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UMI
Octanol/Lipid-Water Partition Coefficients of Chlorobenzenes and Chemical Fate Modelling in Indian lakes

by

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A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy at Department of Chemical Engineering and Applied Chemistry in the University of Toronto

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0-612-36196-9
Dedicated to the memory of my father
ABSTRACT

The octanol-water (K_{OW}) and tricaprylamine-water partition coefficients (K_{TW}) of seven chlorobenzenes (1,2-dichlorobenzene, 1,4-dichlorobenzene, 1,3,5-trichlorobenzene, 1,2,3,4-tetrachlorobenzene, 1,2,3,5-tetrachlorobenzene, pentachlorobenzene and hexachlorobenzene) were measured by a conventional shake-flask, batch contacting method over the temperature range 5 to 45 °C. The results agree well with available literature data obtained with comparable methods. The van't Hoff plots of log K_{OW} versus reciprocal of temperature exhibit linearity with values of K_{OW} increasing by 10% - 14% over this temperature range. The enthalpy of phase change ranges from 17 to 24 kJ/mol. The K_{OW} values from this study are also compared with values calculated from reported measurements of octanol-air partition coefficient (K_{OA}) and air-water partition coefficient (K_{AW}). The agreement between experimentally determined and estimated values of K_{OW} are generally within 11%. This correlation approach can be important in estimating missing data for physical-chemical properties as required by the environmental fate models. The K_{TW} values at 25 °C are somewhat greater than corresponding K_{OW} values. Larger deviations between K_{TW} and K_{OW} are observed for lower molecular mass chlorobenzenes. Generally, the differences are within 4%, with the exception of dichlorobenzenes, for which it was up to 10%. The values of log K_{TW} are satisfactorily correlated in linear form with respective values of log K_{OW} (from this work) as well as with reported values of triolein-water partition coefficients. The van't Hoff plots of log K_{TW} versus
reciprocal of temperature show linear behaviour with log $K_{tw}$ values increasing by 5% - 8% over the temperature range (5 to 45 °C). The enthalpy of phase change ranges from 9.7 to 16 kJ/mol. These data, which are regarded as more accurate than previous data will be of value for assessing the environmental fate of the chlorobenzenes, especially as a function of temperature.

As an illustration of the application of such physical-chemical property data, water quality models were developed for two large lakes in India namely Lake Nainital in the Central Himalayan region and Rihand Reservoir in east central India. The contaminants assessed were lead, copper, 1,4-di, 1,2,3,5-tetra, penta-, and hexachlorobenzene, lindane, $\alpha$-HCH, benzo(a)pyrene, and benzo(b)fluoranthene. Using reported and estimated data for emissions and lake characteristics, a steady state multi-segment QWASI fugacity model gave results which compared well with the reported concentrations. This model is viewed as possibly too complex for general use, especially in regions lacking a sophisticated infrastructure for environmental assessment. Accordingly, two simple models were developed and successfully applied to these chemicals. The role of such models for management of chemicals in developing regions is discussed.
ACKNOWLEDGEMENTS

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1. INTRODUCTION

The need for methods to predict the environmental hazards posed by chemicals is globally recognized, and is being reflected in a wide range of regulatory schemes. An essential element of such schemes is the ability to predict the fate and behaviour of chemicals. The environmental fate of chemicals is largely controlled by their physical-chemical properties and can be best assessed by both monitoring and modelling efforts. The key physical-chemical properties are solubility in water, vapor pressure, octanol-water partition coefficient and the susceptibility of the substance to degradation or transformation reactions. Of these, the dimensionless octanol-water partition coefficient ($K_{OW}$) is one of the most important and frequently used descriptors of chemical partitioning in the environment (Mackay et al., 1992). It provides a direct estimate of hydrophobicity which is widely used to predict the partitioning tendency from water to organic media such as lipids, waxes and natural organic matter present in soils and sediments. It is also an indirect indicator of activity coefficient in aqueous phases. It has proved invaluable for predicting soil adsorption (Karickhoff et al., 1979), biological uptake (Thomann, 1989; Oliver et al., 1985; Gobas et al., 1987, 1988), and biomagnification (Clark and Mackay, 1991; Mackay, 1982).

Although numerous studies have been conducted on the partitioning of organic substances between water and octanol, data on the temperature dependence of partition coefficients are sparse. Inspection of the literature suggests that little attention is normally given to defining or controlling temperature accurately during determinations (Sangster, 1989). The temperature dependence of $K_{OW}$ can be an important factor, but is not often taken into account in environmental models. It is, therefore, important to study the effect of temperature on
partitioning. The knowledge of physicochemical factors such as $K_{ow}$ and its temperature dependence can be used in correlating and estimating partitioning characteristics and for predicting the $K_{ow}$ over a range of environmental temperatures.

Octanol is considered to be a suitable and convenient lipid surrogate for fat, i.e. glycerol, esters (the portion of organism where hydrophobic chemicals tend to bioaccumulate). Few efforts have been made to explore the possibility of using other organic media in place of octanol (Chiou, 1985). It would therefore be interesting to examine the feasibility of substituting other organic media such as tricaprylin (glycerol trioctanoate) as surrogate for 1-octanol, which may represent lipids/ triglycerides/ fats of biota more closely in describing chemical partitioning characteristics.

This thesis has, therefore, two connected parts, experimental and modelling. The experimental section involves the measurements of the temperature dependences of octanol-water ($K_{ow}$) and tricaprylin-water ($K_{rw}$) partitioning of selected chlorobenzenes. The chlorobenzenes were selected for this study first because some of them are environmentally persistent, toxic and bioaccumulative, and they cover a range in hydrophobicity and secondly, because they are among the most studied compounds in terms of physical-chemical properties. The octanol-water and tricaprylin-water partition coefficients were determined by the conventional shake-flask, batch contacting method. Their temperature dependence was measured by determining the partition coefficients at ten degree intervals from 5 to 45 °C. The logarithm of the partition coefficients were correlated with the inverse of temperature to obtain the thermodynamic relationship between $K_{ow}$ and temperature. The present data contribute to the existing data base on temperature dependence and can contribute either to more accurate modelling of the fate and behaviour of chemicals, or for use in situations when data are
unavailable or are suspect. Moreover, such studies permit the estimation of the enthalpy and entropy contributions involved in the partitioning of chemicals between n-octanol/ tricaprylin and water and are thus of thermodynamic interest.

The second part of this thesis deals with the development and application of Quantitative Water-Air-Sediment Interaction (QWASI) fugacity models to elucidate the fate of some chlorinated and persistent chemicals in aquatic environments. Models such as these have been extensively used and validated for the Great Lakes of North America (e.g. Mackay et al., 1983; Jeremiasen et al., 1994; Diamond et al., 1994) and other temperate aquatic environments (Lun, 1995) but not in tropical systems. Therefore, in an attempt to apply these models to tropical conditions, two important Indian lakes for which there are growing concerns over chemical contamination, were selected for this study. There is an urgent need to initiate this work for developing countries such as India where most of the aquatic systems, though heavily contaminated, are still used as a primary source of drinking water, as well as for fishing. A three-segment QWASI model is developed and applied to determine the fate of polycyclic aromatic hydrocarbons (PAHs), hexachlorocyclohexanes (HCHs) as well as selected chlorobenzenes in Rihand Reservoir. The reservoir is located in east central India and is contaminated by effluents from numerous industries in nearby area such as pesticides, aluminum, carbon black, power plants. The physical-chemical properties of chlorobenzenes determined in this work are utilized as model parameters. A simulation was also prepared of the fate of lead, copper, and chlorobenzenes in Lake Nainital, which is a high altitude lake, located in the Central Himalaya mountains, and is one of India’s most popular tourist attractions. The validity of the models is assessed by comparing the chemical concentrations estimated by the model with reported values. The environmental fate and
the behaviour of the chemicals are described through mass balance diagrams, which provide insights into the important processes controlling the overall fate. Finally, the implications for the management of emissions are discussed, and accordingly, some remedial and control measures are suggested.

It is hoped that studies such as this will contribute to the better management of these lakes and help the authorities plan for their remediation, thereby preventing further degradation. The example of the application of the mass balance model may encourage its use for regulatory purposes as well as in other areas for which remedial action plans, similar to the those formulated and implemented for the Areas of Concern in the Great Lakes region of North America, must be drafted.
2. LITERATURE REVIEW AND BACKGROUND

2.1 Physical-Chemical Properties

The assessment of a chemical's fate and partitioning behaviour in multimedia environments requires information on physical-chemical properties. The increasing reliance and use of these in recent decades are reflected in the desire of researchers to generate either new physical-chemical data, or more reliable data. Many organic contaminants are hydrophobic, which implies that they are sparingly soluble in water and prefer to partition into lipid or organic phases. In reality, most organic chemicals are approximately equally soluble in lipid or fat phases but they vary greatly in their solubility in water. A convenient surrogate for lipid and fat to describe the hydrophobic tendency is the octanol-water partition coefficient ($K_{ow}$) which is the ratio of the equilibrium concentration which the chemical adopts in octanol to that in water. Therefore, a low water solubility implies high hydrophobicity and a high octanol-water partition coefficient. A chemical's tendency to partition into the atmosphere is controlled by its vapor pressure. The vapor pressure can be converted into a solubility if it is divided by the gas constant, temperature group RT. The ratio of the solubility in air to solubility in water is essentially an air-water partition coefficient ($K_{aw}$) or a version of Henry's law constant.

2.2 Octanol-Water Partition Coefficients

Although several organic liquid-water partition coefficients such as hexane-water, triolein-water could be used as an indicator of hydrophobicity, the most widely used is $K_{ow}$, largely as a result of the extensive studies and data compilations by Hansch and Leo (1979). Octanol was selected probably because it has a similar carbon to oxygen ratio as lipid, is readily available in pure form, and is only sparingly soluble in water. Moreover, owing to its similarity in polarity with biotic liquids, notably lipids, octanol is considered to be a good representative of lipid/water partition coefficient. The variation in $K_{ow}$ between chemicals is primarily due to the variation in aqueous solubility since the solubility of organic chemicals in octanol tends to be fairly constant. This is indicative of a correlation between aqueous solubility and $K_{ow}$. A linear relationship between aqueous solubility and $K_{ow}$ was first proposed by Hansch et al.
A more quantitative relationship was then developed by Chiou et al. (1977) and subsequently by Yalkowsky and Valvani (1979), Tewari et al. (1982) and Banerjee et al. (1980) for environmental chemicals. Mackay et al. (1980) and Miller et al. (1985) derived the relationship between $K_{OW}$ and aqueous solubility in terms of activity coefficients and fugacity. When a solute partitions between a liquid phase such as octanol (subscript O) and water (subscript W), the fugacity is given as:

$$f = x_{O} \gamma_{O} f_{R} = x_{W} \gamma_{W} f_{R}$$  \hspace{1cm} (1)

or

$$x_{O} \gamma_{O} = x_{W} \gamma_{W}$$  \hspace{1cm} (2)

where $x_{W}$ and $\gamma_{W}$ are respectively the chemical's mole fraction and activity coefficient in water, $x_{O}$ and $\gamma_{O}$ are respectively the chemical's mole fraction and activity coefficient in octanol and $f_{R}$ is the reference state fugacity or approximately the vapor pressure of the pure solute in liquid form at system temperature. In dilute aqueous solution, the concentration $C_{W}$ in mol/m$^3$ is approximately $x_{W}/v_{W}$ where $v_{W}$ is the molar volume of the solution (m$^3$/mol). At saturation, when the concentration is $C_{W}^s$, it is usually assumed that the water dissolved in saturated liquid solute has a negligible effect on the fugacity of the excess liquid solute. Therefore, on equating $f$ to $f_{R}$, the above equation can be written as:

$$\gamma_{W} = 1/ x_{W} = 1/ C_{W} v_{W}$$  \hspace{1cm} (3)

Under equilibrium conditions, $K_{OW}$ is defined as the ratio of solute concentration in octanol saturated with water $C_{OW}$, to its concentration in water saturated with octanol, $C_{WO}$ as shown in following equation:

$$K_{OW} = C_{OW} / C_{WO}$$  \hspace{1cm} (4)

It can also be viewed as a ratio of solubility in octanol and water in which case the solubility in octanol, $C_{O}$ is $1/\gamma_{O}v_{O}$. On substituting for $x_{O}/x_{W}$ from equation (2) and $\gamma_{W}$ from equation (3), the above equation gives:
\[ K_{\text{OW}} = \frac{(x_0 / v_0)}{(x_w / v_w)} = \frac{\gamma_{w} v_{w}}{\gamma_{o} v_{o}} = \frac{1}{\gamma_{o} v_{o} C_{w}^{5}} \] (5)

The above fundamental relationship between \( C_{w}^{5} \) and \( K_{\text{OW}} \) can be converted into the logarithmic form as shown in following equation:

\[ \log K_{\text{OW}} = A - B \log C_{w}^{5} \] (6)

Miller et al. (1985) further examined the relationships between \( K_{\text{OW}} \) and \( C_{w}^{5} \) and experimentally demonstrated that the mutual solubility of water and octanol has a negligible effect on the solubility of chemicals in octanol.

\( K_{\text{OW}} \) is a crucial parameter in studies on fate and distribution of organic pollutants in the environment. The correlations between \( K_{\text{OW}} \) and sorption and mobility of a chemical in sediment and soils defined as \( K_{\text{OC}} \), was studied by Schwarzenbach and Westall (1981) and Karickhoff (1981). The \( K_{\text{OC}} \) can be calculated from \( K_{\text{OW}} \). The importance of \( K_{\text{OW}} \) is further evidenced by its correlation with various lipid/water partitioning processes or properties such as drug behaviour (Hansch and Leo, 1979), fish gill adsorption (Clark et al., 1990), accumulation by terrestrial biota (Kenaga, 1980) and bioconcentration by aquatic biota (Mackay, 1982; Clark and Mackay, 1991). \( K_{\text{OW}} \) is a common index used for chemical hazard assessment particularly in aquatic toxicology because of its good correlation with the bioconcentration factor and chronic toxicities (Neely et al., 1974; Hansch and Leo, 1979; Veith et al., 1983). There are numerous literature on \( K_{\text{OW}} \) measurements of various organic solutes (Chiou et al., 1977; Tewari et al., 1982; Lun et al., 1995). Most of these data are measured at room temperature i.e. 20 to 25 °C.

2.2.1 Temperature Dependence of Octanol-Water Partition Coefficients (\( K_{\text{OW}} \))

Measuring partition coefficients as a function of temperature may require lengthy and accurate experimentation. Temperature dependence of \( K_{\text{OW}} \) can be an important factor but is not often taken into account in environmental models. Temperature variation in water bodies
can range from 0 to over 35 °C. Sangster (1989) has compiled data on temperature
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resorcinol monoalkyl-ethers (Beezer et al., 1980) and p-cresol and phenol (James et al., 1981)
have been measured as a function of temperature. Opperhuizen et al. (1988) investigated the
partitioning of chlorobenzenes in fish-water and octanol-water systems over the temperature
range 13 to 33 °C in an attempt to elucidate the thermodynamics of the partitioning process.
Recently, the temperature dependence of octanol-water partitioning of dibenzofuran and
aqueous solubility of some chlorobenzene and dibenzofuran has been reported over the
temperature range 5 to 45 °C (Shiu et al., 1997). Data have been reported on temperature
dependence of the related octanol-air partition coefficient which is suggested as a valuable
descriptor of air-vegetation and air-soil equilibrium (Harner and Mackay, 1995; Harner and
Bidleman, 1996). The temperature dependence of Henry's law constant has also been
investigated for selected chlorobenzenes, polychlorinated biphenyls and polycyclic aromatic
hydrocarbons in the range of 10 to 55 °C (Hulcher et al., 1992) and for many other organic
chemicals over a temperature range of 10 - 30 °C. The studies on vapor pressure variation with
temperature were conducted for benzene and several chlorobenzenes by Liu and Dickhut
(1994).

The temperature dependence of $K_{ow}$ can be modelled with van't Hoff equation, which
is expressed as:

$$\ln K_{ow} = A + \frac{B}{T} = A + \frac{-\Delta H}{RT}$$

where $A$ and $B$ are regression constant, $\Delta H$ is enthalpy of phase transfer (J/mol), $T$ is
absolute temperature (K), $R$ is gas constant (J/moL.K).

The above equation can be used to estimate enthalpies of phase transfer and subsequently,
the $K_{ow}$'s at other environmental temperatures.
2.3 Substitute for surrogate ‘octanol’

It has been generally assumed that the mechanism leading to the uptake of organic pollutants by organisms is analogous to the partitioning between a non-polar organic phase and water. Hence, values of bioconcentration factor (BCF) of organic compounds from both laboratory bioconcentration testsings and natural water systems have been correlated either with the corresponding octanol-water partition coefficients (log \(K_{ow}\)) or with their water solubilities (log S), to which log \(K_{ow}\) is strongly correlated. Many researchers (Reinert, 1970; Anderson and Fenderson, 1970; Roberts et al., 1977; and Sugiura et al., 1979) found that concentrations of various organic compounds accumulated in fish are determined largely by fish lipid content. Hansen et al. (1971) showed that residual PCB contents vary considerably in different tissues of fish, presumably because of variations in lipid content. BCF values of various chlorinated compounds in laboratory studies with guppies (Könemann and van Leeuwen, 1980) as well as with rainbow trout (Oliver and Nümi, 1983) indicated that the lipid fraction of the fish is an important controlling factor in the bioconcentration of relatively hydrophobic organic compounds. The importance of lipids in bioconcentration has also been investigated in correlation analyses (Chiou, 1981; Mackay, 1982). To better understand the effect of lipids in bioconcentration, it is of both theoretical and practical interest to examine the partitioning characteristics of organic compounds in lipid-water systems. Presumably, this was the basis for validating the use of empirical parameters (such as log \(K_{ow}\) and log S) in the assessment of bioconcentration and in characterizing the lipophilicity of organic compounds in biochemical studies.

