nordic countries. While emission

data for the project are still being collected for Sweden, Norway, and Denmark, the releases in Finland have been assessed.

It has been prohibited to produce or import PCBs to Finland since 1989. PCB containing transformers and condensers will have to be removed from the use by the end of 1994. The approximate annual usage of PCBs in Finland has been about 2 000 tonnes. Information exists on the PCB concentrations in municipal solid waste landfill gas, recycled paper, and metal reclamation plants.

The PAHs are by-products of wood preserving materials used in Finland, e.g. creosote-oil. This material contains e.g. antracene and benzo(a)pyrene. The concentrations of the latter compound vary from 0.03 to 0.12 %. Creosote-oil contains also naphthalenes and alkylated naphthalenes in amounts ranging from 15 to 25 %. The total use of creosote-oil in Finland is between 10 000 and 30 000 tonnes. The estimates of PAH emissions from fossil fuel plants, sewage sludge treatment plants, heat producing plants, and traffic are also available for the country.

An extended information exists on emission rates of dioxins and furans for pulp and mill production, municipal and sewage sludge treatment plants, various combustion installations, wood preserving facilities and metal reclamation plants.

The use and import of the studied pesticides is banned in Finland with the exception of their use for research purposes. The latest permission issued in the country was for lindane to make pharmaceuticals from the seeds of turnip rape. This product is named Gamatin, but its production and usage has been forbidden since 1988. DDT and HCB have been imported to Finland in amounts of about 10 tonnes annually.

4. Modeling of the POP behavior in the environment

Natural and anthropogenic emissions of POPs will undergo transformations, dispersion, and accumulation in the different environmental compartments, such as air, water, soil and biota. Our understanding of the great number of organic pollutants in terms of their sources, chemical and physical properties and transformations and eventually their accumulation and destruction is far from complete. In attempts to assess the fate of POPs and their environmental impacts, models describing the dispersion and transformation, as well as biological effects have become very important tools. The current models used to assess the fate of pollutants are build on a large number of assumptions, simplifications or parameterised values, and therefore need to be verified. The validation of these models with real data is a crucial step in the credibility of the model output in those areas where no measured data exits. Another problem arises from the accumulation of errors in a multistep modeling process. The description of the individual steps in the model may be close to reality, but when summed to a total, the output may be a few orders of magnitude different from the measurements used in the validation procedure.

8

Concerning the scales of the POP models it is important to observe that the persistence of these pollutants would permit their transport with water currents and air masses over long distances. Eventually the POPs are removed; the sinks that have been identified so far are photochemical degradation in the atmosphere, bio-degradation by soil bacteria and micro-organisms and sedimentation and subsequent burial in the sea sediment.

Many of the POPs have vapor pressures high enough to permit volatilisation of the solid or liquid phase, a property that allows them to be dispersed in air. The role of the atmosphere is here in focus due to the relatively high speed at which the atmospheric transport occurs. The atmosphere will therefore redistribute pollutants which have a substantial residence time in the atmosphere, or those which may be resuspended into the atmosphere by some processes.

Some of the pesticides, such as the hexachlorocyclohexanes (HCHs) are water soluble and although the pesticides are applied to the plants or the soil, their substantial part will evaporate. Consequently, they will end up in the water phase or more precisely in the oceans. In a model with three compartments, atmosphere, soil and ocean, Strand and Hov (1994) have studied the fate of HCHs. This low resolution model is not expected to give a detailed information on the regional patterns but rather a general picture. On the global scale, about 99 % of the emissions of HCHs will end in the oceans and the remaining 1 % is found in soils and the atmosphere. The use of lindane has been phased out in the Nordic countries for some time. Nevertheless this compound is a regular component in the atmosphere of the Nordic region due to still extensive use in the lower latitudes.

The basic fugacity model (GENERIC.BAS) of Mackay (1991) was used in the reported study under a new acronym POPFATE. Modifications have been made to fit the conditions for regional modeling in the Nordic countries. It was tacitly assumed that the model is also representative for the temperatures lower than those for which the model was initially developed. In particular, the temperature may influence the degradation rate of the pollutants. There are also extreme seasonal fluctuations in the Nordic countries as compared to the most of temperate regions. The impact of seasonal changes on the chemical behavior of POPs in the environment is poorly understood, but possible quite important. This impact is not reflected in the model at present.

Ten key areas have been selected in the model, which are representative for the Nordic region. These areas differ with respect to the key parameters that govern the partition of POPs. The parameters of the regions are presented in Table 1. Each of the ten regions were divided into six compartments, representing air, water, soil, sediment, suspended particles in water, and fish. The temperature of the compartment is one of the most important parameters. The annual mean temperature of the sea in each region was used in this study. The temperature governs not only the kinetics, e.g. the exchange rates, but also the saturation pressure of a given pollutant. The saturation pressures of the POPs were calculated for the supercooled liquid. The temperature corrected vapour pressure is in some cases a few orders of magnitude larger than the uncorrected.

Although distribution and concentration levels of a number of POPs are studied here, only three substances: fluoranthene, hexachlorobenzene (HCB), and lindane were selected for modeling. These three substances are of anthropogenic origin. Fluoranthene has its major source from combustion and traffic, whereas the other two are pesticides. HCB is also a by-product of combustion. They represent POPs with limited range of volatility, and solubility. A comparison between calculated and actually monitored concentrations is possible for these pollutants. The physico-chemical parameters of the compounds, together with other POPs, are presented in Annex 3.

The fugacity model used in this study can be run at three levels, all assuming the steady-state conditions. The level I does not require information on emission rates of POPs to the different compartments and the physical and chemical transformations of POPs are not taken into account. Model output consists of relative concentrations (equilibrium distributions) of a modeled compound in compartments of an evaluative (or "generic") environment, including Air, Water, Soil, Sediment, Suspended Sediment, and Fish (biota). For the higher levels II and III of the model, the emissions data are required. In level II thermodynamic equilibrium is assumed, similarly to level I but transformations and advection are taken into account. In addition to the steady-state concentrations, reaction and advection rates and residence times are obtained. The obtained concentrations are arbitrary, calculated on the basis of assumed total emission rates, but their ratios are characteristic for the compartment and compound chosen. Level III of the model gives similar output as level II but with greater precision and in non-equilibrium conditions. Estimates of chemical quantities, concentrations, and lifetimes in four compartments (Air, Water, Soil, and Sediment) have been obtained. Concentration in Fish is given (as in Level II) only on the basis of thermodynamic partitioning between biota and water.

POPFATE version of the model has been run at all three levels. For the levels II and III of the model, the emission quantities to the different compartments have been adjusted to fit the actual measured environmental levels. It was found that the calculated levels are sensitive to the partitioning of the assumed emission to the compartments. The calculated partition of fluoranthene in the Baltic Proper and the Skagerrak area differs substantially due to differences in the primary emission rates. However, it should be admitted that there is a lack of detailed information on environmental levels of modeled compounds to allow a fine tuning of emissions. The derived emissions rates agree poorly with our knowledge of the actual emission rates obtained from emission inventories or emission measurements.

For the sea areas with no land there is obviously no soil compartment. For the sake of the computation stability, the soil compartment was not set to zero but a small number was assumed as compared to the other compartments. The soil compartment concentration and fraction calculated in this way have no real interpretation and may be discarded afterwards.

The following properties of a given compound and coefficients were used in the POPFATE model:

- molecular mass,
- melting point,
- boiling point,
- solubility in water (temperature dependence can be taken into account),
- logarithm of the octanol-water partition coefficient (temperature dependence can be taken into account),
- vapor pressure (temperature dependence must be taken into account), and
- half-life time of a compound in a given compartment.

The results of calculations at all three levels of the model for the three compounds selected in the study are presented in Annex 4 for all ten key areas. The emissions, concentration levels, and mass distributions of the modeled POPs estimated by the level III of the model are given in Tables 2 to 4, respectively. Fluoranthene and lindane have rather similar physico-chemical properties, although the solubility of fluoranthene in water is more than one order of magnitude lower. The model calculations show this difference: the calculated levels of fluoranthene in Nordic waters are about one order of magnitude lower than the levels of lindane. Hexachlorobenzene is about three orders of magnitude less soluble in water than lindane: the calculated levels of hexachlorobenzene are here of the same order of magnitude as those of lindane. This shows the limitations of the presently used models.

Soils play an important role in the model calculations. In all model calculations where land and soil is included, this compartment has the major fraction of the compound quantities. This is due to the large amount of organic material in this compartment that dissolves organic compounds.

The measured concentration levels of modeled compounds in different compartments in ten key areas are summarized in Table 5 on the basis of information available from Annex 2. The validation of fugacity models depends strongly of the quality of environmental data. The lack of measured data for some of the compartments does not allow for a complete comparison. In general, there is a fairly good agreement for the compartments such as air and water but less for fish. No environmental data on soil has been included in this study. There are also some uncertainties in the model related to its application in the Nordic area, because the mean temperature in this area is lower and the seasonal changes are larger than in the regions for which the model was originally developed.

The steady-state calculations show that a small emission source will maintain the levels of the pollutants in the environment. The use of many POPs have been phased out in the Nordic countries some time ago. It is therefore likely that the environmental concentrations will decrease with time. A steady-state model is therefore unlikely to describe the chemical and physical behavior of these pollutants as accurate as does a dynamic time-dependent model.

The agreement between the assumed emissions used in the model calculations and the emissions available from emission inventories in the Nordic countries is not as good as the agreement between the the concentration levels measured and calculated. The reason could be an inaccurate estimate of the reaction and advection flows or their corresponding time constants. Another cause may be that the atmospheric transport into and out of the Nordic countries is not properly accounted for. Finally, the emission data from emission inventories, which are often based on assumed emission rates can also be inaccurate.

5. Effects of POPs

Several studies have been carried out to describe the environmental effects and to assess the risk for POPs. A broad review of these studies has been prepared within the UN ECE Task Force for POPs (UN ECE, 1994). Extended studies on the exposure and effects of POPs in the Great Lakes region were reviewed by Swain et al. (1993). The following general conclusions have been reached in these reviews as far as the ecosystem uptake of POPs is of concern.

There is a considerable evidence that POPs bioaccumulate and biomagnify through the ecosystem. They are easily partitioned into biological tissues due to their lipophilic nature and the phospholipid structure of biological membranes. The persistence of POPs permits them to accumulate to relatively high levels in living organisms, even at low exposure rates. Lipophilicy and the persistence are the key factors in the high potential for biomagnification exhibited by these compounds. For these reasons, sustained levels of POPs in the abiotic environment, even if they are very low, may continue to generate concern for adverse chronic effects in biota, particularly in higher trophic level organisms, including humans.

For organisms at higher trophic levels, dietary uptake is more important than direct absorption from the environment. Virtually all major POPs that have been released to the environment in large quantities can be measured in a wide range of marine, terrestrial, and freshwater organisms at all trophic levels. Food chain complexity is a likely factor in the marked differences in contaminant levels between aquatic and terrestrial animals. In the terrestrial food chain, the uptake of particle-associated contaminants is less active than in the aquatic environment. Atmospheric deposition is the main entry of POPs into the terrestrial food chain.

Most of the POPs are eliminated from organisms very slowly due to their resistance to chemical and metabolic degradation. They are generally stored and concentrated in lipids, or in organs such as the liver.

Various ecosystem effects have been described as a result of the ecosystem uptake of POPs. The following evidence has been gathered in the Nordic countries. Concerning fish, since 1974 increased salmon yolk-sac fry mortality has occurred in the Swedish salmon fish hatcheries located in the lower reaches of rivers flowing to the Golf of Bothnia. Until the mid 1980's the mortality of salmon fry remained reasonable but increased significantly afterwards. Almost 100 % mortality has been observed in some hatcheries in Sweden and up to 95 % in

Finland, e.g. the hatcheries in Tornio. The causes of this syndrome, called M74, are still unknown. However, any major diseases, direct genetic defects, or poor quality of water have been rull out as a possible reason.

It should be noted, however, that it is difficult to prove or disprove that a particular POP in the environment has caused a particular disease or change in a terrestrial or aquatic population. Proof of an effect can be obtained from broad evaluation of a variety of data.

The above mentioned salmon fish syndrome and the elevated concentrations of chlorinated hydrocarbons were also observed in the Great Lakes.

In the Baltic Sea dying or malformed fry has also been observed in cod, flatfish, and the Baltic herring populations. Other chlorinated hydrocarbons like dioxins have also been shown to affect metabolism of fish so that the reproduction may be disturbed.

Chlorinated hydrocarbons were suspected to cause syndrome where most of the adult females in a burbot population of the northernmost Bothnian Bay remained immature. However, recent studies could not prove any significant differences between the concentrations of chlorinated hydrocarbons measured in normal and affected populations of burbot.

At the end of 1960's high levels of chlorinated hydrocarbons, particularly DDT and PCBs, measured in the fish of the Baltic Sea were found to biomagnify as very high concentrations (e.g.> 100 ppm in lipid fraction) to their predators ringed seals (Phoca hispida), and grey seals (Halichoenus grypus). Consequently, the reduced reproductive capacity was observed in these populations in the Baltic Proper, the Gulf of Bothnia, and the Golf of Finland. The reason for this was found to be pathological uterine occlusions and stenoses, caused mainly by high PCB concentrations (e.g. Bergman and Olsson, 1986). The older the female, the higher PCB concentrations and the higher the incidence of pathological findings. In the northern Gulf of Bothnia the incidence was the highest at the end of the 1970's when more than a half of the ringed seal females were sterile. In the same area the highest concentrations of DDT in the ringed seals, reaching 115 ppm, and PCBs about 130 ppm were measured in 1976-1977. Lateron the concentrations decreased rapidly and the percentage of sterile females dropped to below 10 %.

In the Gulf of Finland about one third of the ringed seal females in reproductive age were sterile in the period from 1983 thruogh 1988. The grey seal females were not so severely affected. The incidents of sterile females in grey seals were roughly a half of those observed in ringed seals.

In a separate ringed seal population of Lake Saimaa in the eastern part of Finland reproductive disturbances caused solely by chlorinated hydrocarbons have not occurred. Also, the highest PCB concentrations in ringed seal females in this lake were lower than those in normal pregnant females in the Baltic population.

Biomagnification of other POPs, including dibenzofuranes and dioxins from fish to seals has also been studied. However, no biomagnification was observed for these two groups of compounds.

High PCB concentrations have been suggested to explain a decline in otter population in the Baltic Sea. Fertility of the females has decreased due to the same kind of uterine dysfunction as in the seals. In fact, the Baltic otter population has almost disappeared in the last few decades. There are no remaining otters in the Baltic archipelagos. Otters from nearby freshwaters areas have levels of PCBs similar to the levels associated with reproductive impairment of mink under experimental conditions (UN ECE, 1994).

The white-tailed sea eagle is the most affected top predator living around the Baltic Sea. Associations between elevated contaminant residues (PCBs and DDTs) and reduced nesting success, increased chick and embryo mortality, or reduction in population levels have been reported in the Nordic countries (reviewed in Colborn, 1991). Only feeding of eagles with non-contaminated food in wintertime has effectively decreased the concentrations of POPs and nesting results seem to be at the normal level at present.

Information on environmental effects of POPs, collected from measurements and observations in the study area together with information from other regions lead to the following conclusions. A clear dose-response relationship between certain POPs and reproductive failure has been established for several species. These species include seal, otter, and various kinds of fish and birds among others. Often a combination of many congeners of various POP groups have had greater effect on reproduction than single fractions administered alone.

The reproductive effects and abnormalities observed in wildlife are consistent with effects induced in lab animals in experiments using certain POPs, particularly organochlorines.

Finally, POPs have been associated with carcinogenic/tumorigenic effects. Wildlife with high residue levels of these pollutants have been found to have elevated incidence of tumours and lesions on skin and organs (UN ECE, 1994).

It is very difficult to prove that a specific POP at environmental levels has affected human population. The evidence for such impact is less extensive than for wildlife, yet consistent with effects reported in exposed wildlife populations (e.g. Hileman, 1993) and in experimentally exposed animals (Tilson et al., 1990; Rogan et al., 1986). In general, the incidents of accidental organochlorine exposure have demostrated that humans are susceptible to effects from organochlorine contamination.

Concerning the impact of POPs on humans in Scandinavia, it should be mentioned that fish and fish products are the main source of chlorinated hydrocarbons in the human diet in the region. The concentrations of PCBs, DDT, and pesticides in fish vary from one aquatic ecosystem to another. In a recent study in Sweden (Asplund et al., 1994) it was concluded that fatty fish species, e.g. salmon and herring, in the Baltic sea contain high levels of these compounds.

Fish from the Baltic Sea was found to be a major source of exposure to PCBs, DDT, and DDE in Sweden.

In Michigan, Jacobson and coworkers (1990) studied the impact of PCBs on human infants whose mathers were exposed to the these compounds through the intake of contaminated fish. Although slight, the effects were considered as adverse. It should be admitted that the study is not fully conclusive from an epidemiological point of view.

The earlier NMR study (NMR, 1992) on the risk assessment of PCBs has assumed that the conclusions from the Michigan studies and similar work in North Carolina (e.g. Rogan et al., 1986) are valid and that the analytical methods used to determine PCBs in the United States and those used in the Nordic countries are comparable. As a result it was concluded that slight neurotoxic effects in infants can be expected in the Nordic countries.

General conclusions on the impact of POPs on humans, reached by the UN ECE Task Force on POPs (UN ECE, 1994) can be summarized as follows. POPs exerting estrogenic effects can act as hormone mimics, hormone blockers, react with and alter hormones, alter hormone synthesis, and interfere with or promote hormone receptors. In this way POPs can cause reproductive tract anomalies, cancers, some of the immune dysfunctions, and several behavioral abnormalities. However, information on the direct linking of environmental organochlorine exposure to the above mentioned abnormalities is still limited. Only recently some associations have been made between human exposures to POPs and cancers in human populations. Various laboratory studies are quite helpful in this respect indicating that selected organochlorines have genotoxic effects and act as strong tumour promoters.

6. Conclusions and recommendations

During the last two decades an extensive research has been carried out in the Nordic countries with the aim to better understand the sources and fate of POPs in the environment. Major emphasis was placed on obtaining information on the concentration levels of various POPs in individual compartments of the environment. Special emphasis was placed on PCBs, PAHs, and a few pesticides, such as HCHs, DDT, DDE, chlordane, and toxaphene. Recently dioxins and furans have been frequently measured. The results of these studies can be used to characterize the level of contamination by the above compounds in certain regions in the Nordic countries. Concentration trends can also be approached for some POPs in certain regions of the study area.

However, the data obtained so far should be considered as incomplete in order to present the environmental assessment of the whole study area. The degree of the data completeness varies between different groups of POPs and even between various congeners within the same group. Therefore, the application of measured data to study the regional cycling of POPs in the Nordic countries is limited, particularly with respect to the compounds considered and the spatial coverage of the assessment. It should also be noted that various sampling and analytical

procedures have been used throughout the Nordic countries to assess the environmental levels of POPs. This fact can contribute significantly to the quality assurance of the assessment.

The use of a simple multicompartmental mass balance model, such as the fugacity model, is useful to indicate migration of selected POPs through various environmental media or compartment. However, the applicability of this particular model to a geographical area, such as the Nordic countries is limited, first of all because of the exchange of material with the surrounding areas. A rough picture of environmental cycling of hexachlorobenzene, lindane, and fluoranthene in the Nordic countries has been obtained informing about concentrations and percentage mass distribution of the compounds between various environmental compartment in all studied areas. However it is difficult to assess the accuracy of these estimates.

The selection of emission data to be used in the model represented a major problem. Emission data for even most studied POPs in the Nordic countries are quite incomplete and definitely need further improvement. In the reported feasibility study several assumption have been made for emission data on the basis of information on concentration levels in various compartments. The problem with obtaining complete and reliable emission data exists not only in the Nordic countries, but also in other regions worldwide. Various activities within several international organizations and programs to elaborate methodologies to estimate POP emissions hold a promise that improvement of the quality of emission data is feasible and can be expected in the near future.

The fugacity model in this study was run in three versions, all assuming a steady-state conditions. During the project it became obvious that a steady-state model cannot describe accurately the chemical behavior of POPs in the environment. For example, emission data change substantially over time, often declining due to the phase-out of some POPs from further use, e.g. certain pesticides. Steady-state models cannot handle these changes. Indeed, further development of dynamic, time-dependent models is necessary to study the cycling of POPs in the environment. First approaches to obtain such models have already been made with preliminary applications for some POPs in southern part of Norway.

Verification of modeled concentrations by measurements has shown fairly good agreement for some POPs and less so for the others. This agreement is quite promising taking into account difficulties in obtaining good quality and complete environmental data for the study areas and the above described problems in modeling. In future, more refined data are needed to verify the results from models applied in specific regions.

Modeling of global cycling can be performed with the use of the fugacity model applied here for selected POP groups of congeners. It should be realized, however, that the accuracy of this exercise will be lower than the accuracy of the regional cycling model studied here due to even less available emission data and less accurate information on physical and chemical conditions of the global compartments of the environment. The validation of the model result is expected to be more difficult and less reliable than that for the regional estimates due to

scarcity of the environmental measurements worldwide and the variety of sampling and analytical procedures applied at present.

Several studies have been carried in the Nordic countries to assess the environmental and health effects of POPs. Several cases of reproductive tract anomalies, cancers, and behavioral abnormalities have been detected and their relationship to the presence of various POPs is now becoming evident for various species. However, it is still difficult to elaborate direct interactions between the concentration levels of POPs and the causes of the above mentioned effects on humans. The evidence of these interactions is now being collected. Additional complications are either synergistic or antagonistic interactions of various groups of POPs or even various congeners within the same group.

Taking into account the above presented conclusions it is recommended to attempt the improvement of our knowledge on the cycling of POPs and its environmental effects through a study in carefully selected region. The Baltic Sea area could be a good choice for such project for several reasons:

- the Baltic Sea extends over a substantial latitudinal range and should, therefore, reveal differences of chemical behavior between temperate and boreal environments,
- the region is heavily polluted by various POPs,
- the Baltic Sea is a relatively well studied marine region and some necessary input parameters for the model may be relatively easy to obtain, and
- there have been numerous measurements of the POP concentrations in various compartments of the Baltic Sea environment and these data may form a good data set for model validation.

The major tool is such study should be a multimedia dynamic time dependent model. Its results should be verified using a set of reliable measured data from the area. The description of dose - response relationships for the studied POPs should be approached.

8. Acknowledgements

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18

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Tables and figures

Table 1

21
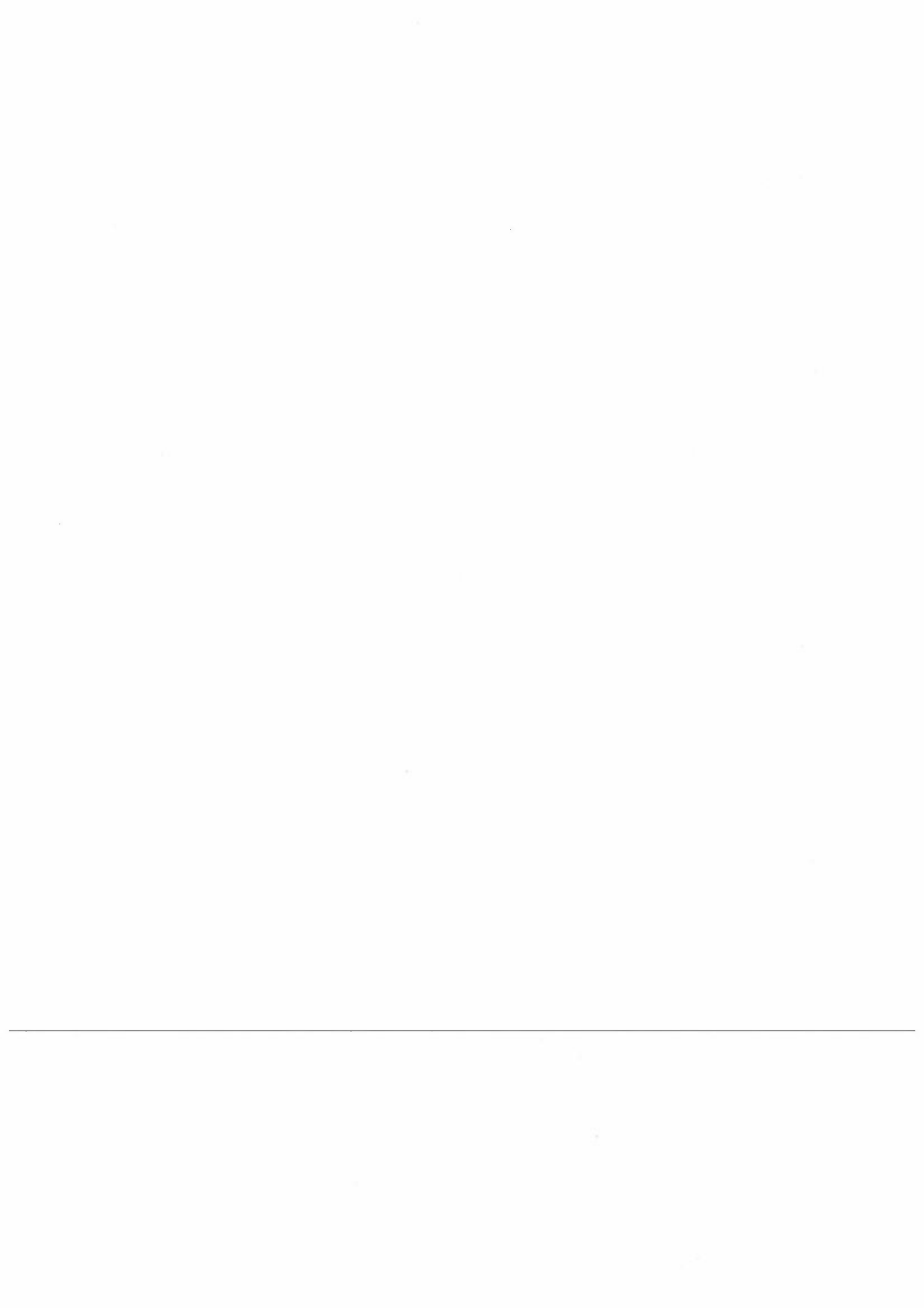
Nordic environments

Parameters for "POPFATE" modelling (Mackay level I+II+III)

Densities kg/m³

Air	1.84503	Water 1000	Soil 2400	Sediment 2300
Susp.sediment	1500	Fish 1000		

Regional parameters (land areas of each country, Σ coastal sea areas 30 km from shore)

Property	Danmark	Finland	Norway	Sweden	Sea areas	Total
Area m²	0.43E+11	3.37E+11	3.24E+11	4.50E+11	3.5E+11	15E+11
Soil area m²	0.424E+11	3.05E+11	3.19E+11	4.11E+11	0	10.7E+11
Water area m²	.0612E+10	3.16E+10	0.5E+10	3.85E+10	35.0E+10	4.26E+11
Ave temp.°C	7.5	2	5	4	6	4
Ann.prec. mm	650	700	1500	900	800	900
Volumes m³						
Air (h 1000 m)	0.43E+14	3.37E+14	3.24E+14	4.50E+14	3.5E+14	15E+14
Water (20/100)	.12E+11	6.32E+11	1.0E+11	7.70E+11	3.5E+13	3.65e+13
Soil (h 0.1 m)	.424E+10	3.05E+10	3.19E+10	4.11E+10	0	10.7E+10
Sedim.(.05)	3.06E+07	1.58E+09	2.5E+08	1.93E+09	1.75E+10	2.13E+10
Fish	.12E+05	6.32E+05	1.0E+05	7.7E+05	3.5E+07	3.65E+07
Frn.org.C						
Soil	.02	.05	.05	.04	.03	.045
Sediment	.04	.08	.08	.06	.05	.05
Susp.sedim.	.20⁻	.30	.30	.25	.40	.30

Special Regions (Sea areas, no lands included, maximum depth considered 200 m)

Property	Bay of Bothnia	Baltic Proper	Skagerrak/North Sea	Barents Sea
Area m²	3.70E+10	2.1E+11	4.5E+10	1.21E+12
Soil area m²	0	0	0	0
Water area m²	3.70E+10	2.1E+11	4.5E+10	1.21E+12
Ave temp.°C	2	7	8	-2
Ann.prec. mm	500	600	700	300
Volumes m³				
Air (h 1000 m)	3.70E+13	2.1E+14	4.5E+13	1.21E+15
Water (h 38-200)	1.39E+12	1.3E+13	5E+12	2.42E+14
Soil (h 0.1 m)	0	0	0	0
Sediment (.05)	1.85E+09	1.05E+10	2.25E+09	2.42E+10 (.02)
Fish	1.39E+06	1.3E+07	4.5E+07	2.42E+08
Frn.org.C				
Soil	0.04	0.03	0.03	0.03
Sediment	0.05	0.05	0.05	0.01
Susp.sedim.	0.15	0.40	0.40	0.02

Table 2

Level III stationary states in Nordic environments

Fluoranthene (annex FLNORDM)

Assumed emission rates kg/h of FLUORANTHENE

Area	Air	Water	Soil	Sediment	Total
Danmark	3	0.4	0	0	3.4
Finland	11	19	2	1	33
Norway	14.5	4	2	0	20.5
Sweden	28	15	5	0	48
$\sum$ Sea areas	11.5	8	0	0	19.5
Total Nordic countr.	60	25	10	0	95
Bay of Bothnia	0.08	0.02	0	0	0.1
Baltic Proper	0.7	4.8	0	0	5.5
Skagerrak/North Sea	0.39	2.2	1.2	.46	4.25
Barents Sea	1	3	0	0	4

Concentrations g/m^3 of FLUORANTHENE

Area	Air	Water	Soil	Sediment	Fish
Danmark	5.1E-09	2.5e-05	7.7E-05	2.5E-02	0.19
Finland	2.0E-09	2.0E-05	8.1E-03	3.2E-02	0.14
Norway	3.1E-09	2.6E-05	8.7E-03	3.8E-02	0.19
Sweden	4.1E-09	1.4E-05	1.4E-02	1.7E-02	0.10
$\sum$ Sea areas	3.0E-09	7.7E-06	3.5E-03	3.0E-02	.052
Total Nordic countr.	2.5E-09	2.5E-06	9.3E-03	9.8E-03	.017
Bay of Bothnia	1.1E-10	6.4E-08	2.8E-04	1.1E-04	.0005
Baltic Proper	1.9E-10	7.4E-07	3.0E-04	2.9E-03	.0050
Skagerrak/North Sea	5.1E-10	1.7E-06	5.2	8.9E-03	.0115
Barents Sea	3.6E-11	1.5E-08	1.4E-04	3.5E-06	1.2E-04

Mass distribution per cents of FLUORANTHENE

Area	Air	Water	Soil	Sediment
Danmark	.349	.486	93.05	6.11
Finland	.095	1.74	62.84	35.32
Norway	.181	.477	90.74	8.60
Sweden	.150	.899	85.13	13.82
$\sum$ Sea areas	.950	4.80	.257	93.99
Total Nordic countr.	.166	.948	80.33	18.55
Bay of Bothnia	.886	10.57	1.13	87.41
Baltic Proper	.0634	4.86	.0086	95.07
Skagerrak/North Sea	.0170	1.12	69.10	29.76
Barents Sea	1.09	88.24	.0647	10.61

Table 3

23

HEXACHLOROBENZENE (annex HCBZNORD)

Assumed emission rates kg/h of HEXACHLOROBENZENE

Area	Air	Water	Soil	Sediment	Total
Danmark	0.15	0.02	0	0	0.17
Finland	0.3	0.43	0.17	0.02	0.92
Norway	0.33	0.01	0.05	0	0.39
Sweden	0.47	0.15	0.04	0.002	0.662
$\sum$ Sea areas	0.33	0.27	0	0	0.60
Total Nordic countr.	1.8	0.3	0.06	0.04	2.20
Bay of Bothnia	0.04	0.012	0	0	0.052
Baltic Proper	0.27	0.15	0	0	0.42
Skagerrak/North Sea	0.17	0.04	0	0.001	0.211
Barents Sea	1.19	1.21	0	0	2.4

Concentrations g/m^3 of HEXACHLOROBENZENE

Area	Air	Water	Soil	Sediment	Fish
Danmark	3.5E-10	7.7E-07	1.8E-05	1.4E-03	0.0010
Finland	1.0E-10	3.1E-07	2.5E-04	8.2E-04	0.0037
Norway	1.0E-10	5.3E-08	7.4E-05	1.3E-10	.00064
Sweden	1.0E-10	9.7E-08	4.9E-05	2.1E-04	.00122
$\sum$ Sea areas	1.0E-10	1.7E-07	5.74E-06	1.1E-03	.00187
Total Nordic countr.	1.1E-10	2.5E-08	3.1E-05	1.8E-04	.00028
Bay of Bothnia	8.4E-11	1.9E-08	6.2E-06	5.5E-05	.00025
Baltic Proper	1.0E-10	2.3E-08	5.5E-06	1.5E-04	.00026
Skagerrak/North Sea	3.0E-10	4.1E-08	1.5E-05	2.7E-04	.00046
Barents Sea	7.0E-11	6.3E-09	6.9E-06	2.8E-06	9.7E-05

Mass distribution per cents of HEXACHLOROBENZENE

Area	Air	Water	Soil	Sediment
Danmark	4.10	2.57	36.95	56.39
Finland	.167	.949	67.26	31.62
Norway	.727	.119	95.51	3.64
Sweden	.818	1.29	62.72	35.16
$\sum$ Sea areas	.912	2.97	7.91	96.11
Total Nordic countr.	1.16	1.49	42.55	1.82
Bay of Bothnia	1.41	6.27	.051	92.27
Baltic Proper	.680	2.98	.0031	96.34
Skagerrak/North Sea	1.06	2.91	.021	96.02
Barents Sea	4.34	78.20	6.40	17.44

Table 4

24

LINDANE (annex LINDNORD)

Assumed emission rates kg/h of LINDANE

Area	Air	Water	Soil	Sediment	Total
Danmark	0.3	0.2	0.1	0.005	0.605
Finland	1.1	0.2	0.6	0.2	2.1
Norway	0.53	0.15	0.11	0.0002	0.7902
Sweden	2.25	1.25	.5	.05	4.05
$\sum$ Sea areas	0.8	1.9	0	0	2.7
Total Nordic countr.	3	18	6	0.3	27.3
Bay of Bothnia	0.08	0.8	0	0	0.88
Baltic Proper	0.45	12.5	0	0.05	13
Skagerrak/North Sea	0.35	2.95	0	0	3.3
Barents Sea	1.2	20	0	0	21.2

Concentrations g/m^3 of LINDANE

Area	Air	Water	Soil	Sediment	Fish
Danmark	4.9E-10	1.7E-05	5.2E-04	9.0E-04	.0053
Finland	1.6E-10	5.0E-07	4.5-04	3.9E-04	.00016
Norway	1.0E-10	1.6E-06	1.2E-04	6.4E-05	.00049
Sweden	2.9E-10	1.8E-06	4.0E-04	1.3E-04	.00055
$\sum$ Sea areas	2.0E-10	2.6E-06	1.3E-04	2.6E-04	.00082
Total Nordic countr.	1.1E-10	2.1E-06	8.0E-04	2.9E-04	.00065
Bay of Bothnia	9.3E-11	1.1E-06	1.1E-04	4.8E-05	.00034
Baltic Proper	1.3E-10	2.8E-06	6.7E-05	3.1E-04	.00088
Skagerrak/North Sea	4.4E-10	3.2E-06	2.0E-04	3.2E-04	.00100
Barents Sea	3.1E-11	8.3E-08	7.0E-05	7.8E-07	2.6E-05

Mass distribution per cents of LINDANE

Area	Air	Water	Soil	Sediment
Danmark	0.491	4.80	91.51	3.19
Finland	.194	1.12	87.86	10.82
Norway	.454	2.17	96.26	1.11
Sweden	.394	4.14	81.57	3.89
$\sum$ Sea areas	2.53	64.89	.243	32.33
Total Nordic countr.	.0928	9.65	83.58	6.68
Bay of Bothnia	.348	81.29	.203	18.16
Baltic Proper	.150	64.55	.00684	35.29
Skagerrak/North Sea	.458	66.38	8.35	33.07
Barents Sea	.187	99.34	6.31	.463

Table 5

"POPFATE" modelling (Mackay level I+II+III).
Environmental concentrations at the POPFATE areas
Nordic countries

Media [units]	Danmark	Finland	Norway	Sweden	Σ Sea areas	Total
HCBz						
Air [g/m^3]			1E-10	1E-10		
Water [mg/L]		3E-7				
Sedim.[mg/kg]			3E-5			
Fish [mg/kg]	1.4E-3	5E-3				
Mussel[mg/kg]	2.3E-4					
LINDANE						
Air [g/m^3]			1.4E-10	3E-10		
Water [mg/L]		5E-7			2.6E-6	2E-6
Sedim.[mg/kg]		5E-4	4E-5			
Fish [mg/kg]	1.7E-3	1.5E-4				
Mussel[mg/kg]	1.5E-3					
FLUORANTH.						
Air [g/m^3]		2E-9	3E-9	4E-9	3E-9	2.5E-9
Water [mg/L]		2E-5				
Sedim.[mg/kg]		2.7E-2				
Fish [mg/kg]		2.5E-5				
Mussel[mg/kg]	5E-3					

Special Regions

Media [units]	Bay of Bothnia	Baltic Proper	Skagerrak/North Sea	Barents Sea
HCBz				
Air [g/m^3]				7E-11
Water [mg/L]	1E-6			
Sedim.[mg/kg]			2E-4	
Fish [mg/kg]	1E-2	4E-3		1E-4
LINDANE				
Air [g/m^3]				3E-11
Water [mg/L]	1.9E-6	2.8E-6	3.2E-6	5E-7
Sedim.[mg/kg]			7E-5	
Fish [mg/kg]	6E-4	9E-4		1E-5
FLUORANTH.				
Air [g/m^3]	1E-10	1.9E-10	5E-10	
Water [mg/L]				
Sedim.[mg/kg]			7E-3	
Fish [mg/kg]	4E-3	5E-3		
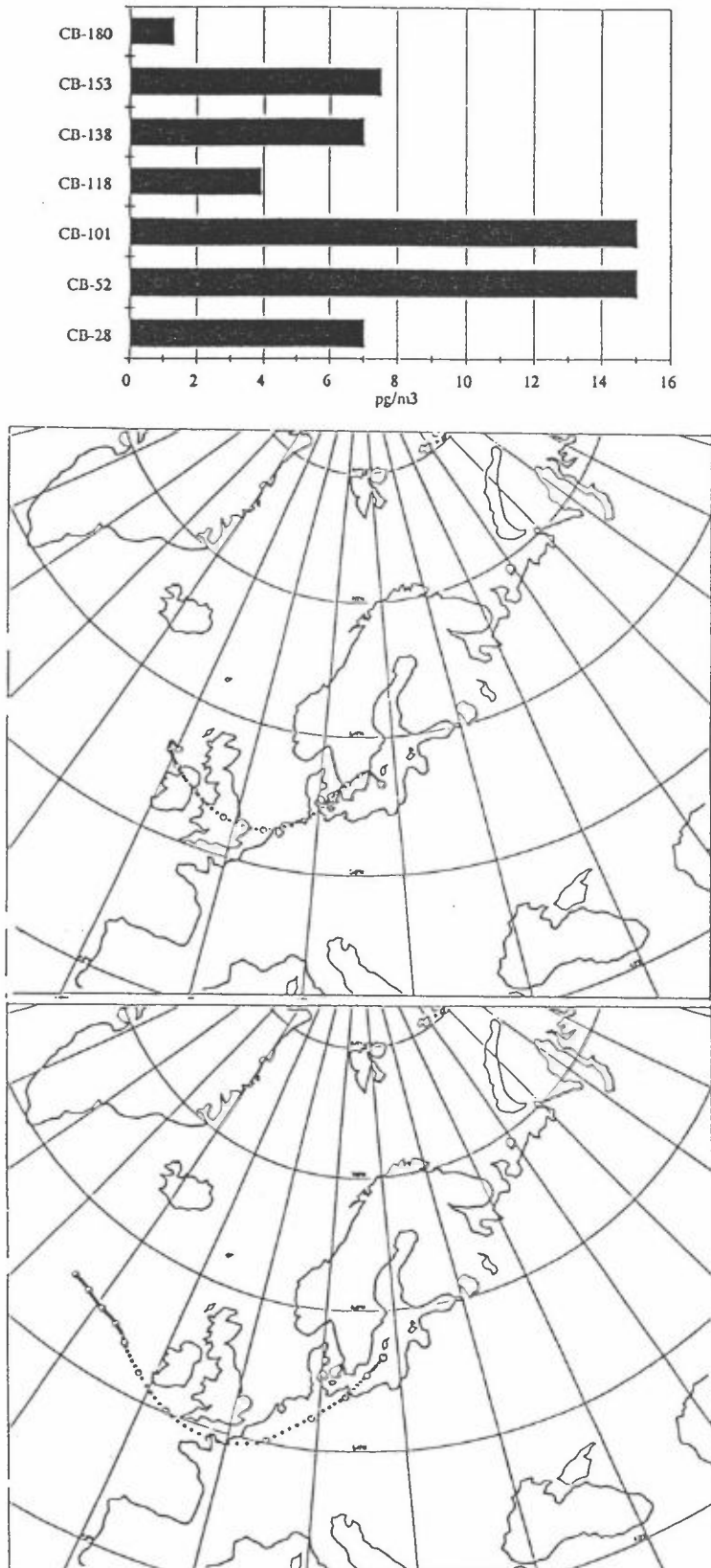
Figure 1. Concentrations of seven PCB congeners in air sampled at Gotland in the Baltic Sea. The sampling time was 48 hours and in the upper map the trajectories for the last 72 hours calculated after 24 hour sampling are shown. In the lower map the corresponding data calculated in the end of the sampling period are given.
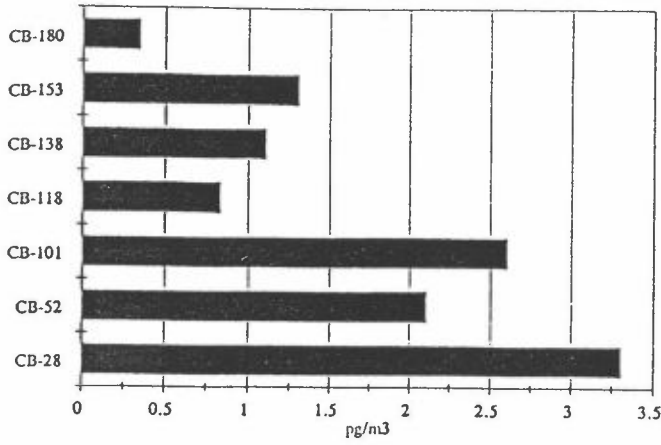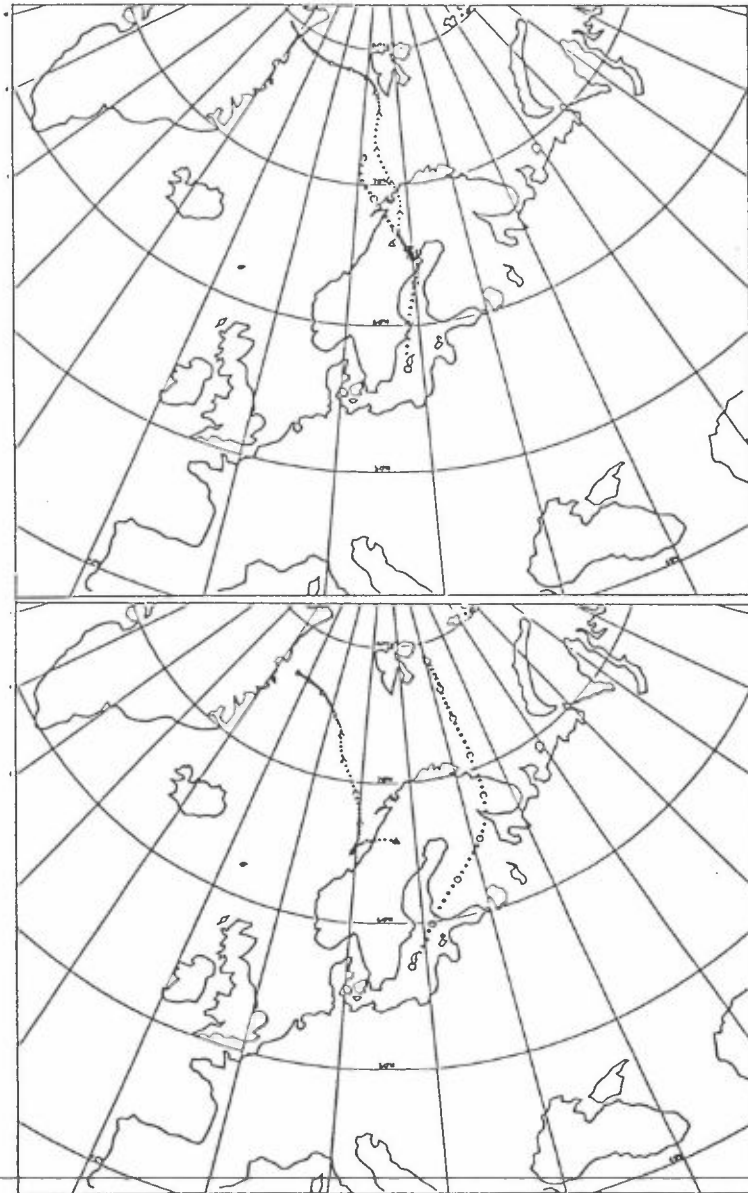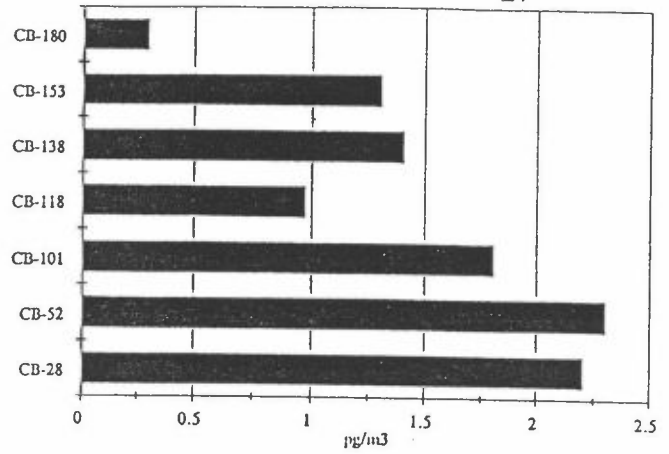
Figure 2. Concentrations of seven PCB congeners in air samples taken at the same time in the mountains in the north of Sweden (left graph) and at Gotland in the Baltic (right graph). The sampling time was 48 hours and in the upper map the trajectories calculated after 24 hours (72 hours back) are shown. The lower map shows the trajectories calculated in the end of the sampling period.
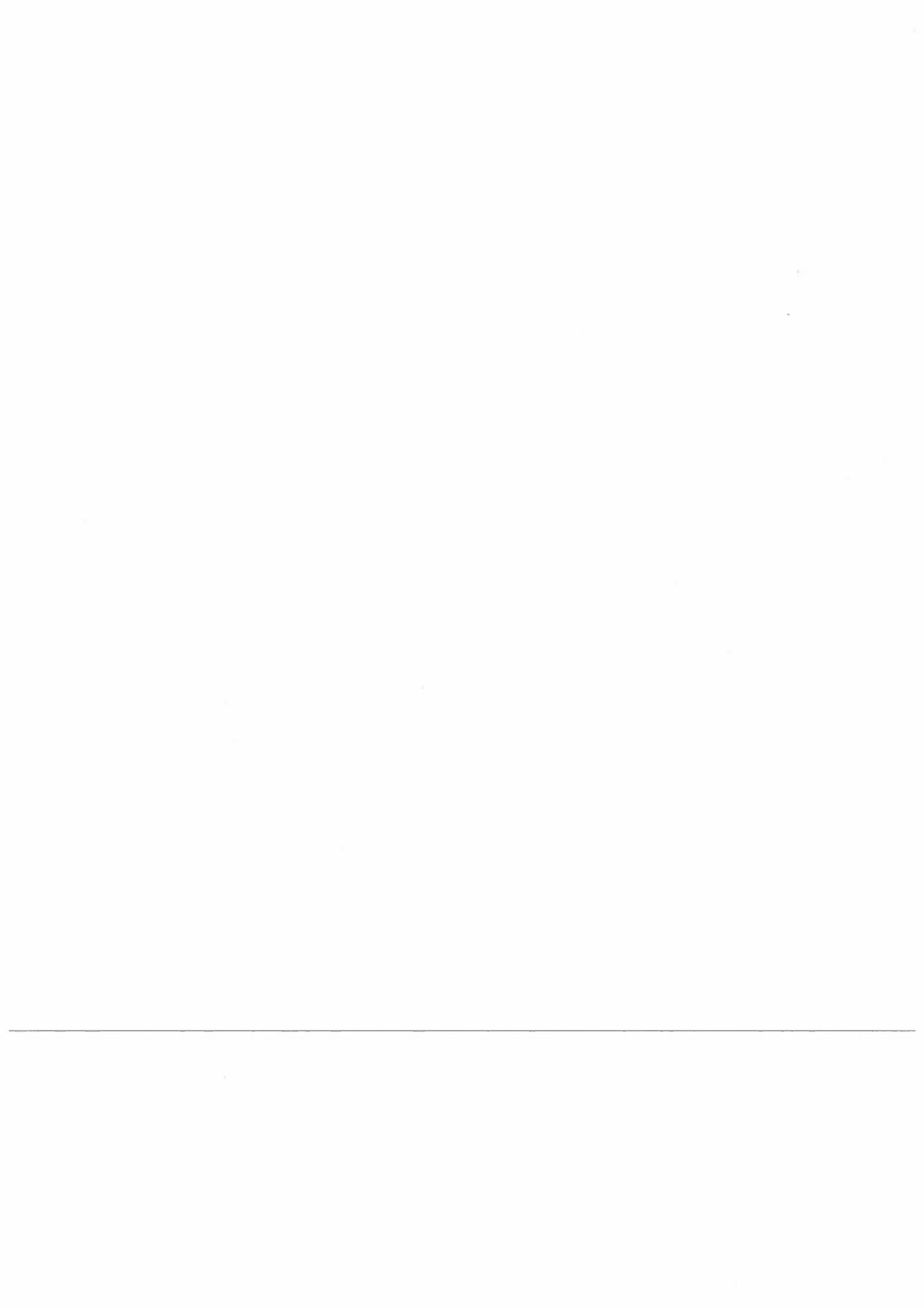
Annex 1