There is some concern about whether the commonly used octanol-water partition coefficient is a good measure of lipid-water partition coefficient, since 1- octanol has some real and potential disadvantages. First, its surfactant properties may cause the formation of emulsions in the analytical method. Secondly, it may not be structurally an ideal surrogate (polar/nonpolar balance). The thermodynamic studies by Beezer et al. (1983) also suggested that octanol was not a satisfactory solvent to mimic a biological lipoidal phase. Apart from only a few studies (Platford, 1979; Chiou, 1985; Nümi, 1991) on partition
coefficient in lipid (triolein)-water system, little efforts have been devoted to find a potentially better lipid surrogate. Triolein (C_{57}H_{104}O_{6}, also known as glycerol tristearate) selected in all the previous studies may still not be a good choice due to problems during gas chromatographic (GC) analysis. Triolein, being a high molar mass triglyceride (MW: 885), which is unsaturated and difficult to purify, does not easily elute from the GC column. It may contaminate the column and eventually reduce the sensitivity of the detector.

Tricaprylin (C_{27}H_{50}O_{6}, also known as glyceryl tricaprylate and glycerol tri-caprylate) is selected in this study as a model lipid to overcome some of these analytical problems. Tricaprylin is relatively a low molar mass triglyceride (MW: 470). The structure is compared with those of triolein and octanol in Figure 2.1. There may be several advantages with the use of this compound, e.g. (1) it is lower molar mass and less viscous compound than triolein. (2) its volatility is also much higher than that of triolein; therefore, less GC analytical problems are expected. As evident from the Figure 2.1, tricaprylin, being a triglyceride, may act more like a naturally occurring lipids. In addition, its overall structural polarity may account for actual partitioning behaviour.
**Triolein** (C\textsubscript{57}H\textsubscript{104}O\textsubscript{6}, also known as glycerol trioleate)

\[
\begin{align*}
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_6\cdot \text{CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{OH} \\
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_6\cdot \text{CH}_3
\end{align*}
\]

**1-Octanol** (C\textsubscript{8}H\textsubscript{18}O)

(C\textsubscript{27}H\textsubscript{50}O\textsubscript{6}, also known as glyceryl tricaprylate)

\[
\begin{align*}
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_7\cdot \text{CH} = \text{CH} \cdot \text{(CH}_2\text{)}_7\cdot \text{CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3\cdot \text{CH} = \text{CH} \cdot \text{(CH}_2\text{)}_7\cdot \text{CH}_3 \\
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_7\cdot \text{CH} = \text{CH} \cdot \text{(CH}_2\text{)}_7\cdot \text{CH}_3
\end{align*}
\]

**Triolein**

(Also known as glycerol trioleate)

\[
\begin{align*}
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_6\cdot \text{CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{CH}_2\cdot \text{OH} \\
\text{CH}_2\cdot \text{O.CO. (CH}_2\text{)}_6\cdot \text{CH}_3
\end{align*}
\]

**Figure 2.1: Chemical structures of tricaprylin, octanol and triolein**
3. EXPERIMENTAL

The partition coefficients of seven chlorobenzenes (CBs) were determined by the conventional shake-flask, batch contacting method with analysis by gas chromatography. The detailed description of the method is given elsewhere (Chiou et al., 1977). Care must be taken to avoid emulsion formed during shaking. The temperature dependence of octanol-water as well as tricaprylin-water partitioning was measured by determining the partition coefficients at ten degree intervals from 5 to 45 °C. The enthalpies of phase transfer from organic-phase to water were thus estimated.

3.1 Materials

1,2-dichlorobenzene 98.6%, 1,4-dichlorobenzene 99%, 1,3,5-trichlorobenzene 98%, 1,2,3,4-tetrachlorobenzene 98%, 1,2,3,5-tetrachlorobenzene 99%, pentachlorobenzene 98%, and n-octanol 99 + % were obtained from Aldrich Chemical Co., 1001 West Saint Paul Avenue, Milwaukee, WI 53223; OAS grade hexachlorobenzene was obtained from BDH Chemicals Ltd., 350 Evans Avenue Toronto, Ontario. Tricaprylin was purchased from Sigma Chemical Co., P.O. Box 14508, St. Louis, with a purity of 97-98%. All chemicals were used as purchased without further purification. Milli-Q ultrapure deionized water (Millipore Corp., Milford, MA) was used for all experiments. HPLC grade hexane was obtained from Caledon Laboratories, Georgetown, Ontario.
3.2 Methods

The procedure used for preparing the solutions as well as for determining the partition coefficients in the tricaprylin-water system is virtually the same as described below for the octanol-water system. The solubility of water in tricaprylin was determined by the standard Karl-Fisher titration method.

Preparation of Solutions

Except for hexachlorobenzene, a stock solution of approximately 1 g/L of the compound in 1-octanol was prepared, this concentration being well below the solubility limit. A 2 mL aliquot of stock solution and 20 mL of water were shaken by a wrist-action shaker (Gilson Differential Respirometer) for 24 hours in a 125 mL Erlenmeyer flask immersed in a temperature controlled bath maintained within ± 0.1 K of the required temperature. The contents were then allowed to equilibrate in the temperature bath for about 48 h for phase separation at the desired temperature. Near-saturated solutions of approximately 0.7 g/L hexachlorobenzene in octanol were prepared in the same manner but using a 15 mL aliquot of stock solution and 150 mL of water in a 250 mL Erlenmeyer flask.

3.3 Gas Chromatographic Measurements

The aqueous phase and octanol phase were first separated. The aqueous phase was extracted with hexane (2 mL) and then a 0.5 µL sample was directly injected (splitless) onto the gas chromatograph column. The octanol phase was diluted 20 to 2000 fold as required to analyze by GC. Analysis was on a Hewlett-Packard 5890 gas chromatograph equipped with a $^{63}$Ni electron capture (EC) detector. A 0.32 mm i.d. by 30 m long J&M DB-17 fused silica
capillary column was used for separation. The make-up and carrier gas was a 95:5 by volume argon-methane mixture. Operating conditions were: injection port at 250 °C, oven in isothermal mode between 110-210 °C depending on the boiling point of the chemical, detector at 300 °C. Carrier gas flow rate was 3.1 mL/min. Peak areas were recorded on a Hewlett-Packard 3392A integrator. Calibration standards were prepared in hexane. The concentration ranges used were 2-50 mg/L (1,2-dichlorobenzene; 1,4-dichlorobenzene), 0.6-25 mg/L (1,3,5-trichlorobenzene), 0.1-4.0 mg/L (1,2,3,4-tetrachlorobenzene; 1,2,3,5-tetrachlorobenzene), 0.06-4 mg/L (pentachlorobenzene), and 0.007-1.6 mg/L (hexachlorobenzene). Calibration plots and calculations for two compounds are shown in Appendix B as examples. The calibration plots were linear for all chemicals and calculations were done similarly.

3.4 Quality Assurance and Control

The following are the major precautions that should be taken in order to ensure high quality data.

(1) The flasks should be shaken gently to avoid emulsion formation.

(2) Sufficient time should be allowed to reach equilibrium and phase separation.

(3) Extreme care should be taken in sample preparations, extraction procedures and analyses.
4. RESULTS AND DISCUSSION

4.1 Octanol-water Partition Coefficient (K\textsubscript{OW})

Table 4.1 summarizes the logarithm of the octanol-water partition coefficients for selected chlorobenzenes at 25 °C. Available literature values for various chlorobenzenes are also included for comparison. The mean K\textsubscript{OW} values as a function of temperature for all the compounds are given in Table 4.2, the data being also depicted in Figures 4.1 and 4.2. Each point represents three or four determinations. The precision (standard deviation) of experimentally determined K\textsubscript{OW} is approximately ± 5%. The van't Hoff plots of log K\textsubscript{OW} versus \(1/T\) exhibit linearity with log K\textsubscript{OW} increasing by 10% - 14% over the temperature range 5 to 45 °C. The variation of log K\textsubscript{OW} with T i.e. \(d(\text{log } K_{\text{OW}})/dT\), given in Table 4.2 was between -0.010 to -0.014 K\(^{-1}\) with a mean value of -0.012 K\(^{-1}\). Sangster (1989) indicated a similar value of approximately -0.01 K\(^{-1}\) for variation of log K\textsubscript{OW} with T. The following more thermodynamically rigorous equation is used to model the experimental data:

\[
\text{log } K_{\text{OW}} = A - \frac{\Delta H}{2.303 RT}
\]  

All of the chemicals showed a satisfactory correlation of log K\textsubscript{OW} with 1/T (correlation coefficients ranging from 0.985 to 0.998). The regression constants A, B, and calculated enthalpies of transfer (\(\Delta H\)) are listed in Table 4.3, the \(\Delta H\) values ranging from 17.1 kJ.mol\(^{-1}\) for 1,4-dichlorobenzene to 24.4 kJ.mol\(^{-1}\) for hexachlorobenzene.

The log octanol-water partition coefficients at 25 °C are in good agreement with more recent (post-1983) and accurate determinations reported in the literature (Table 4.1). For the post-1983 data the average deviation in log K\textsubscript{OW} between the experimental values reported here and previously reported experimental values is 0.14. For earlier data the deviation is 0.21.

The log linear increase in K\textsubscript{OW} with 1/T, though small, clearly indicates the enhanced partitioning to lipid phases at low temperatures. For the chlorobenzene series log K\textsubscript{OW} increases
Table 4.1. Logarithm of Octanol-Water partition coefficients (K_{ow}) of selected chlorobenzenes at 25 °C (with precision expressed as ± standard deviation)

<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>log K_{ow}</th>
<th>literature values at 25 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-di-</td>
<td>3.29 ± 0.05</td>
<td>3.38^{ab}; 3.40^{cd}; 3.34^{c}; 3.55^{f}; 3.43^{g}; 3.49^{h}</td>
</tr>
<tr>
<td>1,4-di-</td>
<td>3.23 ± 0.03</td>
<td>3.37^{ac}; 3.38^{b}; 3.46^{e}; 3.62^{f}; 3.52^{d}; 3.44^{g}</td>
</tr>
<tr>
<td>1,3,5-tri-</td>
<td>4.34 ± 0.04</td>
<td>4.15^{f}; 4.17^{g}; 4.02^{b}; 4.18^{h}; 4.31^{bl}; 4.40^{g}</td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>4.41 ± 0.06</td>
<td>4.46^{f}; 4.37^{d}; 4.60^{bl}; 4.63^{g}; 4.55^{b}; 4.41^{e}; 4.75^{m}</td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>4.55 ± 0.02</td>
<td>4.50^{f}; 4.46^{c}; 4.52^{g}; 4.56^{d}; 4.53^{e}; 4.51^{b}; 4.61^{k}; 4.59^{bl}; 4.66^{g}</td>
</tr>
<tr>
<td>penta-</td>
<td>4.94 ± 0.03</td>
<td>4.88^{f}; 4.94^{ik}; 5.17^{j}; 5.06^{e}; 5.69^{m}; 5.03^{b}; 5.20^{bl}; 5.18^{g}</td>
</tr>
<tr>
<td>hexa-</td>
<td>5.46 ± 0.02</td>
<td>5.0^{i}; 6.22^{n}; 5.50^{h}; 5.66^{o}; 5.40^{b}; 5.47^{b}; 5.60^{o}; 5.64^{p}; 5.73^{e}</td>
</tr>
</tbody>
</table>

\(^{a}\) Wasik et al. 1983; \(^{b}\) Miller et al. 1984; \(^{c}\) Banerjee et al. 1980; \(^{d}\) Wateral et al. 1982; \(^{e}\) Hammers et al. 1982; \(^{f}\) Körmann et al. 1979; \(^{g}\) De Bruijn et al. 1989; \(^{h}\) Pereira et al. 1988; \(^{i}\) Veith et al. 1980; \(^{j}\) Banerjee 1984; \(^{k}\) Garst 1984; \(^{l}\) Chiou 1985; \(^{m}\) Bruggeman et al. 1982; \(^{n}\) McDuffie 1981; \(^{o}\) Brooke et al. 1986; \(^{p}\) Mailhot 1987.
<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>log $K_{ow}$</th>
<th>d($\log K_{ow}$)/dT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5 °C</td>
<td>15 °C</td>
</tr>
<tr>
<td>1,2-di-</td>
<td>3.51 ± 0.05</td>
<td>3.41 ± 0.04</td>
</tr>
<tr>
<td>1,4-di-</td>
<td>3.42 ± 0.01</td>
<td>3.35 ± 0.04</td>
</tr>
<tr>
<td>1,3,5-tri</td>
<td>4.52 ± 0.02</td>
<td>4.43 ± 0.04</td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>4.65 ± 0.02</td>
<td>4.53 ± 0.02</td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>4.80 ± 0.02</td>
<td>4.67 ± 0.04</td>
</tr>
<tr>
<td>penta-</td>
<td>5.20 ± 0.01</td>
<td>5.06 ± 0.03</td>
</tr>
<tr>
<td>hexa-</td>
<td>5.74 ± 0.04</td>
<td>5.60 ± 0.07</td>
</tr>
</tbody>
</table>
Figure 4.1. van't Hoff plot of $\log K_{ow}$ versus reciprocal absolute temperature for 1,2-dichlorobenzene $\Box$, 1,4-dichlorobenzene $\bullet$, 1,3,5-trichlorobenzene $\Delta$, 1,2,3,4-tetrachlorobenzene $\blacksquare$, 1,2,3,5-tetrachlorobenzene $\times$, pentachlorobenzene $\bullet$ and hexachlorobenzene $\ast$. 
by an average of 0.56 log units per chlorine added. The difference in log $K_{ow}$ between isomers is less than 0.15 log unit. Only for 1,3,5-tri-, 1,2,3,4-tetra-, penta- and hexachlorobenzene are there previous measurements of temperature dependence (Opperhuizen et al., 1988). As shown in Figure 4.2, log $K_{ow}$ values are comparable but slopes differ by up to 55%. It is noteworthy that Opperhuizen et al. determined $K_{ow}$ over a narrower temperature range of 13 to 33 °C. The partitioning of all chlorobenzenes from water to octanol is exothermic with a trend of higher enthalpies for more chlorinated benzenes. Figure 4.3 shows a plot of $\Delta H$ as a function of chlorine number which yields the relationship:

$$\Delta H/\text{kJ. mol}^{-1} = 13.5 + 1.8 (\text{Cl No.})$$

where Cl No is number of chlorine atoms in the molecule.

Equation 2 can be used to predict the enthalpies in situations when high accuracy is not required, for example, for environmental assessment purposes. A similar trend in $\Delta H$ was reported by Opperhuizen et al. (1988), however, their enthalpies are generally 16 to 26% higher than the values reported here. The data do not permit any assessment of the effect of temperature on enthalpy. As is apparent from Figure 4.2, the present data are regarded as more accurate than previous reported data and thus permit more reliable estimation of enthalpies of phase transfer.

4.1.1 Comparison between measured and calculated $K_{ow}$'s

The $K_{ow}$ values in this study can also be compared with values calculated from reported measurements of octanol-air partition coefficient ($K_{oa}$) and air-water partition coefficient ($K_{aw}$) since $K_{ow} = K_{oa} \times K_{aw}$. The air-water partition coefficient is calculated from Henry's law constant ($H$) as $K_{aw} = H/RT$. The $H$ and its temperature dependence have already been reported for various compounds including some chlorobenzenes (Ashworth et al., 1988; Hulscher et al., 1992). When no measurements of temperature dependence of $H$ are available, its temperature dependence can be estimated from the reported data on temperature dependence of vapor pressure ($P^s$) and temperature dependence of aqueous solubility ($C^s$).
Figure 4.2. Van't Hoff plot of log $K_{OW}$ versus reciprocal absolute temperature for this work - 1,3,5-trichlorobenzene ■, 1,2,3,4-tetrachlorobenzene †, pentachlorobenzene ▲, hexachlorobenzene ● and previous work (Opperhuizen et al. 1988) - 1,3,5-trichlorobenzene ×, 1,2,3,4-tetrachlorobenzene Δ, pentachlorobenzene □, and hexachlorobenzene ◆.
Table 4.3. Regression constants in equation 1 and enthalpy of phase change

<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>A</th>
<th>B</th>
<th>$\Delta H$/kJ.mol$^{-1}$</th>
<th>$r^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-di-</td>
<td>0.1831</td>
<td>928.2</td>
<td>-17.8</td>
<td>0.998</td>
</tr>
<tr>
<td>1,4-di-</td>
<td>0.2338</td>
<td>892.2</td>
<td>-17.1</td>
<td>0.9923</td>
</tr>
<tr>
<td>1,3,5-tri</td>
<td>1.1228</td>
<td>951.5</td>
<td>-18.2</td>
<td>0.9855</td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>0.6978</td>
<td>1103.7</td>
<td>-21.1</td>
<td>0.9965</td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>1.0159</td>
<td>1053.6</td>
<td>-20.2</td>
<td>0.9989</td>
</tr>
<tr>
<td>penta-</td>
<td>0.9255</td>
<td>1192.5</td>
<td>-22.8</td>
<td>0.997</td>
</tr>
<tr>
<td>hexa-</td>
<td>1.1806</td>
<td>1219.1</td>
<td>-24.4</td>
<td>0.998</td>
</tr>
</tbody>
</table>
Figure 4.3. Relationship between ΔH and number of chlorine atoms.
Temperature dependence of vapor pressure (Liu and Dickhut, 1994) and aqueous solubility (Shiu et al., 1997) have been reported for several chlorinated benzenes. Recently, some values for octanol-air partition coefficients (K_{OA}) over the temperature range -10 to +10 °C for selected chlorobenzenes (Harner and Mackay, 1995) and polychlorinated biphenyls (Harner and Bidleman, 1996) have been published. The observed temperature dependencies of K_{OA} and H have been modelled with the van't Hoff equation. The calculated enthalpies and regression constants resulting from fitting the experimental data for chlorobenzenes are summarized in Table 4.4. The values of regression constants can be used to extrapolate the K_{OA} and H at different temperatures. Only 1,2-di-, 1,2,3,4-tetra-, penta- and hexachlorobenzene were selected for comparison since these chemicals (examined in this study) are common with previous measurements of H and K_{OA}, and their temperature dependence. Table 4.5 summarizes the extrapolated values of K_{OA}, H and K_{AW} at five temperatures, which are then used to calculate the K_{OW} values. The calculated and measured K_{OW} are listed for comparison. In many cases, the agreement between experimentally determined and estimated values of K_{OW} are quite good. Generally, the differences are within 11%. The measurements of K_{OW}, K_{OA} and H are difficult and inevitably involve experimental error. Calculation of K_{OW} from K_{OA} and H thus combines these errors and introduces greater uncertainties into the calculated values of K_{OW}.