Participants of the project

PARTICIPANTS OF THE PROJECT

GROUP 1 ON RELEASES AND DISTRIBUTION

Ms. Eva Brorstrom-Lunden (Sweden - Group leader)
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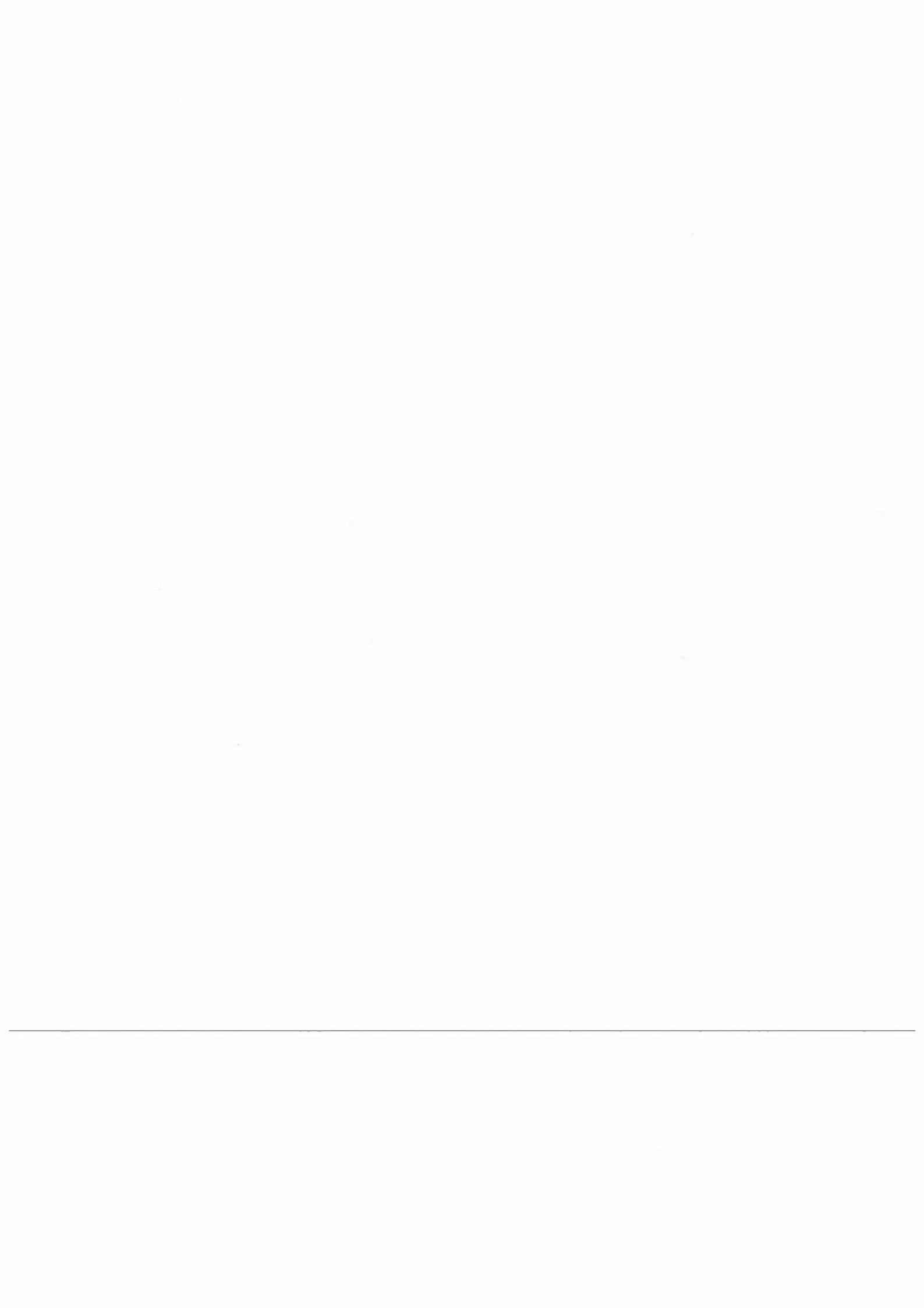
Annex 2

Concentrations of studied POPs in samples of air, deposition, vegetation, sediment, water, and mussels collected in the Nordic countries

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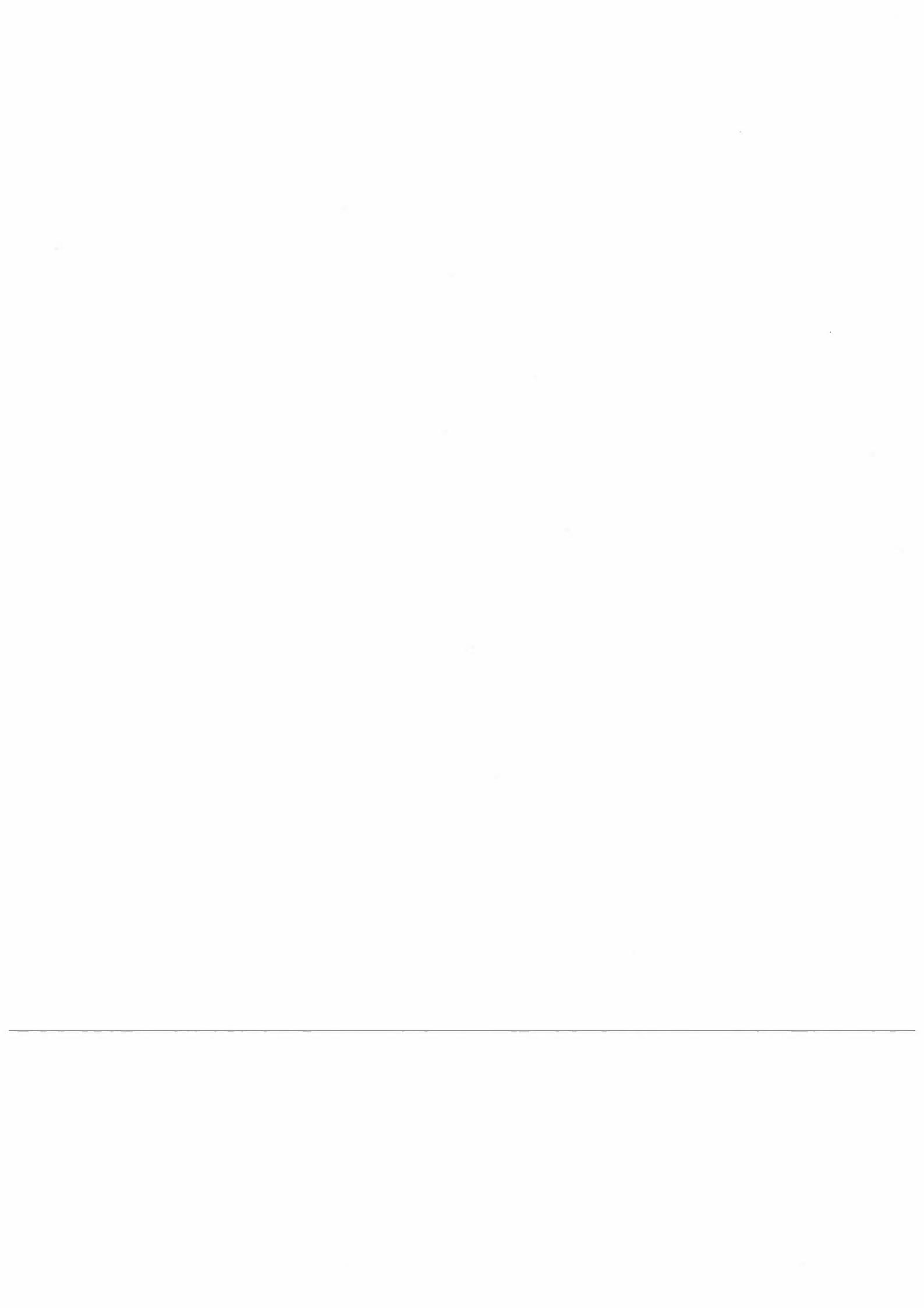
REF	AIR Country	Year	Site (Number)	Seas.	Distrib. Location	PAH ng/m3	PCB pg/m3	HCH alfa, gamma pg/m3	HCB pg/m3	Comment
3	Nor	1981	1 (4-7)	Spring	NILU		·	347-1230, 154-410	55-230	Artic not included
4	Nor	1984	3(12)	Sum	geo.		data Cl5-Cl8	289-1168, 37-705	30-153	Artic not included
4	Nor	1984	3(12)	Winter	geo		data Cl5-Cl8	56-507, 6-43	55-210	Artic not included
5	Nor	1992	3(80)	Spring	geo		data PCB 28-180	40-200, 10-500	55-280	Artic not included
1	Swe	1984-85	1(11)	all	East coast		23-1200(tot)	190-3200, 21->660	54->170	Stockholm not included.
11	Swe	1984-85	14	all	geo		<5-3600(tot)*			from figure
2	Swe	1986-87	5	Win, Spr	East coast	2.8-6.9 (15 PAH)				Stockholm not included.
6	Swe	1988-90	1 (14)	all	West coast					
7	Swe	1988	1(5)	wint	West coast	2.9-25 (11PAH)				
8,9	Swe	1989-90	1(12)	wint-sp.	West coast	1.5-30 (11PAH)	6-120 (Sum7)	14-550, 9-1100		
10	Swe	1991-92	1(11)	spr- sum.	West coast	1-2-2.1(11PAH)	17-69(Sum7)	17-140, 33-518		
28	Swe		1(11)	all	East coast		10-57(Sum 7)**			

*= Data contains extreme values not included   **= gas phase

AIR.XLS

REF	Country	Year	Site (Number)	Seas.	Distrib. Location	Dioxin PCDF, PCDD pg/m3	DDT DDE,DDT pg/m3	Chlord. gamma, alfa pg/m3	Tox. pg/m3	Comment
3	Nor	1981	1 (4-7)	Spring	NILU					
4	Nor	1984	3(12)	Sum	geo.			0.7-3.7, 1.3-7.8		
4	Nor	1984	3(12)	Winter	geo			0.4-3.2, 0.4-3.1		
5	Nor	1992	3(80)	Spring	geo			0.24-2.1 0.4-2.8		
1	Swe	1984-85	1(11)	all	East coast		0.4-41 0.6-100	1.3-10, 1.0-15	5-225	
11	Swe	1984-85	14	all	geo		<2-120			from figure
2	Swe	1986-87	5	Win, Spr	East coast	0.2-0.4				Stockholm not included.
6	Swe	1988-90	1 (14)	all	West coast	0.08-2.2 0.2-3		0.4-1.7, 1-1.9		
7	Swe	1988	1(5)	wint	West coast					
8,9	Swe	1989-90	1(12)	wint-sp.	West coast					
10	Swe	1991-92	1(11)	spr- sum.	West coast			1-1.8, 1.7-3.1		

DEP.XLS

DEPOSITION

REF	Country	Year	Site (Number)	Seas.	Distrib. Location	PAH ug/m day	PCB ng/m2day	HCH alfa, gamma ng/m2day	HCB ng/m2day	Comment
12	Den	1990	2(24)	year				2-25, 5-190		Bulk sampler, from fig
11	Swe	1984-85	14(4)	year	geog.		<10-2800(tot)*			silicone oil net, from fig.
7	Swe	1988	1(5)	wint	West coast	1-7.1(11PAH)				Bulk sampler 1m2
8.9	Swe	1989-90	1(12 -4)	wint-spri.	West coast	0.2-2 11PAH	2.3-4.5 (sum7)	0.11-3.2, 0.8-35		Bulk sampler 1m2
10	Swe	1991-92	3 (34)	year	West coast	0.1-1.5 (11PAH)	0.7-5.8 (sum 7)	0.21-11, 0.2-35		Bulk sampler 1m2

* Data contains some extreme values, not included

REF	Country	Year	Site (Number)	Seas.	Distrib. Location	Dioxin PCDF, PCDD ng/m2day	DDT DDE,DDT ng/m2day	Chlord. gamma, alfa ng/m2day	Tox. ng/m2day	Comment
11	Swe	1984-85	14(4)	year	geog.		<5-110*			silicone oil net, from fig.

* Data contains some extreme values, not included

VEG.XLS

VEGETATION

REF	Country	Year	Site (Number)	Seas.	Distrib. Location	PAH ng/g dw	PCB ng/g dw	HCH alfa, gamma ng/g dw	HCB ng/g dw	Comment
15	Nor.	1986	2(3)		time		4-6* (total)	1-3*		Pine needle 84-86
15	Swe	1986	20(3)		geo, time.		4-8 * (total)	2-6*		Pine needle 84-86
16	Den	1989	1(5)		time			0.35--3.8, 0.37-2.3	0.08-0.59	Pine needle 84-88
16	Swe	1989	1(5)		North, time			0.84-5.6, 0.29-2.0	0.38-1.4	Pine needle 84-88
13,14	Swe	1991-92	1(10)	year	West coast	22-140 (11PAH)	1.3-2.8 (sum7)	0.76-1.2, 1.0-1.5	0.33-0.51	Spruce Needles
17	Swe	1990-91	7(1)		Cent.	190-77(11 PAH)	2-4(Sum7)		0.7-1.1	Mosses

REF	Country	Year	Site (Number)	Seas.	Distrib. Location	Dioxin PCDF, PCDD ng/g dw	DDT DDE,DDT ng/g dw	Chlord. gamma, alfa ng/g dw	Tox. ng/g dw	Comment
15	Nor.	1986	2(3)		time		0.1-0.6*			Pine needle 84-86
15	Swe	1986	20(3)		geo, time.		0.2-1.3*			Pine needle 84-86
16	Den	1989	1(5)		time		0.1-0.31, 0.28-0.55			Pine needle 84-88
16	Swe	1989	1(5)		North, time		0.03-0.21, 0.1-0.19			Pine needle 84-88

SEDIMENT							HCH alfa, gamma		
REF	Country	Year	Site (Number)	Seas.	PAH ug/g dw	PCB ng/g dw	ng/g dw	HCB ng/g dw	Comment
22	Nor	1990	Atlantic outside Nor. (9)		0.17-0.31	0.07-0.64 (sum 7)	<0.01-0.06	0.01-0.05	
21	Nor		North Sea/Skagerrak (10)						
23	Nor	1991	Olensfj. (8)			0.8-3.6 (sum 7)			
24	Swe		Skagerrak (15)		0.4-3 (11PAH)	1.3-3.9 (sum7)	0.01-0.1 <0.04-0.1	0.1-0.3	
20	Swe	1985	Baltic14	winter-spring	1.5-8.6 (18 PAH)				Uban influence
20	Swe	1985	Baltic14	summer	1.1-4.7 (18 PAH)				
Ex	Fin		Average based on few data			10-30(total)	0.2 0.5	1	

EX = Ref from Finland, see separate list from M.Koronen

					Dioxin PCDF, PCDD	DDT DDE,DDT	Chlord. gamma, alfa	Tox.	
REF	Country	Year	Site (Number)	Seas.	pg/g dw	ng/g dw	ng/g dw	ng/g dw	Comment
22	Nor	1990	Atlantic outside Nor. (9)			0.03-0.2	<0.01-0.06		
21	Nor		North Sea/Skagerrak (10)		25-520 29-475				
23	Nor	1991	Olensfj. (8)						
24	Swe		Skagerrak (15)			0.4-1.8	0.04-0.09	0.1-0.6	

WATER.XLS

REF	WATER Year	Site (Number)	Seas.	PAH ng/l	PCB ng/l	HCH alfa, gamma ng/l	HCB ng/l	Comment
18	1983	Baltic	Spring			5-8 2-4		surface 5m
18	1983	Kattegatt	Spring			5-6 4-6		surface 5m
18	1985	Skagerrak	Summer			3.0 3.2		surface 5m
18	1985	Nor. west coast	Summer			1.3-2.7 0.5-2.1		surface 5m
18	1988	Baltic	Spring			4-4.7 1.5-3.9		surface 5m
19	1988	Baltic (9)	Summer	0.5-1.1(11 PAH)				

REF	Year	Site (Number)	Seas.	Dioxin PCDF, PCDD pg/m3	DDT DDE,DDT ng/l	Chlord. gamma, alfa ng/l	Tox. ng/l	Comment
19	1988	Baltic (9)	Summer	242-552				

MUSSELS.XLS

Mussels							alfa, gamma		
REF	Country	Year	Site	PAH	PCB(sum7)	HCH	HCB	Comment
			(Number)					
				ng/g dw	ng/g dw	ng/g dw	ng/g dw	
26	Nor	1990-91	Nor. west coast (5)		2-5.5	0.2-0.5(gamma)	0.04-0.07	50 mussles
23	Nor	1991	Olensfj. (5)		4.3-10.3			
25	Den		Kattegatt, Belt Sea (26)	5.4-110(ww)	4.3-328* (ww)	.3--3.1 0.6-3.4(ww	0.11-0.74(ww)	
27	Swe	1993	Swe. west coast		2.2-11(ww)		<0.3-0.6(ww)	

				Dioxin		gamma, alfa		
REF	Country	Year	Site	PCDF, PCDD	DDT	Chlord.	Tox.	Comment
			(Number)		DDE,DDT			
					ng/g dw	ng/g dw	ng/g dw	
26	Nor	1990-91	Nor. west coast (5)		0.34-26			
23	Nor	1991	Olensfj. (5)					
25	Den		Kattegatt, Belt Sea (26)		2.4-67*(ww)			
27	Swe	1993	Swe. west coast					

* =Data contains one extreme value

42

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CHEMICAL / SPECIMEN	PCBs	PAHs	DioxFur	LIND	aHCH	DDTs	HCB
inlandwater***	<0.1-1ng/l			<2-3ng/l	<3-5ng/l	<0.01-0.02ng/l	
human serum*** (DioxFur/milk)	2.5-3.5ug/l		20-30pg/g lf TEQ	0.7ug/l		1ug/l	0.3ug/l
white tailed eagle*	200ug/g lf		1100pg/g lf TEQ			30-60ug/g lf	1.2-2ug/g lf
ringed seal**	100-150ug/g lf(70s-80s) 40-70ug/g lf(80s-90s)		400pg/g lf TEQ			80-150ug/g lf(70s-80s) 30-70ug/g lf(80s-90s)	
grey seal*	100ug/g lf(70s-80s) 30ug/g lf(80s-90s)		800pg/g lf TEQ			100ug/g lf(70s-80s)	
salmon*** -spawning	3.5-5ug/g lf 4-9ug/g lf		100pg/g lf TEQ	30ng/g lf	50ng/g lf	2-3ug/g lf 4-10ug/g lf	8-50ng/g lf
pike***	6-10ug/g lf(70s-80s) 1-3ug/g lf(80s-90s)	25ng/g fw	0.5-3pg/g fw TEQ	30ng/g lf	30ng/g lf	4ug/g lf(70s-80s) 1-2ug/g lf(80s-90s)	50ng/g lf
Baltic herring***	2-10ug/g lf(70s-80s) 1ug/g lf(80s-90s)	20ng/g fw	0.5-2pg/g fw TEQ	40-60ng/g lf	30-80ng/g lf	2-4ug/g lf(70s-80s) 1ug/g lf(80s-90s)	40-60ng/g lf
Macoma balthica* (PAH/Mytilus e.)	0.5ug/g lf	100ng/g fw	0.3pg/g fw TEQ	15ng/g lf	30ng/g lf	0.3ug/g lf	10ng/g lf
Anodonta piscinalis**	0.4ug/g lf		0.3pg/g fw TEQ	30ng/g lf	20ng/g lf	0.1ug/g lf	10ng/g lf
sediment(surface)*	10-30ng/g dw 20-300ng/g dw	20-300ng/g dw	100-700pg/g dw	0.5ng/g dw	0.2ng/g dw	1.5ng/g dw	1ng/g dw

***=good data, **=some data, *=small data
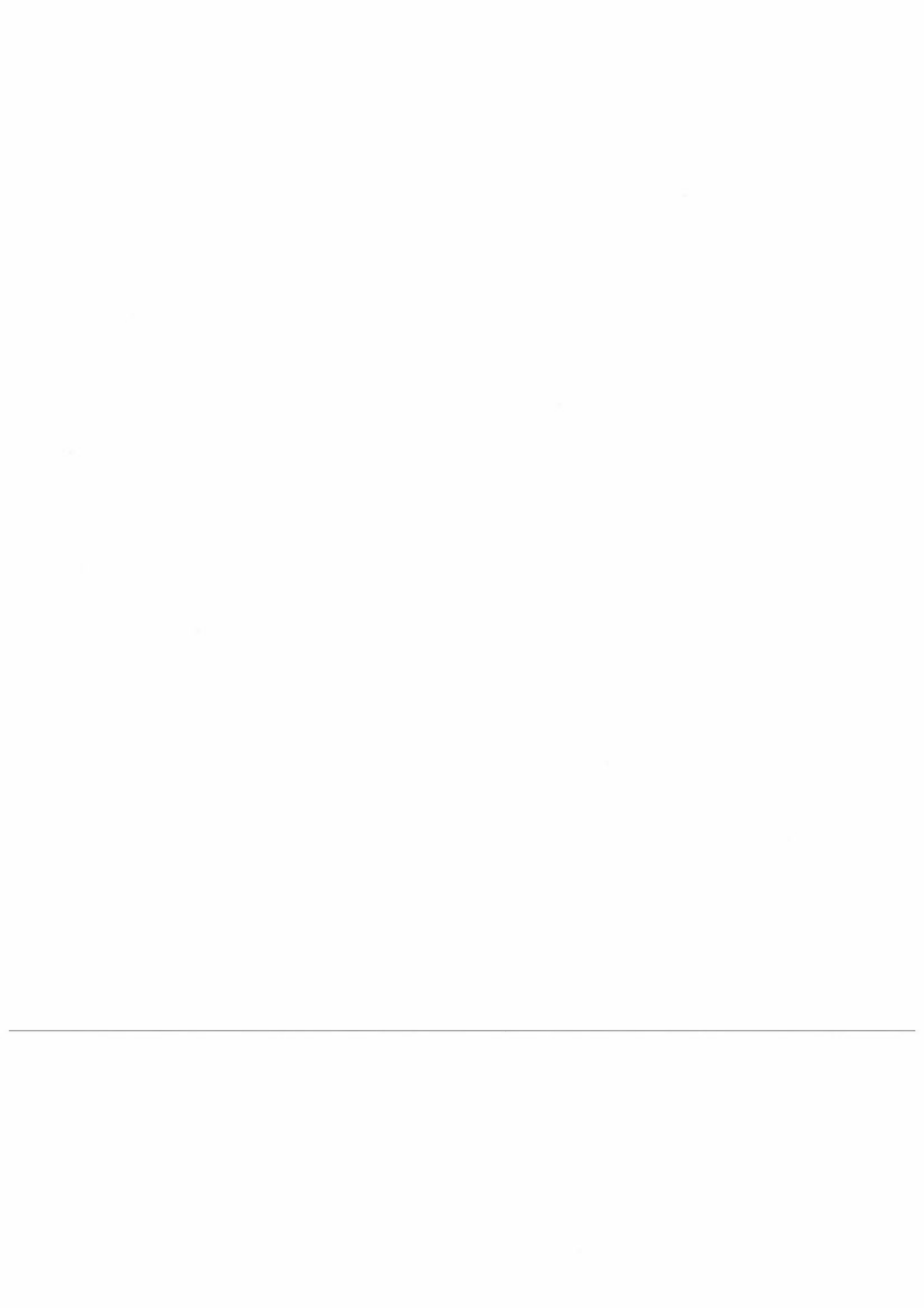
Annex 3

Physico-chemical properties of the studied POPs
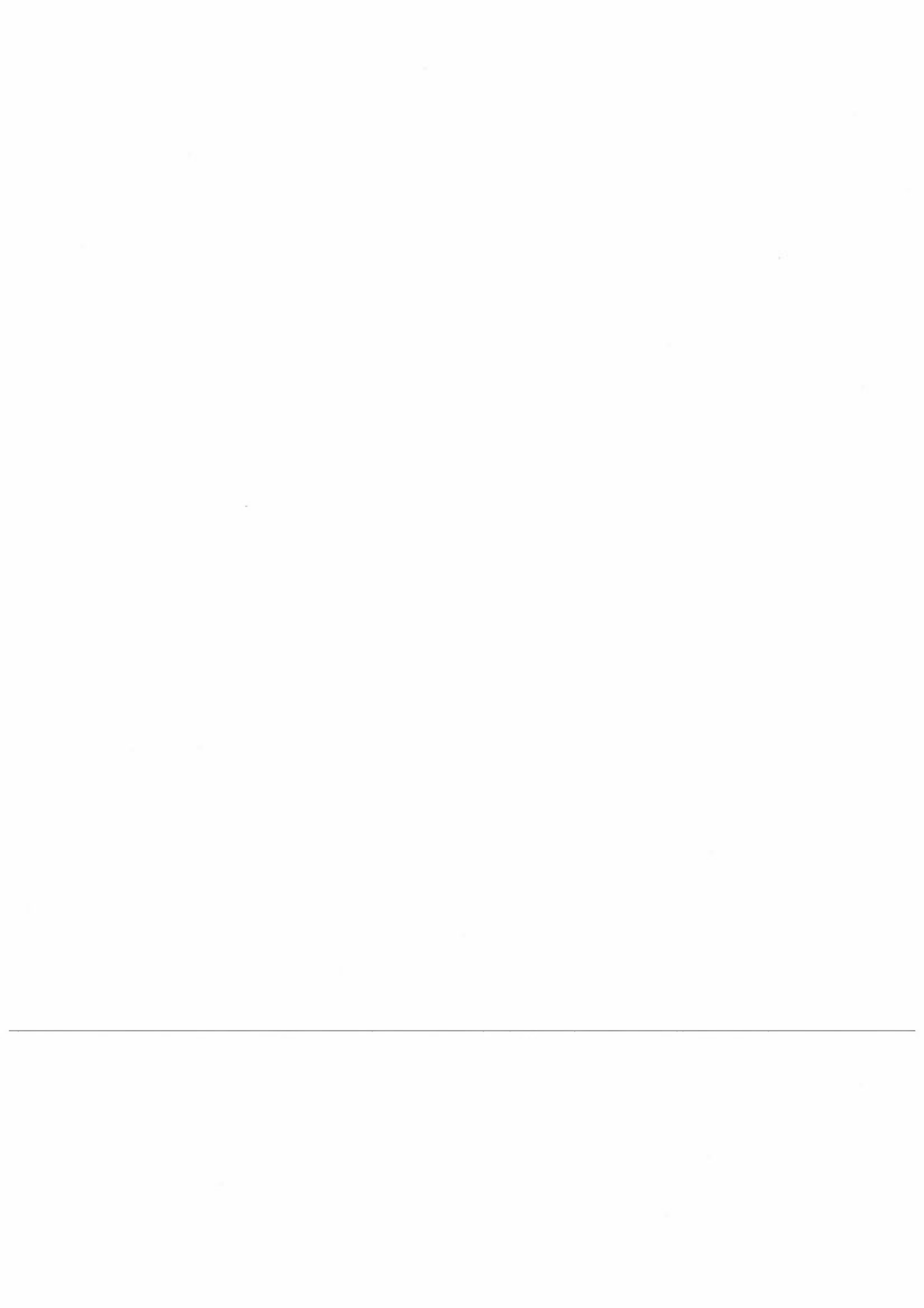
PROPERTIES OF POP's

Compound	M g/mol	MP, ^{o}C	BP, ^{o}C	S, g/m³ 25°C
α-HCH	290.82	158	228	
γ-HCH (lindane)	290.82	112.9 (16)	323	7.3-7.80 (16)
HCBz	284.78	231 (23)	322 (16)	0.005 (16)
Oxychlordane	423.76			
Trans-chlordane	409.77			
Cis-chlordane	409.77			
Trans-nonachlor	444.22			
p,p'-DDE	318.00	88-90 (23)		4×10^{-8} (19)
p,p'-DDT	354.50	108.5-109 (23)	185 (16)	3.2×10^{-9} (19)
				0.8 ng/L (27)
p,p'-DDD	320.00	112 (23)		
TOX1 Octachlorobornane	413.79			
TOX2 Nonachlorobornane	448.24			
PCB28 2,4,4'-trichloro-	257.53	57 (1,3)	337, c (2,3)	0.16±0.1 (3)
				0.117 (25)
PCB52 2,2',5,5´-tetra-	291.98	87 (1,3)	360, c (2,3)	0.030±0.020 (3)
				0.110 (25)
PCB101 2,2',4,5,5'-penta-	326.43	77 (1,3)	381, c (2,3)	0.010±0.010 (3)
				0.00674 (25)
PCB105	326.43			
PCB118 2,3',4,4',5-penta-	326.43	105 (1,3)	381, c (2,3)	
PCB138 2,2',3,4,4',5-hexa-	360.87	79 (1,3)	400, c (2,3)	
PCB153 2,2',4,4',5,5'-hexa-	360.87	103 (1,3)	400, c (2,3)	0.0010±0.00040 (3)
				0.00086 (25)
PCB180 2,2',3,4,4',5,5'-hepta-	395.32			
PAH1 Anthracene	178.21	217.0	340	0.053 (5)
				0.073 (6)
PAH2 Phenanthrene	178.21	100.0	339.0	1.18 (7)
PAH3 Fluoranthene	202.23	111 (16)	375 (16)	0.260 (16)
PAH4 Pyrene	202.23	156 (8)	360.0 (8)	0.135
		150 (9)	404 (9)	
PAH5 Benzo(k)fluoranthene	252.29	217 (34)	481 (34)	0.55 μg/L (18)
				0.0008 (34s)
PAH6 Benzo(a)pyrene	252.29	179, 176 (9)	495 (9)	0.0038
				0.004 (34s)

Compound	M g/mol	MP, °C	BP, °C	S, g/m³ 25°C
DF1 2378-TeCDD	321.966	305 °C (26)	421.2 (34) 446.5 (34)	19.2 20°C (22) 7.91x10⁻⁹ g/L 25°C (26) 0.0193mg/m³ (34s)
DF2 12378-PeCDD	356.413	196	464.7	0.0001
DF3 123478-HxCDD	390.86	273-275 (34)	487.7 (34)	4.4 20°C (22) 0.00442 mg/m³ (34s)
DF4 123678-HxCDD	390.86			
DF5 123789-HxCDD	390.86			
DF6 1234678-HpCDD	425.307	265 (34)	507 (34)	2.4 20°C (22) 0.0024 mg/m³ (34s)
DF7 OCDD	459.754	322 (34)	510 (34)	0.4 20°C (22) 0.000074 mg/m³ (34s)
DF8 2378-TeCDF	305.967	227 (34)	438.3 (34)	0.419 mg/m³ (34s)
DF9 12378-PeCDF	340.414			
DF10 23478-PeCDF	340.414	196 (34)	464.7 (34)	0.236 mg/m³ (34s)
DF11 123789-HxCDF	374.861			
DF12 234678-HxCDF	374.861			
DF13 123678-HxCDF	374.861	232 (34)	487.7 (34)	0.0177 mg/m³ (34s)
DF14 123478-HxCDF	374.861	225.5 (34)	487.7 (34)	0.00825 mg/m³ (34s)
DF15 1234678-HpCDF	409.308	236 (34)	507.2 (34)	0.00135 mg/m³ (34s)
DF16 1234789-HpCDF	409.308	221 (34)	507.2 (34)	
DF 17 OCDF	443.755	258 (34)	537 (34)	0.00116 mg/m³ (34s)

Compound	$\log K_{ow}$	Vapor pressure P(s) , Pa, 25°C
α-HCH	3.8	0.003 (20 °C)
γ-HCH (lindane)	3.85 (10,11,28,29)	8.39×10^{-6} kPa (16)
	3.89 (30)	0.003 Pa 20°C (23)
	4.05 (31)	9.4×10^{-6} mmHg 25°C (32)
		1.9×10^{-5} mmHg 25°C (33)
HCBz	5.47 (17)	0.001 (20 °C)
Oxychlordane		
Trans-chlordane		0.00133
Cis-chlordane		
Trans-nonachlor		
p,p'-DDE	5.7 (23)	3×10^{-6} mmHg (20)
		0.0050 Pa (23)
p,p'-DDT	6.0 (23)	0.00015 Pa (23)
	5.64 (27)	4.3×10^{-7} mmHg (21)
		1.34×10^{-8} kPa (16)
		2.53×10^{-8} kPa 20°C (16)
p,p'-DDD	5.5 (23)	0.00083 Pa (23)
TOX1 Octachlorobornane		0.0005 20°C
TOX2 Nonachlorobornane		0.0001 20°C
PCB28 2,4,4'-trichloro-	5.80±0.20 (3)	0.015
PCB52 2,2',5,5´-tetra-	6.10±0.20 (3)	0.005±0.002 (3) s
PCB101 2,2',4,5,5'-penta-	6.40±0.50 (3)	0.0011±0.0002 (3) s
PCB105		0.00090±0.00005 (3) L
PCB118 2,3',4,4',5-penta-	6.40±0.30 (3)	0.000228 (3) s from P(L)
PCB138 2,2',3,4,4',5-hexa-	7.00±0.50 (3)	0.000145 (3) s from MP
PCB153 2,2',4,4',5,5'-hexa-	6.90±0.20 (3)	0.00012±0.000003 (3) s from P(L)
PCB180 2,2',3,4,4',5,5'-hepta-		0.00013 (3) L
PAH1 Anthracene	4.34-4.54 (10-13)	2.70×10^{-6} (9)
	4.54 (34)	0.001 Pa 25°C (34) s
PAH2 Phenanthrene	4.46-4.52 (10,11,13-15)	1.12×10^{-4} (9)
	4.57 (34)	0.02 Pa 25°C (34) s
PAH3 Fluoranthene	5.22 (8)	1.79×10^{-6} kPa (16)
	5.22 (34)	0.00123 Pa 25°C (34) s
PAH4 Pyrene	4.88-5.03 (10,11,13-15)	2.50×10^{-6} (9)
	5.18 (34)	0.0006 Pa 25° (34) s
PAH5 Benzo(k)fluoranthene	6.00 (34)	5.0×10^{-7} torr 20°C (18)
		5.20×10^{-8} Pa 25°C (34) s
PAH6 Benzo(a)pyrene	6.35 (13)	5.49×10^{-9} (9)
	5.98 (17)	7.00×10^{-7} Pa 25°C (34) s
	6.04 (34)	

Compound	$logK_{OW}$	Vapor pressure P(s) , Pa, 25^0C
DF1 2378-TeCDD	7.02 (22)	2.02×10^{-7} Pa 25^0C (26)
	7.72 (27)	2.00×10^{-7} (34s) s
DF2 12378-PeCDD	7.4	1×10^{-7}
DF3 123478-HxCDD	10.36-10.89, c (4)	5.10×10^{-9} (34s) s
	7.79 (22)	
	9.19 (27)	
DF4 123678-HxCDD		
DF5 123789-HxCDD		
DF6 1234678-HpCDD	11.29-11.90, c (4)	7.50×10^{-10} (34s) s
	8.20 (22)	
DF7 OCDD	12.21-12.97, c (4)	1.10×10^{-10} (34s) s
	10.07 (27)	
	8.60 (22)	
DF8 2378-TeCDF	6.1 (34)	2.00×10^{-6} (34s) s
DF9 12378-PeCDF		
DF10 23478-PeCDF	6.5 (34)	3.50×10^{-7} (34s) s
DF 11 123789-HxCDF		
DF12 234678-HxCDF		
DF13 123678-HxCDF		3.50×10^{-8} (34s) s
DF14 123478-HxCDF	7.0 (34)	3.20×10^{-8} (34s) s
DF15 1234678-HpCDF	7.4 (34)	4.70×10^{-9} (34s) s
DF16 1234789-HpCDF		6.20×10^{-9} (34s) s
DF17 OCDF	13.06-13.78, c (4)	5.0×10^{-10} (34s) s
	8.0 (34)	

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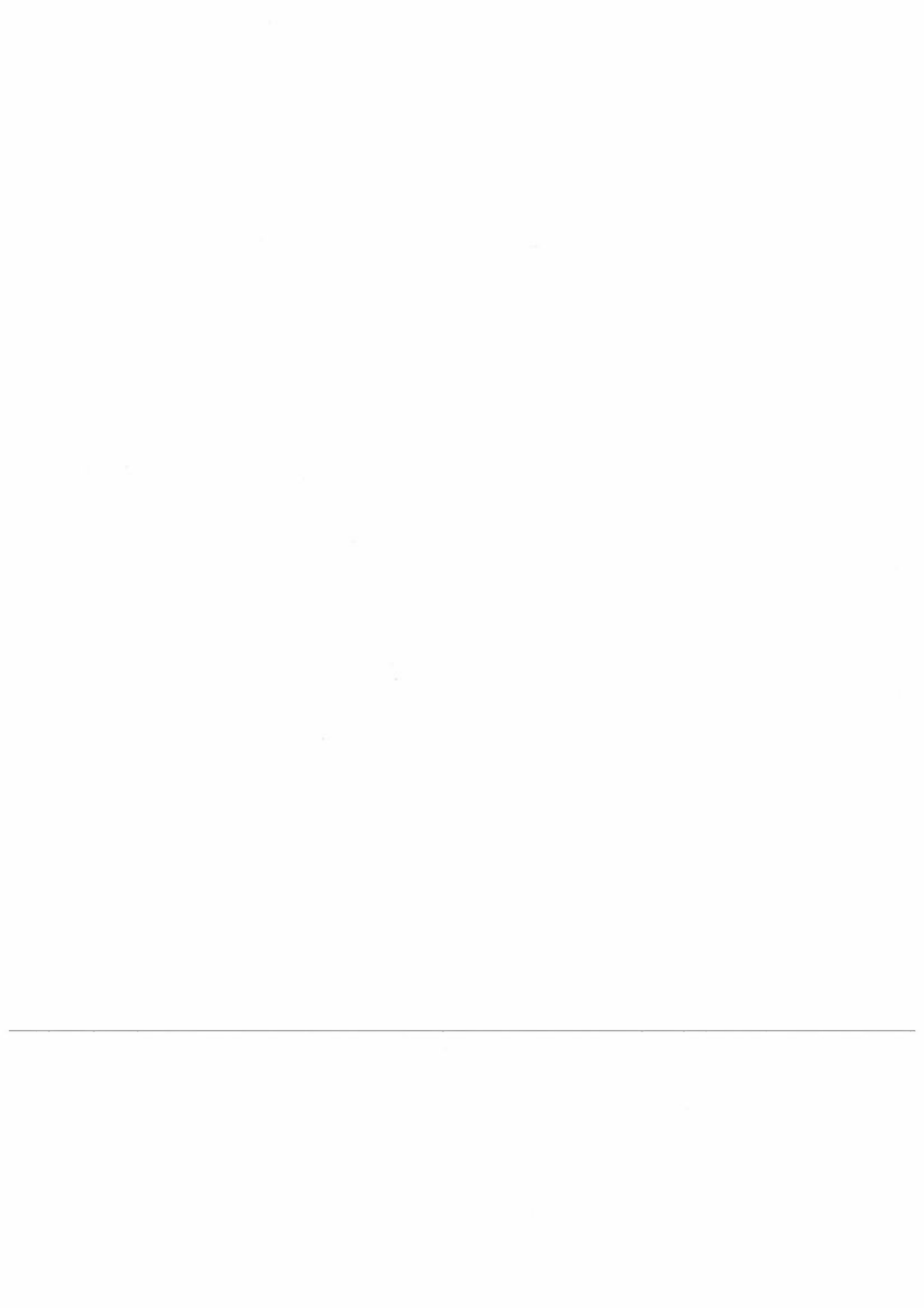
Annex 4