As shown above, the temperature dependence of K_{OW} can be predicted from the data on temperature dependence of K_{OA} and H. This example shows the feasibility of using this correlation approach to estimate missing data for these physical-chemical properties as required by the environmental fate models. The temperature relationship is, of course essential for predicting the values at the desired temperatures.

4.2 Tricaprylin-Water Partition Coefficient (K_{TW})

The logarithm of the tricaprylin-water partition coefficients for the same set of chlorobenzenes at 25 °C are listed in Table 4.6. The values are compared with the corresponding K_{OW} data from this study as well as previously reported literature values. In addition, triolein-water partition coefficients (K_{TW}) from Chiou (1985) are also included. The
<table>
<thead>
<tr>
<th>Property</th>
<th>Chlorobenzene</th>
<th>A</th>
<th>B</th>
<th>$r^2$</th>
<th>$\Delta H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{OA}$ (Harner &amp; Mackay, 1995)</td>
<td>1.2-</td>
<td>-4.3</td>
<td>2574</td>
<td>0.9992</td>
<td>49.3</td>
</tr>
<tr>
<td>Regression Equation:</td>
<td>1.2,3-</td>
<td>-4.6</td>
<td>2909</td>
<td>0.9997</td>
<td>55.7</td>
</tr>
<tr>
<td>$\ln K_{OA} = A + B / T = A + \Delta H_{OA} / RT$</td>
<td>1.2,3,4-</td>
<td>-5.3</td>
<td>3254</td>
<td>0.9998</td>
<td>62.3</td>
</tr>
<tr>
<td>Temp. range:</td>
<td>1.2,4,5-</td>
<td>-5</td>
<td>3176</td>
<td>0.9999</td>
<td>60.8</td>
</tr>
<tr>
<td>-10 to +20 °C (-10,0,+10,+20)</td>
<td>penta-</td>
<td>-6.2</td>
<td>3722</td>
<td>1</td>
<td>71.3</td>
</tr>
<tr>
<td>hexa-</td>
<td>-6.3</td>
<td>3928</td>
<td>1</td>
<td>75.2</td>
<td></td>
</tr>
<tr>
<td>$H$ (Ashworth et al., 1988)</td>
<td>1.2-</td>
<td>-1.518</td>
<td>1422</td>
<td>0.464</td>
<td></td>
</tr>
<tr>
<td>Regression Equation:</td>
<td>1.3-</td>
<td>2.882</td>
<td>2564</td>
<td>0.85</td>
<td></td>
</tr>
<tr>
<td>$\ln H$ (atm.m3/mol) = A - B / T</td>
<td>1.4-</td>
<td>3.373</td>
<td>2720</td>
<td>0.941</td>
<td></td>
</tr>
<tr>
<td>Temp. range:</td>
<td>1.2,4-</td>
<td>7.361</td>
<td>4028</td>
<td>0.819</td>
<td></td>
</tr>
<tr>
<td>10, 15, 20, 25, 30 °C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H$ (Hulscher et al., 1992)</td>
<td>1.2,3,4-</td>
<td>20.282</td>
<td>4750.3</td>
<td>0.9862</td>
<td></td>
</tr>
<tr>
<td>Regression Equation:</td>
<td>penta-</td>
<td>21.659</td>
<td>5184.1</td>
<td>0.9913</td>
<td></td>
</tr>
<tr>
<td>$\ln H$ (Pa.m3/mol) = A - B / T</td>
<td>hexa-</td>
<td>23.139</td>
<td>5736.5</td>
<td>0.9793</td>
<td></td>
</tr>
<tr>
<td>Temp. range:</td>
<td>14.8, 20.1, 22.1, 24.2, 34.8, 50.5 °C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_S$ (Shiu et al., 1997)</td>
<td>1.4-</td>
<td>6.7447</td>
<td>2187.8</td>
<td>0.9999</td>
<td>18.18</td>
</tr>
<tr>
<td>Regression Equation:</td>
<td>1.2,3-</td>
<td>5.825</td>
<td>3962</td>
<td>0.9997</td>
<td>28.80</td>
</tr>
<tr>
<td>$\ln C_S$ (mol/m3) = A - B / T</td>
<td>1.3,5-</td>
<td>6.4868</td>
<td>2648.7</td>
<td>0.9968</td>
<td>22.02</td>
</tr>
<tr>
<td>Temp. range:</td>
<td>1.2,3,5-</td>
<td>6.3791</td>
<td>3161.3</td>
<td>0.9985</td>
<td>26.03</td>
</tr>
<tr>
<td>5, 15, 25, 35, 45 °C</td>
<td>penta-</td>
<td>2.8904</td>
<td>3939.7</td>
<td>0.9946</td>
<td>32.8</td>
</tr>
<tr>
<td>hexa-</td>
<td>11.05</td>
<td>4055.2</td>
<td>0.9969</td>
<td>33.7</td>
<td></td>
</tr>
<tr>
<td>$P_S$ (Liu &amp; Dickhut, 1994)</td>
<td></td>
<td>$C_{\text{vap}}$</td>
<td>$C_{\text{sub}}$</td>
<td>$r^2$</td>
<td>$\Delta H_{\text{vap}}$</td>
</tr>
<tr>
<td>Regression Equation:</td>
<td>1.2-</td>
<td>25.7</td>
<td>NA</td>
<td>0.998</td>
<td>51.2</td>
</tr>
<tr>
<td>$\ln P_S$(Pa) = C$<em>J$ - ($\Delta H</em>{J}$ /RT)</td>
<td>1.4-</td>
<td>14.8</td>
<td>26.4</td>
<td>0.958</td>
<td>35</td>
</tr>
<tr>
<td>Temp. range:</td>
<td>1.2,3-</td>
<td>20.1</td>
<td>31.8</td>
<td>0.998</td>
<td>54.3</td>
</tr>
<tr>
<td>-15, -5, 10, 25, 40 °C</td>
<td>hexa-</td>
<td>25.5</td>
<td>36.4</td>
<td>0.978</td>
<td>81.3</td>
</tr>
</tbody>
</table>

*aEnthalpy of vaporization for liquid or subcooled liquid. bEnthalpy of sublimation for solid; NA - not applicable. cRegression constant for vaporization. dRegression constant for sublimation.
Table 4.5: Comparison of measured $K_{OW}$ with values calculated from reported data on $K_{OA}$, H and their temperature dependence

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Temperature ($^\circ$C)</th>
<th>log $K_{OA}$</th>
<th>H (Pa.m$^3$/mol)</th>
<th>$K_{AW} = H/RT$</th>
<th>log $K_{OW}$ (calcld.)</th>
<th>log $K_{OW}$ (measd.)</th>
<th>difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-dichlorobenzene</td>
<td>5</td>
<td>4.95</td>
<td>133.35</td>
<td>0.057</td>
<td>3.72</td>
<td>3.51</td>
<td>5.64</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>4.64</td>
<td>159.26</td>
<td>0.066</td>
<td>3.46</td>
<td>3.41</td>
<td>1.45</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>4.34</td>
<td>187.97</td>
<td>0.075</td>
<td>3.22</td>
<td>3.29</td>
<td>2.17</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>4.06</td>
<td>219.46</td>
<td>0.085</td>
<td>2.99</td>
<td>3.20</td>
<td>7.03</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>3.79</td>
<td>253.76</td>
<td>0.095</td>
<td>2.78</td>
<td>3.09</td>
<td>11.15</td>
</tr>
<tr>
<td>1,2,3,4-tetrachlorobenzene</td>
<td>5</td>
<td>6.45</td>
<td>24.40</td>
<td>0.010</td>
<td>4.43</td>
<td>4.65</td>
<td>4.96</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>5.99</td>
<td>44.16</td>
<td>0.018</td>
<td>4.26</td>
<td>4.53</td>
<td>6.33</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>5.61</td>
<td>76.81</td>
<td>0.031</td>
<td>4.11</td>
<td>4.41</td>
<td>7.29</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>5.26</td>
<td>128.88</td>
<td>0.050</td>
<td>3.97</td>
<td>4.28</td>
<td>7.80</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>4.93</td>
<td>209.33</td>
<td>0.079</td>
<td>3.83</td>
<td>4.15</td>
<td>8.35</td>
</tr>
<tr>
<td>pentachlorobenzene</td>
<td>5</td>
<td>7.43</td>
<td>20.20</td>
<td>0.009</td>
<td>5.38</td>
<td>5.20</td>
<td>3.34</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>6.72</td>
<td>38.61</td>
<td>0.016</td>
<td>4.93</td>
<td>5.06</td>
<td>2.64</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>6.28</td>
<td>71.02</td>
<td>0.028</td>
<td>4.75</td>
<td>4.94</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>5.88</td>
<td>124.15</td>
<td>0.048</td>
<td>4.57</td>
<td>4.79</td>
<td>4.81</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>5.50</td>
<td>210.98</td>
<td>0.079</td>
<td>4.41</td>
<td>4.66</td>
<td>5.67</td>
</tr>
<tr>
<td>hexachlorobenzene</td>
<td>5</td>
<td>7.82</td>
<td>12.23</td>
<td>0.005</td>
<td>5.55</td>
<td>5.74</td>
<td>3.42</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>7.33</td>
<td>25.04</td>
<td>0.010</td>
<td>5.37</td>
<td>5.60</td>
<td>4.28</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>6.88</td>
<td>48.86</td>
<td>0.019</td>
<td>5.18</td>
<td>5.46</td>
<td>5.41</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>6.45</td>
<td>91.28</td>
<td>0.035</td>
<td>5.01</td>
<td>5.30</td>
<td>5.79</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>6.05</td>
<td>163.97</td>
<td>0.062</td>
<td>4.84</td>
<td>5.17</td>
<td>6.82</td>
</tr>
</tbody>
</table>
Table 4.6. Logarithm of Tricaprylin - Water partition coefficients (K_{TW}) of selected chlorobenzenes at 25 °C (with precision expressed as ± standard deviation); compared with literature values of log K_{TW} and log K_{OW}

<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>log K_{TW}</th>
<th>log K_{OW}</th>
<th>literature values at 25 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>log K_{TW}</td>
<td>log K_{OW}</td>
<td>log K_{TW}</td>
</tr>
<tr>
<td>1,2-di-</td>
<td>3.56 ± 0.07</td>
<td>3.29 ± 0.05</td>
<td>3.51</td>
</tr>
<tr>
<td>1,4-di-</td>
<td>3.61 ± 0.04</td>
<td>3.23 ± 0.03</td>
<td>3.55</td>
</tr>
<tr>
<td>1,3,5-tri-</td>
<td>4.50 ± 0.06</td>
<td>4.34 ± 0.04</td>
<td>4.36</td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>4.63 ± 0.09</td>
<td>4.41 ± 0.06</td>
<td>4.68</td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>4.65 ± 0.05</td>
<td>4.55 ± 0.02</td>
<td>4.69</td>
</tr>
<tr>
<td>penta-</td>
<td>5.09 ± 0.03</td>
<td>4.94 ± 0.03</td>
<td>5.27</td>
</tr>
<tr>
<td>hexa-</td>
<td>5.59 ± 0.02</td>
<td>5.46 ± 0.02</td>
<td>5.50</td>
</tr>
</tbody>
</table>


*Triolein - Water partition Coefficients (Chiou et al., 1985)
mean $K_{TW}$ measurements, calculated from three replicates for each compound, are presented in Table 4.7 over the temperature range 5 to 45 °C. Figure 4.4 shows log $K_{TW}$ values as a function of temperature. The estimated precision expressed as a standard deviation is ± 9%. The van't Hoff plots show linear behaviour with log $K_{TW}$ increasing by 5% - 8% over the temperature range 5 to 45 °C. The variation of log $K_{TW}$ with T i.e. d(log $K_{TW}$)/dT are between -0.006 to -0.010 K$^{-1}$ with a mean of -0.008 K$^{-1}$. The log linear increase in $K_{TW}$ with 1/T is slightly less than (24%) that for log $K_{OW}$. The slopes in Figure 4.4 are lower by up to 50% of the corresponding temperature slopes for $K_{OW}$ (Figure 4.1) and therefore it is less sensitive to temperature variation. The experimental data were regressed using the equation 1 as before and the regression coefficients A, B, and enthalpies of phase transfer (ΔH) are shown in Table 4.8. The partitioning of chlorobenzenes from water to tricaprylin is exothermic with the trend in enthalpy increase being similar to that for octanol-water, i.e. higher enthalpies for higher chlorobenzenes derivatives. The ΔH values range from 9.7 kJ.mol$^{-1}$ for 1,2-dichlorobenzene to 16.1 kJ.mol$^{-1}$ for hexachlorobenzene. The relationship between ΔH and number of chlorine atoms in the molecule is illustrated in Figure 4.5, and can be expressed as:

$$\Delta H/\text{kJ. mol}^{-1} = 6.6 + 1.6 (\text{Cl No.})$$

(3)

The above equation can be useful for estimating the enthalpies for environmental purposes.

As shown in Table 4.6, measured log $K_{TW}$ values are somewhat greater than corresponding log $K_{OW}$ values. Larger deviations between log $K_{TW}$ and log $K_{OW}$ are observed for smaller chlorobenzenes. The log $K_{TW}$ values are greater than log $K_{OW}$ by 0.38 and 0.27 units for 1,4- and 1,2-dichlorobenzene respectively. With increasing molecular size of the solute, e.g., for penta- and hexachlorobenzenes, the log $K_{TW}$ and log $K_{OW}$ values become closer. Generally, the differences are within 4%, with the exception of dichlorobenzenes, for which it was up to 10%. Chiou (1985) also reported higher values for triolein-water partition coefficients and observed larger deviations for less chlorinated benzenes.
<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>log $K_{TW}$</th>
<th>$5, ^\circ C$</th>
<th>$15, ^\circ C$</th>
<th>$25, ^\circ C$</th>
<th>$35, ^\circ C$</th>
<th>$45, ^\circ C$</th>
<th>$d(\log K_{TW})/dT$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-di-</td>
<td>3.65 ± 0.07</td>
<td>3.61 ± 0.04</td>
<td>3.56 ± 0.07</td>
<td>3.51 ± 0.03</td>
<td>3.41 ± 0.05</td>
<td>-0.006</td>
<td></td>
</tr>
<tr>
<td>1,4-di-</td>
<td>3.71 ± 0.03</td>
<td>3.66 ± 0.05</td>
<td>3.61 ± 0.04</td>
<td>3.56 ± 0.03</td>
<td>3.46 ± 0.04</td>
<td>-0.0063</td>
<td></td>
</tr>
<tr>
<td>1,3,5-tri</td>
<td>4.60 ± 0.04</td>
<td>4.58 ± 0.08</td>
<td>4.50 ± 0.06</td>
<td>4.44 ± 0.04</td>
<td>4.35 ± 0.05</td>
<td>-0.0063</td>
<td></td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>4.75 ± 0.06</td>
<td>4.68 ± 0.07</td>
<td>4.63 ± 0.09</td>
<td>4.50 ± 0.06</td>
<td>4.43 ± 0.03</td>
<td>-0.008</td>
<td></td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>4.81 ± 0.07</td>
<td>4.75 ± 0.03</td>
<td>4.65 ± 0.05</td>
<td>4.56 ± 0.05</td>
<td>4.53 ± 0.09</td>
<td>-0.007</td>
<td></td>
</tr>
<tr>
<td>penta-</td>
<td>5.27 ± 0.05</td>
<td>5.22 ± 0.03</td>
<td>5.09 ± 0.03</td>
<td>5.07 ± 0.06</td>
<td>4.91 ± 0.03</td>
<td>-0.009</td>
<td></td>
</tr>
<tr>
<td>hexa-</td>
<td>5.80 ± 0.09</td>
<td>5.63 ± 0.06</td>
<td>5.59 ± 0.02</td>
<td>5.50 ± 0.02</td>
<td>5.39 ± 0.07</td>
<td>-0.0103</td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.4. Van't Hoff plot of log $K_{TW}$ versus reciprocal absolute temperature for 1,2-dichlorobenzene □, 1,4-dichlorobenzene ◆, 1,3,5-trichlorobenzene Δ, 1,2,3,4-tetrachlorobenzene ■, 1,2,3,5-tetrachlorobenzene ×, pentachlorobenzene ● and hexachlorobenzene +.
Table 4.8. Regression constants in equation 1 and enthalpy of phase change