Results of the model estimates for hexachlorobenzene, lindane, and fluoranthene
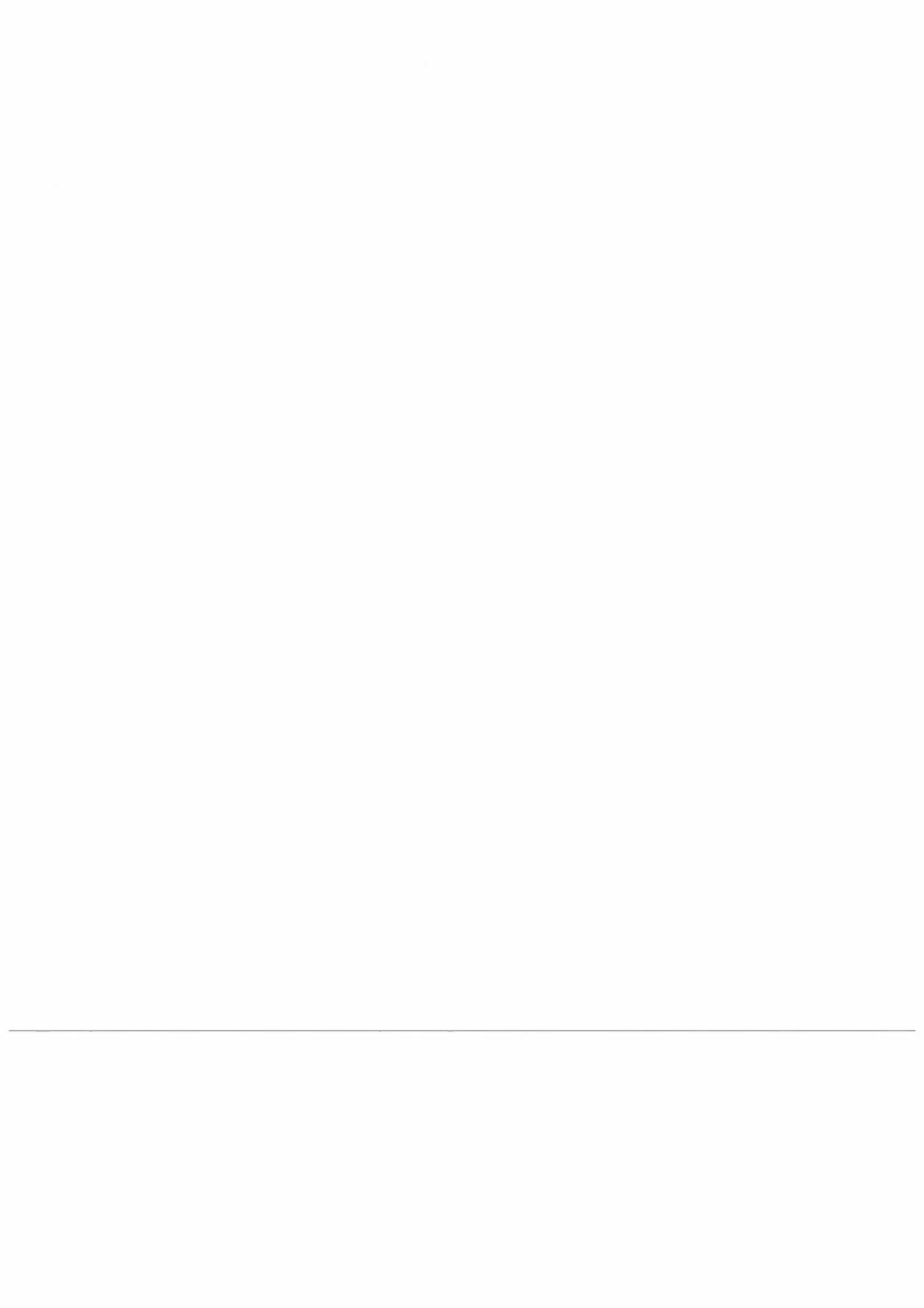
SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Danmark environment

Properties of Fluoranthene :

Temperature deg C	7.5
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	8.175221E-02
Vapor pressure Pa	1.697829E-04
Sub-cooled liquid vapor press Pa	2.076799E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	.1320584
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	5.65967E-05
Soil-water partition coefficient	3266.065
Sedt-water partition coefficient	6259.958
Susp sedt-water partn coeffnt	20412.9
Aerosol-air partition coeff	2.889062E+09
Aerosol Z value	1238174
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	4.645883E-09
Total of VZ products	1.064354E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.3E+13	1.224E+10	4.240001E+09
Density kg/m3	1.25933	1000	2400
Depth m	1000	20	.1
Area m2	4.3E+10	6.12E+08	4.24E+10
Frn org carb			.02
Z mol/m3.Pa	4.285731E-04	7.572405	24731.96
VZ mol/Pa	1.842864E+10	9.268624E+10	1.048635E+14
Fugacity Pa	4.645883E-09	4.645883E-09	4.645883E-09
Conc mol/m3	1.991101E-12	3.518051E-08	1.149018E-04
Conc g/m3	4.026603E-10	7.114554E-06	2.323659E-02
Conc ug/g	3.197417E-07	7.114554E-06	9.681914E-03
Amount mol	85.61732	430.6095	487183.7
Amount kg	17.31439	87.08214	98523.16
Amount %	1.731439E-02	8.708215E-02	98.52316

Phase	Sediment	Susp sedt	Fish
Volume m3	3.06E+07	61200	12240
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	6.12E+08	0	0
Frn org carb	.04	.2	
Z mol/m3.Pa	47402.94	154574.8	62835.28
VZ mol/Pa	1.45053E+12	9.459976E+09	7.691038E+08
Fugacity Pa	4.645883E-09	4.645883E-09	4.645883E-09
Conc mol/m3	2.202285E-04	7.181364E-04	2.919254E-04
Conc g/m3	4.453681E-02	.1452287	5.903607E-02
Conc ug/g	1.936383E-02	9.681914E-02	5.903607E-02

```
      FLNORDM
        58
Amount mol      6738.992        43.94995        3.573166
Amount kg       1362.826        8.887998        .7226015
Amount %        1.362826        8.887997E-03    7.226015E-04


SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Danmark environment

Emission rate of chemical mol/h    21.26292
Emission rate of chemical  kg/h    4.3
Fugacity Pa                        1.290649E-08
Total amount of chemical mol       1373707
Total amount of chemical kg        277804.8

Phase properties,compositions and rates

Phase            Air             Water           Soil
Adv.flow m3/h    4.3E+11         1.224E+07       0
Adv.restime h    100             1000            0
Rct halflife h   17000           55000           55000
Rct rate c.h-1   4.076471E-05    .0000126        .0000126
Fugacity Pa      1.290649E-08    1.290649E-08    1.290649E-08
Conc mol/m3      5.531374E-12    9.773316E-08    3.192028E-04
Conc g/m3        1.11861E-09     1.976458E-05    6.455238E-02
Conc ug/g        8.882579E-07    1.976458E-05    2.689682E-02
Amount mol       237.8491        1196.254        1353420
Amount kg        48.10022        241.9184        273702.1
Amount %         1.731439E-02    8.708215E-02    98.52316
D rct mol/Pa.h   751238.3        1167847         1.321281E+09
D adv mol/Pa.h   1.842865E+08    9.268623E+07    0
Rct rate mol/h   9.695849E-03    .0150728        17.05309
Adv rate mol/h   2.378491        1.196254        0
Rct rate kg/h    1.960791E-03    3.048172E-03    3.448647
Adv rate kg/h    .4810022        .2419184        0
Reaction %       4.559981E-02    7.088773E-02    80.20109
Advection %      11.1861         5.62601         0

Phase            Sediment        Susp sedt       Fish
Adv.flow m3/h    612
Adv.restime h    50000
Rct halflife h   55000
Rct rate c.h-1   .0000126
Fugacity Pa      1.290649E-08    1.290649E-08    1.290649E-08
Conc mol/m3      6.118054E-04    1.995018E-03    8.109828E-04
Conc g/m3        .1237254        .4034524        .164005
Conc ug/g        5.379366E-02    .2689683        .164005
Amount mol       18721.25        122.0951        9.926429
Amount kg        3785.998        24.69129        2.007422
Amount %         1.362827        8.887998E-03    7.226015E-04
D rct mol/Pa.h   1.827668E+07
D adv mol/Pa.h   2.90106E+07
Rct rate mol/h   .2358877
Adv rate mol/h   .3744249
Rct rate kg/h    4.770357E-02
Adv rate kg/h    7.571995E-02
Reaction %       1.109386
Advection %      1.760929

Total advection D value        3.059833E+08
Total reaction D value         1.341476E+09
Total D value                  1.64746E+09
Output by reaction      mol/h  17.31375
Output by advection     mol/h  3.94917
```

Total output by reaction and advection mol/h   21.26292
Output by reaction   kg/h   3.501359
Output by advection   kg/h   .7986406
Total output by reaction and advection kg/h   4.3

Overall residence time   h   64605.78
Reaction residence time   h   79342
Advection residence time h   347847.1

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Danmark environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.3E+13	1.224E+10	7.632E+09
Density kg/m3	1.25933	1000.009	1500.252
Bulk Z value	4.533366E-04	8.408114	12368.25
Bulk VZ	1.949347E+10	1.029153E+11	9.439451E+13
Emission mol/h	14.8346	1.977946	0
Emission kg/h	3	.4	0
Fugacity Pa	5.609315E-08	1.479033E-08	3.084239E-09
Conc mol/m3	2.542908E-11	1.243588E-07	3.814664E-05
Conc g/m3	5.142522E-09	2.514907E-05	7.714395E-03
Conc ug/g	4.083538E-06	2.514886E-05	5.142067E-03
Amount mol	1093.45	1522.151	291135.2
Amount kg	221.1284	307.8246	58876.26
Amount %	.3494717	.4864865	93.04812
Adv.flow m3/h	4.3E+11	1.224E+07	0
D rct mol/Pa.h	794645.8	1296733	1.189371E+09
D adv mol/Pa.h	1.949348E+08	1.029153E+08	0
Rct rate mol/h	4.457418E-02	.0191791	3.668303
Rct rate kg/h	9.014237E-03	3.87859E-03	.741841
Adv rate mol/h	10.9345	1.522151	0
Adv rate kg/h	2.211285	.3078246	0
Reaction %	.2651246	.1140762	21.81885
Advection %	65.03778	9.053665	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.53E+08		
Density kg/m3	1260		
Bulk Z value	9486.644		0
Bulk VZ	1.451457E+12	0	
Emission mol/h	0	16.81254	
Emission kg/h	0	3.4	
Fugacity Pa	1.318393E-08		1.479033E-08
Conc mol/m3	1.250713E-04		9.293542E-04
Conc g/m3	2.529316E-02		.1879433
Conc ug/g	2.007394E-02		.1879433
Amount mol	19135.9	312886.7	
Amount kg	3869.854	63275.07	
Amount %	6.115922		
Adv.flow m3/h	3060		
D rct mol/Pa.h	1.828835E+07		
D adv mol/Pa.h	2.902913E+07		
Rct rate mol/h	.2411124	3.973169	
Rct rate kg/h	4.876015E-02	0	
Adv rate mol/h	.382718	12.83937	
Adv rate kg/h	7.739706E-02	2.596506	

```
        FLNORDM
        60
Reaction %      1.434122
Advection %     2.276384

Overall residence time    h    18610.31
Reaction residence time   h    78749.9
Advection residence time  h    24369.31
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 2.5207E-02	6.0793E+03	4.9017E+09	2.2221E+06	1.2465E-01
Air to soil 7.6054E-01	2.0149E+02	1.4789E+11	6.7045E+07	3.7608E+00
Water to air 3.9005E-03	5.4691E+04	1.5509E+05	1.3041E+06	1.9287E-02
Water to sediment 1.4286E-01	1.4932E+03	5.6806E+06	4.7763E+07	7.0644E-01
Soil to air 2.1449E-03	1.9022E+07	2.7804E+02	3.4389E+06	1.0606E-02
Soil to water 1.6554E-02	2.4648E+06	2.1458E+03	2.6540E+07	8.1855E-02
Sediment to water 1.6705E-02	1.6054E+05	6.6046E+02	6.2656E+06	8.2605E-02

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

```
Individual process D values
Air-water diffusion (air-side)   1311434          Air-water diffusion
(water-side)   2.317156E+08
Air-water diffusion (overall)      1304053
Rain dissolution to water          463431.2       Aerosol deposition to
water          454657.6
Rain dissolution to soil           3.2107E+07     Aerosol deposition to
soil          3.149915E+07
Soil-air diffusion (air-phase)     363430         Soil-air diffusion
(water-phase)   3210700
Soil-air diffusion (bndry layer)   9.085751E+07   Soil-air diffusion
(overall)       3438853
Water-sediment diffusion           463431.2
Water-sediment deposition          4.729989E+07   Sediment-water
resuspension    5802119
Soil-water runoff (water)          1.60535E+07    Soil-water runoff
(solids)       1.048635E+07
```

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Finland environment

Properties of Fluoranthene :

Temperature deg C	2
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	6.789166E-02
Vapor pressure Pa	8.531027E-05
Sub-cooled liquid vapor press Pa	1.256565E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	6.635498E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	2.900641E-05
Soil-water partition coefficient	8165.162
Sedt-water partition coefficient	12519.92
Susp sedt-water partn coeffnt	30619.36
Aerosol-air partition coeff	4.774923E+09
Aerosol Z value	2087309
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	1.21713E-10
Total of VZ products	4.062725E+15

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.37E+14	6.32E+11	3.05E+10
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.37E+11	3.16E+10	3.05E+11
Frn org carb			.05
Z mol/m3.Pa	4.371399E-04	15.07046	123052.7
VZ mol/Pa	1.473162E+11	9.524531E+12	3.753108E+15
Fugacity Pa	1.21713E-10	1.21713E-10	1.21713E-10
Conc mol/m3	5.320562E-14	1.834271E-09	1.497712E-05
Conc g/m3	1.075977E-11	3.709446E-07	3.028823E-03
Conc ug/g	8.376605E-09	3.709446E-07	1.26201E-03
Amount mol	17.93029	1159.259	456802.2
Amount kg	3.626043	234.437	92379.09
Amount %	3.626043E-03	.234437	92.37909

Phase	Sediment	Susp sedt	Fish
Volume m3	1.58E+09	3792000	632000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.16E+10	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	188680.9	461447.8	125053.6
VZ mol/Pa	2.981158E+14	1.74981E+12	7.903387E+10
Fugacity Pa	1.21713E-10	1.21713E-10	1.21713E-10
Conc mol/m3	2.296492E-05	5.61642E-05	1.522065E-05
Conc g/m3	4.644195E-03	1.135809E-02	3.078072E-03
Conc ug/g	2.019215E-03	7.572057E-03	3.078072E-03
Amount mol	36284.57	212.9747	9.619449

```
      FLNORDM
       62
Amount kg        7337.828          43.06987        1.945341
Amount %         7.337827          4.306987E-02    1.945341E-03


SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Finland environment

Emission rate of chemical mol/h      168.1254
Emission rate of chemical  kg/h      34
Fugacity Pa                          2.467663E-09
Total amount of chemical mol         1.002543E+07
Total amount of chemical kg          2027443

Phase properties,compositions and rates

Phase              Air             Water            Soil
Adv.flow m3/h      3.37E+12        6.32E+08         0
Adv.restime h      100             1000             0
Rct halflife h     17000           55000            55000
Rct rate c.h-1     4.076471E-05    .0000126         .0000126
Fugacity Pa        2.467663E-09    2.467663E-09     2.467663E-09
Conc mol/m3        1.078714E-12    3.718881E-08     3.036526E-04
Conc g/m3          2.181483E-10    7.520692E-06     6.140767E-02
Conc ug/g          1.698309E-07    7.520692E-06     2.558653E-02
Amount mol         363.5266        23503.33         9261404
Amount kg          73.51597        4753.078         1872934
Amount %           3.626044E-03    .234437          92.3791
D rct mol/Pa.h     6005300         1.200091E+08     4.728917E+10
D adv mol/Pa.h     1.473162E+09    9.524529E+09     0
Rct rate mol/h     1.481905E-02    .2961419         116.6937
Adv rate mol/h     3.635265        23.50333         0
Rct rate kg/h      2.996857E-03    5.988878E-02     23.59897
Adv rate kg/h      .7351597        4.753077         0
Reaction %         8.814286E-03    .1761435         69.40873
Advection %        2.162235        13.97964         0

Phase              Sediment        Susp sedt        Fish
Adv.flow m3/h      31600
Adv.restime h      50000
Rct halflife h     55000
Rct rate c.h-1     .0000126
Fugacity Pa        2.467663E-09    2.467663E-09     2.467663E-09
Conc mol/m3        4.656007E-04    1.138697E-03     3.085901E-04
Conc g/m3          9.415842E-02    .2302788         6.240616E-02
Conc ug/g          4.093845E-02    .1535192         6.240616E-02
Amount mol         735649.1        4317.941         195.0289
Amount kg          148770.3        873.2172         39.4407
Amount %           7.337829        4.306987E-02     1.945342E-03
D rct mol/Pa.h     3.756259E+09
D adv mol/Pa.h     5.962316E+09
Rct rate mol/h     9.269179
Adv rate mol/h     14.71298
Rct rate kg/h      1.874506
Adv rate kg/h      2.975406
Reaction %         5.513253
Advection %        8.751196

Total advection D value       1.696001E+10
Total reaction D value        5.117144E+10
Total D value                 6.813145E+10
Output by reaction     mol/h  126.2738
Output by advection    mol/h  41.85157
Total output by reaction and advection mol/h   168.1254
```

Output by reaction   kg/h   25.53636
Output by advection   kg/h   8.463643
Total output by reaction and advection kg/h   34

Overall residence time   h   59630.69
Reaction residence time   h   79394.38
Advection residence time h   239547.4

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Finland environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.37E+14	6.32E+11	5.49E+10
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.788861E-04	17.50275	61530.89
Bulk VZ	1.613846E+11	1.106174E+13	3.378046E+15
Emission mol/h	54.39352	93.95243	9.889729
Emission kg/h	11	19	2
Fugacity Pa	2.057604E-08	5.518928E-09	6.511729E-10
Conc mol/m3	9.853579E-12	9.659642E-08	4.006724E-05
Conc g/m3	1.992689E-09	1.953469E-05	8.102799E-03
Conc ug/g	1.551331E-06	1.953453E-05	5.400941E-03
Amount mol	3320.656	61048.94	2199692
Amount kg	671.5363	12345.93	444843.6
Amount %	9.486531E-02	1.744061	62.84132
Adv.flow m3/h	3.37E+12	6.32E+08	0
D rct mol/Pa.h	6578797	1.393779E+08	4.256338E+10
D adv mol/Pa.h	1.613846E+09	1.106174E+10	0
Rct rate mol/h	.1353656	.7692166	27.71612
Rct rate kg/h	2.737498E-02	.1555587	5.60503
Adv rate mol/h	33.20656	61.04894	0
Adv rate kg/h	6.715363	12.34593	0
Reaction %	8.295448E-02	.4713899	16.98494
Advection %	20.34959	37.4119	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	7.900001E+09		
Density kg/m3	1260		
Bulk Z value	37748.23		0
Bulk VZ	2.98211E+14	0	
Emission mol/h	4.944865	163.1805	
Emission kg/h	1	33	
Fugacity Pa	4.145821E-09		5.518928E-09
Conc mol/m3	1.564974E-04		6.901617E-04
Conc g/m3	3.164847E-02		.1395714
Conc ug/g	2.511783E-02		.1395714
Amount mol	1236330	3500391	
Amount kg	250022.9	707884	
Amount %	35.31976		
Adv.flow m3/h	158000		
D rct mol/Pa.h	3.757459E+09		
D adv mol/Pa.h	5.96422E+09		
Rct rate mol/h	15.57775	44.19845	
Rct rate kg/h	3.150288	0	
Adv rate mol/h	24.72659	118.9821	
Adv rate kg/h	5.000458	24.06175	
Reaction %	9.546329		

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        64
Advection %      15.1529

Overall residence time    h    21451.03
Reaction residence time   h    79197.13
Advection residence time  h    29419.48
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 6.4941E-01	7.1662E+02	3.2589E+11	1.5607E+08	3.2112E+00
Air to soil 3.6907E+00	1.2609E+02	1.8521E+12	8.8695E+08	1.8250E+01
Water to air 7.6863E-02	1.1131E+05	3.9347E+06	6.8868E+07	3.8008E-01
Water to sediment 8.1904E+00	1.0446E+03	4.1928E+08	7.3385E+09	4.0501E+01
Soil to air 5.9687E-03	5.1649E+07	7.3662E+02	4.5325E+07	2.9514E-02
Soil to water 7.9688E-02	3.8685E+06	9.8347E+03	6.0514E+08	3.9405E-01
Sediment to water 1.0397E+00	1.6665E+05	3.2851E+04	1.2401E+09	5.1412E+00

Transport velocity parameters		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

```
Individual process D values
Air-water diffusion (air-side)  6.906811E+07      Air-water diffusion
(water-side)   2.381133E+10
Air-water diffusion (overall)      6.886835E+07
Rain dissolution to water          4.762265E+07    Aerosol deposition to
water         3.957539E+07
Rain dissolution to soil           4.59649E+08     Aerosol deposition to
soil          3.819776E+08
Soil-air diffusion (air-phase)     2666553         Soil-air diffusion
(water-phase)   4.59649E+07
Soil-air diffusion (bndry layer)   6.666383E+08    Soil-air diffusion
(overall)       4.532498E+07
Water-sediment diffusion           4.762265E+07
Water-sediment deposition          7.290875E+09    Sediment-water
resuspension      1.192463E+09
Soil-water runoff (water)          2.298245E+08    Soil-water runoff
(solids)        3.753108E+08
```

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Sweden environment

Properties of Fluoranthene :

Temperature deg C	4
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	7.269867E-02
Vapor pressure Pa	1.099162E-04
Sub-cooled liquid vapor press Pa	1.511943E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	8.549368E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	3.7103E-05
Soil-water partition coefficient	6532.129
Sedt-water partition coefficient	9389.936
Susp sedt-water partn coeffnt	25516.13
Aerosol-air partition coeff	3.968404E+09
Aerosol Z value	1722229
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	1.470671E-10
Total of VZ products	3.36232E+15

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+14	7.7E+11	4.11E+10
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+11	3.85E+10	4.11E+11
Frn org carb			.04
Z mol/m3.Pa	4.339854E-04	11.69677	76404.82
VZ mol/Pa	1.952934E+11	9.006515E+12	3.140238E+15
Fugacity Pa	1.470671E-10	1.470671E-10	1.470671E-10
Conc mol/m3	6.382495E-14	1.72021E-09	1.123663E-05
Conc g/m3	1.290732E-11	3.47878E-07	2.272384E-03
Conc ug/g	1.012154E-08	3.47878E-07	9.468267E-04
Amount mol	28.72123	1324.562	461825.6
Amount kg	5.808294	267.8661	93394.99
Amount %	5.808294E-03	.2678661	93.39498

Phase	Sediment	Susp sedt	Fish
Volume m3	1.925E+09	4620001	770000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.85E+10	0	0
Frn org carb	.06	.25	
Z mol/m3.Pa	109831.9	298456.3	97058.98
VZ mol/Pa	2.114265E+14	1.378868E+12	7.473541E+10
Fugacity Pa	1.470671E-10	1.470671E-10	1.470671E-10
Conc mol/m3	1.615266E-05	4.389309E-05	1.427418E-05
Conc g/m3	3.266552E-03	.0088765	2.886667E-03
Conc ug/g	1.42024E-03	5.917666E-03	2.886667E-03
Amount mol	31093.87	202.7861	10.99112
Amount kg	6288.113	41.00943	2.222734

Amount %   6.288113   4.100943E-02   2.222734E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Sweden environment

Emission rate of chemical mol/h   222.5189
Emission rate of chemical kg/h   45
Fugacity Pa   3.867178E-09
Total amount of chemical mol   1.300269E+07
Total amount of chemical kg   2629534

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+12	7.7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	3.867178E-09	3.867178E-09	3.867178E-09
Conc mol/m3	1.678299E-12	4.52335E-08	2.95471E-04
Conc g/m3	3.394023E-10	9.147569E-06	5.975311E-02
Conc ug/g	2.661492E-07	9.147569E-06	2.489713E-02
Amount mol	755.2344	34829.79	1.214386E+07
Amount kg	152.7311	7043.629	2455853
Amount %	5.808294E-03	.2678661	93.39498
D rct mol/Pa.h	7961079	1.134821E+08	3.9567E+10
D adv mol/Pa.h	1.952934E+09	9.006514E+09	0
Rct rate mol/h	3.078691E-02	.4388554	153.0126
Adv rate mol/h	7.552344	34.82979	0
Rct rate kg/h	6.226036E-03	8.874972E-02	30.94375
Adv rate kg/h	1.52731	7.043629	0
Reaction %	1.383564E-02	.1972216	68.76387
Advection %	3.394023	15.65251	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	38500		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	3.867178E-09	3.867178E-09	3.867178E-09
Conc mol/m3	4.247396E-04	1.154184E-03	3.753443E-04
Conc g/m3	8.589509E-02	.2334106	7.590588E-02
Conc ug/g	3.734569E-02	.155607	7.590588E-02
Amount mol	817623.8	5332.329	289.0151
Amount kg	165348.1	1078.357	58.44753
Amount %	6.288113	4.100943E-02	2.222733E-03
D rct mol/Pa.h	2.663974E+09		
D adv mol/Pa.h	4.22853E+09		
Rct rate mol/h	10.30206		
Adv rate mol/h	16.35247		
Rct rate kg/h	2.083385		
Adv rate kg/h	3.306961		
Reaction %	4.629745		
Advection %	7.348801		

Total advection D value   1.518798E+10
Total reaction D value   4.235242E+10
Total D value   5.75404E+10
Output by reaction   mol/h   163.7843
Output by advection   mol/h   58.73461
Total output by reaction and advection mol/h   222.5189
Output by reaction   kg/h   33.12211

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Output by advection   kg/h   11.8779
Total output by reaction and advection kg/h   45.00001

Overall residence time   h   58434.08
Reaction residence time   h   79389.09
Advection residence time h   221380.4

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Sweden environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+14	7.7E+11	7.398E+10
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.6843E-04	13.28611	38205.92
Bulk VZ	2.107935E+11	1.023031E+13	2.826474E+15
Emission mol/h	138.4562	74.17298	24.72433
Emission kg/h	28	15	5
Fugacity Pa	4.291214E-08	5.291446E-09	1.813341E-09
Conc mol/m3	2.010133E-11	7.030274E-08	6.928037E-05
Conc g/m3	4.065092E-09	1.421732E-05	1.401057E-02
Conc ug/g	3.187724E-06	1.42172E-05	9.338791E-03
Amount mol	9045.599	54133.11	5125362
Amount kg	1829.291	10947.34	1036502
Amount %	.1502374	.8990909	85.12656
Adv.flow m3/h	4.5E+12	7.7E+08	0
D rct mol/Pa.h	8592934	1.289019E+08	3.561357E+10
D adv mol/Pa.h	2.107935E+09	1.023031E+10	0
Rct rate mol/h	.3687412	.6820773	64.57956
Rct rate kg/h	7.457052E-02	.1379365	13.05992
Adv rate mol/h	90.45599	54.13311	0
Adv rate kg/h	18.29291	10.94734	0
Reaction %	.1553553	.2873677	27.20818
Advection %	38.11024	22.80696	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	9.625E+09		
Density kg/m3	1260		
Bulk Z value	21975.75		0
Bulk VZ	2.115165E+14	0	
Emission mol/h	0	237.3535	
Emission kg/h	0	48	
Fugacity Pa	3.935069E-09		5.291446E-09
Conc mol/m3	8.647607E-05		5.135823E-04
Conc g/m3	1.748806E-02		.1038617
Conc ug/g	1.387941E-02		.1038617
Amount mol	832332.1	6020872	
Amount kg	168322.5	1217601	
Amount %	13.82411		
Adv.flow m3/h	192500		
D rct mol/Pa.h	2.665109E+09		
D adv mol/Pa.h	4.230331E+09		
Rct rate mol/h	10.48739	76.11777	
Rct rate kg/h	2.120864	0	
Adv rate mol/h	16.64664	161.2358	
Adv rate kg/h	3.36645	32.60671	
Reaction %	4.418467		
Advection %	7.013438		

Overall residence time   h   25366.69
Reaction residence time   h   79099.43
Advection residence time h   37342.04

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 1.4584E+00	8.6927E+02	3.5875E+11	1.6805E+08	7.2114E+00
Air to soil 8.2811E+00	1.5308E+02	2.0371E+12	9.5425E+08	4.0949E+01
Water to air 8.9067E-02	8.5177E+04	6.2647E+06	8.3233E+07	4.4042E-01
Water to sediment 6.1962E+00	1.2244E+03	4.3582E+08	5.7903E+09	3.0639E+01
Soil to air 1.7901E-02	4.0126E+07	1.2777E+03	4.8815E+07	8.8517E-02
Soil to water 2.0330E-01	3.5331E+06	1.4511E+04	5.5439E+08	1.0053E+00
Sediment to water 7.0884E-01	1.6456E+05	4.0533E+04	8.9074E+08	3.5051E+00

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   8.35422E+07   Air-water diffusion
(water-side)   2.251629E+10
Air-water diffusion (overall)   8.323338E+07
Rain dissolution to water   4.503257E+07   Aerosol deposition to
water   3.97835E+07
Rain dissolution to soil   4.807373E+08   Aerosol deposition to
soil   4.247018E+08
Soil-air diffusion (air-phase)   3567360   Soil-air diffusion
(water-phase)   4.807373E+07
Soil-air diffusion (bndry layer)   8.918399E+08   Soil-air diffusion
(overall)   4.881454E+07
Water-sediment diffusion   4.503257E+07
Water-sediment deposition   5.745284E+09   Sediment-water
resuspension   8.457059E+08
Soil-water runoff (water)   2.403687E+08   Soil-water runoff
(solids)   3.140238E+08

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Fate of Fluoranthene at Norway environment

Properties of Fluoranthene :

Temperature deg C	5
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	7.520058E-02
Vapor pressure Pa	1.245946E-04
Sub-cooled liquid vapor press Pa	1.656831E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	9.691066E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	4.190661E-05
Soil-water partition coefficient	8165.162
Sedt-water partition coefficient	12519.92
Susp sedt-water partn coeffnt	30619.36
Aerosol-air partition coeff	3.621372E+09
Aerosol Z value	1565972
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	1.817039E-10
Total of VZ products	2.721387E+15

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.24E+14	1E+11	3.19E+10
Density kg/m3	1.270649	1000	2400
Depth m	1000	20	.1
Area m2	3.24E+11	5E+09	3.19E+11
Frn org carb			.05
Z mol/m3.Pa	4.324251E-04	10.31878	84254.52
VZ mol/Pa	1.401057E+11	1.031878E+12	2.687719E+15
Fugacity Pa	1.817039E-10	1.817039E-10	1.817039E-10
Conc mol/m3	7.857331E-14	1.874962E-09	1.530937E-05
Conc g/m3	1.588988E-11	3.791736E-07	3.096014E-03
Conc ug/g	1.250533E-08	3.791736E-07	1.290006E-03
Amount mol	25.45775	187.4962	488369
Amount kg	5.148321	37.91736	98762.85
Amount %	5.148321E-03	3.791736E-02	98.76284

Phase	Sediment	Susp sedt	Fish
Volume m3	2.5E+08	600000	100000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	5E+09	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	129190.3	315954.5	85624.52
VZ mol/Pa	3.229757E+13	1.895727E+11	8.562451E+09
Fugacity Pa	1.817039E-10	1.817039E-10	1.817039E-10
Conc mol/m3	2.347437E-05	5.741015E-05	1.555831E-05
Conc g/m3	4.747222E-03	1.161006E-02	3.146356E-03
Conc ug/g	2.064009E-03	7.740036E-03	3.146356E-03
Amount mol	5868.593	34.44609	1.555831
Amount kg	1186.806	6.966033	.3146356

Amount %   1.186805   6.966033E-03 3.146356E-04

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Norway environment

Emission rate of chemical mol/h	158.2357
Emission rate of chemical kg/h	32
Fugacity Pa	4.234318E-09
Total amount of chemical mol	1.152322E+07
Total amount of chemical kg	2330340

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.24E+12	1E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.234318E-09	4.234318E-09	4.234318E-09
Conc mol/m3	1.831026E-12	4.369301E-08	3.567605E-04
Conc g/m3	3.702883E-10	8.836037E-06	7.214767E-02
Conc ug/g	2.914168E-07	8.836037E-06	3.006153E-02
Amount mol	593.2523	4369.301	1.138066E+07
Amount kg	119.9734	883.6037	2301511
Amount %	5.148321E-03	3.791737E-02	98.76285
D rct mol/Pa.h	5711369	1.300167E+07	3.386526E+10
D adv mol/Pa.h	1.401057E+09	1.031878E+09	0
Rct rate mol/h	2.418376E-02	.0550532	143.3963
Adv rate mol/h	5.932523	4.369301	0
Rct rate kg/h	4.890681E-03	1.113341E-02	28.99903
Adv rate kg/h	1.199734	.8836037	0
Reaction %	1.528338E-02	.0347919	90.62197
Advection %	3.749169	2.761261	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	5000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.234318E-09	4.234318E-09	4.234318E-09
Conc mol/m3	5.470328E-04	1.337852E-03	3.625614E-04
Conc g/m3	.1106264	.2705538	.0733208
Conc ug/g	4.809845E-02	.1803692	.0733208
Amount mol	136758.2	802.7111	36.25614
Amount kg	27656.61	162.3323	7.332079
Amount %	1.186806	6.966033E-03	3.146356E-04
D rct mol/Pa.h	4.069494E+08		
D adv mol/Pa.h	6.459514E+08		
Rct rate mol/h	1.723153		
Adv rate mol/h	2.735164		
Rct rate kg/h	.3484733		
Adv rate kg/h	.5531321		
Reaction %	1.088979		
Advection %	1.728538		

Total advection D value	3.078887E+09
Total reaction D value	3.429092E+10
Total D value	3.736981E+10
Output by reaction mol/h	145.1987
Output by advection mol/h	13.03699
Total output by reaction and advection mol/h	158.2357
Output by reaction kg/h	29.36353

Output by advection   kg/h   2.63647
Total output by reaction and advection kg/h   32

Overall residence time   h   72823.13
Reaction residence time   h   79361.72
Advection residence time h   883886.6

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Norway environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.24E+14	1E+11	5.742E+10
Density kg/m3	1.270649	1000.009	1500.254
Bulk Z value	4.637446E-04	11.98418	42130.36
Bulk VZ	1.502532E+11	1.198418E+12	2.419125E+15
Emission mol/h	71.70054	19.77946	9.889729
Emission kg/h	14.5	4	2
Fugacity Pa	3.277765E-08	1.083148E-08	1.021554E-09
Conc mol/m3	1.520046E-11	1.298064E-07	4.303845E-05
Conc g/m3	3.073988E-09	2.625076E-05	8.703666E-03
Conc ug/g	2.419227E-06	2.625053E-05	5.801461E-03
Amount mol	4924.948	12980.64	2471268
Amount kg	995.9721	2625.076	499764.5
Amount %	.1808351	.4766256	90.74045
Adv.flow m3/h	3.24E+12	1E+08	0
D rct mol/Pa.h	6125029	1.510006E+07	3.048098E+10
D adv mol/Pa.h	1.502532E+09	1.198418E+09	0
Rct rate mol/h	.200764	.1635561	31.13797
Rct rate kg/h	4.060051E-02	3.307595E-02	6.297032
Adv rate mol/h	49.24948	12.98064	0
Adv rate kg/h	9.959721	2.625075	0
Reaction %	.1980513	.1613461	30.71723
Advection %	48.58401	12.80525	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.25E+09		
Density kg/m3	1260		
Bulk Z value	25846.31		0
Bulk VZ	3.230789E+13	0	
Emission mol/h	0	101.3697	
Emission kg/h	0	20.5	
Fugacity Pa	7.25128E-09		1.083148E-08
Conc mol/m3	1.874188E-04		9.274406E-04
Conc g/m3	3.790171E-02		.1875563
Conc ug/g	3.008072E-02		.1875563
Amount mol	234273.5	2723447	
Amount kg	47377.14	550762.6	
Amount %	8.602096		
Adv.flow m3/h	25000		
D rct mol/Pa.h	4.070794E+08		
D adv mol/Pa.h	6.461578E+08		
Rct rate mol/h	2.951847	34.45414	
Rct rate kg/h	.596952	0	
Adv rate mol/h	4.685471	66.91559	
Adv rate kg/h	.9475428	13.53234	
Reaction %	2.911961		
Advection %	4.62216		

Overall residence time   h   26866.47
Reaction residence time   h   79045.56
Advection residence time h   40699.74

Intermedia Data. transport	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h kg/h
Air to water	5.0490E+03	4.4470E+10	2.0623E+07	6.7597E-01 1.3670E-01
Air to soil	1.5710E+02	1.4293E+12	6.6282E+08	2.1726E+01 4.3936E+00
Water to air	7.7145E+04	8.9831E+05	1.0766E+07	1.1661E-01 2.3581E-02
Water to sediment	1.0446E+03	6.6341E+07	7.9505E+08	8.6115E+00 1.7415E+00
Soil to air	4.9422E+07	8.0515E+02	3.3921E+07	3.4652E-02 7.0077E-03
Soil to water	3.8685E+06	1.0286E+04	4.3336E+08	4.4270E-01 8.9527E-02
Sediment to water	1.6665E+05	5.1980E+03	1.3435E+08	9.7421E-01 1.9701E-01

Transport velocity parameters		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   1.081063E+07   Air-water diffusion
(water-side) 2.579695E+09
Air-water diffusion (overall)   1.076551E+07
Rain dissolution to water   5159391   Aerosol deposition to
water   4697916
Rain dissolution to soil   3.291691E+08 Aerosol deposition to
soil   2.997271E+08
Soil-air diffusion (air-phase)   2758872   Soil-air diffusion
(water-phase) 3.291691E+07
Soil-air diffusion (bndry layer) 6.89718E+08   Soil-air diffusion
(overall)   3.392121E+07
Water-sediment diffusion   5159391
Water-sediment deposition   7.898863E+08 Sediment-water
resuspension   1.291903E+08
Soil-water runoff (water)   1.645846E+08 Soil-water runoff
(solids)   2.687719E+08

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Fate of Fluoranthene at Nordic Sea areas environment

Properties of Fluoranthene :

Temperature deg C	6
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	.0777697
Vapor pressure Pa	1.411061E-04
Sub-cooled liquid vapor press Pa	1.81441E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	.1097534
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	4.729013E-05
Soil-water partition coefficient	4899.097
Sedt-water partition coefficient	7824.946
Susp sedt-water partn coeffnt	40825.81
Aerosol-air partition coeff	3.30686E+09
Aerosol Z value	1424847
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	8.289737E-09
Total of VZ products	5.965045E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.5E+14	7E+11	3E+07
Density kg/m3	1.266097	1000	2400
Depth m	1000	20	.1
Area m2	3.5E+11	3.5E+10	3E+08
Frn org carb			.03
Z mol/m3.Pa	4.308761E-04	9.111332	44637.3
VZ mol/Pa	1.508066E+11	6.377932E+12	1.339119E+12
Fugacity Pa	8.289737E-09	8.289737E-09	8.289737E-09
Conc mol/m3	3.571849E-12	7.553055E-08	3.700315E-04
Conc g/m3	7.22335E-10	1.527454E-05	7.483146E-02
Conc ug/g	5.705211E-07	1.527454E-05	3.117977E-02
Amount mol	1250.147	52871.38	11100.94
Amount kg	252.8172	10692.18	2244.944
Amount %	.2528172	10.69218	2.244944

Phase	Sediment	Susp sedt	Fish
Volume m3	7E+08	4900000	700000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	71295.68	371977.5	75605.19
VZ mol/Pa	4.990698E+13	1.82269E+12	5.292363E+10
Fugacity Pa	8.289737E-09	8.289737E-09	8.289737E-09
Conc mol/m3	5.910225E-04	3.083596E-03	6.267471E-04
Conc g/m3	.1195225	.6235955	.1267471
Conc ug/g	5.196629E-02	.4157303	.1267471
Amount mol	413715.7	15109.62	438.723
Amount kg	83665.72	3055.618	88.72294

Amount %   83.66572   3.055618   8.872294E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Nordic Sea areas environment

Emission rate of chemical mol/h   173.0703
Emission rate of chemical   kg/h   35
Fugacity Pa   1.79975E-08
Total amount of chemical mol   1073559
Total amount of chemical kg   217105.9

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.5E+12	7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	1.79975E-08	1.79975E-08	1.79975E-08
Conc mol/m3	7.754693E-12	1.639812E-07	8.033599E-04
Conc g/m3	1.568231E-09	3.316192E-05	.1624635
Conc ug/g	1.238635E-06	3.316192E-05	6.769311E-02
Amount mol	2714.142	114786.9	24100.8
Amount kg	548.881	23213.35	4873.904
Amount %	.2528172	10.69218	2.244944
D rct mol/Pa.h	6147587	8.036195E+07	1.68729E+07
D adv mol/Pa.h	1.508066E+09	6.377933E+09	0
Rct rate mol/h	.1106412	1.446314	.3036701
Adv rate mol/h	27.14142	114.7869	0
Rct rate kg/h	2.237497E-02	.2924881	.0614112
Adv rate kg/h	5.48881	23.21335	0
Reaction %	6.392849E-02	.8356805	.1754606
Advection %	15.68231	66.32385	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	14000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	1.79975E-08	1.79975E-08	1.79975E-08
Conc mol/m3	1.283144E-03	6.694667E-03	1.360705E-03
Conc g/m3	.2594903	1.353862	.2751753
Conc ug/g	.1128218	.9025749	.2751753
Amount mol	898200.9	32803.87	952.4933
Amount kg	181643.2	6633.926	192.6227
Amount %	83.66572	3.055618	8.872294E-02
D rct mol/Pa.h	6.288279E+08		
D adv mol/Pa.h	9.981395E+08		
Rct rate mol/h	11.31733		
Adv rate mol/h	17.96402		
Rct rate kg/h	2.288704		
Adv rate kg/h	3.632864		
Reaction %	6.539154		
Advection %	10.37961		

Total advection D value   8.884138E+09
Total reaction D value   7.322103E+08
Total D value   9.616348E+09
Output by reaction   mol/h 13.17796
Output by advection   mol/h 159.8923
Total output by reaction and advection mol/h   173.0703
Output by reaction   kg/h 2.664979

Output by advection   kg/h   32.33502
Total output by reaction and advection kg/h   35

Overall residence time   h   6203.025
Reaction residence time   h   81466.28
Advection residence time h   6714.264

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Nordic Sea areas environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.5E+14	7E+11	5.4E+07
Density kg/m3	1.266097	1000.009	1500.253
Bulk Z value	4.59373E-04	11.04683	22321.38
Bulk VZ	1.607805E+11	7.732777E+12	1.205355E+12
Emission mol/h	56.86595	39.55892	0
Emission kg/h	11.5	8	0
Fugacity Pa	3.260878E-08	3.429088E-09	1.175787E-09
Conc mol/m3	1.497959E-11	3.788053E-08	2.624519E-05
Conc g/m3	3.029323E-09	7.66058E-06	5.307564E-03
Conc ug/g	2.392647E-06	7.660516E-06	3.537779E-03
Amount mol	5242.857	26516.37	1417.24
Amount kg	1060.263	5362.406	286.6085
Amount %	.9497617	4.803533	.256738
Adv.flow m3/h	3.5E+12	7E+08	0
D rct mol/Pa.h	6554171	9.743299E+07	1.518747E+07
D adv mol/Pa.h	1.607805E+09	7.732777E+09	0
Rct rate mol/h	.2137235	.3341063	1.785723E-02
Rct rate kg/h	.0432213	6.756632E-02	3.611267E-03
Adv rate mol/h	52.42856	26.51637	0
Adv rate kg/h	10.60263	5.362406	0
Reaction %	.2216477	.346494	1.851932E-02
Advection %	54.37246	27.49952	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.5E+09		
Density kg/m3	1260		
Bulk Z value	14266.43		0
Bulk VZ	4.993249E+13	0	
Emission mol/h	0	96.42487	
Emission kg/h	0	19.5	
Fugacity Pa	1.039086E-08		3.429088E-09
Conc mol/m3	1.482405E-04		2.592569E-04
Conc g/m3	2.997867E-02		5.242951E-02
Conc ug/g	.0237926		5.242951E-02
Amount mol	518841.7	552018.1	
Amount kg	104925.4	111634.6	
Amount %	93.98997		
Adv.flow m3/h	70000		
D rct mol/Pa.h	6.291493E+08		
D adv mol/Pa.h	9.986498E+08		
Rct rate mol/h	6.537405	7.103092	
Rct rate kg/h	1.322059	0	
Adv rate mol/h	10.37683	89.32176	
Adv rate kg/h	2.098507	18.06354	
Reaction %	6.779793		
Advection %	10.76158		

Overall residence time   h   5724.854
Reaction residence time   h   77715.19
Advection residence time h   6180.108

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 9.0252E-01	8.1412E+02	2.9793E+11	1.3686E+08	4.4628E+00
Air to soil 3.6824E-03	1.9953E+05	1.2156E+09	5.5841E+05	1.8209E-02
Water to air 5.2043E-02	7.1405E+04	6.7937E+06	7.5048E+07	2.5735E-01
Water to sediment 4.5363E+00	8.1920E+02	5.9216E+08	6.5415E+09	2.2431E+01
Soil to air 6.7994E-06	2.9211E+07	1.2811E+00	2.8596E+04	3.3622E-05
Soil to water 6.4339E-05	3.0871E+06	1.2122E+01	2.7058E+05	3.1815E-04
Sediment to water 1.1157E+00	6.5171E+04	3.7217E+04	5.3096E+08	5.5171E+00

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side) 7.540331E+07   Air-water diffusion
(water-side) 1.594483E+10
Air-water diffusion (overall)   7.50484E+07
Rain dissolution to water   3.188966E+07   Aerosol deposition to
water   2.992178E+07
Rain dissolution to soil   273340   Aerosol deposition to
soil   256472.4
Soil-air diffusion (air-phase)   2585.256   Soil-air diffusion
(water-phase) 27334
Soil-air diffusion (bndry layer) 646314.1   Soil-air diffusion
(overall)   28595.51
Water-sediment diffusion   3.188966E+07
Water-sediment deposition   6.509607E+09   Sediment-water
resuspension   4.990698E+08
Soil-water runoff (water)   136670   Soil-water runoff
(solids)   133911.9

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Nordic Countries environment

Properties of Fluoranthene :

Temperature deg C	4
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	7.269867E-02
Vapor pressure Pa	1.099162E-04
Sub-cooled liquid vapor press Pa	1.511943E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	8.549368E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	3.7103E-05
Soil-water partition coefficient	4899.097
Sedt-water partition coefficient	7824.947
Susp sedt-water partn coeffnt	40825.81
Aerosol-air partition coeff	3.968404E+09
Aerosol Z value	1722229
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	7.02305E-11
Total of VZ products	7.040908E+15

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.5E+15	8.52E+12	1.07E+11
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	1.5E+12	4.26E+11	1.07E+12
Frn org carb			.03
Z mol/m3.Pa	4.339854E-04	11.69677	57303.62
VZ mol/Pa	6.509781E+11	9.965649E+13	6.131488E+15
Fugacity Pa	7.02305E-11	7.02305E-11	7.02305E-11
Conc mol/m3	3.047901E-14	8.214701E-10	4.024462E-06
Conc g/m3	6.16377E-12	1.661259E-07	8.13867E-04
Conc ug/g	4.833445E-09	1.661259E-07	3.391112E-04
Amount mol	45.71852	6998.926	430617.5
Amount kg	9.245654	1415.393	87083.76
Amount %	9.245654E-03	1.415393	87.08376

Phase	Sediment	Susp sedt	Fish
Volume m3	8.519999E+09	5.964E+07	8520000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.26E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	91526.61	477530.2	97058.98
VZ mol/Pa	7.798067E+14	2.84799E+13	8.269425E+11
Fugacity Pa	7.02305E-11	7.02305E-11	7.02305E-11
Conc mol/m3	6.42796E-06	3.353718E-05	6.816501E-06
Conc g/m3	1.299926E-03	6.782224E-03	1.378501E-03
Conc ug/g	5.651854E-04	4.521483E-03	1.378501E-03
Amount mol	54766.22	2000.158	58.07659
Amount kg	11075.37	404.4919	11.74483

Amount %   11.07537   .4044919   1.174483E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Nordic Countries environment

Emission rate of chemical mol/h   741.7298
Emission rate of chemical kg/h   150
Fugacity Pa   3.529913E-09
Total amount of chemical mol   2.48538E+07
Total amount of chemical kg   5026183

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.5E+13	8.52E+09	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	3.529913E-09	3.529913E-09	3.529913E-09
Conc mol/m3	1.531931E-12	4.128858E-08	2.022768E-04
Conc g/m3	3.098023E-10	8.34979E-06	4.090643E-02
Conc ug/g	2.429377E-07	8.349789E-06	1.704435E-02
Amount mol	2297.896	351778.7	2.164362E+07
Amount kg	464.7035	71140.21	4376988
Amount %	9.245654E-03	1.415392	87.08376
D rct mol/Pa.h	2.653693E+07	1.255672E+09	7.725675E+10
D adv mol/Pa.h	6.509781E+09	9.965649E+10	0
Rct rate mol/h	9.367304E-02	4.432412	272.7096
Adv rate mol/h	22.97896	351.7787	0
Rct rate kg/h	.0189435	.8963667	55.15006
Adv rate kg/h	4.647035	71.14021	0
Reaction %	.012629	.5975778	36.76671
Advection %	3.098023	47.42681	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	170400		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	3.529913E-09	3.529913E-09	3.529913E-09
Conc mol/m3	3.23081E-04	1.68564E-03	3.426097E-04
Conc g/m3	6.533666E-02	.340887	6.928596E-02
Conc ug/g	2.840725E-02	.227258	6.928596E-02
Amount mol	2752650	100531.6	2919.035
Amount kg	556668.3	20330.5	590.3164
Amount %	11.07537	.4044918	1.174483E-02
D rct mol/Pa.h	9.825564E+09		
D adv mol/Pa.h	1.559613E+10		
Rct rate mol/h	34.68339		
Adv rate mol/h	55.05299		
Rct rate kg/h	7.014021		
Adv rate kg/h	11.13337		
Reaction %	4.676014		
Advection %	7.422244		

Total advection D value   1.217624E+11
Total reaction D value   8.836452E+10
Total D value   2.101269E+11
Output by reaction   mol/h   311.919
Output by advection   mol/h   429.8107
Total output by reaction and advection mol/h   741.7298
Output by reaction   kg/h   63.07939

Output by advection   kg/h   86.92062
Total output by reaction and advection kg/h   150

Overall residence time   h   33507.88
Reaction residence time h   79680.28
Advection residence time h   57824.98

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Nordic Countries environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.5E+15	8.52E+12	1.926E+11
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.6843E-04	14.18148	28655.32
Bulk VZ	7.02645E+11	1.208262E+14	5.519014E+15
Emission mol/h	296.6919	123.6216	49.44865
Emission kg/h	60	25	10
Fugacity Pa	2.611643E-08	8.694213E-10	1.612425E-09
Conc mol/m3	1.223372E-11	1.232968E-08	4.620456E-05
Conc g/m3	2.474025E-09	2.493431E-06	9.343948E-03
Conc ug/g	1.940057E-06	2.49341E-06	6.22824E-03
Amount mol	18350.58	105048.9	8898998
Amount kg	3711.037	21244.04	1799644
Amount %	.1656507	.9482767	80.3313
Adv.flow m3/h	1.5E+13	8.52E+09	0
D rct mol/Pa.h	2.864312E+07	1.522411E+09	6.953958E+10
D adv mol/Pa.h	7.02645E+09	1.208262E+11	0
Rct rate mol/h	.748056	1.323616	112.1274
Rct rate kg/h	.1512794	.2676749	22.67552
Adv rate mol/h	183.5058	105.0489	0
Adv rate kg/h	37.11038	21.24404	0
Reaction %	.1592414	.281763	23.86896
Advection %	39.06355	22.36214	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.26E+10		
Density kg/m3	1260		
Bulk Z value	18314.68		0
Bulk VZ	7.802053E+14	0	
Emission mol/h	0	469.7622	
Emission kg/h	0	95	
Fugacity Pa	2.63453E-09		8.694213E-10
Conc mol/m3	4.825058E-05		8.438514E-05
Conc g/m3	9.757714E-03		1.706521E-02
Conc ug/g	7.744218E-03		1.706521E-02
Amount mol	2055475	1.107787E+07	
Amount kg	415678.6	2240278	
Amount %	18.55478		
Adv.flow m3/h	851999.9		
D rct mol/Pa.h	9.830588E+09		
D adv mol/Pa.h	1.560411E+10		
Rct rate mol/h	25.89898	140.098	
Rct rate kg/h	5.237551	0	
Adv rate mol/h	41.10949	329.6642	
Adv rate kg/h	8.313572	66.66798	
Reaction %	5.513212		
Advection %	8.751128		

Overall residence time   h   23581.87
Reaction residence time   h   79072.3
Advection residence time h   33603.51

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
kg/h	h	m3/h	mol/Pa.h	mol/h
Air to water 9.8208E+00	2.6187E+02	3.9695E+12	1.8595E+09	4.8562E+01
Air to soil 1.3121E+01	1.9600E+02	5.3035E+12	2.4843E+09	6.4881E+01
Water to air 1.6193E-01	9.0918E+04	6.4942E+07	9.2097E+08	8.0071E-01
Water to sediment 1.7971E+01	8.1920E+02	7.2074E+09	1.0221E+11	8.8865E+01
Soil to air 4.1440E-02	3.0096E+07	4.4349E+03	1.2708E+08	2.0491E-01
Soil to water 4.0399E-01	3.0871E+06	4.3235E+04	1.2389E+09	1.9977E+00
Sediment to water 4.4201E+00	6.5171E+04	4.5299E+05	8.2963E+09	2.1857E+01

Transport velocity parameters

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   9.243889E+08   Air-water diffusion
(water-side) 2.491412E+11
Air-water diffusion (overall)   9.209718E+08
Rain dissolution to water   4.982825E+08   Aerosol deposition to
water   4.402018E+08
Rain dissolution to soil   1.251554E+09   Aerosol deposition to
soil   1.105671E+09
Soil-air diffusion (air-phase)   9287286   Soil-air diffusion
(water-phase) 1.251555E+08
Soil-air diffusion (bndry layer) 2.321822E+09   Soil-air diffusion
(overall)   1.270841E+08
Water-sediment diffusion   4.982825E+08
Water-sediment deposition   1.017139E+11   Sediment-water
resuspension   7.798067E+09
Soil-water runoff (water)   6.257772E+08   Soil-water runoff
(solids)   6.131488E+08

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Bay of Bothnia environment

Properties of Fluoranthene :

Temperature deg C	2
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	6.789166E-02
Vapor pressure Pa	8.531027E-05
Sub-cooled liquid vapor press Pa	1.256565E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	6.635498E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	2.900641E-05
Soil-water partition coefficient	6532.13
Sedt-water partition coefficient	7824.948
Susp sedt-water partn coeffnt	15309.68
Aerosol-air partition coeff	4.774923E+09
Aerosol Z value	2087309
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	4.918571E-09
Total of VZ products	1.005346E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.7E+13	7.4E+11	1E+07
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.7E+10	3.7E+10	1E+08
Frn org carb			.04
Z mol/m3.Pa	4.371399E-04	15.07046	98442.19
VZ mol/Pa	1.617418E+10	1.115214E+13	9.844219E+11
Fugacity Pa	4.918571E-09	4.918571E-09	4.918571E-09
Conc mol/m3	2.150104E-12	7.412512E-08	4.841949E-04
Conc g/m3	4.348155E-10	1.499032E-05	9.791873E-02
Conc ug/g	3.385088E-07	1.499032E-05	4.079947E-02
Amount mol	79.55383	54852.59	4841.949
Amount kg	16.08817	11092.84	979.1874
Amount %	1.608817E-02	11.09284	.9791874

Phase	Sediment	Susp sedt	Fish
Volume m3	7.4E+08	4440000	740000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.7E+10	0	0
Frn org carb	.05	.15	
Z mol/m3.Pa	117925.5	230723.9	125053.6
VZ mol/Pa	8.726489E+13	1.024414E+12	9.253965E+10
Fugacity Pa	4.918571E-09	4.918571E-09	4.918571E-09
Conc mol/m3	5.800252E-04	1.134832E-03	6.150849E-04
Conc g/m3	.1172985	.229497	.1243886
Conc ug/g	5.099934E-02	.152998	.1243886
Amount mol	429218.6	5038.654	455.1628
Amount kg	86800.88	1018.967	92.04757

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       82
Amount %        86.80088          1.018967          9.204758E-02


SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Bay of Bothnia environment

Emission rate of chemical mol/h    19.77946
Emission rate of chemical  kg/h    4
Fugacity Pa                        1.381991E-09
Total amount of chemical mol       138937.9
Total amount of chemical kg        28097.4

Phase properties,compositions and rates

Phase           Air                Water              Soil
Adv.flow m3/h   3.7E+11            7.4E+08            0
Adv.restime h   100               1000               0
Rct halflife h  17000             55000              55000
Rct rate c.h-1  4.076471E-05      .0000126           .0000126
Fugacity Pa     1.381991E-09      1.381991E-09       1.381991E-09
Conc mol/m3     6.041233E-13      2.082723E-08       1.360462E-04
Conc g/m3       1.221718E-10      4.211891E-06       2.751262E-02
Conc ug/g       9.511217E-08      4.211891E-06       1.146359E-02
Amount mol      22.35256          15412.15           1360.462
Amount kg       4.520358          3116.799           275.1262
Amount %        1.608817E-02      11.09284           .9791873
D rct mol/Pa.h  659335.5          1.40517E+08        1.240372E+07
D adv mol/Pa.h  1.617418E+08      1.115214E+10       0
Rct rate mol/h  9.111955E-04      .1941931           1.714182E-02
Adv rate mol/h  .2235256          15.41215           0
Rct rate kg/h   1.842711E-04      3.927167E-02       3.46659E-03
Adv rate kg/h   4.520358E-02      3.116799           0
Reaction %      4.606777E-03      .9817919           8.666477E-02
Advection %     1.130089          77.91998           0

Phase           Sediment           Susp sedt          Fish
Adv.flow m3/h   14800
Adv.restime h   50000
Rct halflife h  55000
Rct rate c.h-1  .0000126
Fugacity Pa     1.381991E-09      1.381991E-09       1.381991E-09
Conc mol/m3     1.62972E-04       3.188583E-04       1.728229E-04
Conc g/m3       3.295783E-02      6.448271E-02       3.494997E-02
Conc ug/g       1.432949E-02      4.298847E-02       3.494997E-02
Amount mol      120599.3          1415.731           127.8889
Amount kg       24388.79          286.3032           25.86298
Amount %        86.80088          1.018967           9.204758E-02
D rct mol/Pa.h  1.099538E+09
D adv mol/Pa.h  1.745298E+09
Rct rate mol/h  1.519551
Adv rate mol/h  2.411986
Rct rate kg/h   .3072988
Adv rate kg/h   .4877758
Reaction %      7.68247
Advection %     12.1944


Total advection D value       1.305918E+10
Total reaction D value        1.253118E+09
Total D value                 1.43123E+10
Output by reaction      mol/h 1.731797
Output by advection     mol/h 18.04766
Total output by reaction and advection mol/h  19.77946
Output by reaction      kg/h  .3502213
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Output by advection   kg/h   3.649779
Total output by reaction and advection kg/h   4

Overall residence time   h   7024.351
Reaction residence time   h   80227.57
Advection residence time h   7698.386

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Bay of Bothnia environment

Bulk phase properties, compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.7E+13	7.4E+11	1.8E+07
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.788861E-04	16.34913	49225.62
Bulk VZ	1.771878E+10	1.209836E+13	8.860611E+11
Emission mol/h	.3955892	.0988973	0
Emission kg/h	.08	.02	0
Fugacity Pa	1.100306E-09	1.923851E-11	2.818395E-11
Conc mol/m3	5.269212E-13	3.14533E-10	1.387372E-06
Conc g/m3	1.065593E-10	6.3608E-08	2.805683E-04
Conc ug/g	8.295761E-08	6.360746E-08	1.870135E-04
Amount mol	19.49608	232.7544	24.9727
Amount kg	3.942693	47.06993	5.050229
Amount %	.8856101	10.57287	1.134386
Adv.flow m3/h	3.7E+11	7.4E+08	0
D rct mol/Pa.h	722301	1.524393E+08	1.116437E+07
D adv mol/Pa.h	1.771878E+08	1.209836E+10	0
Rct rate mol/h	7.947521E-04	2.932706E-03	3.146561E-04
Rct rate kg/h	1.607227E-04	5.93081E-04	6.36329E-05
Adv rate mol/h	.1949608	.2327544	0
Adv rate kg/h	3.942693E-02	4.706992E-02	0
Reaction %	.1607227	.593081	.0636329
Advection %	39.42693	47.06993	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.7E+09		
Density kg/m3	1260		
Bulk Z value	23597.17		0
Bulk VZ	8.730951E+13	0	
Emission mol/h	0	.4944865	
Emission kg/h	0	9.999999E-02	
Fugacity Pa	2.203891E-11		1.923851E-11
Conc mol/m3	5.200558E-07		2.405845E-06
Conc g/m3	1.051709E-04		4.865341E-04
Conc ug/g	8.346895E-05		4.865341E-04
Amount mol	1924.206	2201.43	
Amount kg	389.1323	445.1952	
Amount %	87.40712		
Adv.flow m3/h	74000		
D rct mol/Pa.h	1.1001E+09		
D adv mol/Pa.h	1.74619E+09		
Rct rate mol/h	.024245	2.828712E-02	
Rct rate kg/h	4.903067E-03	0	
Adv rate mol/h	3.848413E-02	.4661994	
Adv rate kg/h	7.782645E-03	9.427949E-02	
Reaction %	4.903067		
Advection %	7.782645		

Overall residence time   h   4451.952
Reaction residence time   h   77824.2
Advection residence time h   4722.077

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h kg/h
Air to water	6.7196E+01	3.8159E+11	1.8274E+08	2.0107E-01 4.0661E-02
Air to soil	4.2225E+04	6.0725E+08	2.9080E+05	3.1997E-04 6.4708E-05
Water to air	1.0397E+05	4.9322E+06	8.0637E+07	1.5513E-03 3.1373E-04
Water to sediment	1.9389E+03	2.6449E+08	4.3242E+09	8.3190E-02 1.6824E-02
Soil to air	4.1320E+07	3.0189E-01	1.4861E+04	4.1883E-07 8.4700E-08
Soil to water	3.5331E+06	3.5306E+00	1.7379E+05	4.8982E-06 9.9057E-07
Sediment to water	6.5171E+04	3.9344E+04	9.2841E+08	2.0461E-02 4.1379E-03

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   8.087088E+07   Air-water diffusion
(water-side) 2.788035E+10
Air-water diffusion (overall)   8.063698E+07
Rain dissolution to water   5.576069E+07   Aerosol deposition to
water   4.633827E+07
Rain dissolution to soil   150704.6   Aerosol deposition to
soil   125238.6
Soil-air diffusion (air-phase)   874.2799   Soil-air diffusion
(water-phase) 15070.46
Soil-air diffusion (bndry layer) 218570   Soil-air diffusion
(overall)   14860.65
Water-sediment diffusion   5.576069E+07
Water-sediment deposition   4.268392E+09   Sediment-water
resuspension   8.726489E+08
Soil-water runoff (water)   75352.29   Soil-water runoff
(solids)   98442.19

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Baltic Proper environment

Properties of Fluoranthene :

Temperature deg C	7
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	.0804074
Vapor pressure Pa	1.596642E-04
Sub-cooled liquid vapor press Pa	1.98569E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	.124188
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	5.331864E-05
Soil-water partition coefficient	4899.097
Sedt-water partition coefficient	7824.947
Susp sedt-water partn coeffnt	40825.81
Aerosol-air partition coeff	3.02162E+09
Aerosol Z value	1297296
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	1.608052E-09
Total of VZ products	3.075066E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	2.1E+14	4.2E+12	1E+07
Density kg/m3	1.261578	1000	2400
Depth m	1000	20	.1
Area m2	2.1E+11	2.1E+11	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.29338E-04	8.052307	39449.04
VZ mol/Pa	9.016099E+10	3.381969E+13	3.944904E+11
Fugacity Pa	1.608052E-09	1.608052E-09	1.608052E-09
Conc mol/m3	6.903979E-13	1.294853E-08	6.34361E-05
Conc g/m3	1.396192E-10	2.618581E-06	1.282868E-02
Conc ug/g	1.106703E-07	2.618581E-06	5.345284E-03
Amount mol	144.9836	54383.82	634.361
Amount kg	29.32003	10998.04	128.2868
Amount %	2.932003E-02	10.99804	.1282868

Phase	Sediment	Susp sedt	Fish
Volume m3	4.2E+09	2.52E+07	4200000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	2.1E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	63008.88	328742	66817.47
VZ mol/Pa	2.646373E+14	8.284297E+12	2.806334E+11
Fugacity Pa	1.608052E-09	1.608052E-09	1.608052E-09
Conc mol/m3	1.013216E-04	5.286341E-04	1.07446E-04
Conc g/m3	2.049026E-02	.1069057	.0217288
Conc ug/g	8.908808E-03	7.127045E-02	.0217288
Amount mol	425550.5	13321.58	451.2731
Amount kg	86059.07	2694.023	91.26095

Amount %   86.05907   2.694023   9.126095E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Baltic Proper environment

Emission rate of chemical mol/h   103.8422
Emission rate of chemical kg/h   21
Fugacity Pa   2.371733E-09
Total amount of chemical mol   729323.3
Total amount of chemical kg   147491.1

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	2.1E+12	4.2E+09	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	2.371733E-09	2.371733E-09	2.371733E-09
Conc mol/m3	1.018275E-12	1.909792E-08	9.356256E-05
Conc g/m3	2.059258E-10	3.862172E-06	1.892116E-02
Conc ug/g	1.632288E-07	3.862172E-06	7.883816E-03
Amount mol	213.8378	80211.27	935.6257
Amount kg	43.24441	16221.12	189.2116
Amount %	2.932003E-02	10.99804	.1282868
D rct mol/Pa.h	3675386	4.261282E+08	4970579
D adv mol/Pa.h	9.016099E+08	3.381969E+10	0
Rct rate mol/h	8.717033E-03	1.010662	1.178888E-02
Adv rate mol/h	2.138378	80.21126	0
Rct rate kg/h	1.762846E-03	.2043862	2.384066E-03
Adv rate kg/h	.4324441	16.22112	0
Reaction %	8.394503E-03	.9732675	.0113527
Advection %	2.059258	77.24345	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	84000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	2.371733E-09	2.371733E-09	2.371733E-09
Conc mol/m3	1.494402E-04	7.79688E-04	1.584732E-04
Conc g/m3	3.022129E-02	.1576763	3.204803E-02
Conc ug/g	1.313969E-02	.1051175	3.204803E-02
Amount mol	627648.8	19648.14	665.5873
Amount kg	126929.4	3973.443	134.6017
Amount %	86.05907	2.694023	9.126094E-02
D rct mol/Pa.h	3.33443E+09		
D adv mol/Pa.h	5.292746E+09		
Rct rate mol/h	7.908376		
Adv rate mol/h	12.55298		
Rct rate kg/h	1.599311		
Adv rate kg/h	2.538588		
Reaction %	7.615766		
Advection %	12.08852		

Total advection D value   4.001405E+10
Total reaction D value   3.769204E+09
Total D value   4.378325E+10
Output by reaction   mol/h 8.939542
Output by advection   mol/h 94.90261
Total output by reaction and advection mol/h   103.8422
Output by reaction   kg/h 1.807844

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Output by advection   kg/h   19.19215
Total output by reaction and advection kg/h   21

Overall residence time   h   7023.384
Reaction residence time   h   81583.96
Advection residence time h   7684.965

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Baltic Proper environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	2.1E+14	4.2E+12	1.8E+07
Density kg/m3	1.261578	1000.009	1500.252
Bulk Z value	4.55284E-04	9.762834	19726.93
Bulk VZ	9.560964E+10	4.10039E+13	3.550848E+11
Emission mol/h	3.461406	23.73535	0
Emission kg/h	.7	4.8	0
Fugacity Pa	2.083903E-09	3.723011E-10	7.624125E-11
Conc mol/m3	9.487676E-13	3.634714E-09	1.504006E-06
Conc g/m3	1.918693E-10	7.350481E-07	3.041552E-04
Conc ug/g	1.520868E-07	7.350419E-07	2.02736E-04
Amount mol	199.2412	15265.8	27.07211
Amount kg	40.29255	3087.202	5.474793
Amount %	6.341311E-02	4.858693	8.616324E-03
Adv.flow m3/h	2.1E+12	4.2E+09	0
D rct mol/Pa.h	3897499	5.166492E+08	4474069
D adv mol/Pa.h	9.560963E+08	4.10039E+10	0
Rct rate mol/h	8.12201E-03	.1923491	3.411086E-04
Rct rate kg/h	1.642514E-03	3.889875E-02	6.898239E-05
Adv rate mol/h	1.992412	15.2658	0
Adv rate kg/h	.4029255	3.087202	0
Reaction %	2.986389E-02	.70725	1.254225E-03
Advection %	7.325919	56.13095	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	2.1E+10		
Density kg/m3	1260		
Bulk Z value	12608.22		0
Bulk VZ	2.647726E+14	0	
Emission mol/h	0	27.19676	
Emission kg/h	0	5.5	
Fugacity Pa	1.128151E-09		3.723011E-10
Conc mol/m3	1.422397E-05		2.487622E-05
Conc g/m3	2.876514E-03		5.030717E-03
Conc ug/g	2.282948E-03		5.030717E-03
Amount mol	298703.5	314195.6	
Amount kg	60406.8	63539.77	
Amount %	95.06928		
Adv.flow m3/h	420000		
D rct mol/Pa.h	3.336134E+09		
D adv mol/Pa.h	5.295451E+09		
Rct rate mol/h	3.763664	3.96447o	
Rct rate kg/h	.7611257	0	
Adv rate mol/h	5.974069	23.23228	
Adv rate kg/h	1.208136	4.698264	
Reaction %	13.83865		
Advection %	21.96611		

Overall residence time   h   11552.69
Reaction residence time   h   79252.75
Advection residence time h   13524.1

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h kg/h
Air to water	8.4840E+01	1.7154E+12	7.8097E+08	1.6275E+00 3.2912E-01
Air to soil	3.9695E+05	3.6662E+08	1.6692E+05	3.4784E-04 7.0343E-05
Water to air	6.3369E+04	4.5931E+07	4.4841E+08	1.6695E-01 3.3761E-02
Water to sediment	8.1920E+02	3.5530E+09	3.4687E+10	1.2914E+01 2.6116E+00
Soil to air	2.8761E+07	4.3371E-01	8.5558E+03	6.5231E-07 1.3192E-07
Soil to water	3.0871E+06	4.0407E+00	7.9711E+04	6.0772E-06 1.2290E-06
Sediment to water	6.5171E+04	2.2330E+05	2.8155E+09	3.1763E+00 6.4234E-01

Transport velocity parameters   m/h   m/year

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   4.50805E+08   Air-water diffusion
(water-side)   8.454922E+10
Air-water diffusion (overall)   4.48414E+08
Rain dissolution to water   1.690985E+08   Aerosol deposition to
water   1.634593E+08
Rain dissolution to soil   80523.07   Aerosol deposition to
soil   77837.77
Soil-air diffusion (air-phase)   858.676   Soil-air diffusion
(water-phase)   8052.307
Soil-air diffusion (bndry layer)   214669   Soil-air diffusion
(overall)   8555.828
Water-sediment diffusion   1.690985E+08
Water-sediment deposition   3.45179E+10   Sediment-water
resuspension   2.646373E+09
Soil-water runoff (water)   40261.54   Soil-water runoff
(solids)   39449.04

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at North Sea / Skagerrak environment

Properties of Fluoranthene :

Temperature deg C	8
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	8.311476E-02
Vapor pressure Pa	1.805039E-04
Sub-cooled liquid vapor press Pa	2.171743E-03
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	.1403973
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	6.006351E-05
Soil-water partition coefficient	4899.097
Sedt-water partition coefficient	7824.948
Susp sedt-water partn coeffnt	40825.81
Aerosol-air partition coeff	2.762758E+09
Aerosol Z value	1181938
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	8.443683E-09
Total of VZ products	5.85629E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+13	9E+11	1E+07
Density kg/m3	1.25709	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+10	4.5E+10	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.27811E-04	7.122643	34894.52
VZ mol/Pa	1.925149E+10	6.410379E+12	3.489452E+11
Fugacity Pa	8.443683E-09	8.443683E-09	8.443683E-09
Conc mol/m3	3.6123E-12	6.014134E-08	2.946383E-04
Conc g/m3	7.305154E-10	1.216238E-05	.0595847
Conc ug/g	5.81116E-07	1.216238E-05	2.482696E-02
Amount mol	162.5535	54127.21	2946.383
Amount kg	32.87319	10946.14	595.847
Amount %	3.287319E-02	10.94614	.595847

Phase	Sediment	Susp sedt	Fish
Volume m3	9E+08	5400000	900000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	55734.31	290787.7	59103.19
VZ mol/Pa	5.016088E+13	1.570254E+12	5.319287E+10
Fugacity Pa	8.443683E-09	8.443683E-09	8.443683E-09
Conc mol/m3	4.706028E-04	2.455319E-03	4.990486E-04
Conc g/m3	.09517	.4965392	.1009226
Conc ug/g	4.137826E-02	.3310261	.1009226
Amount mol	423542.5	13258.72	449.1437
Amount kg	85653	2681.312	90.83033

Amount %   85.65299   2.681311   9.083032E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at North Sea / Skagerrak environment

Emission rate of chemical mol/h   24.72433
Emission rate of chemical kg/h   5
Fugacity Pa   2.970214E-09
Total amount of chemical mol   173944.3
Total amount of chemical kg   35176.76

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+11	9E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	2.970214E-09	2.970214E-09	2.970214E-09
Conc mol/m3	1.27069E-12	2.115577E-08	1.036442E-04
Conc g/m3	2.569716E-10	4.278332E-06	2.095996E-02
Conc ug/g	2.044178E-07	4.278332E-06	8.733318E-03
Amount mol	57.18104	19040.19	1036.442
Amount kg	11.56372	3850.498	209.5996
Amount %	3.287319E-02	10.94614	.5958469
D rct mol/Pa.h	784781.5	8.077078E+07	4396710
D adv mol/Pa.h	1.925149E+08	6.410379E+09	0
Rct rate mol/h	2.330969E-03	.2399065	1.305917E-02
Adv rate mol/h	.5718105	19.04019	0
Rct rate kg/h	4.713918E-04	4.851628E-02	2.640955E-03
Adv rate kg/h	.1156372	3.850498	0
Reaction %	9.427834E-03	.9703255	.0528191
Advection %	2.312745	77.00996	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	18000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	2.970214E-09	2.970214E-09	2.970214E-09
Conc mol/m3	1.655428E-04	8.637015E-04	1.755491E-04
Conc g/m3	3.347772E-02	.1746664	3.550129E-02
Conc ug/g	1.455553E-02	.1164442	3.550129E-02
Amount mol	148988.5	4663.988	157.9942
Amount kg	30129.94	943.1982	31.95116
Amount %	85.65299	2.681311	9.083032E-02
D rct mol/Pa.h	6.32027E+08		
D adv mol/Pa.h	1.003218E+09		
Rct rate mol/h	1.877255		
Adv rate mol/h	2.97977		
Rct rate kg/h	.3796373		
Adv rate kg/h	.6025989		
Reaction %	7.592747		
Advection %	12.05198		

Total advection D value   7.606111E+09
Total reaction D value   7.179793E+08
Total D value   8.324091E+09
Output by reaction   mol/h 2.132552
Output by advection   mol/h 22.59178
Total output by reaction and advection mol/h   24.72433
Output by reaction   kg/h   .4312659

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Output by advection      kg/h    4.568734
Total output by reaction and advection kg/h    5

Overall residence time    h    7035.351
Reaction residence time   h    81566.28
Advection residence time  h    7699.453
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FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
Fate of Fluoranthene at North Sea / Skagerrak environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+13	9E+11	1.8E+07
Density kg/m3	1.25709	1000.009	1500.252
Bulk Z value	4.514497E-04	8.635684	17449.4
Bulk VZ	2.031524E+10	7.772116E+12	3.140892E+11
Emission mol/h	1.928497	10.8787	5.933838
Emission kg/h	.39	2.2	1.2
Fugacity Pa	5.58546E-09	9.620962E-10	1.470536E-06
Conc mol/m3	2.521554E-12	8.308359E-09	2.565996E-02
Conc g/m3	5.09934E-10	1.680199E-06	5.189214
Conc ug/g	4.056462E-07	1.680185E-06	3.458897
Amount mol	113.47	7477.523	461879.4
Amount kg	22.94703	1512.179	93405.86
Amount %	1.697649E-02	1.118729	69.1028
Adv.flow m3/h	4.5E+11	9E+08	0
D rct mol/Pa.h	828144.6	9.792866E+07	3957523
D adv mol/Pa.h	2.031524E+08	7.772116E+09	0
Rct rate mol/h	4.625569E-03	9.421679E-02	5.81968
Rct rate kg/h	9.354287E-04	1.905346E-02	1.176914
Adv rate mol/h	1.1347	7.477523	0
Adv rate kg/h	.2294703	1.512179	0
Reaction %	2.201009E-02	.4483167	27.69209
Advection %	5.3993	35.58069	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.5E+09		
Density kg/m3	1260		
Bulk Z value	11152.56		0
Bulk VZ	5.018652E+13	0	
Emission mol/h	2.274638	21.01568	
Emission kg/h	.46	4.25	
Fugacity Pa	3.963701E-09		9.620962E-10
Conc mol/m3	4.420541E-05		5.686295E-05
Conc g/m3	8.939658E-03		1.149939E-02
Conc ug/g	7.094967E-03		1.149939E-02
Amount mol	198924.3	668394.6	
Amount kg	40228.47	135169.4	
Amount %	29.76151		
Adv.flow m3/h	89999.99		
D rct mol/Pa.h	6.323501E+08		
D adv mol/Pa.h	1.00373E+09		
Rct rate mol/h	2.506447	8.424969	
Rct rate kg/h	.5068787	0	
Adv rate mol/h	3.978486	12.59071	
Adv rate kg/h	.8045693	2.546219	
Reaction %	11.92656		
Advection %	18.93104		

Overall residence time   h   31804.58
Reaction residence time   h   79334.97
Advection residence time h   53086.35

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
kg/h	h	m3/h	mol/Pa.h	mol/h
Air to water 1.8033E-01	8.8185E+01	3.5363E+11	1.5965E+08	8.9170E-01
Air to soil 1.6924E-04	9.3960E+04	3.3190E+08	1.4983E+05	8.3689E-04
Water to air 1.8616E-02	5.6291E+04	1.1080E+07	9.5683E+07	9.2056E-02
Water to sediment 1.2792E+00	8.1920E+02	7.6135E+08	6.5748E+09	6.3256E+00
Soil to air 2.2873E-03	2.8300E+07	4.4078E-01	7.6914E+03	1.1310E-02
Soil to water 2.0968E-02	3.0871E+06	4.0407E+00	7.0508E+04	1.0368E-01
Sediment to water 4.2777E-01	6.5171E+04	4.7851E+04	5.3366E+08	2.1153E+00

Transport velocity parameters   m/h   m/year

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   9.625746E+07   Air-water diffusion
(water-side) 1.602595E+10
Air-water diffusion (overall)   9.568275E+07
Rain dissolution to water   3.20519E+07   Aerosol deposition to
water   3.191233E+07
Rain dissolution to soil   71226.43   Aerosol deposition to
soil   70916.28
Soil-air diffusion (air-phase)   855.6219   Soil-air diffusion
(water-phase) 7122.643
Soil-air diffusion (bndry layer) 213905.5   Soil-air diffusion
(overall)   7691.391
Water-sediment diffusion   3.20519E+07
Water-sediment deposition   6.542723E+09   Sediment-water
resuspension   5.016088E+08
Soil-water runoff (water)   35613.22   Soil-water runoff
(solids)   34894.52

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Fluoranthene at Barents Sea environment

Properties of Fluoranthene :

Temperature deg C	-2
Molecular mass g/mol	202.23
Melting point deg C	111
Fugacity ratio	5.903125E-02
Vapor pressure Pa	5.081671E-05
Sub-cooled liquid vapor press Pa	8.608442E-04
Solubility g/m3	.26
Solubility mol/m3	1.285665E-03
Henry's law constant Pa.m3/mol	3.952563E-02
Log octanol-water p-coefficient	5.22
Octanol-water partn-coefficient	165958.6
Organic C-water ptn-coefficient	68043.02
Fish-water partition coefficient	8297.929
Air-water partition coefficient	1.753312E-05
Soil-water partition coefficient	4899.097
Sedt-water partition coefficient	1564.989
Susp sedt-water partn coeffnt	2041.29
Aerosol-air partition coeff	6.969902E+09
Aerosol Z value	3091769
Aerosol density kg/m3	2000

Amount of chemical moles	494486.5
Amount of chemical kilograms	100000
Fugacity Pa	6.977546E-11
Total of VZ products	7.086825E+15

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.2E+15	2.4E+14	1E+07
Density kg/m3	1.303452	1000	2400
Depth m	1000	200	.1
Area m2	1.2E+12	1.2E+12	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.435886E-04	25.30004	123947.4
VZ mol/Pa	5.323063E+11	6.07201E+15	1.239474E+12
Fugacity Pa	6.977546E-11	6.977546E-11	6.977546E-11
Conc mol/m3	3.09516E-14	1.765322E-09	8.648484E-06
Conc g/m3	6.259342E-12	3.570011E-07	1.748983E-03
Conc ug/g	4.802128E-09	3.570011E-07	7.287429E-04
Amount mol	37.14192	423677.3	86.48484
Amount kg	7.51121	85680.27	17.48983
Amount %	7.51121E-03	85.68026	1.748983E-02

Phase	Sediment	Susp sedt	Fish
Volume m3	2.4E+10	2.4E+08	2.4E+08
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	1.2E+12	0	0
Frn org carb	.01	.02	
Z mol/m3.Pa	39594.3	51644.73	209938
VZ mol/Pa	9.502631E+14	1.239474E+13	5.038511E+13
Fugacity Pa	6.977546E-11	6.977546E-11	6.977546E-11
Conc mol/m3	2.762711E-06	3.603535E-06	1.464852E-05
Conc g/m3	5.587029E-04	7.287429E-04	2.96237E-03
Conc ug/g	2.429143E-04	4.858286E-04	2.96237E-03
Amount mol	66305.05	864.8483	3515.644
Amount kg	13408.87	174.8983	710.9687

Amount %   13.40887   .1748983   .7109687

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Fluoranthene at Barents Sea environment

Emission rate of chemical mol/h   296.6919
Emission rate of chemical kg/h   60
Fugacity Pa   4.79707E-11
Total amount of chemical mol   339960
Total amount of chemical kg   68750.1

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.2E+13	2.4E+11	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.79707E-11	4.79707E-11	4.79707E-11
Conc mol/m3	2.127925E-14	1.213661E-09	5.945841E-06
Conc g/m3	4.303304E-12	2.454386E-07	1.202427E-03
Conc ug/g	3.301467E-09	2.454386E-07	5.010115E-04
Amount mol	25.5351	291278.6	59.45841
Amount kg	5.163964	58905.27	12.02428
Amount %	7.511209E-03	85.68026	1.748983E-02
D rct mol/Pa.h	2.169931E+07	7.650733E+10	1.561737E+07
D adv mol/Pa.h	5.323063E+09	6.07201E+12	0
Rct rate mol/h	1.040931E-03	3.67011	7.49176E-04
Adv rate mol/h	.255351	291.2786	0
Rct rate kg/h	2.105075E-04	.7422063	1.515059E-04
Adv rate kg/h	5.163963E-02	58.90526	0
Reaction %	3.508458E-04	1.237011	2.525098E-04
Advection %	8.606607E-02	98.17544	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	480000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.79707E-11	4.79707E-11	4.79707E-11
Conc mol/m3	1.899366E-06	2.477434E-06	1.007087E-05
Conc g/m3	3.841088E-04	5.010115E-04	2.036632E-03
Conc ug/g	1.670038E-04	3.340076E-04	2.036632E-03
Amount mol	45584.78	594.5841	2417.009
Amount kg	9218.611	120.2427	488.7917
Amount %	13.40887	.1748983	.7109687
D rct mol/Pa.h	1.197332E+10		
D adv mol/Pa.h	1.900526E+10		
Rct rate mol/h	.5743683		
Adv rate mol/h	.9116956		
Rct rate kg/h	.1161545		
Adv rate kg/h	.1843722		
Reaction %	.1935908		
Advection %	.307287		

Total advection D value   6.096339E+12
Total reaction D value   8.851796E+10
Total D value   6.184857E+12
Output by reaction   mol/h 4.246269
Output by advection   mol/h 292.4456
Total output by reaction and advection mol/h   296.6919
Output by reaction   kg/h   .8587228

Output by advection   kg/h   59.14128
Total output by reaction and advection kg/h   60

Overall residence time   h   1145.835
Reaction residence time   h   80060.88
Advection residence time h   1162.472

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Fluoranthene at Barents Sea environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.2E+15	2.4E+14	1.8E+07
Density kg/m3	1.303452	1000.009	1500.261
Bulk Z value	5.05424E-04	25.76821	61981.27
Bulk VZ	6.065088E+11	6.184369E+15	1.115663E+12
Emission mol/h	4.944865	14.8346	0
Emission kg/h	1	3	0
Fugacity Pa	3.535038E-10	2.803857E-12	1.139424E-11
Conc mol/m3	1.786693E-13	7.225036E-11	7.062297E-07
Conc g/m3	3.613229E-11	1.461119E-08	1.428208E-04
Conc ug/g	2.772047E-08	1.461107E-08	9.519733E-05
Amount mol	214.4032	17340.09	12.71213
Amount kg	43.35875	3506.686	2.570775
Amount %	1.091009	88.23651	6.468678E-02
Adv.flow m3/h	1.2E+13	2.4E+11	0
D rct mol/Pa.h	2.472415E+07	7.792305E+10	1.405735E+07
D adv mol/Pa.h	6.065088E+09	6.184369E+12	0
Rct rate mol/h	8.740081E-03	.2184851	1.601729E-04
Rct rate kg/h	1.767507E-03	4.418424E-02	3.239176E-05
Adv rate mol/h	2.144032	17.34008	0
Adv rate kg/h	.4335875	3.506685	0
Reaction %	4.418766E-02	1.104606	8.097941E-04
Advection %	10.83969	87.66712	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.2E+11		
Density kg/m3	1260		
Bulk Z value	7939.1		0
Bulk VZ	9.526919E+14	0	
Emission mol/h	0	19.77946	
Emission kg/h	0	4	
Fugacity Pa	2.188144E-12		2.803857E-12
Conc mol/m3	1.737189E-08		5.88636E-07
Conc g/m3	3.513118E-06		1.190399E-04
Conc ug/g	2.788189E-06		1.190399E-04
Amount mol	2084.627	19651.83	
Amount kg	421.5741	3974.189	
Amount %	10.6078		
Adv.flow m3/h	2400000		
D rct mol/Pa.h	1.200392E+10		
D adv mol/Pa.h	1.905384E+10		
Rct rate mol/h	.0262663	.2536516	
Rct rate kg/h	5.311834E-03	0	
Adv rate mol/h	4.169254E-02	19.52581	
Adv rate kg/h	8.431481E-03	3.948704	
Reaction %	.1327958		
Advection %	.210787		

Overall residence time   h   993.5472
Reaction residence time   h   77475.65
Advection residence time h   1006.454

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 5.6612E-01	5.3077E+01	1.5668E+13	7.9190E+09	2.7994E+00
Air to soil 3.3023E-05	9.0990E+05	9.1394E+08	4.6193E+05	1.6329E-04
Water to air 1.5065E-03	1.6131E+06	1.0311E+08	2.6569E+09	7.4495E-03
Water to sediment 1.9292E-02	1.2597E+05	1.3203E+09	3.4023E+10	9.5395E-02
Soil to air 5.3970E-08	3.3010E+07	3.7789E-01	2.3422E+04	2.6687E-07
Soil to water 5.7710E-07	3.0871E+06	4.0407E+00	2.5045E+05	2.8537E-06
Sediment to water 5.5485E-03	5.2654E+04	1.5794E+06	1.2539E+10	2.7436E-02

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   2.661532E+09   Air-water diffusion
(water-side)   1.518003E+12
Air-water diffusion (overall)   2.656873E+09
Rain dissolution to water   3.036005E+09   Aerosol deposition to
water   2.226074E+09
Rain dissolution to soil   253000.5   Aerosol deposition to
soil   185506.1
Soil-air diffusion (air-phase)   887.1772   Soil-air diffusion
(water-phase) 25300.04
Soil-air diffusion (bndry layer) 221794.3   Soil-air diffusion
(overall)   23421.81
Water-sediment diffusion   3.036005E+09
Water-sediment deposition   3.098684E+10   Sediment-water
resuspension   9.502631E+09
Soil-water runoff (water)   126500.2   Soil-water runoff
(solids)   123947.4

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
 Fate of HCBz at Danmark environment
Properties of HCBz :

Temperature deg C	7.5
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	4.483631E-03
Vapor pressure Pa	2.618343E-04
Sub-cooled liquid vapor press Pa	5.839784E-02
Solubility g/m3	1.068886E-02
Solubility mol/m3	3.75311E-05
Henry's law constant Pa.m3/mol	6.976462
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	2.989924E-03
Soil-water partition coefficient	6223.356
Sedt-water partition coefficient	11928.1
Susp sedt-water partn coeffnt	38895.98
Aerosol-air partition coeff	1.027435E+08
Aerosol Z value	44033.12
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	9.107876E-08
Total of VZ products	3.855165E+12

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.3E+13	1.224E+10	4.240001E+09
Density kg/m3	1.25933	1000	2400
Depth m	1000	20	.1
Area m2	4.3E+10	6.12E+08	4.24E+10
Frn org carb			.02
Z mol/m3.Pa	4.285731E-04	.1433391	892.0505
VZ mol/Pa	1.842864E+10	1.754471E+09	3.782294E+12
Fugacity Pa	9.107876E-08	9.107876E-08	9.107876E-08
Conc mol/m3	3.903391E-11	1.305515E-08	8.124685E-05
Conc g/m3	1.111686E-08	3.718107E-06	.0231391
Conc ug/g	8.827596E-06	3.718107E-06	9.641292E-03
Amount mol	1678.458	159.795	344486.6
Amount kg	478.0248	45.50962	98109.78
Amount %	.4780248	4.550962E-02	98.10979

Phase	Sediment	Susp sedt	Fish
Volume m3	3.06E+07	61200	12240
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	6.12E+08	0	0
Frn org carb	.04	.2	
Z mol/m3.Pa	1709.764	5575.316	2266.389
VZ mol/Pa	5.231877E+10	3.412094E+08	2.77406E+07
Fugacity Pa	9.107876E-08	9.107876E-08	9.107876E-08
Conc mol/m3	1.557231E-04	5.077928E-04	2.064199E-04
Conc g/m3	4.434995E-02	.1446194	5.878837E-02
Conc ug/g	1.928259E-02	9.641292E-02	5.878837E-02
Amount mol	4765.128	31.07692	2.526579
Amount kg	1357.108	8.850706	.7195696
Amount %	1.357108	8.850706E-03	7.195696E-04

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Danmark environment

Emission rate of chemical mol/h   15.09832
Emission rate of chemical kg/h   4.3
Fugacity Pa   6.392804E-08
Total amount of chemical mol   246453.1
Total amount of chemical kg   70189.85

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.3E+11	1.224E+07	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	6.392804E-08	6.392804E-08	6.392804E-08
Conc mol/m3	2.739784E-11	9.16339E-09	5.702704E-05
Conc g/m3	7.802905E-09	2.609734E-06	.0162413
Conc ug/g	6.196077E-06	2.609734E-06	6.767208E-03
Amount mol	1178.107	112.1599	241794.7
Amount kg	335.5249	31.94314	68863.11
Amount %	.4780248	4.550963E-02	98.10979
D rct mol/Pa.h	751238.3	22106.34	4.765691E+07
D adv mol/Pa.h	1.842865E+08	1754471	0
Rct rate mol/h	4.802519E-02	1.413215E-03	3.046613
Adv rate mol/h	11.78107	.1121599	0
Rct rate kg/h	1.367757E-02	4.024835E-04	.8676752
Adv rate kg/h	3.355249	3.194314E-02	0
Reaction %	.3180831	9.360081E-03	20.17849
Advection %	78.02904	.7428636	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	612		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	6.392804E-08	6.392804E-08	6.392804E-08
Conc mol/m3	1.093018E-04	3.56419E-04	1.448858E-04
Conc g/m3	3.112916E-02	.1015081	4.126347E-02
Conc ug/g	1.353442E-02	6.767208E-02	4.126347E-02
Amount mol	3344.636	21.81284	1.773402
Amount kg	952.5522	6.212297	.5050648
Amount %	1.357108	8.850706E-03	7.195696E-04
D rct mol/Pa.h	659216.5		
D adv mol/Pa.h	1046375		
Rct rate mol/h	4.214242E-02		
Adv rate mol/h	6.689271E-02		
Rct rate kg/h	1.200216E-02		
Adv rate kg/h	1.905105E-02		
Reaction %	.27912		
Advection %	.4430475		

Total advection D value   1.870873E+08
Total reaction D value   4.908947E+07
Total D value   2.361768E+08
Output by reaction   mol/h 3.138193
Output by advection   mol/h 11.96012
Total output by reaction and advection mol/h 15.09832
Output by reaction   kg/h .8937574
Output by advection   kg/h 3.406243
Total output by reaction and advection kg/h   4.3

Overall residence time   h   16323.22
Reaction residence time   h   78533.44
Advection residence time h   20606.24

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Danmark environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.3E+13	1.224E+10	7.632E+09
Density kg/m3	1.25933	1000.009	1500.252
Bulk Z value	4.294538E-04	.1734821	446.0684
Bulk VZ	1.846651E+10	2.123421E+09	3.404393E+12
Emission mol/h	.5266855	7.022473E-02	0
Emission kg/h	.15	.02	0
Fugacity Pa	2.876713E-09	1.566083E-08	1.405804E-10
Conc mol/m3	1.235415E-12	2.716873E-09	6.270845E-08
Conc g/m3	3.518463E-10	7.737654E-07	1.785937E-05
Conc ug/g	2.793917E-07	7.737588E-07	1.190425E-05
Amount mol	53.12287	33.25453	478.5909
Amount kg	15.12939	9.470888	136.3027
Amount %	4.100865	2.567112	36.94524
Adv.flow m3/h	4.3E+11	1.224E+07	0
D rct mol/Pa.h	752782	26755.11	4.289536E+07
D adv mol/Pa.h	1.846651E+08	2123421	0
Rct rate mol/h	2.165538E-03	4.19007E-04	6.030246E-03
Rct rate kg/h	6.167451E-04	1.193332E-04	1.717414E-03
Adv rate mol/h	.5312286	3.325453E-02	0
Adv rate kg/h	.1512939	9.470889E-03	0
Reaction %	.3627913	7.019599E-02	1.010243
Advection %	88.99641	5.571111	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.53E+08		
Density kg/m3	1260		
Bulk Z value	342.0674		0
Bulk VZ	5.233631E+10	0	
Emission mol/h	0	.5969101	
Emission kg/h	0	.17	
Fugacity Pa	1.395662E-08		1.566083E-08
Conc mol/m3	4.774104E-06		3.549352E-05
Conc g/m3	1.359665E-03		1.010855E-02
Conc ug/g	1.079099E-03		1.010855E-02
Amount mol	730.438	1295.406	
Amount kg	208.0287	368.9317	
Amount %	56.38678		
Adv.flow m3/h	3060		
D rct mol/Pa.h	659437.5		
D adv mol/Pa.h	1046726		
Rct rate mol/h	9.203518E-03	1.781831E-02	
Rct rate kg/h	2.621162E-03	0	
Adv rate mol/h	1.460876E-02	.5790919	
Adv rate kg/h	4.160574E-03	.1649254	
Reaction %	1.54186		
Advection %	2.447397		

Overall residence time   h   2170.186
Reaction residence time   h   72700.44
Advection residence time h   2236.961

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 8.4757E-04	1.2370E+04	2.4089E+09	1.0345E+06	2.9760E-03
Air to soil 1.7616E-03	5.9517E+03	5.0068E+09	2.1502E+06	6.1855E-03
Water to air 4.5029E-03	1.4576E+03	5.8195E+06	1.0096E+06	1.5811E-02
Water to sediment 7.6484E-03	8.5813E+02	9.8847E+06	1.7148E+06	2.6855E-02
Soil to air 1.6905E-05	5.5875E+06	9.4657E+02	4.2223E+05	5.9358E-05
Soil to water 2.7310E-05	3.4588E+06	1.5292E+03	6.8211E+05	9.5891E-05
Sediment to water 8.6670E-04	1.6634E+05	6.3744E+02	2.1805E+05	3.0432E-03

	Transport velocity parameters		m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values

Air-water diffusion (air-side)	1311434	Air-water diffusion (water-side)	4386178
Air-water diffusion (overall)	1009578		
Rain dissolution to water	8772.356	Aerosol deposition to water	16168.96
Rain dissolution to soil	607758	Aerosol deposition to soil	1120203
Soil-air diffusion (air-phase)	363430	Soil-air diffusion (water-phase)	60775.8
Soil-air diffusion (bndry layer)	9.085751E+07	Soil-air diffusion (overall)	422234.4
Water-sediment diffusion	8772.356		
Water-sediment deposition	1706047	Sediment-water resuspension	209275.1
Soil-water runoff (water)	303879	Soil-water runoff (solids)	378229.4

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Finland environment

Properties of HCBz :

Temperature deg C	2
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	3.513524E-03
Vapor pressure Pa	1.348626E-04
Sub-cooled liquid vapor press Pa	3.838385E-02
Solubility g/m3	8.688454E-03
Solubility mol/m3	3.050721E-05
Henry's law constant Pa.m3/mol	4.420679
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	1.932455E-03
Soil-water partition coefficient	15558.39
Sedt-water partition coefficient	23856.2
Susp sedt-water partn coeffnt	58343.97
Aerosol-air partition coeff	1.563157E+08
Aerosol Z value	68331.85
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	3.021393E-09
Total of VZ products	1.162125E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.37E+14	6.32E+11	3.05E+10
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.37E+11	3.16E+10	3.05E+11
Frn org carb			.05
Z mol/m3.Pa	4.371399E-04	.2262096	3519.457
VZ mol/Pa	1.473162E+11	1.429645E+11	1.073435E+14
Fugacity Pa	3.021393E-09	3.021393E-09	3.021393E-09
Conc mol/m3	1.320771E-12	6.834681E-10	1.063366E-05
Conc g/m3	3.761557E-10	1.946517E-07	3.028467E-03
Conc ug/g	2.928415E-07	1.946517E-07	1.261861E-03
Amount mol	445.1	431.9518	324326.7
Amount kg	126.7645	123.0199	92368.25
Amount %	.1267645	.1230199	92.36824

Phase	Sediment	Susp sedt	Fish
Volume m3	1.58E+09	3792000	632000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.16E+10	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	5396.501	13197.97	3576.685
VZ mol/Pa	8.526472E+12	5.004669E+10	2.260465E+09
Fugacity Pa	3.021393E-09	3.021393E-09	3.021393E-09
Conc mol/m3	1.630495E-05	3.987624E-05	1.080657E-05
Conc g/m3	4.64365E-03	1.135675E-02	3.077711E-03
Conc ug/g	2.018978E-03	7.571168E-03	3.077711E-03
Amount mol	25761.82	151.2107	6.829752
Amount kg	7336.966	43.06481	1.945113
Amount %	7.336966	4.306481E-02	1.945113E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Finland environment

Emission rate of chemical mol/h   119.382
Emission rate of chemical kg/h   34
Fugacity Pa   3.668301E-08
Total amount of chemical mol   4263025
Total amount of chemical kg   1214109

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.37E+12	6.32E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	3.668301E-08	3.668301E-08	3.668301E-08
Conc mol/m3	1.603561E-11	8.298049E-09	1.291043E-04
Conc g/m3	4.566941E-09	2.363284E-06	.0367689
Conc ug/g	3.555415E-06	2.363284E-06	1.532038E-02
Amount mol	5404	5244.367	3937681
Amount kg	1539.059	1493.596	1121451
Amount %	.1267645	.1230199	92.36824
D rct mol/Pa.h	6005300	1801352	1.352528E+09
D adv mol/Pa.h	1.473162E+09	1.429645E+08	0
Rct rate mol/h	.2202925	6.607902E-02	49.61478
Adv rate mol/h	54.04	5.244367	0
Rct rate kg/h	6.273929E-02	.0188193	14.13029
Adv rate kg/h	15.39059	1.493596	0
Reaction %	.1845273	5.535089E-02	41.55967
Advection %	45.26644	4.392928	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	31600		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	3.668301E-08	3.668301E-08	3.668301E-08
Conc mol/m3	1.979599E-04	4.841411E-04	1.312036E-04
Conc g/m3	5.637898E-02	.1378834	3.736677E-02
Conc ug/g	.0245126	9.192224E-02	3.736677E-02
Amount mol	312776.6	1835.863	82.92064
Amount kg	89078.78	522.8538	23.6158
Amount %	7.336965	.0430648	1.945113E-03
D rct mol/Pa.h	1.074336E+08		
D adv mol/Pa.h	1.705294E+08		
Rct rate mol/h	3.940986		
Adv rate mol/h	6.255533		
Rct rate kg/h	1.122393		
Adv rate kg/h	1.781576		
Reaction %	3.301155		
Advection %	5.239928		

Total advection D value   1.786655E+09
Total reaction D value   1.467768E+09
Total D value   3.254423E+09
Output by reaction   mol/h 53.84214
Output by advection   mol/h 65.5399
Total output by reaction and advection mol/h   119.382
Output by reaction   kg/h   15.33424
Output by advection   kg/h   18.66576
Total output by reaction and advection kg/h   34

Overall residence time   h   35709.1
Reaction residence time   h   79176.36
Advection residence time h   65044.73

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Finland environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.37E+14	6.32E+11	5.49E+10
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.385066E-04	.2957761	1759.797
Bulk VZ	1.477767E+11	1.869305E+11	9.661283E+13
Emission mol/h	1.053371	1.509832	.5969101
Emission kg/h	.3	.43	.17
Fugacity Pa	8.077387E-10	3.631999E-09	4.982657E-10
Conc mol/m3	3.541987E-13	1.074259E-09	8.768463E-07
Conc g/m3	1.008758E-10	3.059489E-07	2.497258E-04
Conc ug/g	7.853295E-08	3.059462E-07	1.664554E-04
Amount mol	119.365	678.9315	48138.86
Amount kg	33.99514	193.3597	13709.95
Amount %	.1667839	.9486439	67.26251
Adv.flow m3/h	3.37E+12	6.32E+08	0
D rct mol/Pa.h	6024074	2355325	1.217322E+09
D adv mol/Pa.h	1.477767E+09	1.869305E+08	0
Rct rate mol/h	4.865877E-03	8.554537E-03	.6065497
Rct rate kg/h	1.385802E-03	2.436332E-03	.1727454
Adv rate mol/h	1.19365	.6789315	0
Adv rate kg/h	.3399514	.1933597	0
Reaction %	.1506306	.2648187	18.77667
Advection %	36.95124	21.01736	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	7.900001E+09		
Density kg/m3	1260		
Bulk Z value	1079.481		0
Bulk VZ	8.527901E+12	0	
Emission mol/h	7.022473E-02	3.230337	
Emission kg/h	.02	.92	
Fugacity Pa	2.653816E-09		3.631999E-09
Conc mol/m3	2.864744E-06		1.299052E-05
Conc g/m3	8.15879E-04		3.699699E-03
Conc ug/g	6.475231E-04		3.699699E-03
Amount mol	22631.48	71568.63	
Amount kg	6445.444	20382.75	
Amount %	31.62206		
Adv.flow m3/h	158000		
D rct mol/Pa.h	1.074516E+08		
D adv mol/Pa.h	1.70558E+08		
Rct rate mol/h	.2851566	.9051267	
Rct rate kg/h	.0812126	0	
Adv rate mol/h	.4526296	2.325211	
Adv rate kg/h	.1289089	.66222	
Reaction %	8.827456		
Advection %	14.01184		

Overall residence time   h   22155.16
Reaction residence time   h   79070.28
Advection residence time h   30779.42

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
kg/h	h	m3/h	mol/Pa.h	mol/h
Air to water 1.3778E-02	1.7099E+03	1.3658E+11	5.9893E+07	4.8378E-02
Air to soil 5.2321E-03	4.5027E+03	5.1866E+10	2.2744E+07	1.8371E-02
Water to air 5.9873E-02	2.2380E+03	1.9570E+08	5.7883E+07	2.1023E-01
Water to sediment 2.1644E-01	6.1910E+02	7.0744E+08	2.0924E+08	7.5997E-01
Soil to air 4.7392E-04	2.0048E+07	1.8978E+03	3.3397E+06	1.6640E-03
Soil to water 2.0128E-03	4.7203E+06	8.0600E+03	1.4184E+07	7.0674E-03
Sediment to water 2.6318E-02	1.6972E+05	3.2257E+04	3.4821E+07	9.2408E-02

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side) 6.906811E+07   Air-water diffusion
(water-side) 3.574112E+08
Air-water diffusion (overall)   5.788257E+07
Rain dissolution to water   714822.3   Aerosol deposition to
water   1295572
Rain dissolution to soil   6899392   Aerosol deposition to
soil   1.250473E+07
Soil-air diffusion (air-phase)   2666553   Soil-air diffusion
(water-phase) 689939.2
Soil-air diffusion (bndry layer)   6.666383E+08   Soil-air diffusion
(overall)   3339677
Water-sediment diffusion   714822.3
Water-sediment deposition   2.085278E+08   Sediment-water
resuspension   3.410589E+07
Soil-water runoff (water)   3449696   Soil-water runoff
(solids)   1.073434E+07

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Norway environment

Properties of HCBz :
Temperature deg C	5
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	4.018081E-03
Vapor pressure Pa	1.942982E-04
Sub-cooled liquid vapor press Pa	4.835596E-02
Solubility g/m3	9.737973E-03
Solubility mol/m3	3.419232E-05
Henry's law constant Pa.m3/mol	5.682509
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	2.45726E-03
Soil-water partition coefficient	15558.39
Sedt-water partition coefficient	23856.2
Susp sedt-water partn coeffnt	58343.97
Aerosol-air partition coeff	1.240799E+08
Aerosol Z value	53655.24
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	3.965075E-09
Total of VZ products	8.85541E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.24E+14	1E+11	3.19E+10
Density kg/m3	1.270649	1000	2400
Depth m	1000	20	.1
Area m2	3.24E+11	5E+09	3.19E+11
Frn org carb			.05
Z mol/m3.Pa	4.324251E-04	.1759786	2737.944
VZ mol/Pa	1.401057E+11	1.759786E+10	8.734041E+13
Fugacity Pa	3.965075E-09	3.965075E-09	3.965075E-09
Conc mol/m3	1.714598E-12	6.977684E-10	1.085615E-05
Conc g/m3	4.883175E-10	1.987244E-07	3.091833E-03
Conc ug/g	3.843057E-07	1.987244E-07	1.288264E-03
Amount mol	555.5298	69.77684	346311.3
Amount kg	158.2149	19.87244	98629.44
Amount %	.1582149	1.987244E-02	98.62945

Phase	Sediment	Susp sedt	Fish
Volume m3	2.5E+08	600000	100000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	5E+09	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	4198.181	10267.29	2782.464
VZ mol/Pa	1.049545E+12	6.160375E+09	2.782463E+08
Fugacity Pa	3.965075E-09	3.965075E-09	3.965075E-09
Conc mol/m3	1.66461E-05	4.071058E-05	1.103268E-05
Conc g/m3	4.74081E-03	1.159437E-02	3.142106E-03
Conc ug/g	2.061222E-03	7.729581E-03	3.142106E-03
Amount mol	4161.526	24.42635	1.103268
Amount kg	1185.203	6.956623	.3142106
Amount %	1.185203	6.956623E-03	3.142106E-04

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Norway environment

Emission rate of chemical mol/h   112.3596
Emission rate of chemical kg/h   32
Fugacity Pa   4.390258E-08
Total amount of chemical mol   3887754
Total amount of chemical kg   1107232

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.24E+12	1E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.390258E-08	4.390258E-08	4.390258E-08
Conc mol/m3	1.898458E-11	7.725915E-09	1.202028E-04
Conc g/m3	5.406808E-09	2.200341E-06	3.423376E-02
Conc ug/g	4.255156E-06	2.200341E-06	1.426407E-02
Amount mol	6151.004	772.5915	3834470
Amount kg	1751.806	220.0341	1092057
Amount %	.1582148	1.987244E-02	98.62944
D rct mol/Pa.h	5711369	221733.1	1.100489E+09
D adv mol/Pa.h	1.401057E+09	1.759786E+07	0
Rct rate mol/h	.2507438	9.734653E-03	48.31432
Adv rate mol/h	61.51004	.7725915	0
Rct rate kg/h	7.141184E-02	2.772429E-03	13.75992
Adv rate kg/h	17.51806	.2200341	0
Reaction %	.223162	8.663841E-03	42.99974
Advection %	54.74393	.6876064	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	5000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.390258E-08	4.390258E-08	4.390258E-08
Conc mol/m3	1.84311E-04	4.507606E-04	1.221573E-04
Conc g/m3	5.249177E-02	.1283766	3.479041E-02
Conc ug/g	2.282251E-02	.0855844	3.479041E-02
Amount mol	46077.75	270.4563	12.21573
Amount kg	13122.94	77.02596	3.479041
Amount %	1.185203	6.956623E-03	3.142106E-04
D rct mol/Pa.h	1.322427E+07		
D adv mol/Pa.h	2.099091E+07		
Rct rate mol/h	.5805796		
Adv rate mol/h	.921555		
Rct rate kg/h	.1653491		
Adv rate kg/h	.2624589		
Reaction %	.5167158		
Advection %	.8201839		

Total advection D value   1.439646E+09
Total reaction D value   1.119647E+09
Total D value   2.559293E+09
Output by reaction   mol/h 49.15538
Output by advection   mol/h 63.20418
Total output by reaction and advection mol/h   112.3596
Output by reaction   kg/h   13.99945
Output by advection   kg/h   18.00055
Total output by reaction and advection kg/h   32

Overall residence time   h   34601.01
Reaction residence time   h   79091.12
Advection residence time h   61511.02

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Norway environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.24E+14	1E+11	5.742E+10
Density kg/m3	1.270649	1000.009	1500.254
Bulk Z value	4.334983E-04	.2300975	1369.025
Bulk VZ	1.404534E+11	2.300975E+10	7.86094E+13
Emission mol/h	1.158708	3.511236E-02	.1755618
Emission kg/h	.33	.01	.05
Fugacity Pa	8.109026E-10	8.118775E-10	1.90109E-10
Conc mol/m3	3.515248E-13	1.86811E-10	2.60264E-07
Conc g/m3	1.001143E-10	5.320377E-08	7.412319E-05
Conc ug/g	7.878988E-08	5.320332E-08	4.940709E-05
Amount mol	113.894	18.6811	14944.36
Amount kg	32.43702	5.320377	4256.154
Amount %	.7278981	.1193911	95.50958
Adv.flow m3/h	3.24E+12	1E+08	0
D rct mol/Pa.h	5725542	289922.9	9.904784E+08
D adv mol/Pa.h	1.404534E+09	2.300975E+07	0
Rct rate mol/h	4.642857E-03	2.353819E-04	.1882989
Rct rate kg/h	1.322286E-03	6.703676E-05	5.362753E-02
Adv rate mol/h	1.138941	.0186811	0
Adv rate kg/h	.3243702	5.320377E-03	0
Reaction %	.3390476	1.718891E-02	13.75065
Advection %	83.17185	1.364199	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.25E+09		
Density kg/m3	1260		
Bulk Z value	839.7771		0
Bulk VZ	1.049721E+12	0	
Emission mol/h	0	1.369382	
Emission kg/h	0	.39	
Fugacity Pa	5.430401E-10		8.118775E-10
Conc mol/m3	4.560326E-07		2.259019E-06
Conc g/m3	1.298781E-04		6.433687E-04
Conc ug/g	1.030779E-04		6.433687E-04
Amount mol	570.0408	15646.98	
Amount kg	162.3476	4456.259	
Amount %	3.643137		
Adv.flow m3/h	25000		
D rct mol/Pa.h	1.322649E+07		
D adv mol/Pa.h	2.099443E+07		
Rct rate mol/h	7.182515E-03	.2003597	
Rct rate kg/h	2.04558E-03	0	
Adv rate mol/h	1.140082E-02	1.169022	
Adv rate kg/h	3.246952E-03	.3329376	
Reaction %	.5245077		
Advection %	.8325518		

Overall residence time   h   11426.31
Reaction residence time   h   78094.4
Advection residence time h   13384.67

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 2.0617E-03	1.0903E+04	2.0593E+10	8.9271E+06	7.2390E-03
Air to soil 4.4313E-03	5.0727E+03	4.4262E+10	1.9188E+07	1.5559E-02
Water to air 2.0066E-03	1.8375E+03	3.7715E+07	8.6782E+06	7.0456E-03
Water to sediment 5.9554E-03	6.1910E+02	1.1194E+08	2.5756E+07	2.0911E-02
Soil to air 1.7891E-04	1.6486E+07	2.4136E+03	3.3043E+06	6.2818E-04
Soil to water 6.2486E-04	4.7203E+06	8.4300E+03	1.1541E+07	2.1940E-03
Sediment to water 6.6289E-04	1.6972E+05	5.1039E+03	4.2862E+06	2.3276E-03

	Transport velocity parameters		m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values

Air-water diffusion (air-side)   1.081063E+07   Air-water diffusion
(water-side)   4.399465E+07
Air-water diffusion (overall)   8678175
Rain dissolution to water   87989.31   Aerosol deposition to
water   160965.7
Rain dissolution to soil   5613718   Aerosol deposition to
soil   1.026961E+07
Soil-air diffusion (air-phase)   2758872   Soil-air diffusion
(water-phase)   561371.8
Soil-air diffusion (bndry layer) 6.89718E+08   Soil-air diffusion
(overall)   3304337
Water-sediment diffusion   87989.31
Water-sediment deposition   2.566823E+07   Sediment-water
resuspension   4198181
Soil-water runoff (water)   2806859   Soil-water runoff
(solids)   8734041

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Sweden environment

Properties of HCBz :
Temperature deg C	4
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	3.84356E-03
Vapor pressure Pa	1.721833E-04
Sub-cooled liquid vapor press Pa	4.479788E-02
Solubility g/m3	9.377321E-03
Solubility mol/m3	3.292599E-05
Henry's law constant Pa.m3/mol	5.229405
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	2.269485E-03
Soil-water partition coefficient	12446.71
Sedt-water partition coefficient	17892.15
Susp sedt-water partn coeffnt	48619.97
Aerosol-air partition coeff	1.339349E+08
Aerosol Z value	58125.8
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	3.350486E-09
Total of VZ products	1.047978E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+14	7.7E+11	4.11E+10
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+11	3.85E+10	4.11E+11
Frn org carb			.04
Z mol/m3.Pa	4.339854E-04	.1912264	2380.139
VZ mol/Pa	1.952934E+11	1.472443E+11	9.782372E+13
Fugacity Pa	3.350486E-09	3.350486E-09	3.350486E-09
Conc mol/m3	1.454062E-12	6.407011E-10	7.974621E-06
Conc g/m3	4.141168E-10	1.824717E-07	2.271172E-03
Conc ug/g	3.24738E-07	1.824717E-07	9.463217E-04
Amount mol	654.3278	493.3399	327757
Amount kg	186.3525	140.5032	93345.18
Amount %	.1863525	.1405032	93.34517

Phase	Sediment	Susp sedt	Fish
Volume m3	1.925E+09	4620001	770000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.85E+10	0	0
Frn org carb	.06	.25	
Z mol/m3.Pa	3421.45	9297.419	3023.551
VZ mol/Pa	6.586292E+12	4.295408E+10	2.328135E+09
Fugacity Pa	3.350486E-09	3.350486E-09	3.350486E-09
Conc mol/m3	1.146352E-05	3.115087E-05	1.013037E-05
Conc g/m3	3.26481E-03	8.871767E-03	2.885128E-03
Conc ug/g	1.419483E-03	5.914511E-03	2.885128E-03
Amount mol	22067.27	143.917	7.800381
Amount kg	6284.759	40.98757	2.221548
Amount %	6.284759	4.098757E-02	2.221548E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Sweden environment

Emission rate of chemical mol/h   158.0056
Emission rate of chemical kg/h   45
Fugacity Pa   4.441746E-08
Total amount of chemical mol   4654853
Total amount of chemical kg   1325702

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+12	7.7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.441746E-08	4.441746E-08	4.441746E-08
Conc mol/m3	1.927653E-11	8.493788E-09	1.057197E-04
Conc g/m3	5.489954E-09	2.419031E-06	3.010898E-02
Conc ug/g	4.305058E-06	2.419031E-06	1.254541E-02
Amount mol	8674.436	6540.217	4345081
Amount kg	2470.479	1862.654	1237479
Amount %	.1863525	.1405032	93.34517
D rct mol/Pa.h	7961079	1855278	1.232579E+09
D adv mol/Pa.h	1.952934E+09	1.472443E+08	0
Rct rate mol/h	.3536108	8.240674E-02	54.74802
Adv rate mol/h	86.74436	6.540217	0
Rct rate kg/h	.1007084	2.346944E-02	15.59224
Adv rate kg/h	24.70479	1.862654	0
Reaction %	.2237964	5.215431E-02	34.64942
Advection %	54.89955	4.139231	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	38500		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.441746E-08	4.441746E-08	4.441746E-08
Conc mol/m3	1.519721E-04	4.129677E-04	1.342985E-04
Conc g/m3	4.328166E-02	.1176132	.0382482
Conc ug/g	1.881811E-02	.0784088	.0382482
Amount mol	292546.3	1907.911	103.4098
Amount kg	83317.19	543.373	29.45111
Amount %	6.28476	4.098757E-02	2.221548E-03
D rct mol/Pa.h	8.298728E+07		
D adv mol/Pa.h	1.317258E+08		
Rct rate mol/h	3.686084		
Adv rate mol/h	5.850927		
Rct rate kg/h	1.049797		
Adv rate kg/h	1.666344		
Reaction %	2.332881		
Advection %	3.702987		

Total advection D value   2.231904E+09
Total reaction D value   1.325383E+09
Total D value   3.557287E+09
Output by reaction   mol/h 58.87012
Output by advection   mol/h 99.13551
Total output by reaction and advection mol/h   158.0056
Output by reaction   kg/h   16.76621
Output by advection   kg/h   28.23379
Total output by reaction and advection kg/h   45

Overall residence time   h   29460.05
Reaction residence time   h   79069.88
Advection residence time h   46954.45

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Sweden environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+14	7.7E+11	7.398E+10
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.351479E-04	.240737	1190.127
Bulk VZ	1.958166E+11	1.853675E+11	8.804561E+13
Emission mol/h	1.650281	.5266855	.1404495
Emission kg/h	.47	.15	.04
Fugacity Pa	8.471026E-10	1.417721E-09	1.445063E-10
Conc mol/m3	3.686149E-13	3.412979E-10	1.719809E-07
Conc g/m3	1.049815E-10	9.720164E-08	4.898015E-05
Conc ug/g	8.232338E-08	9.720082E-08	3.264789E-05
Amount mol	165.8767	262.7994	12723.15
Amount kg	47.24169	74.84527	3623.552
Amount %	.8177988	1.295643	62.72714
Adv.flow m3/h	4.5E+12	7.7E+08	0
D rct mol/Pa.h	7982404	2335631	1.109375E+09
D adv mol/Pa.h	1.958166E+09	1.853675E+08	0
Rct rate mol/h	6.761915E-03	3.311273E-03	.1603116
Rct rate kg/h	1.925793E-03	9.430504E-04	4.565675E-02
Adv rate mol/h	1.658767	.2627994	0
Adv rate kg/h	.4724169	7.484526E-02	0
Reaction %	.2909053	.1424547	6.896791
Advection %	71.36207	11.30593	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	9.625E+09		
Density kg/m3	1260		
Bulk Z value	684.443		0
Bulk VZ	6.587764E+12	0	
Emission mol/h	7.022472E-03	2.324438	
Emission kg/h	.002	.662	
Fugacity Pa	1.082536E-09		1.417721E-09
Conc mol/m3	7.409345E-07		4.286552E-06
Conc g/m3	2.110181E-04		1.22081E-03
Conc ug/g	1.674747E-04		1.22081E-03
Amount mol	7131.494	20283.32	
Amount kg	2031.05	5776.688	
Amount %	35.15941		
Adv.flow m3/h	192500		
D rct mol/Pa.h	8.300583E+07		
D adv mol/Pa.h	1.317553E+08		
Rct rate mol/h	8.985682E-02	.2602417	
Rct rate kg/h	2.559122E-02	0	
Adv rate mol/h	.1426299	2.064197	
Adv rate kg/h	4.062099E-02	.5878832	
Reaction %	3.865744		
Advection %	6.136101		

Overall residence time   h   8726.115
Reaction residence time   h   77940.29
Advection residence time h   9826.252

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 1.6928E-02	1.9339E+03	1.6125E+11	7.0168E+07	5.9440E-02
Air to soil 6.3994E-03	5.1159E+03	6.0957E+10	2.6525E+07	2.2470E-02
Water to air 2.7492E-02	1.8866E+03	2.8284E+08	6.8089E+07	9.6532E-02
Water to sediment 7.2562E-02	7.1481E+02	7.4651E+08	1.7971E+08	2.5478E-01
Soil to air 1.7829E-04	1.4084E+07	3.6401E+03	4.3322E+06	6.2602E-04
Soil to water 5.6433E-04	4.4498E+06	1.1522E+04	1.3712E+07	1.9815E-03
Sediment to water 8.3494E-03	1.6858E+05	3.9567E+04	2.7081E+07	2.9317E-02

Transport velocity parameters		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values

Air-water diffusion (air-side) 8.35422E+07 Air-water diffusion (water-side) 3.681107E+08

Air-water diffusion (overall) 6.80894E+07

Rain dissolution to water 736221.5 Aerosol deposition to water 1342706

Rain dissolution to soil 7859403 Aerosol deposition to soil 1.433382E+07

Soil-air diffusion (air-phase) 3567360 Soil-air diffusion (water-phase) 785940.3

Soil-air diffusion (bndry layer) 8.918399E+08 Soil-air diffusion (overall) 4332154

Water-sediment diffusion 736221.5

Water-sediment deposition 1.789753E+08 Sediment-water resuspension 2.634517E+07

Soil-water runoff (water) 3929702 Soil-water runoff (solids) 9782372

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Nordic Sea areas environment

Properties of HCBz :

Temperature deg C	6
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	4.19919E-03
Vapor pressure Pa	2.190635E-04
Sub-cooled liquid vapor press Pa	5.216803E-02
Solubility g/m3	1.010976E-02
Solubility mol/m3	3.549774E-05
Henry's law constant Pa.m3/mol	6.171194
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	2.65902E-03
Soil-water partition coefficient	9335.034
Sedt-water partition coefficient	14910.12
Susp sedt-water partn coeffnt	77791.96
Aerosol-air partition coeff	1.15013E+08
Aerosol Z value	49556.34
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	1.70082E-07
Total of VZ products	2.064437E+12

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.5E+14	7E+11	3E+07
Density kg/m3	1.266097	1000	2400
Depth m	1000	20	.1
Area m2	3.5E+11	3.5E+10	3E+08
Frn org carb			.03
Z mol/m3.Pa	4.308761E-04	.1620432	1512.679
VZ mol/Pa	1.508066E+11	1.134302E+11	4.538037E+10
Fugacity Pa	1.70082E-07	1.70082E-07	1.70082E-07
Conc mol/m3	7.328426E-11	2.756063E-08	2.572794E-04
Conc g/m3	2.087136E-08	7.849267E-06	7.327318E-02
Conc ug/g	1.64848E-05	7.849267E-06	3.053049E-02
Amount mol	25649.49	19292.44	7718.383
Amount kg	7304.974	5494.487	2198.195
Amount %	7.304973	5.494487	2.198195

Phase	Sediment	Susp sedt	Fish
Volume m3	7E+08	4900000	700000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	2416.084	12605.66	2562.126
VZ mol/Pa	1.691259E+12	6.176772E+10	1.793488E+09
Fugacity Pa	1.70082E-07	1.70082E-07	1.70082E-07
Conc mol/m3	4.109324E-04	2.143995E-03	4.357714E-04
Conc g/m3	.1170335	.6106098	.1241077
Conc ug/g	5.088415E-02	.4070732	.1241077
Amount mol	287652.7	10505.58	305.04
Amount kg	81923.48	2991.988	86.87538
Amount %	81.92348	2.991988	8.687538E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
Fate of HCBz at Nordic Sea areas environment