<table>
<thead>
<tr>
<th>chlorobenzene</th>
<th>A</th>
<th>B</th>
<th>ΔH/kJ.mol⁻¹</th>
<th>r²</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-di-</td>
<td>1.8391</td>
<td>508.9</td>
<td>-9.74</td>
<td>0.949</td>
</tr>
<tr>
<td>1,4-di-</td>
<td>1.8301</td>
<td>527.1</td>
<td>-10.09</td>
<td>0.960</td>
</tr>
<tr>
<td>1,3,5-tri</td>
<td>2.6049</td>
<td>562.6</td>
<td>-10.77</td>
<td>0.995</td>
</tr>
<tr>
<td>1,2,3,4-tetra-</td>
<td>2.1722</td>
<td>722.4</td>
<td>-13.83</td>
<td>0.972</td>
</tr>
<tr>
<td>1,2,3,5-tetra-</td>
<td>2.4254</td>
<td>665.5</td>
<td>-12.74</td>
<td>0.983</td>
</tr>
<tr>
<td>penta-</td>
<td>2.5407</td>
<td>765.7</td>
<td>-14.66</td>
<td>0.941</td>
</tr>
<tr>
<td>hexa-</td>
<td>2.7613</td>
<td>840.0</td>
<td>-16.08</td>
<td>0.965</td>
</tr>
</tbody>
</table>
Figure 4.5. Relationship between $\Delta H$ and number of chlorine atoms.
The values of log $K_{TW}$ can be satisfactorily correlated in linear form with respective values of log $K_{OW}$ (from this work) as well as with the logarithm of the triolein-water partition coefficients from the Chiou data (1985). A plot of log $K_{TW}$ vs. log $K_{OW}$ values at 25 °C is given in Figure 4.6. A hypothetical relationship with a regression coefficient of 1.0 and an intercept of zero is shown by broken lines. The relationship between log $K_{TW}$ and log $K_{OW}$ is linear, which is given by the following equation:

$$\log K_{TW} = 0.90 \log K_{OW} + 0.615 \quad (r^2 = 0.99) \quad (4)$$

The response shown in Figure 4.6 suggests that hydrophobic compounds such as higher chlorinated benzenes (where log $K_{OW} > 5$), which have high activity coefficient in the aqueous phase, behave similarly in the two solvent phases i.e. octanol and tricaprylin. The log $K_{TW}$ values are therefore quite close to log $K_{OW}$ values; the correlation line merges with the hypothetical line log $K_{TW} = \log K_{OW}$, when extended over the upper range of log $K_{TW}$. In contrast, for less hydrophobic compounds, which have lower activity coefficients in the aqueous phase, the differences in the non-polar solvent tend to become a more significant factor; consequently, this results in deviations from the line log $K_{TW} = \log K_{OW}$. But nothing could be convincingly concluded about this trend as mostly, the deviations are within the experimental error. This should be further evaluated and clarified with more compounds and intensive experimental work as the critical analyses of the linearity in plots of log $K_{TW}$ vs. log $K_{OW}$ as well as response of relatively higher values of log $K_{TW}$, would require a large set of data on these properties.

The log $K_{TW}$ values are in close agreement with the log $K_{TW}$ values reported by Chiou (1985). In most cases the agreement is within 2%. Thus, log $K$ values do not appear to show systematic difference between the two triglycerides. When log $K_{TW}$ values are correlated with corresponding log $K_{TW}$ values (Figure 4.7), the result gives

$$\log K_{TW} = 0.94 \log K_{TW} + 0.268 \quad (r^2 = 0.97) \quad (6)$$
Figure 4.6: Correlation of $\log K_{TW}$ with $\log K_{OW}$

Figure 4.7: Correlation of $\log K_{TW}$ with $\log K_{TW}$
The fact that slope is nearly 1 and intercept is small further supports the hypothesis that log $K_{TW}$ and log $K_{TW}$ are approximately equal.

These analyses do not provide any strong evidence that either would demonstrate whether tricaprylin is a sufficiently good model for biological lipids or would convincingly support the importance of substituting it for octanol. However, in hindsight, the selection of 1-octanol as a surrogate for lipids may not have been the best choice whereas tricaprylin which is a real triglyceride and structurally similar to fish lipids could be a better surrogate. The lipid-water partition coefficients investigated from this work together with the Chiou's data suggest that both the triglycerides have almost the same partitioning behaviour. Triolein, which is a high molar mass triglyceride and difficult to purify, creates problems during analytical measurements as indicated earlier. Therefore, tricaprylin appears to be the preferred choice over the triolein because of its ease in analysis and availability in purer form. However, there are some additional advantages of tricaprylin, as listed below:

1. Tricaprylin is less soluble in water than octanol is in water (solubility of tricaprylin in water: $0.0134 \pm 0.003$, g / 100g; solubility of octanol in water (IUPAC, 1984): $0.054 \pm 0.005$, g / 100g at 25 °C).

2. It has lower vapour pressure than octanol (B.P. of tricaprylin: 233 °C; B.P. of octanol: 196 °C).

3. Solubility of water in tricaprylin, (0.4 g / 100g) is less than solubility of water in octanol (4.5 ± 0.1, g / 100g, IUPAC, 1984) at 25 °C.

Tricaprylin could be better for $K_{TA}$ measurements and subsequently related to $K_{AW}$ and $K_{TW}$.

To substantiate the effects of lipids and use of log $K_{TW}$ and log $K_{OW}$ in estimating bioconcentration, further studies are required with more compounds to determine the relationship between log $K_{TW}$ (or log $K_{OW}$) and (lipid-based) BCF and examine whether the correlation of log BCF with log $K_{OW}$ will be statistically different from that of log BCF with log $K_{Tw}$. Investigations on suitability of other lipid surrogate such as methyl esters derived from triglycerides should also be the subject of future studies.
PART II: MODELLING THE FATE OF PERSISTANT CHEMICALS IN THE INDIAN AQUATIC ENVIRONMENT USING MULTI-SEGMENT FUGACITY MODELS

1. LITERATURE REVIEW AND BACKGROUND

1.1 Introduction

Persistent pollutants enter lakes, estuaries and the rivers by direct discharges, riverine inflow and atmospheric deposition. Often the major sources and their relative contributions are not obvious. It is, therefore, necessary to understand and establish a quantitative link between contaminant loadings and the resulting concentrations in water, sediments, and biota which comprise the receiving ecosystem. This helps to ascertain the extent to which loading reduction will translate into reduced concentrations, and how long it will take for the system to respond to such changes. Numerous studies (Mackay, 1989; Trapp et al., 1994; Mackay and Southwood, 1992) have demonstrated that a link between loading and contaminant concentrations can be established by the application of mathematical models developed using the principles of mass balance, chemical thermodynamics and transport phenomena, along with sufficient knowledge of the physical-chemical properties of the chemicals and hydrological and sedimentary characteristics of the receiving environment. Model results can be a useful regulatory tool, particularly, when assessing or implementing remedial measures to treat already-contaminated environments from past and present discharges. Further, the response time of the system can also be assessed. The Canada-U.S. Great Lakes Basin provides numerous examples of "Areas of Concern" degraded by chemical discharges and which are therefore, the subject of "Remediation Action Plan". The use of predictive models was recommended by the Great Lakes Science Advisory Board for making rational and scientifically defensible management decisions (International Joint Commission, 1993).

Most of the fate modelling of persistent chemicals in large water bodies has until now been focused on the Great Lakes of North America (e.g. Mackay, 1989; Jeremiasen et al., 1994; Diamond et al., 1994) and some other temperate aquatic environments such as Finnish lakes, Saguenera Ford in eastern Quebec (Lun, 1995) and the Baltic sea (Wania et al., 1996).
It was hoped that the experimental results on physical-chemical properties of some chlorobenzenes established in this as well as previous studies could be applied to the models simulating Indian aquatic systems. However, for most of these chemicals there is insufficient information on chemical loadings, concentrations and industrial activities for Indian waters to construct a model. The data are sketchy and are not well documented quantitatively. Recently, the National Thermal Power Corporation has conducted an extensive environmental assessment study for a large water body (Rihand reservoir) where some organochlorine compounds such as lindane and its isomers, polychlorinated biphenyls, DDT and some polycyclic aromatic hydrocarbon have been detected. The information on occurrence, loadings and concentrations are documented in their monitoring studies. In this section of the study, the QWASI (Quantitative Water-Air-Sediment Interaction) fugacity models (Mackay, 1991) are used to elucidate the fate of some of these chemicals and to assess the validity of the model. The models have also been applied to another Indian lake (Nainital) for which the data on lead and copper concentrations, emission and hydrological parameters are well documented. In an attempt to apply the same models for the chlorobenzenes in this lake, a simulation was prepared to understand the behavior of these chemicals and to identify the dominant processes. The background information, including descriptions of geography, hydrology and industrial activities, are addressed in separate sub-sections for each of the modelling locations. The application of the QWASI based fugacity model is then described. Finally, the selection of model parameters and the results from modelling efforts are discussed individually for the two locations. The primary objective of this study is not to describe the fate of chemicals in the lake with high accuracy, which would demand considerably more data than are available. Rather it is to illustrate how mass balance models such as this can improve our understanding of
contaminant fate in the Indian lakes, from which recommendations for effective remedial actions can be formulated and justified.

1.2 Background information on status of aquatic pollution in India

India is a riverine country with population of 900 million in the year 1996. It has 14 major rivers, 44 medium rivers and 55 minor rivers besides numerous lakes, ponds and wells which are used as primary sources of drinking water, often without treatment (MOEF, 1997). Rapid industrialization and urbanization has resulted in increased discharge of untreated industrial and domestic waste into these water bodies endangering the quality of scarce water resources. The economic conditions do not permit the development of appropriate facilities for the treatment of domestic waste into smaller cities. Growth of small scale industries, being the primary area of the development, have created an enormous problem of untreated industrial waste water. These industries are incapable of treating the waste on their own and collective treatment is still not feasible. Efforts to develop combined waste water treatment facilities for industrial and domestic waste water are in progress (e.g. common effluent treatment plant, Vapi; National River Conservation Plan; Ganga Action Plan) with the help of international development agencies (World Bank, United Nation Development Program, Asian Development Bank) but the pace of these development is not sufficient to cope with the problem. The surface and ground water have been contaminated beyond their assimilative capacities and there are instances of court ordering the closing of industries in certain areas and ordering the government to take up remediation measures (MOEF, 1997). Trivedi (1988) reviewed water quality problems in approximately 20 Indian rivers, in particular the problems on the Ganges due to waste discharge from tanneries, oil refineries and fertilizer plants. The Central Pollution Control Board of India is conducting water quality monitoring programs: a global level under Global Environmental Monitoring Systems (GEMS) and at the national level under the Monitoring Indian National Aquatic Resources (MINARS) program which covers various lakes, rivers, wells and canals (Chakrabarti and Kumar, 1987). There are numerous studies on groundwater and river pollution due to large quantities of industrial wastes discharged from pulp and paper, cement and other chemical plants (Srivastava et al., 1988; Handa et al., 1983; Biswas and Saha, 1983). Agrawal investigated the pesticide problem and
indicated that DDT was found in almost all the samples collected from Indian rivers and lakes. In recent years, much attention has been focused on monitoring the level of organochlorine compounds and polycyclic aromatic hydrocarbons in the vicinity of pesticide plants, power plants and other chemical industries.

1.2.1 Modelling the fate of persistent pollutants in Indian water bodies

Despite the observation of intense contamination at various aquatic systems through regular sampling and monitoring studies in India, no attempt has been made to describe the fate and behavior of chemicals employing the multimedia modelling approach. The Central Pollution Control Board and Indian Ministry of Environment have set up various stations throughout the country to carry out regular monitoring of rivers and lakes under the inland water quality monitoring program, but the measurements are made only for physico-chemical and biological parameters and no data exist for the persistent chemicals. However, there are a few studies in recent years that have reported the concentrations of some organochlorine substances namely lindane, heptachlor, aldrin, polychlorinated biphenyl and DDT in water (Kumar and Lal, 1988; NTPC, 1995), fish (Bakre et al., 1990) and birds (Misra and Bakre, 1994) of Jaipur lakes and Rihand Reservoir; concentrations of chromium, nickel, cadmium, mercury, copper, manganese and zinc in water, suspended particles, sediments and biota of Hussainsagar and Nainital lake (Prablad and Seenayya, 1986; Seenayya and Prablad 1987; 1988; Srikanth et al., 1993; Pande and Das, 1980); concentrations of methyl isocyanate and its degradation products in water and fish of Bhopal lake (Sen Gupta, 1991).

From analyses of the complete data it was found with regards to system hydrology, sedimentation, loading and chemical characteristics that more comprehensive information was available for Lake Nainital, in the Central Himalaya region and Rihand reservoir, in east central India (Figure 1.1 shows the location of these lakes in India). Hence, these aquatic systems have been selected for the modelling studies. The former receives waste of mainly domestic character due to impact of increasing urbanization in the area whereas latter is contaminated by effluents from pesticides, aluminum, and power plants. As mentioned earlier, it is imperative to understand the dominant processes that control the fate of the
Figure 1.1: Map of India showing the locations of two lakes
pollutants in the system in order to carry out remediation and to chose appropriate technology and methodology for treatment. It is hoped that applying the model to these lakes will encourage the use of models for regulatory purposes. Models are viewed as particularly valuable for preventing future problems of contamination by persistent chemicals.

1.2.1 (a) Lake Nainital and Environs

There are many large and small lakes in the Kumaun region of the Central Himalayas (240 km north east of New Delhi, Figure 1.1) forming the 'Lake district of Kumaun Himalayan' comparable with the Lake District of England, the recreational lakes of Ontario and high altitude lakes of Kashmir. Of these group of lakes, Lake Naini (popularly known as Nainital Lake) in the district of Nainital is well known because of tourism in India. Its natural beauty has attracted tourists, human settlements, government offices and educational institutions in the region.

The cup-shaped water body of the lake (Figure 1.2) is surrounded by the steeply sloping mountains in the catchment (Valdiya, 1988). It is situated at latitude: 29 ° 24 'N, longitude: 79 ° 23 'E, and at an altitude of 1938 m. The total length of the drainage basin is 42 km and the lake has a catchment area of 11.8 km² (Pande et al., 1983). The surface area of the lake is about 48.78 hectares and the volume 10,772,000 m³ (Das and Pande, 1980). It is the only source of potable water for 50,000 people living in Nainital city and approximately 70,000 tourists per year.

Over the years, unplanned urbanization and associated development activities in the area have resulted in serious ecological and environmental problems. Indiscriminate discharge of untreated domestic waste along with refuse and solid waste through open drains has caused severe impairment in lake water quality. The infrastructural facilities such as water supply, sewerage, solid waste disposal, traffic, transportation and tourist facilities have fallen short of requirements. The lake has been also showing signs of accelerated eutrophication due to human influences and anthropogenic activities in the catchment area (NIH, 1994).
Figure 1.2: (a) View of Lake Nainital (b) Sampling in lake (c) Sketch map of lake indicating positions of sampling stations and inlets/outlet
Besides a few seasonal rain-water fed channels, there are two permanent inlet drains that discharge waste water into the lake from neighboring high habitation areas on the hills. Large inputs of municipal waste, including urban runoff from surrounding area and extraneous material such as silt, rubble from house building, leaf-litter, household effluent, garbage, detergents, laundry wash and also some chemical effluent from hospitals, college laboratories and gas stations, are carried into the lake. To prevent excessive outflow of water during the rainy season, a dam has been constructed towards the lower end of the lake. The excess water is discharged from the dam (300 m$^3$/h) through a single outlet (Pant et al., 1981).

The hydrological and limnological status of the lake is well reviewed in previous studies by Singh (1990) and NIH (1994). Recently, the National Institute of Hydrology at Roorkee (India) has performed extensive studies on water balance, sedimentation patterns, hydrodynamics of the lake, soil and surface runoff. There are numerous studies on bacteriological and microbiological contamination and the poor clarity of the lake water (Pant et al., 1979, 1981; Pande et al., 1983; Bisht and Das, 1985; Khulbe and Durgapal, 1994) where mainly physical and biological aspects of pollution are examined. The studies on eutrophication (Pant et al., 1980) and productivity and growth of various plant species at different depths (Khulbe and Bhargava, 1983; Purohit and Singh, 1987) indicated that the lake water was fairly rich in nutrients and that the process of eutrophication has started. The macrobenthic community structure at different depths has also been measured (Gupta and Pant, 1983). Investigation on harmful effects on fish life and other biota was observed as early as 1978 (Das, 1978; Das and Pande, 1978; Das and Upadhaya, 1979). Very high fish mortality and the decline in population of some species were evident in several studies (Das and Pande, 1982; Das and Srivastava, 1984).

The water and sediment of the lake is highly contaminated by numerous metals (GUP, 1989). Pande and Das (1980) and Pant et al. (1981) conducted studies on identification of heavy metals in water and sediments including lead, copper, zinc, manganese and cobalt. Most measured concentrations, particularly of lead, were above the
disposal guidelines of the Indian Ministry of the Environment (concentration of lead ranged from 0.061 to 0.076 mg/L in water, and 110 to 268 mg/kg in sediment).