```
Emission rate of chemical mol/h      122.8933
Emission rate of chemical  kg/h      35
Fugacity Pa                          7.294323E-08
Total amount of chemical mol         150586.7
Total amount of chemical kg          42887.1
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.5E+12	7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	7.294323E-08	7.294323E-08	7.294323E-08
Conc mol/m3	3.142949E-11	1.181995E-08	1.103397E-04
Conc g/m3	8.951117E-09	3.366323E-06	3.142474E-02
Conc ug/g	7.069852E-06	3.366323E-06	1.309364E-02
Amount mol	11000.32	8273.967	3310.19
Amount kg	3132.891	2356.426	942.7421
Amount %	7.304974	5.494487	2.198196
D rct mol/Pa.h	6147587	1429221	571792.6
D adv mol/Pa.h	1.508066E+09	1.134302E+08	0
Rct rate mol/h	.4484248	.104252	.0417084
Adv rate mol/h	110.0032	8.273967	0
Rct rate kg/h	.1277114	2.969097E-02	1.187855E-02
Adv rate kg/h	31.32891	2.356426	0
Reaction %	.3648896	8.483131E-02	3.393872E-02
Advection %	89.51116	6.732644	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	14000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	7.294323E-08	7.294323E-08	7.294323E-08
Conc mol/m3	1.76237E-04	9.194973E-04	1.868897E-04
Conc g/m3	5.019229E-02	.2618728	5.322618E-02
Conc ug/g	2.182273E-02	.1745819	5.322618E-02
Amount mol	123365.9	4505.537	130.8228
Amount kg	35134.6	1283.177	37.25833
Amount %	81.92349	2.991989	8.687539E-02
D rct mol/Pa.h	2.130987E+07		
D adv mol/Pa.h	3.382518E+07		
Rct rate mol/h	1.55441		
Adv rate mol/h	2.467318		
Rct rate kg/h	.442696		
Adv rate kg/h	.7026921		
Reaction %	1.264846		
Advection %	2.007691		

```
Total advection D value          1.655321E+09
Total reaction D value           2.945847E+07
Total D value                    1.68478E+09
Output by reaction      mol/h    2.148795
Output by advection     mol/h    120.7445
Total output by reaction and advection mol/h   122.8933
Output by reaction      kg/h     .6119769
Output by advection     kg/h     34.38802
Total output by reaction and advection kg/h      35
```

```
Overall residence time    h    1225.345
Reaction residence time   h    70079.6
Advection residence time  h    1247.152
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Nordic Sea areas environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.5E+14	7E+11	5.4E+07
Density kg/m3	1.266097	1000.009	1500.253
Bulk Z value	4.318672E-04	.2276336	756.3881
Bulk VZ	1.511535E+11	1.593435E+11	4.084496E+10
Emission mol/h	1.158708	.9480338	0
Emission kg/h	.33	.27	0
Fugacity Pa	8.307837E-10	2.568713E-09	2.666234E-11
Conc mol/m3	3.587882E-13	5.847255E-10	2.016708E-08
Conc g/m3	1.021829E-10	1.665298E-07	5.743583E-06
Conc ug/g	8.070701E-08	1.665284E-07	3.828409E-06
Amount mol	125.5759	409.3078	1.089022
Amount kg	35.76401	116.5709	.3101535
Amount %	.9120428	2.972755	7.90944E-03
Adv.flow m3/h	3.5E+12	7E+08	0
D rct mol/Pa.h	6161728	2007729	514646.5
D adv mol/Pa.h	1.511535E+09	1.593435E+08	0
Rct rate mol/h	5.119063E-03	5.157279E-03	1.372168E-05
Rct rate kg/h	1.457909E-03	1.468793E-03	3.907934E-06
Adv rate mol/h	1.255759	.4093078	0
Adv rate kg/h	.3576401	.1165709	0
Reaction %	.2429849	.2447989	6.513224E-04
Advection %	59.60668	19.42848	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.5E+09		
Density kg/m3	1260		
Bulk Z value	483.3465		0
Bulk VZ	1.691713E+12	0	
Emission mol/h	0	2.106742	
Emission kg/h	0	.6	
Fugacity Pa	7.822053E-09		2.568713E-09
Conc mol/m3	3.780762E-06		6.581366E-06
Conc g/m3	1.076761E-03		1.874373E-03
Conc ug/g	8.54572E-04		1.874373E-03
Amount mol	13232.67	13768.64	
Amount kg	3768.663	3921.308	
Amount %	96.10729		
Adv.flow m3/h	70000		
D rct mol/Pa.h	2.131558E+07		
D adv mol/Pa.h	3.383426E+07		
Rct rate mol/h	.1667316	.1770217	
Rct rate kg/h	4.748516E-02	0	
Adv rate mol/h	.2646533	1.92972	
Adv rate kg/h	7.537326E-02	.5495841	
Reaction %	7.914194		
Advection %	12.56221		

```
Overall residence time    h    6535.514
Reaction residence time   h    77779.35
Advection residence time  h    7135.045
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 1.4474E-02	1.7124E+03	1.4165E+11	6.1173E+07	5.0821E-02
Air to soil 3.9841E-06	6.2209E+06	3.8990E+07	1.6838E+04	1.3989E-05
Water to air 4.3576E-02	1.8539E+03	2.6167E+08	5.9565E+07	1.5301E-01
Water to sediment 1.6180E-01	4.9929E+02	9.7159E+08	2.2117E+08	5.6811E-01
Soil to air 2.3212E-08	9.2597E+06	4.0414E+00	3.0569E+03	8.1503E-08
Soil to water 5.2916E-08	4.0618E+06	9.2131E+00	6.9687E+03	1.8580E-07
Sediment to water 3.8940E-02	6.7069E+04	3.6164E+04	1.7480E+07	1.3673E-01

Transport velocity parameters　　　　　　　　　　　m/h　　　　　　m/year

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values

Air-water diffusion (air-side) 7.540331E+07　　　Air-water diffusion (water-side) 2.835756E+08

Air-water diffusion (overall) 5.956489E+07

Rain dissolution to water 567151.2　　　Aerosol deposition to water 1040683

Rain dissolution to soil 4861.296　　　Aerosol deposition to soil 8920.139

Soil-air diffusion (air-phase) 2585.256　　　Soil-air diffusion (water-phase) 486.1296

Soil-air diffusion (bndry layer) 646314.1　　　Soil-air diffusion (overall) 3056.859

Water-sediment diffusion 567151.2

Water-sediment deposition 2.20599E+08　　　Sediment-water resuspension 1.691259E+07

Soil-water runoff (water) 2430.648　　　Soil-water runoff (solids) 4538.037

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Nordic Countries environment

Properties of HCBz :

Temperature deg C	4
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	3.84356E-03
Vapor pressure Pa	1.721833E-04
Sub-cooled liquid vapor press Pa	4.479788E-02
Solubility g/m3	9.377321E-03
Solubility mol/m3	3.292599E-05
Henry's law constant Pa.m3/mol	5.229405
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	2.269485E-03
Soil-water partition coefficient	9335.035
Sedt-water partition coefficient	14910.12
Susp sedt-water partn coeffnt	77791.95
Aerosol-air partition coeff	1.339349E+08
Aerosol Z value	58125.8
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	1.607034E-09
Total of VZ products	2.184917E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.5E+15	8.52E+12	1.07E+11
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	1.5E+12	4.26E+11	1.07E+12
Frn org carb			.03
Z mol/m3.Pa	4.339854E-04	.1912264	1785.105
VZ mol/Pa	6.509781E+11	1.629248E+12	1.910062E+14
Fugacity Pa	1.607034E-09	1.607034E-09	1.607034E-09
Conc mol/m3	6.974294E-13	3.073073E-10	2.868725E-06
Conc g/m3	1.986279E-10	8.752112E-08	8.170128E-04
Conc ug/g	1.557581E-07	8.752112E-08	3.40422E-04
Amount mol	1046.144	2618.258	306953.5
Amount kg	297.9418	745.68	87420.35
Amount %	.2979418	.74568	87.42035