The main sources of lead were identified to be white lead (lead oxide) used for boat paints and lead-acid batteries manufactured around the lake (Pant and Das, 1980; GUP, 1989). The other sources are leachate from soil and rocks, and effluents from chemical laboratories, hospitals and gas stations around the catchment. Data on chemical loadings, environmental and hydrological parameters were used to develop a fugacity model that adequately simulates lake Nainital. Two chemicals: lead and copper have sufficiently complete data sets for calibrating and testing the water quality model. Therefore, the model was first applied to elucidate the fate of these chemicals. It was then used to predict the behavior of 1,4-dichlorobenzene, 1,2,3,5-tetrachlorobenzene, pentachlorobenzene and hexachlorobenzene assuming an illustrative loading of 1000 kg/year and same hydrological parameters. The fates of these compounds were simulated by a 3 segment quantitative water-air-sediment interaction model. Segment 1 is the north basin (near Mallital) which receives most of the discharges. Segment 2 is the middle portion i.e. mid-basin of the lake, while the south basin at Tallital is segment 3.

1.2.1 (b) Rihand Reservoir

Several river valley projects have been constructed in the country, which have led to the creation of a many big and small impoundments. Some of these reservoirs are intended for irrigation and power generation. The Rihand reservoir is one of the important reservoirs in India developed for hydroelectric power generation. It is located in east central India (Figure 1.1), approximately - 700 km south east of New Delhi (latitude: 24 °52´N; longitude: 83 °5´E). It was formed by the construction of a dam during 1956-62 across the Rihand river in Mirzapur district of north Indian state. The Rihand river is a tributary of the Sone river which finally joins the Ganges. It originates in the hills of Rewa division in Madhaya Pradesh draining a catchment area of 13,344 km². The reservoir is a principal source of water for the irrigation of approximately, 65000 hectares of land, the source of water for five power plants generating 6370 MW power and for a host of other
chemicals industries in the region. The reservoir is also used for supplying potable water to 500,000 inhabitants in villages and townships located around it.

The reservoir has a surface area of $46.5 \times 10^7$ m$^2$ when full with a shoreline of 250 km. It has maximum length of 48 km and maximum width of 20 km. The mean volume over last few years was estimated to be $7 \times 10^9$ m$^3$ with a mean depth of 23 m (Konar et al., 1991).

Figure 1.3 is the map of the reservoir and surrounding area. It shows perennial and non-perennial rivers as well as urbanized zones and industrial townships (Singrauli, Renukut, Pipri, Muipur, Rihand and Waidan) in the region. As shown in the figure, there are 7 tributaries flowing into the reservoir. The reservoir receives most of its water input from 3 major rivers namely Rihand, Mayur and Kanchan to the south basin, and secondarily from minor streams: Balia, Matwani, Baran & Ajir into middle basin. The water is discharged from the Pipri dam at the north end of the reservoir (Gosse, 1990a). The average flow of the upstream Rihand river on entry into reservoir is estimated at $52.2 \times 10^4$ m$^3$/h and flow from other streams is $5.8 \times 10^4$ m$^3$/h. The average discharge of the Rihand at the dam is estimated to be $54 \times 10^4$ m$^3$/h (Gosse, 1990a). The mean residence time of water crossing the reservoir is estimated to be about one and half years ($7 \times 10^9 / 54 \times 10^4 \approx 12962$ h or 1.47 years). The construction of Rihand Dam has changed the ground-water flow in the surrounding area. As the reservoir filled, water seeped into the subsurface, causing a rise in the water table. Hydrological studies conducted by the Central Ground-water Board reported that the water table was between 5 to 10 m in the vicinity of the dam. The high water table indicates that reservoir water recharges the local ground-water system. However, ground-water discharge for the local drainage basin around the reservoir has been estimated at $1.71 \times 10^4$ m$^3$/h (NTPC, 1995), less than 4% of the average annual inflow to the reservoir. Therefore, ground-water recharge or discharge can be assumed to be negligible for the purpose of the model.
Figure 1.3: Map of Rihand Reservoir and surrounding region indicating perennial and non-perennial rivers
Industrial activities

Large quantities of readily available reservoir water and the abundant availability of coal from nearby open cast mines led to the installation of five coal-fired thermal power plants, namely: Singrauli, Vindhayachal, Rihand, Renusagar and Anapara. These are situated just at the bank of the reservoir (pictures of some power plants and coal mines are shown in Figure 1.4). Further, the development of a electric power facility and other natural resources in the vicinity promoted the commissioning of various chemical industries in the region such as aluminum, chlor-alkali, pesticide, carbon black, cement etc., located at the north end of the reservoir. The location of main the industries along the reservoir are illustrated in Figure 1.5. Hindalco, a major aluminum producer in the country transforms bauxite into aluminum products. The bauxite is obtained from mines in the nearby region of Bihar and Madhya Pradesh. Kanoria Chemicals manufactures caustic soda, liquid chlorine, hydrochloric acid and technical grade lindane. The Hi-tech carbon plant produces various types of carbon black mainly for tire and rubber industries.

For modelling purposes, the Rihand reservoir is divided into three segments, as shown in Figure 1.6. Segment 1 i.e. the south basin (lotic sector) is located in the upper part of the reservoir. It receives inflowing water from larger the rivers Rihand, Mayur and Kanchan as well as effluents from two power plants (Singrauli and Vindhayachal). Downstream from segment 1 is segment 2 which is the middle basin (intermediate sector). Two power plants (Rihand and Renusagar) located in this area discharge their effluent into the reservoir. Segment 3 (north-west basin) is the lower part i.e. lentic sector of reservoir. The area is close to the dam and is highly influenced by industrial activities in this region. The effluents from various chemical industries (Hindalco, Kanoria Chemicals, Hi-tech Carbon) and a power plant (Anapara) are discharged into this part via the Dongia river.

Previous studies

The ecological survey of Rihand reservoir was undertaken (1971-81) by the Central Inland Fisheries Research Institute (CIFRI) to understand the physico-chemical
Renusagar Power plant

Hindalco Aluminum plant

Overburden dumps of Jayant mine

and excavation of Bina open cast mine.

Vindhyachal and Singrauli power plants.

Figure 1.4: Pictures of some power plants and coal mines around Rihand reservoir
Figure 1.5: Location of main industries around Rihand reservoir.
Figure 1.6: Segmentation of reservoir for modelling purpose
characteristics of water, plankton/ fish population and its production potential (Natrajam and Tripathi, 1981). This study has given rise to many other investigations including water quality, limnological (Singh, 1985) and biological (Singh et al., 1980; Natrajam et al., 1976) status of the reservoir.

There are several studies on pollution effects of industrial effluents from chemical and thermal power plants on the Rihand reservoir ecosystem (Panwar et al., 1979; Chandra et al., 1985). Agarwal and Kumar (1978) have reported high concentrations of mercury in the effluent of the chlor-alkali factory which discharges into reservoir. It was also reported that there was a likelihood of heavy metals and PAHs leaching into the reservoir from the ash ponds of various power plants located around it. Many reports have indicated that the reservoir receives substantial effluents from pesticide and other chemical industries which is responsible for heavy fish mortality and toxic effects on other aquatic organisms (Arora et al., 1970; Konar et al., 1991).

In recent years, NTPC (India) and their consultant Electricité de France (EDF) International have performed one year extensive sampling surveys of the reservoir and the surrounding region with the intent of preparing environmental impact assessment studies. Their studies present detailed data on various aspects of hydrology, air and water quality, sediments, ecology, meteorology and existing industries and shed more light on exact sources of pollution in the reservoir and identification of persistent and toxic chemicals. These reports confirm that reservoir sediments are highly contaminated with numerous chemicals. Predominant contaminants have found to be mercury, PAHs, lindane and its isomers. Higher values persisted particularly in the north-west sector of the reservoir which receives direct effluent discharged from aluminum, caustic soda, pesticide and carbon black plants. Table 1.1 outlines the type of industries, important contaminants and their main sources of emission into the reservoir. High mercury content, with a maximum value of 47 mg/kg, was detected in sediments samples of this sector due to Chlor-alkali plant discharges. Average mercury concentration in fish was 0.84 mg/kg. The concentration of total HCH ranged from 48 to 127 μg/kg in sediments, and 1.6 to 7.1
<table>
<thead>
<tr>
<th>Type of industry</th>
<th>Raw material (tones/year)</th>
<th>Production capacity (MW or tones/year)</th>
<th>Main sources of emission</th>
<th>Chemicals of concern</th>
</tr>
</thead>
<tbody>
<tr>
<td>coal fired power plants</td>
<td>coal: 17.9x10^6</td>
<td>electricity: 6763 MW</td>
<td>- atmospheric emission from boiler stack</td>
<td>- PAHs, SO₂, NOₓ</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td>- over flow from ash ponds</td>
<td>- PAHs, metals</td>
</tr>
<tr>
<td>chlor-alkali &amp; pesticide</td>
<td>benzene: 446 kl</td>
<td>caustic soda: 33x10^3</td>
<td>- mercury cell</td>
<td>- Hg</td>
</tr>
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<td></td>
<td>liq.chlorine: 1271x10^6</td>
<td>HCH: 16x10^3</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>Hg: 6.8</td>
<td>lindane: 400</td>
<td>- effluent from HCH plant</td>
<td></td>
</tr>
<tr>
<td></td>
<td>coal: 11388x10^6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>aluminum plant</td>
<td>bauxite: 90x10^4</td>
<td>aluminum: 15x10^4</td>
<td>- aluminum smelters</td>
<td>- PAHs, HF, NO₂, SO₂,</td>
</tr>
<tr>
<td></td>
<td>alumna: 30x10^3</td>
<td></td>
<td>- over flow from ash ponds</td>
<td>- PAHs</td>
</tr>
<tr>
<td></td>
<td>coal: 2x10^3</td>
<td></td>
<td>- red mud discharge</td>
<td>- Pb, Cu, Cd, As</td>
</tr>
<tr>
<td></td>
<td>coke: 27x10^3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>carbon black plant</td>
<td>fuel oil LSHS: 7500</td>
<td>carbon black product: 20x10^3</td>
<td>- stock emissions from reactor, boiler, rotary dryer and gas filter</td>
<td>- PAHs</td>
</tr>
<tr>
<td></td>
<td>LDO(m³): 900</td>
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</table>
mg/kg (average of 4.48) in fish from this area of the reservoir. This is approximately 10 times more than the US Food & Drug Administration recommended level for lindane in edible fish tissue (0.3 mg/kg). The concentration of total PAH in sediments ranged from 235 to 670 µg/kg.

Based on available information and monitoring data on chemical loadings, concentration and system hydrology, two chemicals: HCH and PAHs were selected for the modelling exercise as more comprehensive information is documented for only these. Moreover, there has been a great concern about these compounds in recent years. This is reviewed in the following paragraphs along with some discussion on the source, generation and presence of these two group of chemicals in the environment.

1.3 Concern over HCHs and PAHs and their source, generation and presence in environment

Environmental impact of some of the potential carcinogenic chemicals such as HCHs and PAHs has been the focus of much scientific attention throughout the world. Monitoring of organochlorine pesticides (OCP) and polycyclic aromatic hydrocarbons (PAHs) residues has always been considered important for controlling the human exposure. The large scale use of OCP in developing countries has caused serious concern due to their persistence in the environment. This persistence leads to bioaccumulation in biota and their food chains such that species at the top of food chains contain relatively high concentrations and there may be toxic and physiological effects from the compounds. Consumption of food and wildlife with high contaminant concentrations is the major route of exposure for humans. As compared to several other countries, the higher body burden of OCP in the Indian population (Jani et al., 1988a) is indicative of higher exposure to these chemicals.

To understand the environmental fate of OCPs in tropics, India offers an ideal example of a developing country where HCHs and DDT have been extensively used in agriculture and public health programs (Gupta, 1986). Annual consumption of HCH range
from 22,000 to 47,000 tons (ICS, 1986). Technical HCH is a mixture of 60-70% α-HCH, 5-12% β-HCH, 10-15% γ-HCH, and minor percentages of other isomers (Iwata et al., 1993). Lindane (pure γ-HCH) is the active ingredient of hexachlorocyclohexane. Several studies from India have shown high residues of HCH in vegetables and other food commodities (Siddiqui and Saxena, 1983; Dikshit et al., 1989) including human breast milk (Ramkrishnan et al., 1985; Jani et al., 1988b; UNEP/WHO, 1983) and tissues of goat, buffalo, chicken (Kaphalia and Seth, 1981) and birds (Kaphalia et al., 1981). Recent studies have shown the occurrence of these pesticides in soil (Kumari et al., 1996; Kawano et al., 1992), water (Bakre et al., 1990; Dikshit et al., 1990; Dua et al., 1996; Kumari et al., 1996), sediments of Ganges (Ahmad et al., 1996) and other rivers (Mahapatra et al., 1995). Lindane has been detected at relatively low concentrations (i.e. generally $< 10^3$ ng/L) in surface waters in numerous countries (Kucklick et al., 1994; Iwata et al., 1994; Gomme et al., 1991; Nerin et al., 1992; Nwankwoala and Osibanjo, 1992). Moreover, the presence of lindane in atmosphere and precipitations from sites remote from industrial and human activities indicates that long-range atmospheric transport of this pesticide occurs (Atlas and Giam, 1981; Kurtz and Atlas, 1990). HCHs migrate to colder regions also, as proposed in global condensation hypothesis and model (Mackay and Wania, 1995; Wania and Mackay, 1995), to such an extent that is the most abundant organochlorine compound found in the high Arctic (Barrie et., 1992). Concentration of lindane in various lakes, rivers and ponds of India as well as some European countries are summarized in Table 1.2.

PAHs are another group of contaminants of concern that pose a potential hazard to human life. Some PAHs, namely benzo(a)pyrene, benzo(b)fluoranthene and dibenzo(a,h)anthracene, are highly potent carcinogens, which have been linked to the etiology of some human cancers (Conney, 1982). The distribution of PAHs throughout the world is strongly correlated with, and has been attributed to anthropogenic combustion of organic material. PAH appear in a large number of industrial processes, mainly due to high temperature treatment of coal tar and pitch as well as incomplete combustion or pyrolysis of organic material in general. Coal tar products, derived from the carbonization of bituminous
Table 1.2: Concentrations of lindane and PAHs in various lakes, ponds and rivers of India and some other countries

<table>
<thead>
<tr>
<th>System</th>
<th>Location</th>
<th>Water conc. (μg/L)</th>
<th>Sediment conc. (mg/kg)</th>
<th>Fish conc. (μg/kg)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Lindane</strong></td>
<td></td>
<td></td>
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<tr>
<td>Lake orsjoen</td>
<td>Norway</td>
<td>-</td>
<td>0.0001 - 0.312</td>
<td>0.08 - 104</td>
<td>Brevik et al., 1996</td>
</tr>
<tr>
<td>Yonne river</td>
<td>Bassin de, Paris, France</td>
<td>0.022 - 0.036</td>
<td>-</td>
<td>11.25</td>
<td>Bintein &amp; Devillers, 1996</td>
</tr>
<tr>
<td>Various other rivers</td>
<td>France</td>
<td>0.013 - 0.078</td>
<td>-</td>
<td>12.25 - 29.25</td>
<td>Bintein &amp; Devillers, 1996</td>
</tr>
<tr>
<td>Ganges river</td>
<td>U.P India</td>
<td>0.2</td>
<td>0.002 - 0.014</td>
<td>-</td>
<td>Ahmad et al., 1996</td>
</tr>
<tr>
<td>Ponds in Hisar, Sirsa &amp; Rohtak</td>
<td>Haryana, India</td>
<td>0.2 - 3.0</td>
<td>-</td>
<td>-</td>
<td>Kumari et al., 1996</td>
</tr>
<tr>
<td>Ponds in district Shahjanpur</td>
<td>U.P India</td>
<td>-</td>
<td>-</td>
<td>12 - 418</td>
<td>Dua et al., 1996</td>
</tr>
<tr>
<td>Drinking water</td>
<td>Ahmadabad city, India</td>
<td>0.0166 - 1.8</td>
<td>-</td>
<td>-</td>
<td>Jani et al., 1991</td>
</tr>
<tr>
<td>Ponds in Bhopal</td>
<td>Bhopal, India</td>
<td>109 - 3608</td>
<td>-</td>
<td>-</td>
<td>Dikshit et al., 1990</td>
</tr>
<tr>
<td>Madras Coast</td>
<td>Madras, India</td>
<td>6 - 2538</td>
<td>0.001 - 2.208</td>
<td>-</td>
<td>Sivaswamy, 1989</td>
</tr>
<tr>
<td><strong>PAHs</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ganges river</td>
<td>U.P India</td>
<td>BaP: 0.001</td>
<td>BaP: 8.0</td>
<td>-</td>
<td>Ahmad et al., 1996</td>
</tr>
<tr>
<td>Ponds/ wells water</td>
<td>Ahmadabad city, India</td>
<td>BaP: 0.052 - 0.386</td>
<td>BaP: 100 - 260</td>
<td>-</td>
<td>Jani et al., 1991</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BbF: 0.021 - 0.398</td>
<td>BbF: 100 - 900</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Sagueneay Fjord</td>
<td>Québec, Canada</td>
<td>-</td>
<td>BaP: 60 - 170</td>
<td>-</td>
<td>Martel et al., 1986</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>BbF: 60 - 170</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Cayuga lake</td>
<td>Ithaca, New York</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Heit, 1985</td>
</tr>
<tr>
<td>St. Lawrence River</td>
<td>Québec, Canada</td>
<td>total PAHs: 0.014 - 0.045</td>
<td>BaP: 0.11±0.17</td>
<td>-</td>
<td>Pham et al., 1993</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>BbF: 0.091±0.13</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Lake Superior</td>
<td>various, USA</td>
<td>BaP: 0.39x10⁻³±0.18</td>
<td>-</td>
<td>-</td>
<td>Baker &amp; Eisenreich, 1990</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BbF: 0.07x10⁻³±0.10</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
coal, are the most important sources of PAH emissions in the work environment (Bjorseth and Becher, 1986). In many industrial processes these products are heated to high temperatures, thereby releasing PAHs into the work atmosphere. In particular, coking operations and aluminum production have been recognized as major contributors to airborne PAH burden and are documented occupational hazards. Several other industries including iron and steel production, petroleum processing and asphalt production also contribute to the production of PAHs (Bjorseth and Becher, 1986).