Phase	Sediment	Susp sedt	Fish
Volume m3	8.519999E+09	5.964E+07	8520000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.26E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	2851.209	14875.87	3023.551
VZ mol/Pa	2.42923E+13	8.871969E+11	2.576066E+10
Fugacity Pa	1.607034E-09	1.607034E-09	1.607034E-09
Conc mol/m3	4.58199E-06	2.390604E-05	4.858951E-06
Conc g/m3	1.304951E-03	6.808439E-03	1.383829E-03
Conc ug/g	5.673699E-04	4.538959E-03	1.383829E-03
Amount mol	39038.56	1425.756	41.39826
Amount kg	11118.18	406.0553	11.79023
Amount %	11.11818	.4060553	1.179022E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Nordic Countries environment

Emission rate of chemical mol/h   526.6855
Emission rate of chemical kg/h   150
Fugacity Pa   4.626256E-08
Total amount of chemical mol   1.010798E+07
Total amount of chemical kg   2878753

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.5E+13	8.52E+09	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.626256E-08	4.626256E-08	4.626256E-08
Conc mol/m3	2.007727E-11	8.846619E-09	8.25835E-05
Conc g/m3	5.718007E-09	2.519517E-06	2.351978E-02
Conc ug/g	4.483891E-06	2.519517E-06	9.799909E-03
Amount mol	30115.91	75373.2	8836434
Amount kg	8577.011	21466.28	2516616
Amount %	.2979418	.7456799	87.42035
D rct mol/Pa.h	2.653693E+07	2.052853E+07	2.406678E+09
D adv mol/Pa.h	6.509781E+09	1.629249E+09	0
Rct rate mol/h	1.227666	.9497022	111.3391
Adv rate mol/h	301.1591	75.3732	0
Rct rate kg/h	.3496394	.2704752	31.70937
Adv rate kg/h	85.77011	21.46629	0
Reaction %	.2330929	.1803168	21.13958
Advection %	57.18008	14.31086	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	170400		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.626256E-08	4.626256E-08	4.626256E-08
Conc mol/m3	1.319042E-04	6.881958E-04	1.398772E-04
Conc g/m3	3.756631E-02	.1959982	3.983703E-02
Conc ug/g	1.633318E-02	.1306654	3.983703E-02
Amount mol	1123824	41044	1191.754
Amount kg	320065	11689.33	339.4115
Amount %	11.11818	.4060553	1.179022E-02
D rct mol/Pa.h	3.06083E+08		
D adv mol/Pa.h	4.858459E+08		
Rct rate mol/h	14.16018		
Adv rate mol/h	22.47647		
Rct rate kg/h	4.032819		
Adv rate kg/h	6.401299		
Reaction %	2.688546		
Advection %	4.267533		

Total advection D value   8.624876E+09
Total reaction D value   2.759827E+09
Total D value   1.13847E+10
Output by reaction   mol/h   127.6766
Output by advection   mol/h   399.0088
Total output by reaction and advection mol/h   526.6854
Output by reaction   kg/h   36.3623
Output by advection   kg/h   113.6377
Total output by reaction and advection kg/h   150

Overall residence time   h   19191.69
Reaction residence time   h   79168.63
Advection residence time h   25332.74

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Nordic Countries environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.5E+15	8.52E+12	1.926E+11
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.351479E-04	.2686293	892.6098
Bulk VZ	6.527219E+11	2.288721E+12	1.719166E+14
Emission mol/h	6.320225	1.053371	.2106742
Emission kg/h	1.8	.3	.06
Fugacity Pa	8.874043E-10	3.24591E-10	1.232373E-10
Conc mol/m3	3.861521E-13	8.719462E-11	1.100028E-07
Conc g/m3	1.099761E-10	2.483303E-08	3.13288E-05
Conc ug/g	8.623999E-08	2.483282E-08	2.088232E-05
Amount mol	579.2281	742.8982	21186.54
Amount kg	164.9642	211.5774	6033.927
Amount %	1.163167	1.491838	42.54539
Adv.flow m3/h	1.5E+13	8.52E+09	0
D rct mol/Pa.h	2.660802E+07	2.883789E+07	2.16615E+09
D adv mol/Pa.h	6.527219E+09	2.288721E+09	0
Rct rate mol/h	2.361207E-02	9.360518E-03	.2669504
Rct rate kg/h	6.724716E-03	2.665875E-03	7.602748E-02
Adv rate mol/h	5.792282	.7428983	0
Adv rate kg/h	1.649642	.2115774	0
Reaction %	.305669	.1211762	3.455795
Advection %	74.98372	9.617156	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.26E+10		
Density kg/m3	1260		
Bulk Z value	570.3946		0
Bulk VZ	2.429881E+13	0	
Emission mol/h	.1404495	7.72472	
Emission kg/h	.04	2.2	
Fugacity Pa	1.123052E-09		3.24591E-10
Conc mol/m3	6.40583E-07		9.814174E-07
Conc g/m3	1.82438E-04		2.795077E-04
Conc ug/g	1.447921E-04		2.795077E-04
Amount mol	27288.83	49797.5	
Amount kg	7771.859	14182.33	
Amount %	54.7996		
Adv.flow m3/h	851999.9		
D rct mol/Pa.h	3.06165E+08		
D adv mol/Pa.h	4.859762E+08		
Rct rate mol/h	.3438393	.6437623	
Rct rate kg/h	9.792542E-02	0	
Adv rate mol/h	.5457766	7.080957	
Adv rate kg/h	.1554372	2.016656	
Reaction %	4.451156		
Advection %	7.065327		

Overall residence time   h   6446.513
Reaction residence time   h   77353.86
Advection residence time h   7032.595

Intermedia Data. transport kg/h	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h
Air to water 1.9622E-01	5.8260E+02	1.7842E+12	7.7641E+08	6.8899E-01
Air to soil 1.7453E-02	6.5503E+03	1.5870E+11	6.9056E+07	6.1281E-02
Water to air 6.9647E-02	2.1052E+03	2.8046E+09	7.5340E+08	2.4455E-01
Water to sediment 2.9367E-01	4.9929E+02	1.1826E+10	3.1767E+09	1.0311E+00
Soil to air 3.9585E-04	1.0563E+07	1.2635E+04	1.1278E+07	1.3899E-03
Soil to water 1.0295E-03	4.0618E+06	3.2860E+04	2.9331E+07	3.6147E-03
Sediment to water 8.0303E-02	6.7069E+04	4.4017E+05	2.5107E+08	2.8196E-01

		Transport velocity parameters	m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   9.243889E+08   Air-water diffusion (water-side)   4.073121E+09
Air-water diffusion (overall)   7.534048E+08
Rain dissolution to water   8146243   Aerosol deposition to water   1.485695E+07
Rain dissolution to soil   2.046122E+07   Aerosol deposition to soil   3.731676E+07
Soil-air diffusion (air-phase)   9287286   Soil-air diffusion (water-phase)   2046122
Soil-air diffusion (bndry layer)   2.321822E+09   Soil-air diffusion (overall)   1.127836E+07
Water-sediment diffusion   8146243
Water-sediment deposition   3.168561E+09   Sediment-water resuspension   2.42923E+08
Soil-water runoff (water)   1.023061E+07   Soil-water runoff (solids)   1.910062E+07

HCBZNORD

Fate of HCBz at Bay of Bothnia environment

Properties of HCBz :
Temperature deg C   2
Molecular mass g/mol   284.8
Melting point deg C   231
Fugacity ratio   3.513524E-03
Vapor pressure Pa   1.348626E-04
Sub-cooled liquid vapor press Pa   3.838385E-02
Solubility g/m3   8.688454E-03
Solubility mol/m3   3.050721E-05
Henry's law constant Pa.m3/mol   4.420679
Log octanol-water p-coefficient   5.5
Octanol-water partn-coefficient   316227.5
Organic C-water ptn-coefficient   129653.3
Fish-water partition coefficient   15811.37
Air-water partition coefficient   1.932455E-03
Soil-water partition coefficient   12446.71
Sedt-water partition coefficient   14910.12
Susp sedt-water partn coeffnt   29171.98
Aerosol-air partition coeff   1.563157E+08
Aerosol Z value   68331.85
Aerosol density kg/m3   2000

Amount of chemical moles   351123.6
Amount of chemical kilograms   100000
Fugacity Pa   1.281682E-07
Total of VZ products   2.739553E+12

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.7E+13	7.4E+11	1E+07
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.7E+10	3.7E+10	1E+08
Frn org carb			.04
Z mol/m3.Pa	4.371399E-04	.2262096	2815.566
VZ mol/Pa	1.617418E+10	1.673951E+11	2.815566E+10
Fugacity Pa	1.281682E-07	1.281682E-07	1.281682E-07
Conc mol/m3	5.602744E-11	2.899288E-08	3.60866E-04
Conc g/m3	1.595661E-08	8.257171E-06	.1027746
Conc ug/g	1.242241E-05	8.257171E-06	4.282277E-02
Amount mol	2073.015	21454.73	3608.66
Amount kg	590.3947	6110.307	1027.746
Amount %	.5903947	6.110307	1.027746

Phase	Sediment	Susp sedt	Fish
Volume m3	7.4E+08	4440000	740000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.7E+10	0	0
Frn org carb	.05	.15	
Z mol/m3.Pa	3372.813	6598.983	3576.685
VZ mol/Pa	2.495882E+12	2.929948E+10	2.646747E+09
Fugacity Pa	1.281682E-07	1.281682E-07	1.281682E-07
Conc mol/m3	4.322875E-04	8.457798E-04	4.584173E-04
Conc g/m3	.1231155	.2408781	.1305572
Conc ug/g	5.352846E-02	.1605854	.1305572
Amount mol	319892.7	3755.262	339.2288
Amount kg	91105.43	1069.499	96.61234
Amount %	91.10543	1.069499	9.661234E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
Fate of HCBz at Bay of Bothnia environment

Emission rate of chemical mol/h   14.04495
Emission rate of chemical kg/h   4
Fugacity Pa   3.395567E-08
Total amount of chemical mol   93023.37
Total amount of chemical kg   26493.06

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.7E+11	7.4E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	3.395567E-08	3.395567E-08	3.395567E-08
Conc mol/m3	1.484338E-11	7.681098E-09	9.560442E-05
Conc g/m3	4.227395E-09	2.187577E-06	2.722814E-02
Conc ug/g	3.291075E-06	2.187577E-06	1.134506E-02
Amount mol	549.205	5684.013	956.0442
Amount kg	156.4136	1618.807	272.2814
Amount %	.5903947	6.110307	1.027746
D rct mol/Pa.h	659335.5	2109178	354761.3
D adv mol/Pa.h	1.617418E+08	1.673951E+08	0
Rct rate mol/h	2.238818E-02	7.161856E-02	1.204616E-02
Adv rate mol/h	5.49205	5.684013	0
Rct rate kg/h	6.376154E-03	2.039697E-02	3.430746E-03
Adv rate kg/h	1.564136	1.618807	0
Reaction %	.1594039	.5099242	8.576864E-02
Advection %	39.10339	40.47017	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	14800		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	3.395567E-08	3.395567E-08	3.395567E-08
Conc mol/m3	1.145261E-04	2.240729E-04	1.214487E-04
Conc g/m3	3.261704E-02	6.381595E-02	.0345886
Conc ug/g	1.418132E-02	4.254397E-02	.0345886
Amount mol	84749.34	994.8836	89.87206
Amount kg	24136.61	283.3428	25.59556
Amount %	91.10543	1.069499	9.661234E-02
D rct mol/Pa.h	3.144811E+07		
D adv mol/Pa.h	4.991764E+07		
Rct rate mol/h	1.067842		
Adv rate mol/h	1.694987		
Rct rate kg/h	.3041213		
Adv rate kg/h	.4827323		
Reaction %	7.603033		
Advection %	12.06831		

Total advection D value   3.790545E+08
Total reaction D value   3.457139E+07
Total D value   4.136259E+08
Output by reaction   mol/h   1.173895
Output by advection   mol/h   12.87105
Total output by reaction and advection mol/h   14.04495
Output by reaction   kg/h   .3343252
Output by advection   kg/h   3.665675
Total output by reaction and advection kg/h   4

```
Overall residence time    h    6623.263
Reaction residence time   h    79243.37
Advection residence time  h    7227.334
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Bay of Bothnia environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.7E+13	7.4E+11	1.8E+07
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.385066E-04	.2627812	1407.851
Bulk VZ	1.622474E+10	1.944581E+11	2.534132E+10
Emission mol/h	.1404495	4.213484E-02	0
Emission kg/h	.04	.012	0
Fugacity Pa	6.753726E-10	2.499802E-10	1.552756E-11
Conc mol/m3	2.961553E-13	6.56901E-11	2.186049E-08
Conc g/m3	8.434502E-11	1.870854E-08	6.225867E-06
Conc ug/g	6.566356E-08	1.870838E-08	4.149867E-06
Amount mol	10.95775	48.61067	.3934888
Amount kg	3.120766	13.84432	.1120656
Amount %	1.412685	6.266943	5.072902E-02
Adv.flow m3/h	3.7E+11	7.4E+08	0
D rct mol/Pa.h	661396.8	2450172	319300.6
D adv mol/Pa.h	1.622474E+08	1.944581E+08	0
Rct rate mol/h	4.466893E-04	6.124944E-04	4.957958E-06
Rct rate kg/h	1.272171E-04	1.744384E-04	1.412026E-06
Adv rate mol/h	.1095775	4.861067E-02	0
Adv rate kg/h	3.120766E-02	1.384432E-02	0
Reaction %	.2446483	.3354585	2.715435E-03
Advection %	60.01473	26.62369	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.7E+09		
Density kg/m3	1260		
Bulk Z value	674.7436		0
Bulk VZ	2.496551E+12	0	
Emission mol/h	0	.1825843	
Emission kg/h	0	.052	
Fugacity Pa	2.866779E-10		2.499802E-10
Conc mol/m3	1.934341E-07		8.941003E-07
Conc g/m3	5.509002E-05		2.546398E-04
Conc ug/g	4.372224E-05		2.546398E-04
Amount mol	715.7061	775.668	
Amount kg	203.8331	220.9102	
Amount %	92.26964		
Adv.flow m3/h	74000		
D rct mol/Pa.h	3.145655E+07		
D adv mol/Pa.h	4.993103E+07		
Rct rate mol/h	9.017897E-03	1.008204E-02	
Rct rate kg/h	2.568297E-03	0	
Adv rate mol/h	1.431412E-02	.1725022	
Adv rate kg/h	4.076662E-03	4.912864E-02	
Reaction %	4.939033		
Advection %	7.839734		

```
Overall residence time    h    4248.274
Reaction residence time   h    76934.87
Advection residence time  h    4496.565
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
kg/h	h	m3/h	mol/Pa.h	mol/h
Air to water 1.3489E-02	1.6033E+02	1.5992E+11	7.0128E+07	4.7362E-02
Air to soil 1.4343E-06	1.5078E+06	1.7005E+07	7.4570E+03	5.0362E-06
Water to air 4.8251E-03	1.9884E+03	2.5791E+08	6.7774E+07	1.6942E-02
Water to sediment 8.7511E-03	1.0963E+03	4.6776E+08	1.2292E+08	3.0727E-02
Soil to air 4.8423E-09	1.6038E+07	7.7776E-01	1.0950E+03	1.7002E-08
Soil to water 1.7453E-08	4.4498E+06	2.8033E+00	3.9466E+03	6.1281E-08
Sediment to water 2.1061E-03	6.7069E+04	3.8231E+04	2.5796E+07	7.3951E-03

Transport velocity parameters   m/h   m/year

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values

Air-water diffusion (air-side)   8.087088E+07   Air-water diffusion
(water-side)   4.184878E+08

Air-water diffusion (overall)   6.777388E+07

Rain dissolution to water   836975.5   Aerosol deposition to
water   1516967

Rain dissolution to soil   2262.096   Aerosol deposition to
soil   4099.911

Soil-air diffusion (air-phase)   874.2799   Soil-air diffusion
(water-phase)   226.2096

Soil-air diffusion (bndry layer)   218570   Soil-air diffusion
(overall)   1094.976

Water-sediment diffusion   836975.5

Water-sediment deposition   1.220812E+08   Sediment-water
resuspension   2.495882E+07

Soil-water runoff (water)   1131.048   Soil-water runoff
(solids)   2815.566

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Baltic Proper environment

Properties of HCBz :
Temperature deg C   7
Molecular mass g/mol   284.8
Melting point deg C   231
Fugacity ratio   4.38708E-03
Vapor pressure Pa   2.467744E-04
Sub-cooled liquid vapor press Pa   5.625025E-02
Solubility g/m3   1.049292E-02
Solubility mol/m3   3.684312E-05
Henry's law constant Pa.m3/mol   6.697976
Log octanol-water p-coefficient   5.5
Octanol-water partn-coefficient   316227.5
Organic C-water ptn-coefficient   129653.3
Fish-water partition coefficient   15811.37
Air-water partition coefficient   2.875696E-03
Soil-water partition coefficient   9335.034
Sedt-water partition coefficient   14910.12
Susp sedt-water partn coeffnt   77791.96
Aerosol-air partition coeff   1.066662E+08
Aerosol Z value   45795.85
Aerosol density kg/m3   2000

Amount of chemical moles   351123.6
Amount of chemical kilograms   100000
Fugacity Pa   3.381647E-08
Total of VZ products   1.038321E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	2.1E+14	4.2E+12	1E+07
Density kg/m3	1.261578	1000	2400
Depth m	1000	20	.1
Area m2	2.1E+11	2.1E+11	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.29338E-04	.1492988	1393.71
VZ mol/Pa	9.016099E+10	6.270551E+11	1.39371E+10
Fugacity Pa	3.381647E-08	3.381647E-08	3.381647E-08
Conc mol/m3	1.45187E-11	5.048759E-09	4.713034E-05
Conc g/m3	4.134924E-09	1.437887E-06	1.342272E-02
Conc ug/g	3.277582E-06	1.437886E-06	.0055928
Amount mol	3048.926	21204.79	471.3034
Amount kg	868.3341	6039.123	134.2272
Amount %	.8683341	6.039123	.1342272

Phase	Sediment	Susp sedt	Fish
Volume m3	4.2E+09	2.52E+07	4200000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	2.1E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	2226.064	11614.25	2360.62
VZ mol/Pa	9.349469E+12	2.926791E+11	9.914601E+09
Fugacity Pa	3.381647E-08	3.381647E-08	3.381647E-08
Conc mol/m3	7.527762E-05	3.927528E-04	7.982781E-05
Conc g/m3	2.143907E-02	.111856	2.273496E-02
Conc ug/g	9.321332E-03	7.457066E-02	2.273496E-02
Amount mol	316166	9897.372	335.2768
Amount kg	90044.07	2818.772	95.48683
Amount %	90.04407	2.818771	9.548682E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Baltic Proper environment

```
Emission rate of chemical mol/h    73.73596
Emission rate of chemical  kg/h    21
Fugacity Pa                        3.996075E-08
Total amount of chemical mol       414921.1
Total amount of chemical kg        118169.5
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	2.1E+12	4.2E+09	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	3.996075E-08	3.996075E-08	3.996075E-08
Conc mol/m3	1.715667E-11	5.966094E-09	5.569369E-05
Conc g/m3	4.88622E-09	1.699144E-06	1.586156E-02
Conc ug/g	3.873103E-06	1.699144E-06	6.608984E-03
Amount mol	3602.901	25057.6	556.9369
Amount kg	1026.106	7136.403	158.6156
Amount %	.868334	6.039123	.1342272
D rct mol/Pa.h	3675386	7900895	175607.4
D adv mol/Pa.h	9.016099E+08	6.270551E+08	0
Rct rate mol/h	.1468712	.3157257	7.017405E-03
Adv rate mol/h	36.02901	25.0576	0
Rct rate kg/h	4.182892E-02	8.991868E-02	1.998557E-03
Adv rate kg/h	10.26106	7.136402	0
Reaction %	.1991853	.4281841	9.516937E-03
Advection %	48.86219	33.98287	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	84000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	3.996075E-08	3.996075E-08	3.996075E-08
Conc mol/m3	8.895519E-05	4.641141E-04	9.433213E-05
Conc g/m3	2.533444E-02	.1321797	2.686579E-02
Conc ug/g	1.101497E-02	8.811979E-02	2.686579E-02
Amount mol	373611.8	11695.68	396.195
Amount kg	106404.6	3330.928	112.8363
Amount %	90.04405	2.818771	9.548682E-02
D rct mol/Pa.h	1.178033E+08		
D adv mol/Pa.h	1.869894E+08		
Rct rate mol/h	4.707509		
Adv rate mol/h	7.472236		
Rct rate kg/h	1.340698		
Adv rate kg/h	2.128093		
Reaction %	6.384278		
Advection %	10.13377		

```
Total advection D value          1.715654E+09
Total reaction D value           1.295552E+08
Total D value                    1.84521E+09
Output by reaction      mol/h    5.177123
Output by advection     mol/h    68.55884
Total output by reaction and advection mol/h   73.73596
Output by reaction      kg/h     1.474445
Output by advection     kg/h     19.52556
Total output by reaction and advection kg/h    21
```

Overall residence time   h   5627.12
Reaction residence time   h   80145.11
Advection residence time h   6052.044

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Baltic Proper environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	2.1E+14	4.2E+12	1.8E+07
Density kg/m3	1.261578	1000.009	1500.252
Bulk Z value	4.30254E-04	.2097307	696.8998
Bulk VZ	9.035334E+10	8.808689E+11	1.25442E+10
Emission mol/h	.9480338	.5266855	0
Emission kg/h	.27	.15	0
Fugacity Pa	8.548917E-10	3.840708E-10	2.781046E-11
Conc mol/m3	3.678205E-13	8.055144E-11	1.93811E-08
Conc g/m3	1.047553E-10	2.294105E-08	5.519737E-06
Conc ug/g	8.303516E-08	2.294085E-08	3.679206E-06
Amount mol	77.24231	338.3161	.3488598
Amount kg	21.99861	96.35242	9.935526E-02
Amount %	.6803419	2.979851	3.072719E-03
Adv.flow m3/h	2.1E+12	4.2E+09	0
D rct mol/Pa.h	3683227	1.109895E+07	158056.9
D adv mol/Pa.h	9.035333E+08	8.808689E+08	0
Rct rate mol/h	3.14876E-03	4.262783E-03	4.395634E-06
Rct rate kg/h	8.967668E-04	1.214041E-03	1.251876E-06
Adv rate mol/h	.7724231	.338316	0
Adv rate kg/h	.2199861	.0963524	0
Reaction %	.2135159	.2890573	2.980658E-04
Advection %	52.37765	22.94105	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	2.1E+10		
Density kg/m3	1260		
Bulk Z value	445.3323		0
Bulk VZ	9.351977E+12	0	
Emission mol/h	0	1.474719	
Emission kg/h	0	.42	
Fugacity Pa	1.169544E-09		3.840708E-10
Conc mol/m3	5.208356E-07		9.06645E-07
Conc g/m3	1.48334E-04		2.582125E-04
Conc ug/g	1.177254E-04		2.582125E-04
Amount mol	10937.55	11353.46	
Amount kg	3115.014	3233.464	
Amount %	96.33673		
Adv.flow m3/h	420000		
D rct mol/Pa.h	1.178349E+08		
D adv mol/Pa.h	1.870395E+08		
Rct rate mol/h	.1378131	.145229	
Rct rate kg/h	3.924917E-02	0	
Adv rate mol/h	.218751	1.32949	
Adv rate kg/h	6.230027E-02	.3786388	
Reaction %	9.345041		
Advection %	14.8334		

Overall residence time   h   7698.724
Reaction residence time   h   78176.15
Advection residence time h   8539.706

Intermedia Data. transport kg/h	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h
Air to water 8.7413E-02	1.7440E+02	8.3445E+11	3.5903E+08	3.0693E-01
Air to soil 1.2768E-06	1.1940E+07	1.2188E+07	5.2440E+03	4.4831E-06
Water to air 3.8297E-02	1.7435E+03	1.6694E+09	3.5012E+08	1.3447E-01
Water to sediment 1.3374E-01	4.9929E+02	5.8295E+09	1.2226E+09	4.6958E-01
Soil to air 7.9463E-09	8.6648E+06	1.4396E+00	1.0033E+03	2.7901E-08
Soil to water 1.6951E-08	4.0618E+06	3.0710E+00	2.1402E+03	5.9520E-08
Sediment to water 3.2186E-02	6.7069E+04	2.1698E+05	9.6630E+07	1.1301E-01

Transport velocity parameters		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values

Air-water diffusion (air-side) 4.50805E+08   Air-water diffusion (water-side) 1.567638E+09

Air-water diffusion (overall)   3.501208E+08

Rain dissolution to water   3135276   Aerosol deposition to water   5770277

Rain dissolution to soil   1492.988   Aerosol deposition to soil   2747.751

Soil-air diffusion (air-phase)   858.676   Soil-air diffusion (water-phase) 149.2988

Soil-air diffusion (bndry layer) 214669   Soil-air diffusion (overall)   1003.264

Water-sediment diffusion   3135276

Water-sediment deposition   1.219496E+09 Sediment-water resuspension   9.349469E+07

Soil-water runoff (water)   746.4941   Soil-water runoff (solids)   1393.71

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at North Sea / Skagerrak environment

Properties of HCBz :

Temperature deg C	8
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	4.58195E-03
Vapor pressure Pa	2.777545E-04
Sub-cooled liquid vapor press Pa	6.061929E-02
Solubility g/m3	1.088773E-02
Solubility mol/m3	3.822938E-05
Henry's law constant Pa.m3/mol	7.265473
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	3.108249E-03
Soil-water partition coefficient	9335.034
Sedt-water partition coefficient	14910.13
Susp sedt-water partn coeffnt	77791.96
Aerosol-air partition coeff	9.89784E+07
Aerosol Z value	42344.05
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	1.702235E-07
Total of VZ products	2.062721E+12

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+13	9E+11	1E+07
Density kg/m3	1.25709	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+10	4.5E+10	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.27811E-04	.1376373	1284.849
VZ mol/Pa	1.925149E+10	1.238736E+11	1.284849E+10
Fugacity Pa	1.702235E-07	1.702235E-07	1.702235E-07
Conc mol/m3	7.28235E-11	2.342911E-08	2.187115E-04
Conc g/m3	2.074013E-08	6.672609E-06	6.228904E-02
Conc ug/g	1.649852E-05	6.672609E-06	2.595377E-02
Amount mol	3277.057	21086.2	2187.115
Amount kg	933.3059	6005.348	622.8903
Amount %	.9333059	6.005348	.6228903

Phase	Sediment	Susp sedt	Fish
Volume m3	9E+08	5400000	900000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	2052.189	10707.07	2176.235
VZ mol/Pa	1.84697E+12	5.78182E+10	1.958611E+09
Fugacity Pa	1.702235E-07	1.702235E-07	1.702235E-07
Conc mol/m3	3.493309E-04	1.822596E-03	3.704464E-04
Conc g/m3	9.948944E-02	.5190754	.1055031
Conc ug/g	4.325628E-02	.3460502	.1055031
Amount mol	314397.8	9842.019	333.4017
Amount kg	89540.49	2803.007	94.95281
Amount %	89.54049	2.803007	.0949528

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at North Sea / Skagerrak environment

Emission rate of chemical mol/h   17.55618
Emission rate of chemical kg/h   5
Fugacity Pa   4.630928E-08
Total amount of chemical mol   95523.11
Total amount of chemical kg   27204.98

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+11	9E+08	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	4.630928E-08	4.630928E-08	4.630928E-08
Conc mol/m3	1.981162E-11	6.373884E-09	5.950043E-05
Conc g/m3	5.642349E-09	1.815282E-06	1.694572E-02
Conc ug/g	4.488419E-06	1.815282E-06	7.060717E-03
Amount mol	891.5228	5736.495	595.0042
Amount kg	253.9057	1633.754	169.4572
Amount %	.9333058	6.005348	.6228904
D rct mol/Pa.h	784781.5	1560807	161891
D adv mol/Pa.h	1.925149E+08	1.238736E+08	0
Rct rate mol/h	3.634266E-02	7.227985E-02	7.497053E-03
Adv rate mol/h	8.915228	5.736495	0
Rct rate kg/h	1.035039E-02	.0205853	2.135161E-03
Adv rate kg/h	2.539057	1.633754	0
Reaction %	.2070078	.411706	4.270321E-02
Advection %	50.78113	32.67507	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	18000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	4.630928E-08	4.630928E-08	4.630928E-08
Conc mol/m3	9.503541E-05	4.958369E-04	1.007799E-04
Conc g/m3	2.706608E-02	.1412143	2.870211E-02
Conc ug/g	1.176786E-02	9.414289E-02	2.870211E-02
Amount mol	85531.87	2677.519	90.70188
Amount kg	24359.48	762.5575	25.83189
Amount %	89.54049	2.803007	9.495281E-02
D rct mol/Pa.h	2.327183E+07		
D adv mol/Pa.h	3.693941E+07		
Rct rate mol/h	1.077702		
Adv rate mol/h	1.710637		
Rct rate kg/h	.3069294		
Adv rate kg/h	.4871895		
Reaction %	6.138588		
Advection %	9.743789		

Total advection D value   3.533279E+08
Total reaction D value   2.577931E+07
Total D value   3.791072E+08
Output by reaction   mol/h   1.193821
Output by advection   mol/h   16.36236
Total output by reaction and advection mol/h   17.55618
Output by reaction   kg/h   .3400002
Output by advection   kg/h   4.66
Total output by reaction and advection kg/h   5

Overall residence time   h   5440.996
Reaction residence time   h   80014.6
Advection residence time h   5837.979

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at North Sea / Skagerrak environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+13	9E+11	1.8E+07
Density kg/m3	1.25709	1000.009	1500.252
Bulk Z value	4.286579E-04	.1933489	642.4658
Bulk VZ	1.92896E+10	1.74014E+11	1.156438E+10
Emission mol/h	.5969101	.1404495	0
Emission kg/h	.17	.04	0
Fugacity Pa	2.42403E-09	7.472084E-10	7.998447E-11
Conc mol/m3	1.03908E-12	1.444719E-10	5.138728E-08
Conc g/m3	2.959299E-10	4.11456E-08	1.46351E-05
Conc ug/g	2.354086E-07	4.114525E-08	9.755096E-06
Amount mol	46.75859	130.0247	.9249711
Amount kg	13.31684	37.03104	.2634318
Amount %	1.047668	2.91332	.0207248
Adv.flow m3/h	4.5E+11	9E+08	0
D rct mol/Pa.h	786335	2192577	145711.2
D adv mol/Pa.h	1.92896E+08	1.74014E+08	0
Rct rate mol/h	.0019061	1.638311E-03	1.165464E-05
Rct rate kg/h	5.428572E-04	4.665911E-04	3.31924E-06
Adv rate mol/h	.4675858	.1300247	0
Adv rate kg/h	.1331684	3.703104E-02	0
Reaction %	.2572783	.2211332	.0015731
Advection %	63.11301	17.55026	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.5E+09		
Density kg/m3	1260		
Bulk Z value	410.548		0
Bulk VZ	1.847466E+12	0	
Emission mol/h	3.511236E-03	.7408708	
Emission kg/h	.001	.211	
Fugacity Pa	2.319612E-09		7.472084E-10
Conc mol/m3	9.523119E-07		1.626101E-06
Conc g/m3	2.712184E-04		4.631135E-04
Conc ug/g	2.152527E-04		4.631135E-04
Amount mol	4285.404	4463.112	
Amount kg	1220.483	1271.094	
Amount %	96.01829		
Adv.flow m3/h	89999.99		
D rct mol/Pa.h	2.327807E+07		
D adv mol/Pa.h	3.694931E+07		
Rct rate mol/h	5.399608E-02	5.755215E-02	
Rct rate kg/h	1.537808E-02	0	
Adv rate mol/h	8.570806E-02	.6833186	
Adv rate kg/h	2.440966E-02	.1946091	
Reaction %	7.288192		
Advection %	11.56856		

Overall residence time   h   6024.144
Reaction residence time   h   77548.87
Advection residence time h   6531.523

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 5.1912E-02	1.7777E+02	1.7542E+11	7.5195E+07	1.8228E-01
Air to soil 3.3867E-06	2.7249E+06	1.1444E+07	4.9057E+03	1.1892E-05
Water to air 1.5627E-02	1.6422E+03	3.7979E+08	7.3433E+07	5.4870E-02
Water to sediment 5.1398E-02	4.9929E+02	1.2492E+09	2.4153E+08	1.8047E-01
Soil to air 2.2521E-08	8.1060E+06	1.5389E+00	9.8867E+02	7.9078E-08
Soil to water 4.4945E-08	4.0618E+06	3.0710E+00	1.9730E+03	1.5781E-07
Sediment to water 1.2611E-02	6.7069E+04	4.6497E+04	1.9089E+07	4.4279E-02

Transport velocity parameters

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   9.625746E+07   Air-water diffusion
(water-side)   3.096839E+08
Air-water diffusion (overall)   7.343274E+07
Rain dissolution to water   619367.8   Aerosol deposition to
water   1143289
Rain dissolution to soil   1376.373   Aerosol deposition to
soil   2540.643
Soil-air diffusion (air-phase)   855.6219   Soil-air diffusion
(water-phase)   137.6373
Soil-air diffusion (bndry layer)   213905.5   Soil-air diffusion
(overall)   988.6682
Water-sediment diffusion   619367.8
Water-sediment deposition   2.409092E+08 Sediment-water
resuspension   1.84697E+07
Soil-water runoff (water)   688.1864   Soil-water runoff
(solids)   1284.849

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of HCBz at Barents Sea environment

Properties of HCBz :

Temperature deg C	-2
Molecular mass g/mol	284.8
Melting point deg C	231
Fugacity ratio	2.924396E-03
Vapor pressure Pa	8.184572E-05
Sub-cooled liquid vapor press Pa	2.798722E-02
Solubility g/m3	7.433665E-03
Solubility mol/m3	2.610136E-05
Henry's law constant Pa.m3/mol	3.135689
Log octanol-water p-coefficient	5.5
Octanol-water partn-coefficient	316227.5
Organic C-water ptn-coefficient	129653.3
Fish-water partition coefficient	15811.37
Air-water partition coefficient	1.390956E-03
Soil-water partition coefficient	9335.034
Sedt-water partition coefficient	2982.025
Susp sedt-water partn coeffnt	3889.598
Aerosol-air partition coeff	2.143836E+08
Aerosol Z value	95098.1
Aerosol density kg/m3	2000

Amount of chemical moles	351123.6
Amount of chemical kilograms	100000
Fugacity Pa	3.461664E-09
Total of VZ products	1.01432E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.2E+15	2.4E+14	1E+07
Density kg/m3	1.303452	1000	2400
Depth m	1000	200	.1
Area m2	1.2E+12	1.2E+12	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.435886E-04	.3189092	2977.028
VZ mol/Pa	5.323063E+11	7.653821E+13	2.977028E+10
Fugacity Pa	3.461664E-09	3.461664E-09	3.461664E-09
Conc mol/m3	1.535555E-12	1.103957E-09	1.030547E-05
Conc g/m3	4.37326E-10	3.144068E-07	2.934998E-03
Conc ug/g	3.355137E-07	3.144068E-07	1.222916E-03
Amount mol	1842.665	264949.5	103.0547
Amount kg	524.7911	75457.63	29.34998
Amount %	.5247911	75.45762	2.934998E-02

Phase	Sediment	Susp sedt	Fish
Volume m3	2.4E+10	2.4E+08	2.4E+08
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	1.2E+12	0	0
Frn org carb	.01	.02	
Z mol/m3.Pa	950.9951	1240.429	5042.393
VZ mol/Pa	2.282388E+13	2.977028E+11	1.210174E+12
Fugacity Pa	3.461664E-09	3.461664E-09	3.461664E-09
Conc mol/m3	3.292026E-06	4.293947E-06	1.745507E-05
Conc g/m3	9.375688E-04	1.222916E-03	4.971204E-03
Conc ug/g	4.076387E-04	8.152773E-04	4.971204E-03
Amount mol	79008.61	1030.547	4189.216
Amount kg	22501.65	293.4998	1193.089
Amount %	22.50165	.2934998	1.193089

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of HCBz at Barents Sea environment

Emission rate of chemical mol/h   210.6742
Emission rate of chemical kg/h   60
Fugacity Pa   2.520274E-09
Total amount of chemical mol   255636.5
Total amount of chemical kg   72805.28

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.2E+13	2.4E+11	0
Adv.restime h	100	1000	0
Rct halflife h	17000	55000	55000
Rct rate c.h-1	4.076471E-05	.0000126	.0000126
Fugacity Pa	2.520274E-09	2.520274E-09	2.520274E-09
Conc mol/m3	1.117965E-12	8.037385E-10	7.502927E-06
Conc g/m3	3.183963E-10	2.289047E-07	2.136834E-03
Conc ug/g	2.442716E-07	2.289047E-07	8.903472E-04
Amount mol	1341.558	192897.2	75.02927
Amount kg	382.0756	54937.13	21.36834
Amount %	.5247911	75.45762	2.934998E-02
D rct mol/Pa.h	2.169931E+07	9.643814E+08	375105.6
D adv mol/Pa.h	5.323063E+09	7.65382E+10	0
Rct rate mol/h	.0546882	2.430505	9.453688E-04
Adv rate mol/h	13.41558	192.8972	0
Rct rate kg/h	.0155752	.6922078	2.69241E-04
Adv rate kg/h	3.820756	54.93713	0
Reaction %	2.595866E-02	1.15368	4.48735E-04
Advection %	6.367926	91.56188	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	480000		
Adv.restime h	50000		
Rct halflife h	55000		
Rct rate c.h-1	.0000126		
Fugacity Pa	2.520274E-09	2.520274E-09	2.520274E-09
Conc mol/m3	2.396768E-06	3.126219E-06	1.270821E-05
Conc g/m3	6.825995E-04	8.903472E-04	3.619298E-03
Conc ug/g	2.967824E-04	5.935648E-04	3.619298E-03
Amount mol	57522.43	750.2926	3049.97
Amount kg	16382.39	213.6833	868.6314
Amount %	22.50165	.2934998	1.193089
D rct mol/Pa.h	2.875809E+08		
D adv mol/Pa.h	4.564777E+08		
Rct rate mol/h	.7247826		
Adv rate mol/h	1.150449		
Rct rate kg/h	.2064181		
Adv rate kg/h	.3276478		
Reaction %	.3440301		
Advection %	.5460796		

Total advection D value   8.231774E+10
Total reaction D value   1.274037E+09
Total D value   8.359178E+10
Output by reaction   mol/h 3.210921
Output by advection   mol/h 207.4632
Total output by reaction and advection mol/h   210.6742
Output by reaction   kg/h .9144703
Output by advection   kg/h 59.08553
Total output by reaction and advection kg/h   60

```
Overall residence time    h    1213.421
Reaction residence time   h    79614.69
Advection residence time  h    1232.201
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of HCBz at Barents Sea environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.2E+15	2.4E+14	1.8E+07
Density kg/m3	1.303452	1000.009	1500.261
Bulk Z value	4.454906E-04	.3301537	1488.61
Bulk VZ	5.345886E+11	7.92369E+13	2.679498E+10
Emission mol/h	4.178371	4.248596	0
Emission kg/h	1.19	1.21	0
Fugacity Pa	5.551012E-10	6.740808E-11	1.631826E-11
Conc mol/m3	2.472923E-13	2.225503E-11	2.429152E-08
Conc g/m3	7.042885E-11	6.338232E-09	6.918225E-06
Conc ug/g	5.403256E-08	6.338179E-09	4.611348E-06
Amount mol	296.7507	5341.207	.4372474
Amount kg	84.5146	1521.176	.124528
Amount %	4.344715	78.20038	6.40172E-03
Adv.flow m3/h	1.2E+13	2.4E+11	0
D rct mol/Pa.h	2.179235E+07	9.983849E+08	337616.7
D adv mol/Pa.h	5.345886E+09	7.923689E+10	0
Rct rate mol/h	1.209696E-02	6.729921E-02	5.509317E-06
Rct rate kg/h	3.445214E-03	1.916681E-02	1.569053E-06
Adv rate mol/h	2.967507	5.341207	0
Adv rate kg/h	.8451461	1.521176	0
Reaction %	.1435506	.7986173	6.537723E-05
Advection %	35.21442	63.38232	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.2E+11		
Density kg/m3	1260		
Bulk Z value	190.4542		0
Bulk VZ	2.28545E+13	0	
Emission mol/h	0	8.426967	
Emission kg/h	0	2.4	
Fugacity Pa	5.214556E-11		6.740808E-11
Conc mol/m3	9.931338E-09		3.39898E-07
Conc g/m3	2.828445E-06		9.680295E-05
Conc ug/g	2.244798E-06		9.680295E-05
Amount mol	1191.76	6830.155	
Amount kg	339.4133	1945.228	
Amount %	17.44851		
Adv.flow m3/h	2400000		
D rct mol/Pa.h	2.879666E+08		
D adv mol/Pa.h	4.570899E+08		
Rct rate mol/h	1.501618E-02	9.441786E-02	
Rct rate kg/h	4.276608E-03	0	
Adv rate mol/h	2.383521E-02	8.33255	
Adv rate kg/h	6.788268E-03	2.37311	
Reaction %	.178192		
Advection %	.2828445		

```
Overall residence time    h    810.5116
Reaction residence time   h    72339.57
Advection residence time  h    819.6957
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h kg/h
Air to water 3.8626E-01	1.5163E+02	5.4844E+12	2.4433E+09	1.3563E+00
Air to soil 1.5959E-06	3.6700E+07	2.2659E+07	1.0095E+04	5.6035E-06
Water to air 4.4856E-02	2.3501E+04	7.0771E+09	2.3365E+09	1.5750E-01
Water to sediment 1.5023E-02	7.0172E+04	2.3702E+09	7.8253E+08	5.2749E-02
Soil to air 5.5749E-09	1.5480E+07	8.0583E-01	1.1996E+03	1.9575E-08
Soil to water 2.1246E-08	4.0618E+06	3.0710E+00	4.5716E+03	7.4600E-08
Sediment to water 3.9579E-03	5.9428E+04	1.3993E+06	2.6651E+08	1.3897E-02

Transport velocity parameters

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values

Air-water diffusion (air-side)	2.661532E+09	Air-water diffusion (water-side)	1.913455E+10
Air-water diffusion (overall)	2.33653E+09		
Rain dissolution to water	3.82691E+07	Aerosol deposition to water	6.847063E+07
Rain dissolution to soil	3189.092	Aerosol deposition to soil	5705.886
Soil-air diffusion (air-phase)	887.1772	Soil-air diffusion (water-phase)	318.9092
Soil-air diffusion (bndry layer)	221794.3	Soil-air diffusion (overall)	1199.563
Water-sediment diffusion	3.82691E+07		
Water-sediment deposition	7.442571E+08	Sediment-water resuspension	2.282388E+08
Soil-water runoff (water)	1594.546	Soil-water runoff (solids)	2977.028

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Danmark environment
Properties of Lindane :

Temperature deg C	7.5
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	7.807933E-02
Vapor pressure Pa	1.425394E-03
Sub-cooled liquid vapor press Pa	1.825571E-02
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	6.795155E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	2.912221E-05
Soil-water partition coefficient	124.1725
Sedt-water partition coefficient	237.9972
Susp sedt-water partn coeffnt	776.0778
Aerosol-air partition coeff	3.286643E+08
Aerosol Z value	140856.7
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	4.269389E-08
Total of VZ products	8.054526E+12

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.3E+13	1.224E+10	4.240001E+09
Density kg/m3	1.25933	1000	2400
Depth m	1000	20	.1
Area m2	4.3E+10	6.12E+08	4.24E+10
Frn org carb			.02
Z mol/m3.Pa	4.285731E-04	14.71637	1827.367
VZ mol/Pa	1.842864E+10	1.801283E+11	7.748038E+12
Fugacity Pa	4.269389E-08	4.269389E-08	4.269389E-08
Conc mol/m3	1.829745E-11	6.282989E-07	7.801742E-05
Conc g/m3	5.320899E-09	1.827093E-04	2.268746E-02
Conc ug/g	4.225182E-06	1.827093E-04	9.453109E-03
Amount mol	786.7904	7690.378	330793.9
Amount kg	228.7986	2236.362	96194.86
Amount %	.2287986	2.236362	96.19486

Phase	Sediment	Susp sedt	Fish
Volume m3	3.06E+07	61200	12240
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	6.12E+08	0	0
Frn org carb	.04	.2	
Z mol/m3.Pa	3502.454	11421.05	4642.702
VZ mol/Pa	1.071751E+11	6.98968E+08	5.682667E+07
Fugacity Pa	4.269389E-08	4.269389E-08	4.269389E-08
Conc mol/m3	1.495334E-04	4.876088E-04	1.98215E-04
Conc g/m3	.0434843	.1417966	5.764091E-02
Conc ug/g	1.890622E-02	9.453109E-02	5.764091E-02
Amount mol	4575.721	29.84166	2.426151
Amount kg	1330.62	8.677954	.7055248
Amount %	1.33062	8.677955E-03	7.055248E-04

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Danmark environment