The PAH emissions in aluminum processing (Bjorseth and Becher, 1986) and effluents from the coal fired power plants (Daisey et al., 1986; Heit, 1985) have been well documented and are of much scientific concern. In the aluminum industry, there are two processes: Söderberg and prebake anode, which are widely different with respect to PAH emissions. The former, which is most commonly used, is the main cause of PAH exposure in aluminum plants. The electrolytic reduction of alumina in molten cryolite which involves several combustion steps takes place at very high temperature. Subsequently, large amounts of PAH are liberated from the electrodes which contain coal tar pitch. Studies by Martel et al. (1986) and Smith and Levy (1990) have shown that direct emission of PAHs in the aluminum plant’s effluent or scrubber liquors contribute to the overall release and accumulation of PAHs in the aquatic environment. The environmental impacts arising from the high level of PAHs in the Saguenay Fjord, located in eastern Québec, Canada have been studied recently (De Marco, 1992; Lun, 1995). It is a highly industrialized area, and aluminum smelters located along the length of the Saguenay Fjord are the major source of PAH to the river (Smith and Levy, 1990). Large discharges of PAHs along with high concentrations of organic matter from pulp and paper effluents, have resulted in the contamination of sediment in the Saguenay Fjord (Martel et al., 1986).

Power plants are also a potential source of PAH emissions. Fly ash, which is generated during the combustion of coal, contains many metals and polycyclic aromatic hydrocarbons (Natusch et al., 1974). During combustion, organic and inorganic constituents of coal condense on fly ash particles. The constituents of fly ash depend on the type of coal used. Studies (Zwoździak et al., 1984; Davison et al., 1974) have shown that power plant fly ash contains
1.15% of organic particulate matter, in which PAH account for some 23%. At elevated temperatures the majority of PAH may be found in the vapor phase, but when the temperature drops, they are adsorbed on the surface of the fly ash (Zwoździak and Zwoździak, 1985).

There are numerous studies on detailed characterization and identification of the different PAHs in solid and gaseous emissions from the coal fired power plants (Natusch, 1974; Bonfanti et al., 1988; Zwoździak and Zwoździak, 1985). A study by Heit, 1985 examines the relationship of a coal-fired power station to the distribution of PAHs and related organic compounds in the sediments of Cayuga lake, Ithaca, New York. Various PAHs have also been identified in the fly ash from a coal fired power plant located in the metro area of New Delhi (Srivastava et al., 1985). PAH compounds were also measured in the main process vent gas from a carbon black plant (Serth and Hughes, 1980). Loads and distribution of PAH that are emitted from power plants and petroleum shipping activities have been estimated in the sediments of Lake Michigan (Helfrich and Armstrong, 1986). Sources and concentration of PAHs in St. Lawrence river, originating from various industrial activities, have also been determined (Pham et al., 1993). Recently, some PAHs, mainly benzo(a)pyrene and phenanthrene were also measured in the sediments of Ganges river, India (Ahmad, 1996). Table 1.2 lists the concentration of some PAH compounds detected in rivers and lakes in India and other countries.
2. MODEL STRUCTURE

The multi-segment steady-state model applied to the Indian lakes is based on the quantitative water-air-sediment interaction (QWASI) fugacity model developed by Mackay and co-workers (e.g., Mackay et al., 1983). The basic concepts of fugacity approach are fully described elsewhere (Mackay, 1991), therefore, only a brief description is presented here.

2.1 Fugacity and Equivalence Concepts

The fugacity has been successfully used as a phase-equilibrium criterion in environmental fate models (e.g., Mackay 1989, 1991; Mackay and Diamond, 1989; Lun, 1995). For each chemical and each medium, a linear relationship between fugacity and concentration is given as: \( C = Z \times f \), where \( C \) is concentration (mol/m\(^3\)), \( Z \) is the "fugacity capacity" with units of mol/m\(^3\).Pa, (defined as the capacity of each compartment to hold a chemical) and \( f \) denotes fugacity (Pa). Each chemical has a unique value of \( Z \) for each phase at a defined temperature. Phases of high \( Z \) (e.g., sediments and fish) are able to absorb much greater quantity of material, with minimal increase in fugacity. It follows that the pollutants tend to partition into these high \( Z \) phases and achieve elevated concentrations. Conversely, phases of low \( Z \) values will tend to experience a large increase of fugacity following absorption of limited quantities of pollutants (Mackay, 1991).

\( Z \) values can be estimated from partition coefficients. A partition coefficient \( K_{12} \) between two phases, 1 and 2, can be shown to be \( Z_1/ Z_2 \). The use of fugacity as a surrogate for concentration in environmental modeling is very convenient for organic chemicals with measurable vapor pressures, but it is inconvenient for chemicals with negligible or unknown vapor pressures. In case of chemicals with negligible or unknown vapor pressure like metals, polymers, an equilibrium criterion "equivalence" is preferred which is analogous to fugacity, having units of mol/m\(^3\). It enables the fugacity equation to be applied with only slight re-definition of \( Z \) values (Mackay and Diamond, 1989). Equivalence is derived by dividing \( f \) by the chemical's Henry's law constant H
The $Z$ value is multiplied by $H$ and becomes an equivalence $Z'$. The expressions used to calculate $Z$ and equivalence $Z'$ values are given in Table 2.1.

2.2 D Values

Rates of transport and transformation processes are expressed as the product of $f$ and a rate parameter $D$ (mol/hPa), i.e., $Df$ (mol/h). There are mainly three types of $D$ values depending on the nature of transport process: advective, diffusive, and reaction. $D$ values can be readily deduced for these processes by simply writing the conventional rate expression in concentration form and then replacing $C$ by $Zf$ and grouping all the terms except $f$ as the $D$ value. The $D$ values considered in the model are listed in Table 2.2.

2.3 The QWASI Model

The basic unit of the QWASI model is shown in Figure 2.1 which comprises three compartments: a well-mixed sediment compartment underlying a well mixed water column which is exposed to the atmosphere. Each compartment is assumed to have homogeneous environmental conditions and chemical concentrations. A chemical enters the water column by direct emissions, via inflow of particles and water, and from air by absorption, deposition (wet and dry) and precipitation. The chemical is transferred out of the system by outflow of water and suspended particles. The chemical movement with the sediment takes place through diffusion, deposition, resuspension and chemical may leave the system through sediment burial to inaccessible depths. The chemical may be lost by volatilization to air, through bio-degradation, and abiotic reactions. Bulk phase $Z$ values are calculated for the three primary media which also include the contribution of dispersed phases within each media. The air compartment is treated as an air-aerosol mixture, water as water plus suspended particles and sediment as solids and pore water. The model locations are subdivided into three such QWASI compartments with specific hydrological and physical dimensions.
Table 2.1: Definition of Z values (Z) and Aquivences (Z')

<table>
<thead>
<tr>
<th>COMPARTMENT</th>
<th>DEFINITION OF Z (mol/m³.Pa)</th>
<th>DEFINITION OF Z' (dimensionless)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>( Z_A = \frac{1}{RT} )</td>
<td>( Z'<em>A = K</em>{AW} )</td>
</tr>
<tr>
<td>Water</td>
<td>( Z_W = \frac{1}{H} ) or ( \frac{C^S}{P^S} )</td>
<td>( Z'_W = 1 )</td>
</tr>
<tr>
<td>Solid Sorbent</td>
<td>( Z_S = K_{SW}D_S/H )</td>
<td>( Z'<em>S = K'</em>{SW} )</td>
</tr>
<tr>
<td>Aerolsos</td>
<td>( Z_Q = Z_AK_{XA} = 6 \times 10^6/PRT )</td>
<td>( Z'<em>Q = K</em>{XA}Z'_A )</td>
</tr>
<tr>
<td>Z for Bulk Water</td>
<td>( Z_{WT} = Z_W(1-VFP) + Z_PVFP )</td>
<td>( Z'_{WT} = Z'_W(1-VFP) + Z'_PVFP )</td>
</tr>
<tr>
<td>Z for Bulk Sediment</td>
<td>( Z_{ST} = Z_W(1-VFS) + Z_SVFS )</td>
<td>( Z'_{ST} = Z'_W(1-VFS) + Z'_SVFS )</td>
</tr>
<tr>
<td>Z for Bulk Air</td>
<td>( Z_{AT} = Z_A(1-VFQ) + Z_QVFQ )</td>
<td>( Z'_{AT} = Z'_A(1-VFQ) + Z'_QVFQ )</td>
</tr>
</tbody>
</table>

\( R = 8.314 \text{ Pa.m}^3/\text{mol.K} \)
\( T = \text{Temperature in K} \)
\( K_{AW} = \text{Air-water Partition Coefficient} \)
\( H = \text{Henry's Law Constant (Pa.m}^3/\text{mol)} \)
\( C^S = \text{Aqueous Solubility (mol/m}^3) \)
\( P^S = \text{Vapor Pressure (Pa)} \)
\( K_{SW} = \text{Partition Coefficient (L/kg)} \)
\( D_S = \text{Phase Density (kg/L)} \)
\( K'_{SW} = \text{Dimensionless} \)
\( P = \text{Sub-cooled Liquid Vapor Pressure (Pa)} \)
\( K_{XA} = \text{Aerosol/air Part. Coeff.} \)
Table 2.2: Process D-values and rate expressions used in the model

<table>
<thead>
<tr>
<th>Processes</th>
<th>D Values ($m^3/h$)</th>
<th>Rates (mol/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sediment Burial</td>
<td>$D_1$ or $D_8$</td>
<td>$GB.CS$ or $(G_B.Z_S).f_S$ or $D_1.f_S$</td>
</tr>
<tr>
<td>Sediment Transformation</td>
<td>$D_2$ or $D_3$</td>
<td>$V_S.C_S.K_S$ or $(V_S.Z_S.K_S).f_S$ or $D_2.f_S$</td>
</tr>
<tr>
<td>Sediment Resuspension</td>
<td>$D_3$ or $D_R$</td>
<td>$G_B.C_S$ or $(G_S.Z_S).f_S$ or $D_3.f_S$</td>
</tr>
<tr>
<td>Sediment to Water Diffusion</td>
<td>$D_4$ or $D_T$</td>
<td>$K_T.A_S.C/K_{SW}$ or $(K_T.A_S.Z_W).f_s$ or $D_4.f_A$</td>
</tr>
<tr>
<td>Water to sediment Diffusion</td>
<td>$D_4$ or $D_T$</td>
<td>$K_T.A_S.C_W$ or $(K_T.A_S.Z_W).f_W$ or $D_4.f_W$</td>
</tr>
<tr>
<td>Sediment Deposition</td>
<td>$D_5$ or $D_D$</td>
<td>$G_D.C_P$ or $(G_D.Z_P).f_W$ or $D_5.f_W$</td>
</tr>
<tr>
<td>Water Transformation</td>
<td>$D_6$ or $D_W$</td>
<td>$V_W.C_W.K_W$ or $(V_W.Z_W.K_W).f_W$ or $D_6.f_W$</td>
</tr>
<tr>
<td>Volatilization</td>
<td>$D_7$ or $D_V$</td>
<td>$K_V.A_W.C_W$ or $(K_V.A_W.Z_W).f_W$ or $D_7.f_W$</td>
</tr>
<tr>
<td>Absorption</td>
<td>$D_7$ or $D_V$</td>
<td>$K_V.A_W.C_A/K_{AW}$ or $(K_V.A_W.Z_W).f_A$ or $D_7.f_A$</td>
</tr>
<tr>
<td>Water Outflow</td>
<td>$D_7$ or $D_V$</td>
<td>$G_J.C_W$ or $(G_J.Z_W).f_W$ or $D_7.f_W$</td>
</tr>
<tr>
<td>Water Particle Outflow</td>
<td>$D_7$ or $D_V$</td>
<td>$G_J.C_P$ or $(G_J.Z_P).f_W$ or $D_7.f_W$</td>
</tr>
<tr>
<td>Rain Dissolution</td>
<td>$D_9$ or $D_M$</td>
<td>$G_M.C_A/K_{AW}$ or $(G_M.Z_W).f_A$ or $D_9.f_A$</td>
</tr>
<tr>
<td>Wet Particle Deposition</td>
<td>$D_{10}$ or $D_C$</td>
<td>$G_C.C_Q$ or $(G_C.Z_Q).f_A$ or $D_{10}.f_A$</td>
</tr>
<tr>
<td>Dry Particle Deposition</td>
<td>$D_{11}$ or $D_Q$</td>
<td>$G_Q.C_Q$ or $(G_Q.Z_Q).f_A$ or $D_{11}.f_A$</td>
</tr>
<tr>
<td>Water Inflow</td>
<td>$D_L$</td>
<td>$G_i.C_i$ or $(G_i.Z_W).f_i$ or $D_L.f_i$</td>
</tr>
<tr>
<td>Water Particle Inflow</td>
<td>$D_X$</td>
<td>$G_X.C_X$ or $(G_X.Z_P).f_W$ or $D_X.f_W$</td>
</tr>
<tr>
<td>Direct Emission</td>
<td>-</td>
<td>$E_W$</td>
</tr>
</tbody>
</table>

Notes:
Groups in Parentheses are D values (mol/h·Pa), e.g. $D_1$ is $(G_B.Z_S)$. Z values are fugacity capacities (mol/m³). The rate is the product of D and fugacity i.e. $Df$.

G values are flow rates ($m^3/h$) of a phase, e.g. $G_B$ is the sediment burial rate.

C represents concentration in sediment (S), water (W), air (A), aerosol (Q), water particles (P), water inflow (I), water particle inflow (X), water outflow (J) and particle outflow (Y).

$f_w$, $f_s$, $f_A$ and $f_i$ are fugacities of water, sediment, air and water inflow.

$K_W$ and $K_S$ are water and sediment transformation rate constant ($h^{-1}$).

$K_{SW}$ is equivalent to ratio of Z values in the two compartments $Z_S/Z_W$ is a dimensionless sediment-water partition coefficient. $K_{AW}$ is $Z_A/Z_W$, dimensionless air-water partition coefficient.

$K_T$ is sediment-water mass transfer coefficient and $K_V$ is the water side overall mass transfer coefficient (m/h).

$A_W$ and $A_S$ are air-water and water-sediment areas ($m^2$). $V_W$ and $V_S$ are water and sediment volumes ($m^3$).
Figure 2.1: QWASI Model

Figure 2.2: QWASI Model Process
2.4 Mass Balance Equations

For each water and sediment segments a differential mass balance equations can be written in terms of fugacity and D values previously defined as follows:

**Water**

\[ V_w Z_{WT} \frac{df_w}{dt} = E_w + f_S(D_3 + D_4) + f_A D_8 \pm f_{w1} D_1 - f_w(D_4 + D_3 + D_6 + D_7 + D_1) \]  \hspace{1cm} (1)

**Sediment**

\[ V_s Z_s \frac{df_s}{dt} = f_w(D_4 + D_3) - f_s(D_1 + D_2 + D_3 + D_4) \]  \hspace{1cm} (2)

where \( V \) is the volume of each phase; \( Z_{WT} \) is the bulk phase Z value; \( f \) is the fugacity; \( E_w \) is chemical discharge or input into the water column; subscripts A, W and S refer to air, water and sediment respectively. The term \( \Sigma f_{w}D_{i} \) represents the sum of advective inflows from adjacent water compartments.

The steady-state solution to these equation is obtained when the derivatives are set to zero (condition which will be reached after prolonged exposure of the system to constant input conditions):

\[ f_w = \frac{E_w + f_A D_8 \pm f_{w1} D_1}{D_0 + D_3 + D_7 + \frac{(D_4 + D_3)(D_1 + D_2)}{D_1 + D_2 + D_3 + D_4}} \]  \hspace{1cm} (3)

\[ f_w = \frac{E_w + f_A D_8 \pm f_{w1} D_1}{D_0 + DE} = \frac{l \pm f_{w1} D_1}{DT} \]  \hspace{1cm} (4)

\[ f_s = \frac{f_w(D_4 + D_3)}{D_1 + D_2 + D_3 + D_4} \]  \hspace{1cm} (5)
The terms in the numerator of equation 3 are the input to the segment from the point source discharges \((E_w)\), atmosphere \((f_{i,D_i})\) and from the advective flow of particles and water from adjacent segments \((\Sigma f_{w,D_i})\). The denominator represents \(D\) values of transport processes out of the water column. \(DE\) (shown in Eq. 4) is the sum of all loss terms excluding advective outflows of water and particles. \(DE\) is also includes a term that describes a net loss to the sediment; algebraically it is the transfer rate to sediment by deposition \((D_4)\) and diffusion \((D_5)\) multiplied by the fraction permanently lost from the sediment by burial and transformation \((D_1+D_2)/(D_1+D_2+D_3+D_4)\). The term \(DT\) is an overall loss \(D\) value from water column i.e. outflows to other segments \((D_0)\), net loss to sediment through deposition and diffusion \((D_4+D_5)\), evaporation into air \((D_7)\) as well as transformation \((D_6)\) and thus is \((D_0+DE)\). The solution is greatly facilitated by first grouping various \(D\) values as illustrated in Figure 2.2.

For developing the models in this study, the aquatic system is treated as series of connected lakes or sub-basins, each of which is assumed to be a QWASI system as shown in Figure 2.3. The term \(I_i\) represents input into water column from outside sources including point source discharges, river inputs and atmospheric deposition but excluding advective input from adjacent compartments. The net outputs from water column are designated \(DT_i\), which includes transfer to adjacent segments and to sediment, volatilization and reaction. \(DE_i\) values are output terms excluding advection. \(D_{ij}\) terms are advective flows of water and particles from segments \(i\) to \(j\). The steady state mass balance equation for the three compartments of Figure 2.3 are as follows (subscript 4 refers to the ultimate receiving water body in the downstream for which the concentration of the chemical is defined):

\[
I_1 + f_{w_1}D_{21} = f_{w_1}(D_{e_1} + D_{12}) = f_{w_1}DT_1 \tag{6}
\]
\[
I_2 + f_{w_1}D_{12} + f_{w_2}D_{32} = f_{w_2}(DE_2 + D_{21} + D_{23}) = f_{w_2}DT_2 \tag{7}
\]
\[
I_3 + f_{w_2}D_{23} + f_{w_4}D_{43} = f_{w_3}(DE_3 + D_{32} + D_{34}) = f_{w_3}DT_3 \tag{8}
\]

This system of three linear equation can be solved numerically for the three unknown water fugacities \(f_{w_i}\). The solution for various segments are:
Figure 2.3: D Values for 3-Segment Model
\[
\begin{align*}
    f_{w1} &= \frac{(I_1 + f_{w2} D_{21})}{DT_1}; \\
    f_{w2} &= \frac{(I_2 + K1 + f_{w3} D_{32})}{K2}; \\
    f_{w3} &= \frac{I_3 + \frac{D_{23}(I_1 + K1 + f_{w3} D_{32})}{K2} + f_{w4} D_{43}}{K3}
\end{align*}
\]

where \( K1 = \frac{I_1 D_{12}}{DT_1}; \) \( K2 = DT_2 - \frac{D_{12} D_{21}}{DT_1}; \) \( K3 = DT_3 - \frac{D_{23} D_{32}}{K2}. \)

Once the fugacities in water are known, it is then possible to calculate the sediment fugacities \( f_S \) using equation 5. Finally, concentrations, amounts, and rates of transport and transformation are determined employing the \( Z \) and \( D \)-values. A computer program has been written in GW Basic language which processes various \( Z \) values, volume, area, flows, input parameters, \( D \) values etc. to give the steady-state algebraic solution. The computer programs and outputs are listed in Appendix A.
3. MODEL PARAMETERS AND PROCEDURES

3.1 Physical-Chemical Properties

Physical -chemical properties are listed in Table 3.1. The values are taken from Mackay et al. (1992, 1993, 1997) with the exceptions of aqueous solubility and octanol-water partition coefficient ($K_{OW}$) for chlorobenzenes, particle-water partition coefficient ($K_p$) for metals and the degradation half lives. For chlorobenzenes, the experimentally measured values of $K_{OW}$ (this study) and aqueous solubility (Shiu et al., 1997) were used. The $K_p$ for Pb and Cu were taken from Diamond et al. (1994). Transformation and metabolic half lives for organic chemicals were either unavailable in the literature or based on laboratory measurements with limited applicability to the condition in the lakes. Therefore, the values of degradation half lives in water and sediments are based on suggested order of magnitudes by Mackay et al.(1992, 1993, 1997) and the compilation by Howard et al. (1991).

Since monitoring studies for Nainital lake indicated that temperature ranges from 6 to 21 °C with an average of 15 °C, a temperature correction was employed for solubility, octanol-water partition coefficient and vapor pressure, being the temperature dependent properties. The vant Hoff’s correlation of temperature dependence:

$$\ln B = A - \frac{\Delta H}{R(J/mol.K)}T$$

developed for $K_{OW}$ in this work and aqueous solubility (Shiu et al., 1997) for chlorobenzenes were used to account for temperature variation, where B is $K_{OW}$ or solubility, $T$ is the system temperature, and A and $\Delta H$ are the regression constant and the enthalpy of phase change respectively. The temperature correction for vapor pressure was incorporated using Clapeyron-Clausius type relationship developed by Liu and Dickhut (1994) for chlorobenzenes.
<table>
<thead>
<tr>
<th>Compounds</th>
<th>Atomic/Mol. Wt. g/mol</th>
<th>Melting Point, °C</th>
<th>Aqueous Solubility (g/m³)</th>
<th>Vapor Pressure, Pa</th>
<th>Henry's Law Constant, Pa.mol/m³</th>
<th>Log Kow or Log Kp</th>
<th>Half-life in water, hours</th>
<th>Half-life in sediment, hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>lead</td>
<td>207.19</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>5.82</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>copper</td>
<td>63.55</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>6.12</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>1,4-dichlorobenzene</td>
<td>147</td>
<td>53.1</td>
<td>63.0</td>
<td>90.2</td>
<td>210.46</td>
<td>3.35</td>
<td>2000</td>
<td>8000</td>
</tr>
<tr>
<td>1,2,3,5-tetrachlorobenzene</td>
<td>215.9</td>
<td>54.5</td>
<td>2.43</td>
<td>9.8</td>
<td>870.70</td>
<td>4.67</td>
<td>6000</td>
<td>14000</td>
</tr>
<tr>
<td>pentachlorobenzene</td>
<td>250.3</td>
<td>86</td>
<td>0.254</td>
<td>0.889</td>
<td>876.05</td>
<td>5.06</td>
<td>10000</td>
<td>17000</td>
</tr>
<tr>
<td>hexachlorobenzene</td>
<td>284.8</td>
<td>230</td>
<td>0.0035</td>
<td>0.0023</td>
<td>187.15</td>
<td>5.60</td>
<td>50000</td>
<td>55000</td>
</tr>
<tr>
<td>lindane (γ-HCH)</td>
<td>290.85</td>
<td>112.5</td>
<td>7.3</td>
<td>0.0073</td>
<td>0.291</td>
<td>3.7</td>
<td>6000</td>
<td>17000</td>
</tr>
<tr>
<td>α-HCH</td>
<td>290.85</td>
<td>158</td>
<td>1.63</td>
<td>0.0033</td>
<td>0.589</td>
<td>3.8</td>
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<td>10000</td>
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<tr>
<td>benzo(a)pyrene</td>
<td>252.32</td>
<td>175</td>
<td>0.002</td>
<td>1.5E-07</td>
<td>0.046</td>
<td>6.04</td>
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<td>30000</td>
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<tr>
<td>benzo(b)fluoranthene</td>
<td>252.32</td>
<td>168</td>
<td>0.0015</td>
<td>5.0E-07</td>
<td>0.054</td>
<td>6.50</td>
<td>12000</td>
<td>35000</td>
</tr>
</tbody>
</table>
There is little temperature variation in Rihand Reservoir over the year, except the two months in winter, and the average temperature is close to 25 °C. Therefore, no adjustment for temperature is required in properties of modelled chemicals for this system.

3.2 Hydrologic and Limnologic Parameters

3.2.1 Lake Nainital

The lake parameters are listed Table 3.2. The area, mean depth and volume were documented in Das and Pande (1982). Suspended particle concentrations and organic carbon (OC) concentrations of suspended particles and sediment solids were experimentally measured by Dr. Bhishm Kumar by periodic sampling at the various monitoring stations. The data were obtained in 1994-95 by personal communication with Dr. Bhism Kumar of the National Institute of Hydrology, who is currently working on hydrological studies of this lake. Water inflows from municipal, surface runoff and other sources were also supplied by Dr. Kumar. The particle density was assumed to be 2.0 g/cm³.

Average concentration of suspended particulate matter in air was experimentally measured at Mallikadevi site near Nainital (Mahadevan et al., 1989). Annual precipitation varies between 2245 to 2480 mm (Pant et al., 1981). Sediment accumulation rates were determined by Das et al. (1994), employing Pb - 210 dating to the sediment cores. The higher burial rate of about 2.5 g/m²/day was found to be related to faster erosion in the catchment aided by greater anthropogenic activity. The average sediment deposition rate in the lake has been estimated from limited sediment trap data to be about 5.5 g/m²/day (Kumar, 1995; unpublished data). There was no information on particle resuspension. Deposition and resuspension rates in each segment were adjusted based on model calibration using Pb concentrations in water and sediment. The high deposition and low resuspension rates in the north basin were attributed to higher particle inputs, low turbulence and greater depth. The deposition rates decrease from north to south basin while resuspension rates increase. This is due to the higher turbulence, and lower depth and particle inputs in middle and south basin. Inter-segmental water exchanges were not available in the literature and thus the flow to upstream segments were estimated to be 5% of the total flow downstream.
### Table 3.2: Characteristics of Lake Nainital

<table>
<thead>
<tr>
<th></th>
<th>Segment 1</th>
<th>Segment 2</th>
<th>Segment 3</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Dimensions</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Area (m²)</td>
<td>$1.5 \times 10^5$</td>
<td>$1.55 \times 10^5$</td>
<td>$1.55 \times 10^5$</td>
<td>Das and Pande, 1982</td>
</tr>
<tr>
<td>Depth (m)</td>
<td>18</td>
<td>18</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td><strong>Particles</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Suspended particle density (g/cm²)</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>estimated</td>
</tr>
<tr>
<td>Suspended particle concentration (mg/L) in water</td>
<td>25</td>
<td>30</td>
<td>40</td>
<td>Kumar, 1995</td>
</tr>
<tr>
<td>Organic content of suspended particle (g/g)</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>Kumar, 1995</td>
</tr>
<tr>
<td><strong>Sediments</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment solid density (g/cm²)</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>estimated</td>
</tr>
<tr>
<td>Organic content of sediment solid (g/g)</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>Kumar, 1995</td>
</tr>
<tr>
<td><strong>Flows</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water inflow rates (m²/h)</td>
<td>250</td>
<td>100</td>
<td>-</td>
<td>Kumar, 1995</td>
</tr>
<tr>
<td><strong>Particle movement</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Particle deposition rates (g/m²/day)</td>
<td>5.5</td>
<td>5.0</td>
<td>5.0</td>
<td>Kumar, 1995</td>
</tr>
<tr>
<td>Particle resuspension rate (g/m²/day)</td>
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<td>2.0</td>
<td>2.0</td>
<td>estimated</td>
</tr>
<tr>
<td>Particle burial rate (g/m²/day)</td>
<td>2.5</td>
<td>1.8</td>
<td>1.3</td>
<td>Das et al., 1994</td>
</tr>
<tr>
<td><strong>Atmosphere properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Avg. concentration of suspended particulate matter in air (µg/m³)</td>
<td>68</td>
<td>68</td>
<td>68</td>
<td>Mahadevan et al., 1989</td>
</tr>
<tr>
<td>Avg. precipitation (m/yr)</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>Pant et al., 1981</td>
</tr>
</tbody>
</table>
3.2.2 Rihand Reservoir

The dimensions of the area, depth and various physical and hydrological specifications for Rihand Reservoir presented in Table 3.3 were obtained from EIA studies conducted by National Thermal Power Corporation, India and their consultant, EDF, France (NTPC, 1995 and references therein). Most of these values have been taken from the data collected for hydrological and limnological studies of the system. Their hydrological surveys include estimation of drainage basin area, river discharges, water losses, contribution of run off, annual inflow and outflow and the water balance of the reservoir.

3.2.2 (a) Dimensions and Flows

Area, capacity and water depth data were first recorded in 1960 by the Irrigation Department of Uttar Pradesh, India (Garg, 1960). Basin areas, listed in Table 3.3, were obtained by digital estimates of surface areas calculated from Geological Survey of India (GSI) topographic maps (Bonsode and Pitale, 1983). Water depths at different parts of reservoir are based on bathymetric estimates of depth.

During the annual set of measurements from 1989 to 1990, several on-site studies were conducted in the field of surface hydrology. Eighty three discharge measurements were taken over the year on a monthly basis in the Rihand river and seven tributaries flowing into the reservoir, both to examine the distribution of discharges over the time and to check the water balance computation of the reservoir. To secure a more accurate knowledge of the contribution of the local drainage basin rivers of the reservoir, gauging stations fitted with continuous limnigraph were installed (Figure 3.1) at Rihand upstream (near Karkota village and railway bridge) and other major rivers (Kanchan, Mayur, Balia). A gauging station was also installed at some ¾ km upstream of the dam near Pipri bridge to measure the total discharge. The mean annual discharge at this location was estimated to be 150 m³/s, which is close to the inflow, estimated to be 161 m³/s (Gosse, 1990a). The monthly discharge data for various rivers were averaged over the year. Based on location of discharge point of each river, their mean annual flows were
### Table 3.3: Characteristics of Rihand Reservoir

<table>
<thead>
<tr>
<th></th>
<th>Segment 1</th>
<th>Segment 2</th>
<th>Segment 3</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
</tr>
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<td>$14.8 \times 10^7$</td>
<td>$19.9 \times 10^7$</td>
<td>$11.6 \times 10^7$</td>
</tr>
<tr>
<td>Depth (m)</td>
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<td>22</td>
<td>25</td>
</tr>
<tr>
<td><strong>Particles</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Suspended particle density (g/cm²)</td>
<td>1.8</td>
<td>2</td>
<td>2</td>
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<tr>
<td>Suspended particle concentration (mg/L) in water</td>
<td>96</td>
<td>81</td>
<td>19</td>
</tr>
<tr>
<td>Organic content of suspended particle (g/g)</td>
<td>0.1</td>
<td>0.1</td>
<td>0.15</td>
</tr>
<tr>
<td><strong>Sediments</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Sediment solid density (g/cm²)</td>
<td>1.8</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Organic content of sediment solid (g/g)</td>
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<td>0.08</td>
<td>0.1</td>
</tr>
<tr>
<td><strong>Flows</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Water inflow rates (m²/h)</td>
<td>$5.65 \times 10^5$</td>
<td>$1.18 \times 10^4$</td>
<td>$1.1 \times 10^3$</td>
</tr>
<tr>
<td><strong>Particle movement</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Particle deposition rates (g/m²/day)</td>
<td>15</td>
<td>13</td>
<td>10</td>
</tr>
<tr>
<td>Particle resuspension rate (g/m²/day)</td>
<td>1.2</td>
<td>0.6</td>
<td>0.2</td>
</tr>
<tr>
<td>Particle burial rate (g/m²/day)</td>
<td>6.5</td>
<td>4.7</td>
<td>2.5</td>
</tr>
<tr>
<td><strong>Atmosphere properties</strong></td>
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<td></td>
</tr>
<tr>
<td>Avg. concentration of suspended particulate matter in air (µg/m³)</td>
<td>165</td>
<td>165</td>
<td>165</td>
</tr>
<tr>
<td>Avg. precipitation (m/yr)</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>
Figure 3.1: Locations of gauging stations (indicated by cross lines) on various rivers flowing into reservoir
added to estimate the total inflow into each reservoir segment. Inter-segmental water exchange are not well defined due to complex hydrology within the system. Backmixing were estimated to be 10% of the total flow downstream.

3.2.2 (b) Particles and Sediments

The reservoir receives a high load of particles from Rihand river, its major tributaries (Mayur, Kanchan and Balia) as well as the overflows from ash ponds. Particle inputs are greatest in the south basin followed by the middle and north basin, due to high inputs from Rihand river, particularly in rainy seasons.

Concentration as well as its organic content of suspended solid were measured at fourteen stations (seven in river water and seven in reservoir water) on a monthly basis under one-year water quality monitoring survey of Rihand region. The sampling stations (labeled 1 to 14) are shown in Figure 3.2. This monitoring campaign provided a complete analysis of reservoir and river water including water quality parameters such as dissolved oxygen, pH, conductivity, hardness, nitrate and phosphate concentration, BOD/COD, potassium and fluoride content, concentration of metals, trace elements and organic contaminants. The nitrate content of the water is low throughout the year.

The reservoir receives close to 50% of the annual water supplies during rainy season from June to October. Consequently, it is expected that water quality of Rihand and its tributaries during this season has a great influence on water quality of the reservoir. The reservoir itself is highly turbid, with suspended particle concentration ranging from 12 to 120 mg/L (Gosse, 1999b; Gosse et al., 1991). A noticeable horizontal gradient was observed between the profiles of suspended solid (SS) concentration in the upper and lower region of reservoir. Highest concentrations were observed in upstream stations 2 and 3 followed by furthest stations 5 and 6. The north basin i.e. segment 3 and downstream Rihand have lower suspended solids as most of the incoming particles slowly settle down at the bottom of the reservoir while moving from the south to north basin. The difference in the profiles of organic component of suspended solids (OSS) was less
Figure 3.2: Positions of sampling stations (labeled 1 to 14) of the water quality monitoring program.
apparent. Most upstream and central stations have comparable levels of OSS. However, the OSS concentrations were slightly higher at most downstream and bank stations in the north basin.

To assess the magnitude of deposition rate of suspended solids, three sediment traps were placed at different locations (one in each segment) in the reservoir. The average sediment deposition rate estimated from the sediment trap data is about 15 g/m²/day (the value decreases from south to north basin). This value was further verified by applying suspended solids input-output balance in the reservoir. The total SS inflow into the reservoir over the hydrological year 1989-1990 was estimated to be 3.0 Mtonnes, whereas SS flow conveyed by reservoir at the dam outlet was 0.45 Mtonnes. This gives the deposition rate of about 2.55 Mtonnes/year (≈ 15 g/m²/day), assuming the resuspension rate to be negligibly small. Rates of sediment burial of 2.5 to 6.5 g/m²/day were determined by Pb-210 dating. There was no information on particle resuspension rate, therefore, deposition and resuspension rates were revised to maximize the correspondence between estimated and measured lindane concentrations.