```
Emission rate of chemical mol/h    14.7868
Emission rate of chemical  kg/h    4.3
Fugacity Pa                        2.107021E-08
Total amount of chemical mol       169710.6
Total amount of chemical kg        49351.83
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.3E+11	1.224E+07	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	2.107021E-08	2.107021E-08	2.107021E-08
Conc mol/m3	9.030125E-12	3.100769E-07	3.850302E-05
Conc g/m3	2.62596E-09	9.017037E-05	1.119668E-02
Conc ug/g	2.085204E-06	9.017037E-05	4.665281E-03
Amount mol	388.2954	3795.342	163252.8
Amount kg	112.9163	1103.685	47473.91
Amount %	.2287986	2.236362	96.19482
D rct mol/Pa.h	7670301	7342879	3.158465E+08
D adv mol/Pa.h	1.842865E+08	1.801283E+08	0
Rct rate mol/h	.1616148	.154716	6.654952
Adv rate mol/h	3.882954	3.795342	0
Rct rate kg/h	4.699759E-02	4.499141E-02	1.93526
Adv rate kg/h	1.129163	1.103685	0
Reaction %	1.092967	1.046312	45.00604
Advection %	26.2596	25.6671	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	612		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	2.107021E-08	2.107021E-08	2.107021E-08
Conc mol/m3	7.379744E-05	2.406438E-04	9.782269E-05
Conc g/m3	.0214603	6.997922E-02	2.844684E-02
Conc ug/g	9.330563E-03	4.665282E-02	2.844684E-02
Amount mol	2258.202	14.7274	1.19735
Amount kg	656.685	4.282728	.3481893
Amount %	1.33062	8.677953E-03	7.055246E-04
D rct mol/Pa.h	4368961		
D adv mol/Pa.h	2143502		
Rct rate mol/h	9.205492E-02		
Adv rate mol/h	4.516404E-02		
Rct rate kg/h	2.676957E-02		
Adv rate kg/h	.0131337		
Reaction %	.6225481		
Advection %	.3054349		

```
Total advection D value        3.665583E+08
Total reaction D value         3.352287E+08
Total D value                  7.017869E+08
Output by reaction     mol/h   7.063338
Output by advection    mol/h   7.723459
Total output by reaction and advection mol/h   14.7868
Output by reaction     kg/h    2.054019
Output by advection    kg/h    2.245982
Total output by reaction and advection kg/h    4.3
```

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Overall residence time   h   11477.17
Reaction residence time   h   24026.97
Advection residence time h   21973.39

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Danmark environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.3E+13	1.224E+10	7.632E+09
Density kg/m3	1.25933	1000.009	1500.252
Bulk Z value	4.313903E-04	14.77811	918.0987
Bulk VZ	1.854978E+10	1.808841E+11	7.00693E+12
Emission mol/h	1.031637	.687758	.343879
Emission kg/h	.3	.2	.1
Fugacity Pa	3.918697E-09	3.940282E-09	1.935234E-09
Conc mol/m3	1.690487E-12	5.822993E-08	1.776736E-06
Conc g/m3	4.915937E-10	1.693326E-05	5.166747E-04
Conc ug/g	3.903614E-07	1.693312E-05	3.44392E-04
Amount mol	72.69096	712.7343	13560.05
Amount kg	21.13853	207.2631	3943.261
Amount %	.4905421	4.809762	91.50758
Adv.flow m3/h	4.3E+11	1.224E+07	0
D rct mol/Pa.h	7720720	7373688	2.856354E+08
D adv mol/Pa.h	1.854978E+08	1.808841E+08	0
Rct rate mol/h	3.025516E-02	.0290544	.5527713
Rct rate kg/h	.0087982	8.449021E-03	.1607459
Adv rate mol/h	.7269096	.7127343	0
Adv rate kg/h	.2113853	.2072631	0
Reaction %	1.454248	1.396532	26.56957
Advection %	34.93972	34.25837	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.53E+08		
Density kg/m3	1260		
Bulk Z value	712.264		0
Bulk VZ	1.089764E+11	0	
Emission mol/h	1.719395E-02	2.080468	
Emission kg/h	.005	.605	
Fugacity Pa	4.340619E-09		3.940282E-09
Conc mol/m3	3.091666E-06		1.829355E-05
Conc g/m3	8.990564E-04		5.319765E-03
Conc ug/g	7.135369E-04		5.319764E-03
Amount mol	473.0249	14818.5	
Amount kg	137.5556	4309.219	
Amount %	3.192125		
Adv.flow m3/h	3060		
D rct mol/Pa.h	4442390		
D adv mol/Pa.h	2179528		
Rct rate mol/h	1.928272E-02	.6313635	
Rct rate kg/h	5.607415E-03	0	
Adv rate mol/h	9.460498E-03	1.449104	
Adv rate kg/h	2.751113E-03	.4213995	
Reaction %	.9268455		
Advection %	.4547294		

Overall residence time   h   7122.676
Reaction residence time   h   23470.62
Advection residence time h   10225.97

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water	5.6881E+03	5.2389E+09	2.2600E+06	8.8562E-03
2.5754E-03				
Air to soil	1.7820E+02	1.6722E+11	7.2137E+07	2.8268E-01
8.2204E-02				
Water to air	9.5863E+04	8.8484E+04	1.3076E+06	5.1524E-03
1.4983E-03				
Water to sediment	2.8519E+04	2.9743E+05	4.3955E+06	1.7319E-02
5.0365E-03				
Soil to air	7.8882E+05	6.7049E+03	6.1558E+06	1.1913E-02
3.4643E-03				
Soil to water	1.5187E+05	3.4826E+04	3.1974E+07	6.1876E-02
1.7994E-02				
Sediment to water	5.6811E+04	1.8664E+03	1.3293E+06	5.7702E-03
1.6780E-03				

Transport velocity parameters   m/h   m/year

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   1311434   Air-water diffusion
(water-side)   4.503209E+08
Air-water diffusion (overall)   1307626
Rain dissolution to water   900641.6   Aerosol deposition to
water   51722.57
Rain dissolution to soil   6.23974E+07   Aerosol deposition to
soil   3583394
Soil-air diffusion (air-phase)   363430   Soil-air diffusion
(water-phase)   6239740
Soil-air diffusion (bndry layer) 9.085751E+07   Soil-air diffusion
(overall)   6155791
Water-sediment diffusion   900641.6
Water-sediment deposition   3494840   Sediment-water
resuspension   428700.4
Soil-water runoff (water)   3.11987E+07   Soil-water runoff
(solids)   774803.8

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Finland environment

Properties of Lindane :

Temperature deg C	2
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	6.478188E-02
Vapor pressure Pa	5.719487E-04
Sub-cooled liquid vapor press Pa	8.828836E-03
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	2.726601E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	1.191906E-05
Soil-water partition coefficient	310.4311
Sedt-water partition coefficient	475.9944
Susp sedt-water partn coeffnt	1164.117
Aerosol-air partition coeff	6.795913E+08
Aerosol Z value	297076.5
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	8.633033E-10
Total of VZ products	3.983293E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.37E+14	6.32E+11	3.05E+10
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.37E+11	3.16E+10	3.05E+11
Frn org carb			.05
Z mol/m3.Pa	4.371399E-04	36.6757	11385.28
VZ mol/Pa	1.473162E+11	2.317904E+13	3.47251E+14
Fugacity Pa	8.633033E-10	8.633033E-10	8.633033E-10
Conc mol/m3	3.773843E-13	3.166225E-08	9.828948E-06
Conc g/m3	1.097434E-10	9.207381E-06	2.858258E-03
Conc ug/g	8.543645E-08	9.207381E-06	1.190941E-03
Amount mol	127.1785	20010.54	299782.9
Amount kg	36.98351	5819.066	87176.86
Amount %	3.698351E-02	5.819066	87.17686

Phase	Sediment	Susp sedt	Fish
Volume m3	1.58E+09	3792000	632000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.16E+10	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	17457.43	42694.8	11570.4
VZ mol/Pa	2.758273E+13	1.618987E+11	7.312496E+09
Fugacity Pa	8.633033E-10	8.633033E-10	8.633033E-10
Conc mol/m3	1.507105E-05	3.685856E-05	9.988768E-06
Conc g/m3	4.382663E-03	1.071847E-02	2.904734E-03
Conc ug/g	1.905505E-03	7.145645E-03	2.904734E-03
Amount mol	23812.27	139.7677	6.312902
Amount kg	6924.607	40.64443	1.835792
Amount %	6.924607	4.064443E-02	1.835792E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Finland environment

Emission rate of chemical mol/h   116.9189
Emission rate of chemical kg/h   34
Fugacity Pa   2.817998E-09
Total amount of chemical mol   1122491
Total amount of chemical kg   326420.3

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.37E+12	6.32E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	2.817998E-09	2.817998E-09	2.817998E-09
Conc mol/m3	1.231859E-12	1.03352E-07	3.208368E-05
Conc g/m3	3.582246E-10	3.005477E-05	9.329934E-03
Conc ug/g	2.78882E-07	3.005477E-05	3.887472E-03
Amount mol	415.1365	65318.48	978552.2
Amount kg	120.7217	18994.61	284563
Amount %	3.698351E-02	5.819066	87.17686
D rct mol/Pa.h	6.131537E+07	9.448868E+08	1.415558E+10
D adv mol/Pa.h	1.473162E+09	2.317904E+10	0
Rct rate mol/h	.1727866	2.662689	39.8904
Adv rate mol/h	4.151365	65.31848	0
Rct rate kg/h	5.024633E-02	.7743098	11.60013
Adv rate kg/h	1.207217	18.99461	0
Reaction %	.1477833	2.277382	34.11802
Advection %	3.550639	55.86652	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	31600		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	2.817998E-09	2.817998E-09	2.817998E-09
Conc mol/m3	4.919498E-05	1.203138E-04	3.260537E-05
Conc g/m3	.0143059	3.498726E-02	9.481641E-03
Conc ug/g	6.219956E-03	2.332484E-02	9.481641E-03
Amount mol	77728.07	456.23	20.60659
Amount kg	22603.32	132.6717	5.992398
Amount %	6.924606	4.064443E-02	1.835792E-03
D rct mol/Pa.h	1.124402E+09		
D adv mol/Pa.h	5.516546E+08		
Rct rate mol/h	3.168562		
Adv rate mol/h	1.554561		
Rct rate kg/h	.9214178		
Adv rate kg/h	.4520665		
Reaction %	2.710053		
Advection %	1.329607		

Total advection D value   2.520386E+10
Total reaction D value   1.628619E+10
Total D value   4.149005E+10
Output by reaction   mol/h   45.89443
Output by advection   mol/h   71.02441
Total output by reaction and advection mol/h   116.9188
Output by reaction   kg/h   13.3461
Output by advection   kg/h   20.6539
Total output by reaction and advection kg/h   34

```
Overall residence time    h    9600.599
Reaction residence time   h    24458.11
Advection residence time  h    15804.3
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Finland environment

Bulk phase properties, compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.37E+14	6.32E+11	5.49E+10
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.430815E-04	36.90074	5703.642
Bulk VZ	1.493185E+11	2.332127E+13	3.131299E+14
Emission mol/h	3.782669	.687758	2.063274
Emission kg/h	1.1	.2	.6
Fugacity Pa	1.263874E-09	4.679718E-11	2.726797E-10
Conc mol/m3	5.599992E-13	1.726851E-09	1.555267E-06
Conc g/m3	1.628478E-10	5.021681E-07	4.522717E-04
Conc ug/g	1.267788E-07	5.021638E-07	3.014629E-04
Amount mol	188.7197	1091.37	85384.18
Amount kg	54.8797	317.3703	24829.72
Amount %	.1941892	1.123	87.85879
Adv.flow m3/h	3.37E+12	6.32E+08	0
D rct mol/Pa.h	6.214877E+07	9.506847E+08	1.276465E+10
D adv mol/Pa.h	1.493184E+09	2.332127E+10	0
Rct rate mol/h	7.854821E-02	4.448936E-02	3.480661
Rct rate kg/h	2.284182E-02	.0129375	1.012176
Adv rate mol/h	1.887197	1.091369	0
Adv rate kg/h	.5487969	.3173702	0
Reaction %	1.087706	.6160716	48.19887
Advection %	26.13319	15.11287	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	7.900001E+09		
Density kg/m3	1260		
Bulk Z value	3520.826		0
Bulk VZ	2.781452E+13	0	
Emission mol/h	.687758	7.221459	
Emission kg/h	.2	2.1	
Fugacity Pa	3.781894E-10		4.679718E-11
Conc mol/m3	1.331539E-06		5.414622E-07
Conc g/m3	3.872115E-04		1.574572E-04
Conc ug/g	3.073107E-04		1.574572E-04
Amount mol	10519.16	97183.41	
Amount kg	3058.971	28260.94	
Amount %	10.82403		
Adv.flow m3/h	158000		
D rct mol/Pa.h	1.133851E+09		
D adv mol/Pa.h	5.562905E+08		
Rct rate mol/h	.4288104	4.032509	
Rct rate kg/h	.124698	0	
Adv rate mol/h	.2103831	3.18895	
Adv rate kg/h	6.117942E-02	.9273466	
Reaction %	5.938002		
Advection %	2.913305		

```
Overall residence time    h    13457.59
Reaction residence time   h    24099.99
Advection residence time  h    30475.05
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 7.0020E-02	5.4315E+02	4.2997E+11	1.9051E+08	2.4079E-01
Air to soil 4.6703E-01	8.1433E+01	2.8679E+12	1.2707E+09	1.6060E+00
Water to air 9.3880E-04	2.3427E+05	1.8695E+06	6.8986E+07	3.2283E-03
Water to sediment 1.0757E-02	2.0446E+04	2.1422E+07	7.9047E+08	3.6992E-02
Soil to air 7.7500E-03	2.2202E+06	1.7136E+04	9.7736E+07	2.6651E-02
Soil to water 4.7104E-02	3.6530E+05	1.0415E+05	5.9403E+08	1.6198E-01
Sediment to water 2.4880E-02	8.5204E+04	6.4254E+04	2.2623E+08	8.5556E-02

Transport velocity parameters

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   6.906811E+07   Air-water diffusion
(water-side)   5.794761E+10
Air-water diffusion (overall)   6.898589E+07
Rain dissolution to water   1.158952E+08   Aerosol deposition to
water   5632570
Rain dissolution to soil   1.118609E+09   Aerosol deposition to
soil   5.436499E+07
Soil-air diffusion (air-phase)   2666553   Soil-air diffusion
(water-phase)   1.118609E+08
Soil-air diffusion (bndry layer) 6.666383E+08   Soil-air diffusion
(overall)   9.773645E+07
Water-sediment diffusion   1.158952E+08
Water-sediment deposition   6.745778E+08   Sediment-water
resuspension   1.103309E+08
Soil-water runoff (water)   5.593043E+08   Soil-water runoff
(solids)   3.472509E+07

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Norway environment

Properties of Lindane :
Temperature deg C	5
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	7.179233E-02
Vapor pressure Pa	9.454027E-04
Sub-cooled liquid vapor press Pa	1.316857E-02
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	4.506936E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	1.948912E-05
Soil-water partition coefficient	310.4311
Sedt-water partition coefficient	475.9944
Susp sedt-water partn coeffnt	1164.117
Aerosol-air partition coeff	4.556302E+08
Aerosol Z value	197025.9
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	1.530133E-09
Total of VZ products	2.24738E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.24E+14	1E+11	3.19E+10
Density kg/m3	1.270649	1000	2400
Depth m	1000	20	.1
Area m2	3.24E+11	5E+09	3.19E+11
Frn org carb			.05
Z mol/m3.Pa	4.324251E-04	22.18802	6887.853
VZ mol/Pa	1.401057E+11	2.218802E+12	2.197225E+14
Fugacity Pa	1.530133E-09	1.530133E-09	1.530133E-09
Conc mol/m3	6.616679E-13	3.395062E-08	1.053933E-05
Conc g/m3	1.92413E-10	9.872841E-06	3.064837E-03
Conc ug/g	1.51429E-07	9.872841E-06	1.277015E-03
Amount mol	214.3804	3395.062	336204.6
Amount kg	62.34181	987.2841	97768.31
Amount %	6.234182E-02	.9872841	97.7683

Phase	Sediment	Susp sedt	Fish
Volume m3	2.5E+08	600000	100000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	5E+09	0	0
Frn org carb	.08	.3	
Z mol/m3.Pa	10561.37	25829.45	6999.851
VZ mol/Pa	2.640344E+12	1.549767E+10	6.999851E+08
Fugacity Pa	1.530133E-09	1.530133E-09	1.530133E-09
Conc mol/m3	1.616031E-05	3.952249E-05	1.07107E-05
Conc g/m3	4.699417E-03	1.149314E-02	3.114672E-03
Conc ug/g	2.043225E-03	7.662093E-03	3.114672E-03
Amount mol	4040.077	23.71349	1.07107
Amount kg	1174.854	6.895884	.3114672
Amount %	1.174854	6.895884E-03	3.114672E-04

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
Fate of Lindane at Norway environment

```
Emission rate of chemical mol/h    110.0413
Emission rate of chemical  kg/h    32
Fugacity Pa                        8.539609E-09
Total amount of chemical mol       1919174
Total amount of chemical kg        558095.9
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.24E+12	1E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	8.539609E-09	8.539609E-09	8.539609E-09
Conc mol/m3	3.692742E-12	1.89477E-07	5.881958E-05
Conc g/m3	1.073849E-09	5.509992E-05	1.710473E-02
Conc ug/g	8.451188E-07	5.509992E-05	7.126971E-03
Amount mol	1196.448	18947.7	1876344
Amount kg	347.9271	5509.992	545640.9
Amount %	6.234182E-02	.9872841	97.76832
D rct mol/Pa.h	5.831428E+07	9.044882E+07	8.956923E+09
D adv mol/Pa.h	1.401057E+09	2.218802E+09	0
Rct rate mol/h	.4979812	.7723975	76.48862
Adv rate mol/h	11.96448	18.9477	0
Rct rate kg/h	.1448129	.2246132	22.24289
Adv rate kg/h	3.479271	5.509992	0
Reaction %	.4525403	.7019162	69.50903
Advection %	10.87272	17.21873	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	5000		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	8.539609E-09	8.539609E-09	8.539609E-09
Conc mol/m3	9.019001E-05	2.205734E-04	5.977599E-05
Conc g/m3	2.622725E-02	6.414275E-02	1.738286E-02
Conc ug/g	1.140315E-02	4.276183E-02	1.738286E-02
Amount mol	22547.5	132.344	5.977599
Amount kg	6556.813	38.48565	1.738286
Amount %	1.174854	6.895885E-03	3.114673E-04
D rct mol/Pa.h	1.076328E+08		
D adv mol/Pa.h	5.280687E+07		
Rct rate mol/h	.9191422		
Adv rate mol/h	.4509501		
Rct rate kg/h	.2672866		
Adv rate kg/h	.1311363		
Reaction %	.8352704		
Advection %	.4098008		

```
Total advection D value      3.672666E+09
Total reaction D value       9.213318E+09
Total D value                1.288598E+10
Output by reaction    mol/h  78.67814
Output by advection   mol/h  31.36314
Total output by reaction and advection mol/h  110.0413
Output by reaction    kg/h   22.8796
Output by advection   kg/h   9.120399
Total output by reaction and advection kg/h   32
```

Overall residence time   h   17440.49
Reaction residence time   h   24392.73
Advection residence time h   61192.04

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Norway environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.24E+14	1E+11	5.742E+10
Density kg/m3	1.270649	1000.009	1500.254
Bulk Z value	4.363657E-04	22.32417	3450.583
Bulk VZ	1.413825E+11	2.232417E+12	1.981325E+14
Emission mol/h	1.822559	.5158185	.3782669
Emission kg/h	.53	.15	.11
Fugacity Pa	7.945637E-10	2.411181E-10	1.201322E-10
Conc mol/m3	3.467203E-13	5.382762E-09	4.145261E-07
Conc g/m3	1.008263E-10	1.565307E-06	1.205442E-04
Conc ug/g	7.935023E-08	1.565294E-06	8.034917E-05
Amount mol	112.3374	538.2762	23802.09
Amount kg	32.66771	156.5307	6921.646
Amount %	.4543016	2.176833	96.25758
Adv.flow m3/h	3.24E+12	1E+08	0
D rct mol/Pa.h	5.884567E+07	9.100381E+07	8.076812E+09
D adv mol/Pa.h	1.413825E+09	2.232417E+09	0
Rct rate mol/h	4.675664E-02	2.194267E-02	.9702849
Rct rate kg/h	1.359683E-02	6.380928E-03	.2821589
Adv rate mol/h	1.123374	.5382761	0
Adv rate kg/h	.3266771	.1565307	0
Reaction %	1.720682	.8075078	35.70727
Advection %	41.34106	19.80899	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.25E+09		
Density kg/m3	1260		
Bulk Z value	2130.026		0
Bulk VZ	2.662532E+12	0	
Emission mol/h	6.877579E-04	2.717332	
Emission kg/h	.0002	.7902	
Fugacity Pa	1.032068E-10		2.411181E-10
Conc mol/m3	2.198331E-07		1.687791E-06
Conc g/m3	6.392745E-05		4.908096E-04
Conc ug/g	5.073607E-05		4.908096E-04
Amount mol	274.7913	24727.49	
Amount kg	79.90931	7190.754	
Amount %	1.111279		
Adv.flow m3/h	25000		
D rct mol/Pa.h	1.085373E+08		
D adv mol/Pa.h	5.325064E+07		
Rct rate mol/h	1.120179E-02	1.050186	
Rct rate kg/h	3.25748E-03	0	
Adv rate mol/h	5.495827E-03	1.667146	
Adv rate kg/h	1.598186E-03	.484806	
Reaction %	.4122348		
Advection %	.2022508		

Overall residence time   h   9099.915
Reaction residence time   h   23545.82
Advection residence time h   14832.23

Intermedia Data. transport kg/h	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h
Air to water 5.1930E-03	4.3595E+03	5.1504E+10	2.2475E+07	1.7858E-02
Air to soil 1.8761E-01	1.2067E+02	1.8607E+12	8.1196E+08	6.4516E-01
Water to air 7.5654E-04	1.4338E+05	4.8331E+05	1.0790E+07	2.6016E-03
Water to sediment 5.3056E-03	2.0446E+04	3.3895E+06	7.5668E+07	1.8245E-02
Soil to air 2.3215E-03	2.0662E+06	1.9259E+04	6.6453E+07	7.9832E-03
Soil to water 1.3131E-02	3.6530E+05	1.0893E+05	3.7587E+08	4.5154E-02
Sediment to water 6.4993E-04	8.5204E+04	1.0167E+04	2.1655E+07	2.2350E-03

Transport velocity parameters   m/h   m/year

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   1.081063E+07   Air-water diffusion (water-side)   5.547006E+09
Air-water diffusion (overall)   1.07896E+07
Rain dissolution to water   1.109401E+07   Aerosol deposition to water   591077.8
Rain dissolution to soil   7.077979E+08   Aerosol deposition to soil   3.771077E+07
Soil-air diffusion (air-phase)   2758872   Soil-air diffusion (water-phase)   7.077978E+07
Soil-air diffusion (bndry layer)   6.89718E+08   Soil-air diffusion (overall)   6.645332E+07
Water-sediment diffusion   1.109401E+07
Water-sediment deposition   6.457363E+07   Sediment-water resuspension   1.056137E+07
Soil-water runoff (water)   3.53899E+08   Soil-water runoff (solids)   2.197225E+07

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Sweden environment

Properties of Lindane :

Temperature deg C	4
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	6.939218E-02
Vapor pressure Pa	8.005514E-04
Sub-cooled liquid vapor press Pa	1.153662E-02
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	3.816399E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	1.656261E-05
Soil-water partition coefficient	248.3449
Sedt-water partition coefficient	356.9958
Susp sedt-water partn coeffnt	970.0972
Aerosol-air partition coeff	5.200829E+08
Aerosol Z value	225708.4
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	1.123962E-09
Total of VZ products	3.059526E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+14	7.7E+11	4.11E+10
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+11	3.85E+10	4.11E+11
Frn org carb			.04
Z mol/m3.Pa	4.339854E-04	26.20271	6507.31
VZ mol/Pa	1.952934E+11	2.017609E+13	2.674504E+14
Fugacity Pa	1.123962E-09	1.123962E-09	1.123962E-09
Conc mol/m3	4.87783E-13	2.945084E-08	7.313967E-06
Conc g/m3	1.418473E-10	8.564305E-06	2.126902E-03
Conc ug/g	1.112324E-07	8.564304E-06	8.862089E-04
Amount mol	219.5023	22677.15	300604
Amount kg	63.83127	6594.515	87415.65
Amount %	6.383127E-02	6.594515	87.41565

Phase	Sediment	Susp sedt	Fish
Volume m3	1.925E+09	4620001	770000
Density kg/m3	2300	1500	1000
Depth m	.05	0	0
Area m2	3.85E+10	0	0
Frn org carb	.06	.25	
Z mol/m3.Pa	9354.257	25419.18	8266.4
VZ mol/Pa	1.800694E+13	1.174366E+11	6.365128E+09
Fugacity Pa	1.123962E-09	1.123962E-09	1.123962E-09
Conc mol/m3	1.051383E-05	2.857018E-05	9.291116E-06
Conc g/m3	3.057421E-03	8.308209E-03	2.701857E-03
Conc ug/g	1.329313E-03	5.538806E-03	2.701857E-03
Amount mol	20239.11	131.9943	7.154159
Amount kg	5885.534	38.38393	2.08043
Amount %	5.885534	3.838393E-02	2.080429E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
Fate of Lindane at Sweden environment

Emission rate of chemical mol/h   154.7455
Emission rate of chemical kg/h   45
Fugacity Pa   4.417578E-09
Total amount of chemical mol   1351569
Total amount of chemical kg   393036.3

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+12	7.7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	4.417578E-09	4.417578E-09	4.417578E-09
Conc mol/m3	1.917164E-12	1.157525E-07	2.874655E-05
Conc g/m3	5.575113E-10	3.366083E-05	8.359495E-03
Conc ug/g	4.371838E-07	3.366083E-05	3.483123E-03
Amount mol	862.7238	89129.43	1181483
Amount kg	250.8801	25918.84	343575.2
Amount %	6.383127E-02	6.594516	87.41566
D rct mol/Pa.h	8.128429E+07	8.224723E+08	1.090254E+10
D adv mol/Pa.h	1.952934E+09	2.017609E+10	0
Rct rate mol/h	.3590796	3.633335	48.16281
Adv rate mol/h	8.627238	89.12942	0
Rct rate kg/h	.1044204	1.056574	14.00574
Adv rate kg/h	2.508801	25.91884	0
Reaction %	.2320452	2.347942	31.12387
Advection %	5.575112	57.59741	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	38500		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	4.417578E-09	4.417578E-09	4.417578E-09
Conc mol/m3	4.132315E-05	1.122912E-04	3.651746E-05
Conc g/m3	1.201677E-02	3.265428E-02	1.061928E-02
Conc ug/g	5.224684E-03	2.176952E-02	1.061928E-02
Amount mol	79547.07	518.7854	28.11845
Amount kg	23132.29	150.8628	8.176844
Amount %	5.885535	3.838393E-02	2.08043E-03
D rct mol/Pa.h	7.340478E+08		
D adv mol/Pa.h	3.601389E+08		
Rct rate mol/h	3.242713		
Adv rate mol/h	1.590941		
Rct rate kg/h	.9429809		
Adv rate kg/h	.4626458		
Reaction %	2.095513		
Advection %	1.028102		

Total advection D value   2.248916E+10
Total reaction D value   1.254034E+10
Total D value   3.50295E+10
Output by reaction   mol/h   55.39794
Output by advection   mol/h   99.3476
Total output by reaction and advection mol/h   154.7456
Output by reaction   kg/h   16.10972
Output by advection   kg/h   28.89028
Total output by reaction and advection kg/h   45

Overall residence time   h   8734.139
Reaction residence time   h   24397.47
Advection residence time h   13604.45

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Sweden environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+14	7.7E+11	7.398E+10
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.384996E-04	26.33807	3261.516
Bulk VZ	1.973248E+11	2.028032E+13	2.412869E+14
Emission mol/h	7.737277	4.298487	1.719395
Emission kg/h	2.25	1.25	.5
Fugacity Pa	2.243327E-09	2.29857E-10	4.268595E-10
Conc mol/m3	9.836978E-13	6.053991E-09	1.392209E-06
Conc g/m3	2.860593E-10	1.760501E-06	4.048543E-04
Conc ug/g	2.243192E-07	1.760486E-06	2.69857E-04
Amount mol	442.664	4661.573	102995.6
Amount kg	128.7267	1355.586	29951.12
Amount %	.3935566	4.144437	91.56969
Adv.flow m3/h	4.5E+12	7.7E+08	0
D rct mol/Pa.h	8.212978E+07	8.267211E+08	9.835991E+09
D adv mol/Pa.h	1.973248E+09	2.028032E+10	0
Rct rate mol/h	.184244	.1900277	4.198586
Rct rate kg/h	5.357814E-02	5.526004E-02	1.220949
Adv rate mol/h	4.42664	4.661573	0
Adv rate kg/h	1.287267	1.355585	0
Reaction %	1.322917	1.364446	30.14688
Advection %	31.78437	33.47125	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	9.625E+09		
Density kg/m3	1260		
Bulk Z value	1891.814		0
Bulk VZ	1.820871E+13	0	
Emission mol/h	.1719395	13.9271	
Emission kg/h	.05	4.05	
Fugacity Pa	2.404345E-10		2.29857E-10
Conc mol/m3	4.548572E-07		1.90009E-06
Conc g/m3	1.322725E-04		5.525461E-04
Conc ug/g	1.049781E-04		5.525461E-04
Amount mol	4378	112477.9	
Amount kg	1273.122	32708.56	
Amount %	3.892322		
Adv.flow m3/h	192500		
D rct mol/Pa.h	7.422726E+08		
D adv mol/Pa.h	3.641741E+08		
Rct rate mol/h	.1784679	4.751325	
Rct rate kg/h	5.189847E-02	0	
Adv rate mol/h	.08756	9.175772	
Adv rate kg/h	2.546245E-02	2.668315	
Reaction %	1.281444		
Advection %	.6287024		

Overall residence time   h   8076.187
Reaction residence time   h   23672.94
Advection residence time h   12258.13

Intermedia Data. transport kg/h	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h
Air to water 1.2362E-01	7.2162E+02	4.3215E+11	1.8950E+08	4.2511E-01
Air to soil 8.0339E-01	1.1104E+02	2.8085E+12	1.2315E+09	2.7627E+00
Water to air 5.5749E-03	1.6851E+05	3.1667E+06	8.3404E+07	1.9171E-02
Water to sediment 3.9450E-02	2.3813E+04	2.2409E+07	5.9020E+08	1.3566E-01
Soil to air 1.2279E-02	1.6904E+06	3.0329E+04	9.8920E+07	4.2225E-02
Soil to water 7.0160E-02	2.9584E+05	1.7330E+05	5.6521E+08	2.4127E-01
Sediment to water 1.2089E-02	7.2979E+04	9.1398E+04	1.7291E+08	4.1573E-02

Transport velocity parameters		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   8.35422E+07   Air-water diffusion (water-side)   5.044022E+10
Air-water diffusion (overall)   8.340406E+07
Rain dissolution to water   1.008804E+08   Aerosol deposition to water   5213863
Rain dissolution to soil   1.076932E+09   Aerosol deposition to soil   5.565968E+07
Soil-air diffusion (air-phase)   3567360   Soil-air diffusion (water-phase)   1.076932E+08
Soil-air diffusion (bndry layer) 8.918399E+08   Soil-air diffusion (overall)   9.891988E+07
Water-sediment diffusion   1.008804E+08
Water-sediment deposition   4.893192E+08   Sediment-water resuspension   7.202778E+07
Soil-water runoff (water)   5.384658E+08   Soil-water runoff (solids)   2.674504E+07

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Nordic Sea areas environment

```
Properties of Lindane :
Temperature deg C                       6
Molecular mass g/mol                    290.8
Melting point deg C                     112.9
Fugacity ratio                          7.425733E-02
Vapor pressure Pa                       1.115135E-03
Sub-cooled liquid vapor press Pa        1.501717E-02
Solubility g/m3                         6.1
Solubility mol/m3                       2.097662E-02
Henry's law constant Pa.m3/mol          5.316086E-02
Log octanol-water p-coefficient         3.8
Octanol-water partn-coefficient         6309.576
Organic C-water ptn-coefficient         2586.926
Fish-water partition coefficient        315.4788
Air-water partition coefficient         2.290574E-05
Soil-water partition coefficient        186.2587
Sedt-water partition coefficient        297.4965
Susp sedt-water partn coeffnt           1552.156
Aerosol-air partition coeff         3.995427E+08
Aerosol Z value                     172153.4
Aerosol density kg/m3               2000


Amount of chemical moles                343879
Amount of chemical kilograms            100000
Fugacity Pa                             1.966368E-08
Total of VZ products                    1.748803E+13
```

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.5E+14	7E+11	3E+07
Density kg/m3	1.266097	1000	2400
Depth m	1000	20	.1
Area m2	3.5E+11	3.5E+10	3E+08
Frn org carb			.03
Z mol/m3.Pa	4.308761E-04	18.81083	3503.681
VZ mol/Pa	1.508066E+11	1.316758E+13	1.051104E+11
Fugacity Pa	1.966368E-08	1.966368E-08	1.966368E-08
Conc mol/m3	8.472607E-12	3.698901E-07	6.889525E-05
Conc g/m3	2.463834E-09	1.075641E-04	2.003474E-02
Conc ug/g	1.946008E-06	1.075641E-04	8.347808E-03
Amount mol	2965.412	258923.1	2066.857
Amount kg	862.3419	75294.82	601.0421
Amount %	.8623419	75.29483	.6010421

Phase	Sediment	Susp sedt	Fish
Volume m3	7E+08	4900000	700000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	5596.157	29197.34	5934.419
VZ mol/Pa	3.91731E+12	1.43067E+11	4.154093E+09
Fugacity Pa	1.966368E-08	1.966368E-08	1.966368E-08
Conc mol/m3	1.10041E-04	5.741271E-04	1.166925E-04
Conc g/m3	3.199993E-02	.1669561	3.393417E-02
Conc ug/g	1.391301E-02	.1113041	3.393417E-02
Amount mol	77028.71	2813.223	81.68474
Amount kg	22399.95	818.0851	23.75392
Amount %	22.39995	.8180851	2.375392E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
Fate of Lindane at Nordic Sea areas environment

```
Emission rate of chemical mol/h     120.3576
Emission rate of chemical  kg/h     35
Fugacity Pa                         7.756248E-09
Total amount of chemical mol        135641.5
Total amount of chemical kg         39444.54
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.5E+12	7E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	7.756248E-09	7.756248E-09	7.756248E-09
Conc mol/m3	3.341981E-12	1.459015E-07	2.717542E-05
Conc g/m3	9.718481E-10	4.242815E-05	7.90261E-03
Conc ug/g	7.675938E-07	4.242815E-05	3.292754E-03
Amount mol	1169.693	102131	815.2625
Amount kg	340.1468	29699.7	237.0783
Amount %	.8623418	75.29483	.6010421
D rct mol/Pa.h	6.276815E+07	5.367726E+08	4284796
D adv mol/Pa.h	1.508066E+09	1.316758E+10	0
Rct rate mol/h	.4868453	4.163341	3.323393E-02
Adv rate mol/h	11.69693	102.131	0
Rct rate kg/h	.1415746	1.2107	9.664426E-03
Adv rate kg/h	3.401468	29.6997	0
Reaction %	.4044989	3.459142	2.761265E-02
Advection %	9.718479	84.85629	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	14000		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	7.756248E-09	7.756248E-09	7.756248E-09
Conc mol/m3	4.340518E-05	2.264618E-04	4.602882E-05
Conc g/m3	1.262222E-02	6.585509E-02	1.338518E-02
Conc ug/g	5.487924E-03	4.390339E-02	1.338518E-02
Amount mol	30383.62	1109.663	32.22017
Amount kg	8835.557	322.6899	9.369626
Amount %	22.39995	.8180851	2.375392E-02
D rct mol/Pa.h	1.59688E+08		
D adv mol/Pa.h	7.83462E+07		
Rct rate mol/h	1.23858		
Adv rate mol/h	.6076725		
Rct rate kg/h	.3601789		
Adv rate kg/h	.1767111		
Reaction %	1.029083		
Advection %	.504889		

```
Total advection D value          1.4754E+10
Total reaction D value           7.635136E+08
Total D value                    1.551751E+10
Output by reaction     mol/h     5.922
Output by advection    mol/h     114.4356
Total output by reaction and advection mol/h    120.3576
Output by reaction      kg/h     1.722117
Output by advection     kg/h     33.27788
Total output by reaction and advection kg/h     35
```

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Overall residence time	h	1126.987
Reaction residence time	h	22904.68
Advection residence time	h	1185.308

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
Fate of Lindane at Nordic Sea areas environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.5E+14	7E+11	5.4E+07
Density kg/m3	1.266097	1000.009	1500.253
Bulk Z value	4.343191E-04	18.96275	1757.484
Bulk VZ	1.520117E+11	1.327393E+13	9.490412E+10
Emission mol/h	2.751032	6.533701	0
Emission kg/h	.8	1.9	0
Fugacity Pa	1.611982E-09	4.734776E-10	2.483241E-10
Conc mol/m3	7.001146E-13	8.978438E-09	4.364256E-07
Conc g/m3	2.035933E-10	2.61093E-06	1.269126E-04
Conc ug/g	1.608039E-07	2.610907E-06	8.459409E-05
Amount mol	245.0401	6284.907	23.56698
Amount kg	71.25765	1827.651	6.853278
Amount %	2.530153	64.89457	.24334
Adv.flow m3/h	3.5E+12	7E+08	0
D rct mol/Pa.h	6.326973E+07	5.411077E+08	3868739
D adv mol/Pa.h	1.520117E+09	1.327393E+10	0
Rct rate mol/h	.1019897	.2562024	9.607011E-04
Rct rate kg/h	2.965859E-02	7.450364E-02	2.793719E-04
Adv rate mol/h	2.450401	6.284907	0
Adv rate kg/h	.7125765	1.827651	0
Reaction %	1.098466	2.759395	1.034711E-02
Advection %	26.39172	67.69078	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.5E+09		
Density kg/m3	1260		
Bulk Z value	1134.28		0
Bulk VZ	3.96998E+12	0	
Emission mol/h	0	9.284732	
Emission kg/h	0	2.7	
Fugacity Pa	7.887398E-10		4.734776E-10
Conc mol/m3	8.946518E-07		2.809814E-06
Conc g/m3	2.601647E-04		8.170938E-04
Conc ug/g	2.0648E-04		8.170938E-04
Amount mol	3131.281	9684.795	
Amount kg	910.5766	2816.338	
Amount %	32.33193		
Adv.flow m3/h	70000		
D rct mol/Pa.h	1.618351E+08		
D adv mol/Pa.h	7.93996E+07		
Rct rate mol/h	.1276458	.4867985	
Rct rate kg/h	3.711939E-02	0	
Adv rate mol/h	6.262563E-02	8.797932	
Adv rate kg/h	1.821153E-02	2.558439	
Reaction %	1.374792		
Advection %	.6745013		

Overall residence time	h	1043.088
Reaction residence time	h	19894.87
Advection residence time	h	1100.804

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 6.7823E-02	7.2810E+02	3.3313E+11	1.4468E+08	2.3323E-01
Air to soil 3.0441E-04	1.6222E+05	1.4952E+09	6.4939E+05	1.0468E-03
Water to air 1.0358E-02	1.2227E+05	3.9673E+06	7.5231E+07	3.5620E-02
Water to sediment 7.9417E-02	1.5948E+04	3.0417E+07	5.7679E+08	2.7310E-01
Soil to air 3.9052E-06	1.2161E+06	3.0771E+01	5.4080E+04	1.3429E-05
Soil to water 2.1135E-05	2.2472E+05	1.6653E+02	2.9267E+05	7.2678E-05
Sediment to water 2.4086E-02	2.6199E+04	9.2579E+04	1.0501E+08	8.2826E-02

Transport velocity parameters

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values

Air-water diffusion (air-side) 7.540331E+07   Air-water diffusion (water-side) 3.291896E+10
Air-water diffusion (overall)   7.523098E+07
Rain dissolution to water   6.583792E+07   Aerosol deposition to water   3615221
Rain dissolution to soil   564325   Aerosol deposition to soil   30987.6
Soil-air diffusion (air-phase)   2585.256   Soil-air diffusion (water-phase) 56432.5
Soil-air diffusion (bndry layer) 646314.1   Soil-air diffusion (overall)   54079.53
Water-sediment diffusion   6.583792E+07
Water-sediment deposition   5.109535E+08   Sediment-water resuspension   3.91731E+07
Soil-water runoff (water)   282162.5   Soil-water runoff (solids)   10511.04

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Nordic Countries environment

Properties of Lindane :

Temperature deg C	4
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	6.939218E-02
Vapor pressure Pa	8.005514E-04
Sub-cooled liquid vapor press Pa	1.153662E-02
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	3.816399E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	1.656261E-05
Soil-water partition coefficient	186.2587
Sedt-water partition coefficient	297.4965
Susp sedt-water partn coeffnt	1552.156
Aerosol-air partition coeff	5.200829E+08
Aerosol Z value	225708.4
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	4.219266E-10
Total of VZ products	8.150209E+14

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.5E+15	8.52E+12	1.07E+11
Density kg/m3	1.275233	1000	2400
Depth m	1000	20	.1
Area m2	1.5E+12	4.26E+11	1.07E+12
Frn org carb			.03
Z mol/m3.Pa	4.339854E-04	26.20271	4880.482
VZ mol/Pa	6.509781E+11	2.232471E+14	5.222116E+14
Fugacity Pa	4.219266E-10	4.219266E-10	4.219266E-10
Conc mol/m3	1.8311E-13	1.105562E-08	2.059205E-06
Conc g/m3	5.324838E-11	3.214974E-06	5.988169E-04
Conc ug/g	4.175579E-08	3.214974E-06	2.49507E-04
Amount mol	274.665	94193.88	220335
Amount kg	79.87257	27391.58	64073.4
Amount %	7.987256E-02	27.39158	64.0734

Phase	Sediment	Susp sedt	Fish
Volume m3	8.519999E+09	5.964E+07	8520000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.26E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	7795.215	40670.68	8266.4
VZ mol/Pa	6.641523E+13	2.4256E+12	7.042972E+10
Fugacity Pa	4.219266E-10	4.219266E-10	4.219266E-10
Conc mol/m3	3.289009E-06	1.716004E-05	3.487814E-06
Conc g/m3	9.564436E-04	4.990141E-03	1.014256E-03
Conc ug/g	4.158451E-04	3.32676E-03	1.014256E-03
Amount mol	28022.35	1023.425	29.71617
Amount kg	8148.899	297.612	.8.641463
Amount %	8.1489	.297612	8.641462E-03

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Nordic Countries environment

```
Emission rate of chemical mol/h     515.8185
Emission rate of chemical  kg/h     150
Fugacity Pa                         1.950519E-09
Total amount of chemical mol        1589713
Total amount of chemical kg         462288.7
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.5E+13	8.52E+09	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	1.950519E-09	1.950519E-09	1.950519E-09
Conc mol/m3	8.464965E-13	5.110888E-08	9.519471E-06
Conc g/m3	2.461612E-10	1.486246E-05	2.768262E-03
Conc ug/g	1.930323E-07	1.486246E-05	1.153442E-03
Amount mol	1269.745	435447.7	1018583
Amount kg	369.2418	126628.2	296204
Amount %	7.987256E-02	27.39158	64.0734
D rct mol/Pa.h	2.709477E+08	9.100602E+09	2.12878E+10
D adv mol/Pa.h	6.509781E+09	2.232471E+11	0
Rct rate mol/h	.5284884	17.7509	41.52225
Adv rate mol/h	12.69745	435.4477	0
Rct rate kg/h	.1536844	5.16196	12.07467
Adv rate kg/h	3.692418	126.6282	0
Reaction %	.1024563	3.441307	8.049781
Advection %	2.461612	84.41878	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	170400		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	1.950519E-09	1.950519E-09	1.950519E-09
Conc mol/m3	1.520471E-05	7.932892E-05	1.612377E-05
Conc g/m3	4.42153E-03	2.306885E-02	4.688791E-03
Conc ug/g	1.922404E-03	1.537923E-02	4.688791E-03
Amount mol	129544.1	4731.177	137.3745
Amount kg	37671.43	1375.826	39.9485
Amount %	8.148898	.297612	8.641462E-03
D rct mol/Pa.h	2.707397E+09		
D adv mol/Pa.h	1.328304E+09		
Rct rate mol/h	5.280828		
Adv rate mol/h	2.590882		
Rct rate kg/h	1.535665		
Adv rate kg/h	.7534285		
Reaction %	1.023777		
Advection %	.5022857		

```
Total advection D value       2.310852E+11
Total reaction D value        3.336675E+10
Total D value                 2.64452E+11
Output by reaction      mol/h  65.08247
Output by advection     mol/h  450.736
Total output by reaction and advection mol/h   515.8184
Output by reaction      kg/h   18.92598
Output by advection     kg/h   131.074
Total output by reaction and advection kg/h    150
```

```
Overall residence time    h    3081.924
Reaction residence time   h    24426.14
Advection residence time  h    3526.928
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Nordic Countries environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.5E+15	8.52E+12	1.926E+11
Density kg/m3	1.275233	1000.009	1500.255
Bulk Z value	4.384996E-04	26.41433	2448.102
Bulk VZ	6.577493E+11	2.250501E+14	4.715044E+14
Emission mol/h	10.31637	61.89822	20.63274
Emission kg/h	3	18	6
Fugacity Pa	8.93199E-10	2.715988E-10	1.122495E-09
Conc mol/m3	3.916673E-13	7.1741E-09	2.747983E-06
Conc g/m3	1.138969E-10	2.086228E-06	7.991134E-04
Conc ug/g	8.931452E-08	2.08621E-06	5.326518E-04
Amount mol	587.501	61123.33	529261.5
Amount kg	170.8453	17774.66	153909.2
Amount %	9.277495E-02	9.652262	83.5781
Adv.flow m3/h	1.5E+13	8.52E+09	0
D rct mol/Pa.h	2.73766E+08	9.174101E+09	1.922074E+10
D adv mol/Pa.h	6.577494E+09	2.250501E+11	0
Rct rate mol/h	.2445275	2.491675	21.57519
Rct rate kg/h	7.110858E-02	.7245789	6.274065
Adv rate mol/h	5.875011	61.12333	0
Adv rate kg/h	1.708453	17.77466	0
Reaction %	.260471	2.654136	22.98192
Advection %	6.25807	65.10866	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.26E+10		
Density kg/m3	1260		
Bulk Z value	1580.005		0
Bulk VZ	6.730821E+13	0	
Emission mol/h	1.031637	93.87896	
Emission kg/h	.3	27.3	
Fugacity Pa	6.281781E-10		2.715988E-10
Conc mol/m3	9.925245E-07		2.245144E-06
Conc g/m3	2.886261E-04		6.528878E-04
Conc ug/g	2.290684E-04		6.528878E-04
Amount mol	42281.55	633253.9	
Amount kg	12295.47	184150.2	
Amount %	6.676871		
Adv.flow m3/h	851999.9		
D rct mol/Pa.h	2.743799E+09		
D adv mol/Pa.h	1.346164E+09		
Rct rate mol/h	1.723595	26.03499	
Rct rate kg/h	.5012213	0	
Adv rate mol/h	.8456309	67.84397	
Adv rate kg/h	.2459095	19.72903	
Reaction %	1.835976		
Advection %	.9007672		

```
Overall residence time    h    6745.43
Reaction residence time   h    24323.19
Advection residence time  h    9333.974
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water	2.1739E+02	4.7817E+12	2.0968E+09	1.8728E+00
5.4462E-01				
Air to soil	1.4217E+02	7.3116E+12	3.2061E+09	2.8637E+00
8.3277E-01				
Water to air	1.6900E+05	3.4938E+07	9.2286E+08	2.5065E-01
7.2888E-02				
Water to sediment	1.5948E+04	3.7022E+08	9.7791E+09	2.6560E+00
7.7236E-01				
Soil to air	1.2688E+06	1.0520E+05	2.5753E+08	2.8907E-01
8.4063E-02				
Soil to water	2.2472E+05	5.9396E+05	1.4541E+09	1.6322E+00
4.7464E-01				
Sediment to water	2.6199E+04	1.1268E+06	1.7804E+09	1.1184E+00
3.2523E-01				

Transport velocity parameters   m/h   m/year

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side) 9.243889E+08 Air-water diffusion
(water-side) 5.581177E+11
Air-water diffusion (overall) 9.228604E+08
Rain dissolution to water 1.116236E+09 Aerosol deposition to
water 5.769105E+07
Rain dissolution to soil 2.80369E+09 Aerosol deposition to
soil 1.449048E+08
Soil-air diffusion (air-phase) 9287286 Soil-air diffusion
(water-phase) 2.80369E+08
Soil-air diffusion (bndry layer) 2.321822E+09 Soil-air diffusion
(overall) 2.575286E+08
Water-sediment diffusion 1.116236E+09
Water-sediment deposition 8.662856E+09 Sediment-water
resuspension 6.641523E+08
Soil-water runoff (water) 1.401845E+09 Soil-water runoff
(solids) 5.222116E+07

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Bay of Bothnia environment

Properties of Lindane :

Temperature deg C	2
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	6.478188E-02
Vapor pressure Pa	5.719487E-04
Sub-cooled liquid vapor press Pa	8.828836E-03
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	2.726601E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	1.191906E-05
Soil-water partition coefficient	248.3449
Sedt-water partition coefficient	297.4965
Susp sedt-water partn coeffnt	582.0584
Aerosol-air partition coeff	6.795913E+08
Aerosol Z value	297076.5
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	9.707329E-09
Total of VZ products	3.542467E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	3.7E+13	7.4E+11	1E+07
Density kg/m3	1.284503	1000	2400
Depth m	1000	20	.1
Area m2	3.7E+10	3.7E+10	1E+08
Frn org carb			.04
Z mol/m3.Pa	4.371399E-04	36.6757	9108.222
VZ mol/Pa	1.617418E+10	2.714002E+13	9.108222E+10
Fugacity Pa	9.707329E-09	9.707329E-09	9.707329E-09
Conc mol/m3	4.243461E-12	3.560231E-07	8.841651E-05
Conc g/m3	1.233999E-09	1.035315E-04	2.571152E-02
Conc ug/g	9.606819E-07	1.035315E-04	1.071313E-02
Amount mol	157.0081	263457.1	884.1651
Amount kg	45.65794	76613.31	257.1152
Amount %	4.565794E-02	76.61331	.2571152

Phase	Sediment	Susp sedt	Fish
Volume m3	7.4E+08	4440000	740000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	3.7E+10	0	0
Frn org carb	.05	.15	
Z mol/m3.Pa	10910.89	21347.4	11570.4
VZ mol/Pa	8.07406E+12	9.478244E+10	8.562099E+09
Fugacity Pa	9.707329E-09	9.707329E-09	9.707329E-09
Conc mol/m3	1.059156E-04	2.072262E-04	1.123177E-04
Conc g/m3	3.080026E-02	6.026138E-02	3.266199E-02
Conc ug/g	1.339142E-02	4.017425E-02	.032662
Amount mol	78377.55	920.0844	83.11511
Amount kg	22792.19	267.5605	24.16987
Amount %	22.79219	.2675605	2.416988E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Bay of Bothnia environment

Emission rate of chemical mol/h   13.75516
Emission rate of chemical kg/h   4
Fugacity Pa   4.75806E-10
Total amount of chemical mol   16855.27
Total amount of chemical kg   4901.513

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	3.7E+11	7.4E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	4.75806E-10	4.75806E-10	4.75806E-10
Conc mol/m3	2.079938E-13	1.745052E-08	4.333747E-06
Conc g/m3	6.048459E-11	5.074611E-06	1.260254E-03
Conc ug/g	4.708794E-08	5.07461E-06	5.251056E-04
Amount mol	7.69577	12913.38	43.33747
Amount kg	2.23793	3755.212	12.60254
Amount %	4.565794E-02	76.61331	.2571152
D rct mol/Pa.h	6731955	1.106355E+09	3712940
D adv mol/Pa.h	1.617418E+08	2.714002E+10	0
Rct rate mol/h	3.203104E-03	.5264103	1.766639E-03
Adv rate mol/h	.0769577	12.91338	0
Rct rate kg/h	9.314626E-04	.1530801	5.137386E-04
Adv rate kg/h	.0223793	3.755211	0
Reaction %	2.328657E-02	3.827002	1.284347E-02
Advection %	.5594824	93.88028	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	14800		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	4.75806E-10	4.75806E-10	4.75806E-10
Conc mol/m3	5.191467E-06	1.015722E-05	5.505268E-06
Conc g/m3	1.509679E-03	2.953719E-03	1.600932E-03
Conc ug/g	6.56382E-04	1.969146E-03	1.600932E-03
Amount mol	3841.686	45.09806	4.073898
Amount kg	1117.162	13.11451	1.18469
Amount %	22.79219	.2675605	2.416987E-02
D rct mol/Pa.h	3.291367E+08		
D adv mol/Pa.h	1.614812E+08		
Rct rate mol/h	.1566052		
Adv rate mol/h	7.683371E-02		
Rct rate kg/h	4.554079E-02		
Adv rate kg/h	2.234324E-02		
Reaction %	1.13852		
Advection %	.5585811		

Total advection D value   2.746324E+10
Total reaction D value   1.445936E+09
Total D value   2.890918E+10
Output by reaction   mol/h   .6879851
Output by advection   mol/h   13.06717
Total output by reaction and advection mol/h   13.75516
Output by reaction   kg/h   .2000661
Output by advection   kg/h   3.799934
Total output by reaction and advection kg/h   4

```
Overall residence time    h    1225.378
Reaction residence time   h    24499.48
Advection residence time  h    1289.894
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Bay of Bothnia environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	3.7E+13	7.4E+11	1.8E+07
Density kg/m3	1.284503	1000.009	1500.257
Bulk Z value	4.430815E-04	36.794	4565.114
Bulk VZ	1.639401E+10	2.722756E+13	8.217205E+10
Emission mol/h	.2751032	2.751032	0
Emission kg/h	.08	.8	0
Fugacity Pa	7.185153E-10	1.0113E-10	8.375248E-11
Conc mol/m3	3.183608E-13	3.720979E-09	3.823396E-07
Conc g/m3	9.257931E-11	1.082061E-06	1.111844E-04
Conc ug/g	7.207405E-08	1.082051E-06	7.411021E-05
Amount mol	11.77935	2753.524	6.882113
Amount kg	3.425434	800.7248	2.001318
Amount %	.3477333	81.28565	.203164
Adv.flow m3/h	3.7E+11	7.4E+08	0
D rct mol/Pa.h	6823454	1.109924E+09	3349720
D adv mol/Pa.h	1.639401E+08	2.722756E+10	0
Rct rate mol/h	4.902756E-03	.1122466	2.805473E-04
Rct rate kg/h	1.425721E-03	3.264131E-02	8.158315E-05
Adv rate mol/h	.1177935	2.753524	0
Adv rate kg/h	3.425434E-02	.8007249	0
Reaction %	.1620138	3.70924	9.270813E-03
Advection %	3.892539	90.99146	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	3.7E+09		
Density kg/m3	1260		
Bulk Z value	2211.519		0
Bulk VZ	8.18262E+12	0	
Emission mol/h	0	3.026135	
Emission kg/h	0	.88	
Fugacity Pa	7.519363E-11		1.0113E-10
Conc mol/m3	1.662921E-07		1.170115E-06
Conc g/m3	4.835775E-05		3.402695E-04
Conc ug/g	3.837916E-05		3.402695E-04
Amount mol	615.2809	3387.466	
Amount kg	178.9237	985.0751	
Amount %	18.16345		
Adv.flow m3/h	74000		
D rct mol/Pa.h	3.335621E+08		
D adv mol/Pa.h	1.636524E+08		
Rct rate mol/h	2.508174E-02	.1425117	
Rct rate kg/h	7.29377E-03	0	
Adv rate mol/h	1.230562E-02	2.883623	
Adv rate kg/h	3.578473E-03	.8385576	
Reaction %	.8288375		
Advection %	.4066447		

```
Overall residence time    h    1119.404
Reaction residence time   h    23769.73
Advection residence time  h    1174.726
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water	5.0930E+01	5.0345E+11	2.2307E+08	1.6028E-01
4.6609E-02				
Air to soil	2.7269E+04	9.4029E+08	4.1663E+05	2.9935E-04
8.7052E-05				
Water to air	2.3360E+05	2.1953E+06	8.0775E+07	8.1687E-03
2.3755E-03				
Water to sediment	3.5559E+04	1.4422E+07	5.3063E+08	5.3662E-02
1.5605E-02				
Soil to air	1.7771E+06	7.0195E+00	3.2045E+04	2.6838E-06
7.8046E-07				
Soil to water	2.9584E+05	4.2165E+01	1.9249E+05	1.6121E-05
4.6881E-06				
Sediment to water	2.6199E+04	9.7870E+04	2.1644E+08	1.6275E-02
4.7328E-03				

Transport velocity parameters   m/h   m/year

		m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   8.087088E+07   Air-water diffusion
(water-side) 6.785004E+10
Air-water diffusion (overall)   8.07746E+07
Rain dissolution to water   1.357001E+08   Aerosol deposition to
water   6595097
Rain dissolution to soil   366757   Aerosol deposition to
soil   17824.59
Soil-air diffusion (air-phase)   874.2799   Soil-air diffusion
(water-phase) 36675.7
Soil-air diffusion (bndry layer) 218570   Soil-air diffusion
(overall)   32044.74
Water-sediment diffusion   1.357001E+08
Water-sediment deposition   3.949269E+08   Sediment-water
resuspension   8.07406E+07
Soil-water runoff (water)   183378.5   Soil-water runoff
(solids)   9108.222

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Baltic Proper environment

```
Properties of Lindane :
Temperature deg C                      7
Molecular mass g/mol                   290.8
Melting point deg C                    112.9
Fugacity ratio                         7.678851E-02
Vapor pressure Pa                      1.313793E-03
Sub-cooled liquid vapor press Pa       1.710924E-02
Solubility g/m3                        6.1
Solubility mol/m3                      2.097662E-02
Henry's law constant Pa.m3/mol         6.263132E-02
Log octanol-water p-coefficient        3.8
Octanol-water partn-coefficient        6309.576
Organic C-water ptn-coefficient        2586.926
Fish-water partition coefficient       315.4788
Air-water partition coefficient        2.689001E-05
Soil-water partition coefficient       186.2587
Sedt-water partition coefficient       297.4965
Susp sedt-water partn coeffnt          1552.156
Aerosol-air partition coeff       3.506877E+08
Aerosol Z value                   150563.6
Aerosol density kg/m3             2000


Amount of chemical moles               343879
Amount of chemical kilograms           100000
Fugacity Pa                            3.917754E-09
Total of VZ products                   8.777452E+13
```

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	2.1E+14	4.2E+12	1E+07
Density kg/m3	1.261578	1000	2400
Depth m	1000	20	.1
Area m2	2.1E+11	2.1E+11	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.29338E-04	15.96645	2973.89
VZ mol/Pa	9.016099E+10	6.705911E+13	2.97389E+10
Fugacity Pa	3.917754E-09	3.917754E-09	3.917754E-09
Conc mol/m3	1.682041E-12	6.255263E-08	1.165097E-05
Conc g/m3	4.891374E-10	1.81903E-05	3.388102E-03
Conc ug/g	3.877189E-07	1.81903E-05	1.411709E-03
Amount mol	353.2286	262721.1	116.5097
Amount kg	102.7189	76399.28	33.88102
Amount %	.1027189	76.39928	3.388102E-02

Phase	Sediment	Susp sedt	Fish
Volume m3	4.2E+09	2.52E+07	4200000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	2.1E+11	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	4749.964	24782.42	5037.078
VZ mol/Pa	1.994985E+13	6.245171E+11	2.115573E+10
Fugacity Pa	3.917754E-09	3.917754E-09	3.917754E-09
Conc mol/m3	1.860919E-05	9.709142E-05	1.973403E-05
Conc g/m3	5.411552E-03	2.823419E-02	5.738655E-03
Conc ug/g	2.352849E-03	1.882279E-02	5.738655E-03
Amount mol	78158.6	2446.704	82.88292
Amount kg	22728.52	711.5015	24.10235
Amount %	22.72852	.7115015	2.410235E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Baltic Proper environment

```
Emission rate of chemical mol/h    72.21458
Emission rate of chemical  kg/h    21
Fugacity Pa                        1.003742E-09
Total amount of chemical mol       88102.99
Total amount of chemical kg        25620.35
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	2.1E+12	4.2E+09	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	1.003742E-09	1.003742E-09	1.003742E-09
Conc mol/m3	4.309447E-13	1.60262E-08	2.985019E-06
Conc g/m3	1.253187E-10	4.66042E-06	8.680435E-04
Conc ug/g	9.933492E-08	4.66042E-06	3.616848E-04
Amount mol	90.49839	67310.06	29.85019
Amount kg	26.31693	19573.76	8.680434
Amount %	.1027189	76.39928	3.388102E-02
D rct mol/Pa.h	3.752647E+07	2.733645E+09	1212298
D adv mol/Pa.h	9.016099E+08	6.705911E+10	0
Rct rate mol/h	.0376669	2.743875	1.216834E-03
Adv rate mol/h	.9049839	67.31005	0
Rct rate kg/h	1.095353E-02	.7979187	3.538554E-04
Adv rate kg/h	.2631693	19.57376	0
Reaction %	5.215969E-02	3.799613	1.685026E-03
Advection %	1.253187	93.2084	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	84000		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	1.003742E-09	1.003742E-09	1.003742E-09
Conc mol/m3	4.767739E-06	2.487516E-05	5.055928E-06
Conc g/m3	1.386458E-03	7.233696E-03	1.470264E-03
Conc ug/g	6.02808E-04	4.822464E-03	1.470264E-03
Amount mol	20024.5	626.8541	21.2349
Amount kg	5823.126	182.2892	6.175108
Amount %	22.72852	.7115015	2.410236E-02
D rct mol/Pa.h	8.132497E+08		
D adv mol/Pa.h	3.98997E+08		
Rct rate mol/h	.816293		
Adv rate mol/h	.4004901		
Rct rate kg/h	.237378		
Adv rate kg/h	.1164625		
Reaction %	1.130372		
Advection %	.5545835		

```
Total advection D value             6.835972E+10
Total reaction D value              3.585633E+09
Total D value                       7.194535E+10
Output by reaction      mol/h       3.599051
Output by advection     mol/h       68.61553
Total output by reaction and advection mol/h   72.21458
Output by reaction      kg/h        1.046604
Output by advection     kg/h        19.95339
Total output by reaction and advection kg/h    21
```

Overall residence time   h   1220.017
Reaction residence time   h   24479.51
Advection residence time h   1284.01

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Baltic Proper environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	2.1E+14	4.2E+12	1.8E+07
Density kg/m3	1.261578	1000.009	1500.252
Bulk Z value	4.323493E-04	16.0954	1491.735
Bulk VZ	9.079336E+10	6.76007E+13	2.685123E+10
Emission mol/h	1.547455	42.98487	0
Emission kg/h	.45	12.5	0
Fugacity Pa	1.039112E-09	6.022071E-10	1.605285E-10
Conc mol/m3	4.492596E-13	9.692767E-09	2.39466E-07
Conc g/m3	1.306447E-10	2.818657E-06	6.963672E-05
Conc ug/g	1.035566E-07	2.818633E-06	4.641667E-05
Amount mol	94.34451	40709.62	4.310389
Amount kg	27.43538	11838.36	1.253461
Amount %	.1496056	64.55477	6.835145E-03
Adv.flow m3/h	2.1E+12	4.2E+09	0
D rct mol/Pa.h	3.778967E+07	2.755723E+09	1094583
D adv mol/Pa.h	9.079335E+08	6.76007E+10	0
Rct rate mol/h	3.926772E-02	1.659516	1.757117E-04
Rct rate kg/h	1.141905E-02	.4825872	5.109697E-05
Adv rate mol/h	.943445	40.70962	0
Adv rate kg/h	.2743538	11.83836	0
Reaction %	8.783884E-02	3.712209	3.930536E-04
Advection %	2.110414	91.06427	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	2.1E+10		
Density kg/m3	1260		
Bulk Z value	962.766		0
Bulk VZ	2.021809E+13	0	
Emission mol/h	.1719395	44.70427	
Emission kg/h	.05	13	
Fugacity Pa	1.100691E-09		6.022071E-10
Conc mol/m3	1.059708E-06		3.033364E-06
Conc g/m3	3.08163E-04		8.821022E-04
Conc ug/g	2.445738E-04		8.821022E-04
Amount mol	22253.87	63062.14	
Amount kg	6471.424	18338.47	
Amount %	35.28879		
Adv.flow m3/h	420000		
D rct mol/Pa.h	8.241843E+08		
D adv mol/Pa.h	4.043617E+08		
Rct rate mol/h	.9071722	2.606131	
Rct rate kg/h	.2638057	0	
Adv rate mol/h	.4450773	42.09814	
Adv rate kg/h	.1294285	12.24214	
Reaction %	2.029274		
Advection %	.9956036		

Overall residence time   h   1410.651
Reaction residence time   h   24197.61
Advection residence time h   1497.979

Intermedia Data. transport kg/h	Half times h	Equiv flows m3/h	D values mol/Pa.h	Rates of mol/h
Air to water 2.4291E-01	7.8272E+01	1.8593E+12	8.0386E+08	8.3530E-01
Air to soil 5.5691E-05	3.4140E+05	4.2628E+08	1.8430E+05	1.9151E-04
Water to air 7.8734E-02	1.0420E+05	2.7933E+07	4.4960E+08	2.7075E-01
Water to sediment 5.1441E-01	1.5948E+04	1.8250E+08	2.9374E+09	1.7690E+00
Soil to air 7.2834E-07	1.1926E+06	1.0459E+01	1.5602E+04	2.5046E-06
Soil to water 3.8655E-06	2.2472E+05	5.5510E+01	8.2806E+04	1.3293E-05
Sediment to water 1.7118E-01	2.6199E+04	5.5548E+05	5.3479E+08	5.8864E-01

	Transport velocity parameters	m/h	m/year
1	air side air-water MTC	5	43800
2	water side air-water MTC	.05	438
3	rain rate	.0001	.876
4	aerosol deposition velocity	6E-10	5.256E-06
5	soil air phase diffusion MTC	.02	175.2
6	soil water phase diffusion MTC	.00001	.0876
7	soil air boundary layer MTC	5	43800
8	sediment-water diffusion MTC	.0001	.876
9	sediment deposition velocity	.0000005	.00438
10	sediment resuspension velocity	.0000002	.001752
11	soil water runoff rate	.00005	.438
12	soil solids runoff rate	1E-08	.0000876

Individual process D values

Air-water diffusion (air-side)   4.50805E+08   Air-water diffusion (water-side)   1.676478E+11

Air-water diffusion (overall)   4.49596E+08

Rain dissolution to water   3.352955E+08   Aerosol deposition to water   1.897101E+07

Rain dissolution to soil   159664.5   Aerosol deposition to soil   9033.814

Soil-air diffusion (air-phase)   858.676   Soil-air diffusion (water-phase)   15966.45

Soil-air diffusion (bndry layer)   214669   Soil-air diffusion (overall)   15602.27

Water-sediment diffusion   3.352955E+08

Water-sediment deposition   2.602154E+09   Sediment-water resuspension   1.994985E+08

Soil-water runoff (water)   79832.27   Soil-water runoff (solids)   2973.89

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at North Sea / Skagerrak environment

Properties of Lindane :

Temperature deg C	8
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	.0793871
Vapor pressure Pa	1.546027E-03
Sub-cooled liquid vapor press Pa	1.947453E-02
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	7.370238E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	3.153068E-05
Soil-water partition coefficient	186.2587
Sedt-water partition coefficient	297.4965
Susp sedt-water partn coeffnt	1552.156
Aerosol-air partition coeff	3.080947E+08
Aerosol Z value	131806.3
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	2.148413E-08
Total of VZ products	1.600619E+13

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	4.5E+13	9E+11	1E+07
Density kg/m3	1.25709	1000	2400
Depth m	1000	20	.1
Area m2	4.5E+10	4.5E+10	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.27811E-04	13.56808	2527.173
VZ mol/Pa	1.925149E+10	1.221128E+13	2.527173E+10
Fugacity Pa	2.148413E-08	2.148413E-08	2.148413E-08
Conc mol/m3	9.191146E-12	2.914985E-07	5.429412E-05
Conc g/m3	2.672785E-09	8.476775E-05	1.578873E-02
Conc ug/g	2.126168E-06	8.476775E-05	6.578637E-03
Amount mol	413.6016	262348.6	542.9412
Amount kg	120.2753	76290.98	157.8873
Amount %	.1202753	76.29098	.1578873

Phase	Sediment	Susp sedt	Fish
Volume m3	9E+08	5400000	900000
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	4.5E+10	0	0
Frn org carb	.05	.4	
Z mol/m3.Pa	4036.457	21059.78	4280.443
VZ mol/Pa	3.632812E+12	1.137228E+11	3.852398E+09
Fugacity Pa	2.148413E-08	2.148413E-08	2.148413E-08
Conc mol/m3	8.671978E-05	4.52451E-04	9.196158E-05
Conc g/m3	2.521811E-02	.1315727	2.674243E-02
Conc ug/g	.0109644	8.771515E-02	2.674243E-02
Amount mol	78047.8	2443.235	82.76542
Amount kg	22696.3	710.4928	24.06819
Amount %	22.6963	.7104928	2.406818E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at North Sea / Skagerrak environment

```
Emission rate of chemical mol/h    17.19395
Emission rate of chemical  kg/h    5
Fugacity Pa                        1.30938E-09
Total amount of chemical mol       20958.17
Total amount of chemical kg        6094.637
```

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	4.5E+11	9E+08	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	1.30938E-09	1.30938E-09	1.30938E-09
Conc mol/m3	5.60167E-13	1.776577E-08	3.309029E-06
Conc g/m3	1.628966E-10	5.166287E-06	9.622657E-04
Conc ug/g	1.295822E-07	5.166287E-06	4.00944E-04
Amount mol	25.20752	15989.2	33.09029
Amount kg	7.330345	4649.658	9.622656
Amount %	.1202753	76.29098	.1578873
D rct mol/Pa.h	8012784	4.977891E+08	1030195
D adv mol/Pa.h	1.925149E+08	1.221128E+10	0
Rct rate mol/h	1.049178E-02	.6517949	1.348916E-03
Adv rate mol/h	.2520751	15.9892	0
Rct rate kg/h	3.051009E-03	.1895419	3.922648E-04
Adv rate kg/h	7.330345E-02	4.649658	0
Reaction %	6.102018E-02	3.790839	7.845296E-03
Advection %	1.466069	92.99316	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	18000		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	1.30938E-09	1.30938E-09	1.30938E-09
Conc mol/m3	5.285255E-06	2.757524E-05	5.604725E-06
Conc g/m3	1.536952E-03	8.01888E-03	1.629854E-03
Conc ug/g	6.682401E-04	5.34592E-03	1.629854E-03
Amount mol	4756.73	148.9063	5.044252
Amount kg	1383.257	43.30195	1.466868
Amount %	22.6963	.7104928	2.406819E-02
D rct mol/Pa.h	1.480905E+08		
D adv mol/Pa.h	7.265623E+07		
Rct rate mol/h	.1939067		
Adv rate mol/h	9.513459E-02		
Rct rate kg/h	5.638806E-02		
Adv rate kg/h	2.766514E-02		
Reaction %	1.127761		
Advection %	.5533028		

```
Total advection D value          1.247645E+10
Total reaction D value           6.549226E+08
Total D value                    1.313137E+10
Output by reaction     mol/h     .8575422
Output by advection    mol/h     16.33641
Total output by reaction and advection mol/h    17.19395
Output by reaction     kg/h      .2493733
Output by advection    kg/h      4.750626
Total output by reaction and advection kg/h     5
```

```
Overall residence time    h    1218.928
Reaction residence time   h    24439.82
Advection residence time  h    1282.912
```

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at North Sea / Skagerrak environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	4.5E+13	9E+11	1.8E+07
Density kg/m3	1.25709	1000.009	1500.252
Bulk Z value	4.304471E-04	13.67766	1267.657
Bulk VZ	1.937012E+10	1.23099E+13	2.281783E+10
Emission mol/h	1.203577	10.14443	0
Emission kg/h	.35	2.95	0
Fugacity Pa	3.533834E-09	8.065983E-10	5.474836E-10
Conc mol/m3	1.521128E-12	1.103238E-08	6.940214E-07
Conc g/m3	4.423441E-10	3.208216E-06	2.018214E-04
Conc ug/g	3.518793E-07	3.208189E-06	1.345251E-04
Amount mol	68.45078	9929.142	12.49239
Amount kg	19.90549	2887.394	3.632786
Amount %	.4576503	66.38455	8.352196E-02
Adv.flow m3/h	4.5E+11	9E+08	0
D rct mol/Pa.h	8062158	5.018093E+08	930162.1
D adv mol/Pa.h	1.937012E+08	1.23099E+10	0
Rct rate mol/h	2.849032E-02	.4047586	5.092485E-04
Rct rate kg/h	8.284985E-03	.1177038	1.480894E-04
Adv rate mol/h	.6845078	9.929141	0
Adv rate kg/h	.1990548	2.887394	0
Reaction %	.2510602	3.566782	4.48756E-03
Advection %	6.031966	87.49681	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	4.5E+09		
Density kg/m3	1260		
Bulk Z value	818.146		0
Bulk VZ	3.681657E+12	0	
Emission mol/h	0	11.34801	
Emission kg/h	0	3.3	
Fugacity Pa	1.343667E-09		8.065983E-10
Conc mol/m3	1.099316E-06		3.452598E-06
Conc g/m3	3.19681E-04		1.004015E-03
Conc ug/g	2.537151E-04		1.004015E-03
Amount mol	4946.921	14957.01	
Amount kg	1438.564	4349.497	
Amount %	33.07427		
Adv.flow m3/h	89999.99		
D rct mol/Pa.h	1.500817E+08		
D adv mol/Pa.h	7.363313E+07		
Rct rate mol/h	.2016598	.6354179	
Rct rate kg/h	5.864266E-02	0	
Adv rate mol/h	.0989384	10.71259	
Adv rate kg/h	2.877129E-02	3.11522	
Reaction %	1.77705		
Advection %	.8718572		

```
Overall residence time    h    1318.03
Reaction residence time   h    23538.85
Advection residence time  h    1396.209
```

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water	8.3599E+01	3.7303E+11	1.6057E+08	5.6743E-01
1.6501E-01				
Air to soil	8.5445E+04	3.6497E+08	1.5710E+05	5.5517E-04
1.6144E-04				
Water to air	8.8904E+04	7.0154E+06	9.5955E+07	7.7397E-02
2.2507E-02				
Water to sediment	1.5948E+04	3.9108E+07	5.3490E+08	4.3145E-01
1.2547E-01				
Soil to air	1.1702E+06	1.0659E+01	1.3513E+04	7.3979E-06
2.1513E-06				
Soil to water	2.2472E+05	5.5510E+01	7.0368E+04	3.8525E-05
1.1203E-05				
Sediment to water	2.6199E+04	1.1903E+05	9.7384E+07	1.3085E-01
3.8052E-02				

Transport velocity parameters   m/h   m/year

			m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   9.625746E+07   Air-water diffusion
(water-side)   3.052819E+10
Air-water diffusion (overall)   9.595491E+07
Rain dissolution to water   6.105638E+07   Aerosol deposition to
water   3558770
Rain dissolution to soil   135680.9   Aerosol deposition to
soil   7908.377
Soil-air diffusion (air-phase)   855.6219   Soil-air diffusion
(water-phase)   13568.08
Soil-air diffusion (bndry layer)   213905.5   Soil-air diffusion
(overall)   13512.55
Water-sediment diffusion   6.105638E+07
Water-sediment deposition   4.73845E+08   Sediment-water
resuspension   3.632812E+07
Soil-water runoff (water)   67840.43   Soil-water runoff
(solids)   2527.173

SIX COMPARTMENT FUGACITY LEVEL I CALCULATION
Fate of Lindane at Barents Sea environment

Properties of Lindane :

Temperature deg C	-2
Molecular mass g/mol	290.8
Melting point deg C	112.9
Fugacity ratio	.0562884
Vapor pressure Pa	2.876289E-04
Sub-cooled liquid vapor press Pa	5.109914E-03
Solubility g/m3	6.1
Solubility mol/m3	2.097662E-02
Henry's law constant Pa.m3/mol	1.371188E-02
Log octanol-water p-coefficient	3.8
Octanol-water partn-coefficient	6309.576
Organic C-water ptn-coefficient	2586.926
Fish-water partition coefficient	315.4788
Air-water partition coefficient	6.082434E-06
Soil-water partition coefficient	186.2587
Sedt-water partition coefficient	59.4993
Susp sedt-water partn coeffnt	77.60778
Aerosol-air partition coeff	1.174188E+09
Aerosol Z value	520856.5
Aerosol density kg/m3	2000

Amount of chemical moles	343879
Amount of chemical kilograms	100000
Fugacity Pa	1.952221E-11
Total of VZ products	1.761476E+16

Phase properties and compositions

Phase	Air	Water	Soil
Volume m3	1.2E+15	2.4E+14	1E+07
Density kg/m3	1.303452	1000	2400
Depth m	1000	200	.1
Area m2	1.2E+12	1.2E+12	1E+08
Frn org carb			.03
Z mol/m3.Pa	4.435886E-04	72.92946	13583.74
VZ mol/Pa	5.323063E+11	1.750307E+16	1.358374E+11
Fugacity Pa	1.952221E-11	1.952221E-11	1.952221E-11
Conc mol/m3	8.659828E-15	1.423744E-09	2.651847E-07
Conc g/m3	2.518278E-12	4.140247E-07	7.71157E-05
Conc ug/g	1.932007E-09	4.140247E-07	3.213154E-05
Amount mol	10.39179	341698.5	2.651847
Amount kg	3.021933	99365.92	.771157
Amount %	3.021933E-03	99.36591	7.711569E-04

Phase	Sediment	Susp sedt	Fish
Volume m3	2.4E+10	2.4E+08	2.4E+08
Density kg/m3	2300	1500	1000
Depth m	.02	0	0
Area m2	1.2E+12	0	0
Frn org carb	.01	.02	
Z mol/m3.Pa	4339.252	5659.894	23007.7
VZ mol/Pa	1.04142E+14	1.358374E+12	5.521847E+12
Fugacity Pa	1.952221E-11	1.952221E-11	1.952221E-11
Conc mol/m3	8.471176E-08	1.104936E-07	4.49161E-07
Conc g/m3	2.463418E-05	3.213154E-05	1.30616E-04
Conc ug/g	1.071051E-05	2.142103E-05	1.30616E-04
Amount mol	2033.082	26.51846	107.7986
Amount kg	591.2203	7.711569	31.34784
Amount %	.5912203	7.711569E-03	3.134784E-02

SIX COMPARTMENT FUGACITY LEVEL II CALCULATION
 Fate of Lindane at Barents Sea environment

Emission rate of chemical mol/h   206.3274
Emission rate of chemical kg/h   60
Fugacity Pa   1.131897E-11
Total amount of chemical mol   199381
Total amount of chemical kg   57979.99

Phase properties,compositions and rates

Phase	Air	Water	Soil
Adv.flow m3/h	1.2E+13	2.4E+11	0
Adv.restime h	100	1000	0
Rct halflife h	1665	17000	17000
Rct rate c.h-1	4.162162E-04	4.076471E-05	4.076471E-05
Fugacity Pa	1.131897E-11	1.131897E-11	1.131897E-11
Conc mol/m3	5.020968E-15	8.254866E-10	1.537541E-07
Conc g/m3	1.460097E-12	2.400515E-07	4.471168E-05
Conc ug/g	1.120177E-09	2.400515E-07	1.862986E-05
Amount mol	6.025161	198116.8	1.53754
Amount kg	1.752117	57612.36	.4471168
Amount %	3.021933E-03	99.36593	7.711569E-04
D rct mol/Pa.h	2.215545E+08	7.135075E+11	5537374
D adv mol/Pa.h	5.323063E+09	1.750307E+13	0
Rct rate mol/h	2.50777E-03	8.076172 •	6.267738E-05
Adv rate mol/h	6.025161E-02	198.1168	0
Rct rate kg/h	7.292594E-04	2.348551	1.822658E-05
Adv rate kg/h	1.752117E-02	57.61236	0
Reaction %	1.215432E-03	3.914251	3.037764E-05
Advection %	2.920194E-02	96.02058	0

Phase	Sediment	Susp sedt	Fish
Adv.flow m3/h	480000		
Adv.restime h	50000		
Rct halflife h	17000		
Rct rate c.h-1	4.076471E-05		
Fugacity Pa	1.131897E-11	1.131897E-11	1.131897E-11
Conc mol/m3	4.911587E-08	6.406418E-08	2.604235E-07
Conc g/m3	1.42829E-05	1.862986E-05	7.573116E-05
Conc ug/g	6.209955E-06	1.241991E-05	7.573116E-05
Amount mol	1178.781	15.3754	62.50164
Amount kg	342.7894	4.471167	18.17548
Amount %	.5912202	7.711569E-03	3.134784E-02
D rct mol/Pa.h	4.245319E+09		
D adv mol/Pa.h	2.082841E+09		
Rct rate mol/h	4.805265E-02		
Adv rate mol/h	2.357562E-02		
Rct rate kg/h	1.397371E-02		
Adv rate kg/h	6.855789E-03		
Reaction %	2.328951E-02		
Advection %	1.142631E-02		

Total advection D value   1.751048E+13
Total reaction D value   7.179799E+11
Total D value   1.822845E+13
Output by reaction   mol/h   8.126796
Output by advection   mol/h   198.2006
Total output by reaction and advection mol/h   206.3274
Output by reaction   kg/h   2.363272
Output by advection   kg/h   57.63673
Total output by reaction and advection kg/h   60.00001

Overall residence time   h   966.3331
Reaction residence time   h   24533.78
Advection residence time h   1005.956

FOUR COMPARTMENT FUGACITY LEVEL III CALCULATION
 Fate of Lindane at Barents Sea environment

Bulk phase properties,compositions and rates

Phase	Air	Water	Soil
Bulk vol m3	1.2E+15	2.4E+14	1.8E+07
Density kg/m3	1.303452	1000.009	1500.261
Bulk Z value	4.540058E-04	72.98077	6813.751
Bulk VZ	5.448069E+11	1.751538E+16	1.226475E+11
Emission mol/h	4.126548	68.7758	0
Emission kg/h	1.2	20	0
Fugacity Pa	2.369124E-10	3.924337E-12	3.557759E-11
Conc mol/m3	1.075596E-13	2.864011E-10	2.424168E-07
Conc g/m3	3.127832E-11	8.328544E-08	7.049481E-05
Conc ug/g	2.399653E-08	8.328473E-08	4.698837E-05
Amount mol	129.0715	68736.26	4.363503
Amount kg	37.53399	19988.5	1.268907
Amount %	.1865467	99.34436	6.30656E-03
Adv.flow m3/h	1.2E+13	2.4E+11	0
D rct mol/Pa.h	2.267575E+08	7.140095E+11	4999690
D adv mol/Pa.h	5.448068E+09	1.751538E+13	0
Rct rate mol/h	5.372164E-02	2.802014	1.778769E-04
Rct rate kg/h	1.562225E-02	.8148255	5.17266E-05
Adv rate mol/h	1.290715	68.73626	0
Adv rate kg/h	.3753398	19.98851	0
Reaction %	7.368986E-02	3.843516	2.439934E-04
Advection %	1.770471	94.28539	0

Bulk phase properties, compositions and rates

Phase	Sediment	Total	Fish
Bulk vol m3	1.2E+11		
Density kg/m3	1260		
Bulk Z value	926.1939		0
Bulk VZ	1.111433E+14	0	
Emission mol/h	0	72.90235	
Emission kg/h	0	21.2	
Fugacity Pa	2.881011E-12		3.924337E-12
Conc mol/m3	2.668375E-09		9.028994E-08
Conc g/m3	7.759633E-07		2.625632E-05
Conc ug/g	6.158438E-07		2.625632E-05
Amount mol	320.2049	69189.9	
Amount kg	93.11558	20120.42	
Amount %	.4627914		
Adv.flow m3/h	2400000		
D rct mol/Pa.h	4.530722E+09		
D adv mol/Pa.h	2.222865E+09		
Rct rate mol/h	1.305306E-02	2.868966	
Rct rate kg/h	3.795829E-03	0	
Adv rate mol/h	6.404098E-03	70.03338	
Adv rate kg/h	1.862312E-03	20.36571	
Reaction %	1.790485E-02		
Advection %	8.784488E-03		

Overall residence time   h   949.0765
Reaction residence time   h   24116.67
Advection residence time h   987.9561

Intermedia Data. transport	Half times	Equiv flows	D values	Rates of
	h	m3/h	mol/Pa.h	mol/h
kg/h				
Air to water 8.1202E-01	3.2033E+01	2.5961E+13	1.1786E+10	2.7924E+00
Air to soil 5.6213E-05	4.6272E+05	1.7972E+09	8.1593E+05	1.9330E-04
Water to air 3.0355E-03	4.5634E+06	3.6447E+07	2.6599E+09	1.0438E-02
Water to sediment 1.3863E-02	9.9923E+05	1.6645E+08	1.2147E+10	4.7671E-02
Soil to air 5.7300E-07	1.5346E+06	8.1283E+00	5.5384E+04	1.9704E-06
Soil to water 3.9132E-06	2.2472E+05	5.5510E+01	3.7823E+05	1.3457E-05
Sediment to water 8.2045E-03	7.8651E+03	1.0573E+07	9.7930E+09	2.8214E-02

	Transport velocity parameters		m/h	m/year
1	air side air-water MTC		5	43800
2	water side air-water MTC		.05	438
3	rain rate		.0001	.876
4	aerosol deposition velocity		6E-10	5.256E-06
5	soil air phase diffusion MTC		.02	175.2
6	soil water phase diffusion MTC		.00001	.0876
7	soil air boundary layer MTC		5	43800
8	sediment-water diffusion MTC		.0001	.876
9	sediment deposition velocity		.0000005	.00438
10	sediment resuspension velocity		.0000002	.001752
11	soil water runoff rate		.00005	.438
12	soil solids runoff rate		1E-08	.0000876

Individual process D values
Air-water diffusion (air-side)   2.661532E+09   Air-water diffusion (water-side)   4.375768E+12
Air-water diffusion (overall)   2.659914E+09
Rain dissolution to water   8.751534E+09   Aerosol deposition to water   3.750167E+08
Rain dissolution to soil   729294.6   Aerosol deposition to soil   31251.39
Soil-air diffusion (air-phase)   887.1772   Soil-air diffusion (water-phase)   72929.46
Soil-air diffusion (bndry layer) 221794.3   Soil-air diffusion (overall)   55383.98
Water-sediment diffusion   8.751534E+09
Water-sediment deposition   3.395936E+09   Sediment-water resuspension   1.04142E+09
Soil-water runoff (water)   364647.3   Soil-water runoff (solids)   13583.74

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TITLE	PROJECT LEADER
Regional and Global Cycling of Persistent Organic Pollutants (POPs): An Assessment and a Feasibility Study in a Nordic Perspective	J.M. Pacyna
	NILU PROJECT NO. O-93078

AUTHOR(S)	CLASSIFICATION *
J.M. Pacyna, E. Brorström-Lunden, M. Cleeman, B. Jansson, M. Korhonen, M. Oehme, J. Paasivirta, M. Erecius Poulsen, S. Sinkkonen, A. Zuber	A
	CLIENT'S REF.

CLIENT
Nordic Council of Ministers
Copenhagen

ABSTRACT
Studies on the fate, behaviour, and environmental and health effects of POPs in Scandinavia are reviewed. The fugacity model was used to assess the migration of hexachlorobenzene, lindane, and fluoranthene. Modeled concentrations were compared with measurements in some compartments of the environment. Fairly good agreement was observed for air and water but less so for fish. More refined data are needed to verify the results from models applied in specific regions. Several cases of reproductive tract anomalies, cancers, and behavioral abnormalities have been detected and their relationship to the presence of various POPs is now becoming evident for various species.

NORWEGIAN TITLE

DESCRIPTORS		
Persistent organice compounds	Emission sources	Environmental migration

ABSTRACT (in Norwegian)

* Classification   A   Unclassified (can be ordered from NILU)
                       B   Restricted distribution
                       C   Classified (not to be distributed)