The data regarding the sediments of the reservoir come from two sources: (1) granulometric and chemical analyses performed as part of CIFRI's study (NTPC, 1995) on surface sediment samples, collected with bottom grab at 30 sites during “Aquatic Ecology” program and (2) a study carried by Hydroexpert (NTPC, 1995) on 130 sediment samples as part of “sediment” program. These studies provide detailed data on water content, sandy fraction, organic and mineral matter including the concentration and spatial distribution of various metals, organochlorine pesticides and PAH in the top 10 cm sediment layer. About 60% water content is present in the sediments. Rest 40% is sandy fraction where clay is the main component. Sediment organic carbon content values ranged from 0.07 to about 0.1 g/g, lower values being observed in south and middle basin. The sediments from lower region near the dam are richest in organic carbon.
3.2.2 (c) Air Quality

Ambient air quality study of the Rihand region includes an experimental study carried out by NTPC (1995) on site for one year (1989-90). The field measurement have been performed with the help of fixed air quality stations (located at three sites: AQ1, AQ2, AQ3) as well as continuous monitoring by a mobile laboratory van. The locations of fixed air quality stations are shown in Figure 3.3. These measurements provide a detailed data on concentration of suspended particulate matter (SPM), gaseous pollutants such as SO$_2$, NO$_2$, NO$_x$, CO, chlorine, fluorine etc. and chemical analysis of SPM for metals and organic contaminants (HCHs, PAHs etc.). Rainfall data recorded at four stations over the year ranged from 938 to 2000 cm. The annual mean concentration of SPM ranged from 150 to 200 $\mu$g/m$^3$ depending on the site and time of measurements.

3.3 Sources and Emissions

There are mainly three type of sources and emission information required by the model: (1) An estimate of direct discharge rate into water column, which includes industrial, urban sources, sewage effluent treatment plant etc.. (2) Average background concentration in riverine inflow and (3) average airborne concentration.

3.3.1 Lake Nainital

Table 3.4 lists all input loading data used to estimate chemical fates. Average airborne concentrations of Pb and Cu listed in the table were experimentally measured at Mallikadevi site near Nainital (Mahadevan et al., 1989). Information on direct releases (point source discharge) of Pb and Cu into the lake is not clearly available. The values used are roughly estimated (Kumar, 1995; unpubl. data) on the basic information of loading assessments. The background concentration of metals in inflows were assumed to be almost the same as reported concentrations in the lake water. Illustrative total inputs of 1000 kg/year (atmospheric, effluents and river inflow) were used for chlorobenzenes, HCHs and PAHs.
Figure 3.3: Locations of air quality stations
3.3.2 Rihand Reservoir

All chemical loadings for lindane, HCH, B(a)P and B(b)F and summarized in Table 3.5. The major sources of lindane and α-HCH emission are the industrial discharges from the pesticide plant. Liquid effluents from HCH plant are directly released after some preliminary treatment into north west sector of reservoir. Therefore, there is a point source discharge only into segment 3 which has been estimated from available data on effluent outflow of the treatment plant and chemical concentration in the effluent. The effluent flow rate of 106 m³/h with the corresponding lindane and α-HCH concentration of 7 and 7.6 g/m³ in the effluent respectively implied a total point source loading of 6500 kg lindane and 7000 kg α-HCH annually.

The point source loading of PAH into the reservoir could not be directly estimated firstly, because there are many sources of industrial emission into the reservoir and secondly, the information on PAH concentration in effluent and corresponding effluent flow rate of each industry are insufficient. The values listed in table 3.5 are rough estimates based on various emission factors. Table 3.6 lists the emission factors and corresponding emission sources of PAHs such as coal-fired power plants, aluminum and carbon plants etc. The value of emission factor which is taken from the literature are mainly dependent on the type of process and raw material used. Total discharge of BaP and BbF in kg/year have been calculated from emission factors which is mg of PAH/kg of coal or aluminum produced. Emission factor when multiplied by the percentage of BaP or BbF present in total PAH emitted times the amount of coal used or aluminum produced gives the total amount of BaP/BbF emitted. The point source discharge into the water column is then estimated by assuming that only some percentage of total discharge in actually going into the liquid effluent. Rest is present in the airborne particulates in the atmosphere which would finally reach the water body and surrounding catchment area via atmospheric deposition. In case of coal fired power plants, it is assumed that 10% of the total PAHs emitted is lost to atmosphere and the remaining 90% is trapped in the particles and the fly ash which is collected through the electrostatic precipitator (ESP) or other devices. The particles and fly ash are collected in ash ponds that are located along the
### Table 3.4: Chemical loadings to Lake Nainital

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Sources</th>
<th>Segment 1</th>
<th>Segment 2</th>
<th>Segment 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lead</td>
<td>Point (kg/year)</td>
<td>450</td>
<td>250</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>Inflow (g/m³)</td>
<td>0.05</td>
<td>0.05</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Air (ng/m³)</td>
<td>0.84</td>
<td>0.84</td>
<td>0.84</td>
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<tr>
<td>Copper</td>
<td>Point (kg/year)</td>
<td>100</td>
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<td></td>
<td>Inflow (g/m³)</td>
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<td>0.001</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Air (ng/m³)</td>
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<td>0.76</td>
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### Table 3.5: Chemical loadings to Rihand Reservoir

<table>
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<tr>
<th>Chemical</th>
<th>Sources</th>
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<th>Segment 2</th>
<th>Segment 3</th>
</tr>
</thead>
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<tr>
<td>lindane</td>
<td>Point (kg/year)</td>
<td>-</td>
<td>-</td>
<td>6500</td>
</tr>
<tr>
<td></td>
<td>Inflow (g/m³)</td>
<td>0.2 x 10⁻³</td>
<td>0.15 x 10⁻²</td>
<td>0.15 x 10⁻²</td>
</tr>
<tr>
<td></td>
<td>Air (ng/m³)</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>α-HCH</td>
<td>Point (kg/year)</td>
<td>-</td>
<td>-</td>
<td>7000</td>
</tr>
<tr>
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<td>Inflow (g/m³)</td>
<td>0.18 x 10⁻³</td>
<td>0.20 x 10⁻²</td>
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</tr>
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<td></td>
<td>Air (ng/m³)</td>
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<td>0.5</td>
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<td>benzo(a)pyrene</td>
<td>Point (kg/year)</td>
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<td>Inflow (g/m³)</td>
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<td>0.9 x 10⁻⁴</td>
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<td>Air (ng/m³)</td>
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<td>11</td>
<td>11</td>
</tr>
<tr>
<td>benzo(b)fluoranthene</td>
<td>Point (kg/d)</td>
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<td>14.1</td>
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<td>Inflow (g/m³)</td>
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<td>Air (ng/m³)</td>
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### Table 3.6: Estimation of PAHs (benzo(a)pyrene and benzo(b)fluoranthene) discharges using emission factors

<table>
<thead>
<tr>
<th>Emission Sources</th>
<th>Capacity (Tones/year)</th>
<th>Emission factors (Total PAH: mg/kg)</th>
<th>Reference</th>
<th>Discharge (kg/year)</th>
<th>BaP</th>
<th>BbF</th>
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<tbody>
<tr>
<td>(1) Power Plants:</td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Vindhavachal</td>
<td>2.2x10^6</td>
<td>0.5</td>
<td>(BaP : 2%)</td>
<td>22</td>
<td>55</td>
<td></td>
</tr>
<tr>
<td>• Singrauli</td>
<td>2.7x10^6</td>
<td></td>
<td>(BbF : 5%)</td>
<td>27</td>
<td>67.5</td>
<td></td>
</tr>
<tr>
<td>• Rihand</td>
<td>3.1x10^6</td>
<td></td>
<td></td>
<td>31</td>
<td>77.5</td>
<td></td>
</tr>
<tr>
<td>• Renusagar</td>
<td>3.0x10^6</td>
<td></td>
<td></td>
<td>30</td>
<td>75</td>
<td></td>
</tr>
<tr>
<td>• Anapara</td>
<td>6.9x10^6</td>
<td></td>
<td></td>
<td>69</td>
<td>172.5</td>
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<td>(2) Aluminum Production:</td>
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<td>400</td>
<td>Axenfeld et al.,</td>
<td>300</td>
<td>480</td>
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<tr>
<td>• Smelters/Pot rooms</td>
<td></td>
<td>(BaP : 0.5%)</td>
<td>1992</td>
<td></td>
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</tr>
<tr>
<td>(Söderberg and</td>
<td></td>
<td>(BbF : 0.8%)</td>
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<td>Prebake processes)</td>
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<td>(BaP : 0.5%)</td>
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</tr>
<tr>
<td></td>
<td>(BbF : 0.5%)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Coal fired boilers</td>
<td>Coal: 2.62x10^5</td>
<td>0.5</td>
<td>(BaP : 2%)</td>
<td>2.6</td>
<td>6.55</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(BbF : 5%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) Carbon Black Production</td>
<td>Carbon black: 1.3x10^5</td>
<td>1.9</td>
<td>Serth &amp; Hughes,</td>
<td>4.0</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(BaP : 1.6%)</td>
<td>1980</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(BbF : 1.6%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4) Chlor-alkali</td>
<td></td>
<td></td>
<td>Axenfeld et al.,</td>
<td>78</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>• Coal fired boilers</td>
<td>Coal: 7.8x10^6</td>
<td>0.5</td>
<td>1992</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(BaP : 2%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(BbF : 5%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.4 Model Calibration and Testing

The models were primarily parameterised and calibrated using available data on measured concentrations of chemical. Lindane and Pb having sufficiently complete data sets were chosen to calibrate the model developed for Rihand reservoir and Lake Nainital respectively. The calibration criterion was correspondence between measured and estimated concentrations in water and sediment. The calibration involved adjustment of sediment deposition and resuspension rates. Although sediments traps were deployed primarily during summer at only few places the catches were not representative of annual average values required. The calibrated models were then tested by comparing the model estimates of α-HCH, BaP, BbF and Cu concentration with the reported values.

3.5 Sensitivity Analysis

Sensitivity analyses were undertaken and various parameters e.g. emission rates, sediment deposition and resuspension rates, suspended solid concentration, half-lives etc. were varied by doubling and halving the original values. The effects upon concentration in water and sediment were obtained. An example is shown for lindane in Rihand reservoir as Table 3.6 (Appendix C). Major parameters identified to be half-life in water, emission and deposition rate. Similarly, the analyses can be repeated for other chemicals and lake.
4.0 RESULTS AND DISCUSSION

The models developed in this study for the aquatic environment in India such as Lake Nainital and Rihand reservoir are used to assess the fate of some persistent contaminants, namely chlorobenzenes, HCHs, PAHs, Pb and Cu. As mentioned before, there were no input data available for CBs. Consequently, the model results for these are only illustrative. The discussion focuses on model validation, details of environmental fate and use of these models in formulating remedial actions to improve the water quality of the systems. The validity of models is assessed by comparing the estimated chemical concentrations with reported values in water and sediment. The environmental fate and behavior of these chemicals in the above lakes are described and illustrated with mass balance diagrams. Accordingly, the various transports, transformation processes and residence times of the chemicals in the system are outlined. Two simple modelling approaches are also developed and applied to these chemicals. Lastly, some examples are given where these models can be a useful tool in regulating emissions. Implications for the better management of emissions and planning the remedial and control measures are discussed briefly. Approaches to reduce loadings are suggested.

4.1 Validation of Models

4.1.1 Nainital Lake

Das and Pande (1980) measured water and sediment concentration of several metals, including Pb and Cu. Simulated results from the study are compared with reported values in Table 4.1. Model results are generally in good agreement with measured values.

High sediment concentrations of lead and copper were found in north basin which receives largest inputs through run off and municipal discharges. The model underestimates the water concentration for Pb by 35% in the segment 3 (south basin), whereas estimated values are within 10% of the measured values in segment 1 and 2 (north-west and middle basin). Sediment concentration is underestimated by 15% in
Table 4.1: Comparison of measured and model estimated chemical concentrations in water and sediment of Lake Nainital

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Variable</th>
<th>1</th>
<th>Segment 2</th>
<th>Segment 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lead</td>
<td>Water (mg/L)</td>
<td>measured: 0.060</td>
<td>0.060</td>
<td>0.070</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated: 0.054</td>
<td>0.056</td>
<td>0.045</td>
</tr>
<tr>
<td></td>
<td>Sediment (μg/g)</td>
<td>measured: 268</td>
<td>164</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated: 226</td>
<td>164</td>
<td>113</td>
</tr>
<tr>
<td>Copper</td>
<td>Water (mg/L)</td>
<td>measured: 0.0017</td>
<td>0.0008</td>
<td>0.004</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated: 0.009</td>
<td>0.008</td>
<td>0.008</td>
</tr>
<tr>
<td></td>
<td>Sediment (μg/g)</td>
<td>measured: 60.03</td>
<td>28.56</td>
<td>19.37</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated: 41.6</td>
<td>25.5</td>
<td>21.10</td>
</tr>
</tbody>
</table>
segment 1 but it is very close (within 3%) to measured values in segment 2 and 3. For Cu, model estimated sediment concentrations are similar (within 10%) to the experimental measurements in segment 2 and 3; it is underestimated by 30% in segment 1. However, estimated water concentration in all segments showed a significant deviation from measured values. The values are overestimated by a factor of 5, 10 and 2 in segment 1, 2, and 3 respectively. The discrepancy is probably associated with the uncertainty in having a correct value of particle-water partition coefficient, $K_p$ for Cu. The effect of increase in $K_p$ by a factor of 5 was to reduce the water concentration by a factor of 3.

4.1.2 Riband Reservoir

The concentrations of various pollutants in the water and sediments of the reservoir have been experimentally measured during one year water quality monitoring and sediment survey programs by CIFRI and NTPC (1994). The validity of the model was evaluated by comparing the calculated compartment concentrations with the range of measured concentration levels. The estimated concentrations of lindane, $\alpha$-HCH, BaP, and BbF in water and sediments of various segments are compared in Table 4.2. Most predicted values are in good agreement with the measured values. In most cases the calculated value is within the range of measured values. Lindane concentration in water is overestimated by 41% in the south basin, whereas it is very close to the measured value (within 8%) in the north-west basin. Sediment concentrations in segment 1 and 2 are well within the range of reported values. Lindane sediment concentration in segment 3 is higher (13%) than the upper range of reported value. For $\alpha$-HCH, sediment concentration in segment 1 is close (within 30%) to measured value whereas in segment 2 and 3, concentrations are close to lower (within 4%) and upper (within 10%) ranges of the reported values respectively. The water concentrations of $\alpha$-HCH in segment 1 and 2 are almost 3 and 5 times higher respectively. However, concentration in segment 3 is in good agreement with the measured value. Regrettably, there are insufficient monitoring data for PAHs concentration in the reservoir water column to permit comparison. Therefore, only sediment concentrations of BaP and BbF are compared. The estimated sediment BaP concentration in the segment 3 is close (4%) to the upper range of measured value but
<table>
<thead>
<tr>
<th>Chemical</th>
<th>Variable</th>
<th>1</th>
<th>Segment</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lindane (γ-HCH)</td>
<td>Water (μg/L)</td>
<td>measured</td>
<td>0.07</td>
<td></td>
<td>0.90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>0.12</td>
<td></td>
<td>0.82</td>
</tr>
<tr>
<td></td>
<td>Sediment (ng/g)</td>
<td>measured</td>
<td>1.5</td>
<td>0.7 - 2.0</td>
<td>3 - 14</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>1.57</td>
<td></td>
<td>16.1</td>
</tr>
<tr>
<td>α-HCH</td>
<td>Water (μg/L)</td>
<td>measured</td>
<td>0.36</td>
<td></td>
<td>0.90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>0.11</td>
<td></td>
<td>0.87</td>
</tr>
<tr>
<td></td>
<td>Sediment (ng/g)</td>
<td>measured</td>
<td>1.2</td>
<td>2 - 10</td>
<td>2 - 23</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>1.71</td>
<td></td>
<td>20.6</td>
</tr>
<tr>
<td>Benzo(a)pyrene</td>
<td>Water (μg/L)</td>
<td>measured</td>
<td>-</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>0.017</td>
<td>0.023</td>
<td>0.027</td>
</tr>
<tr>
<td></td>
<td>Sediment (ng/g)</td>
<td>measured</td>
<td>12</td>
<td>14</td>
<td>13 - 132</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>16.8</td>
<td>29.7</td>
<td>128</td>
</tr>
<tr>
<td>Benzo(b)fluoranthene</td>
<td>Water (μg/L)</td>
<td>measured</td>
<td>-</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>0.018</td>
<td>0.024</td>
<td>0.026</td>
</tr>
<tr>
<td></td>
<td>Sediment (ng/g)</td>
<td>measured</td>
<td>17</td>
<td>14</td>
<td>12 - 172</td>
</tr>
<tr>
<td></td>
<td></td>
<td>estimated</td>
<td>21.1</td>
<td>37.9</td>
<td>188</td>
</tr>
</tbody>
</table>
model overestimated the values by 30% and 53% in segment 1 and 2 respectively. Similarly, for BbF, sediment concentrations are overestimated by 20% and 63% in segment 1 and 2 respectively whereas, it is close (within 9%) to the upper range of measured value in segment 3.

Given the circumstances, there is a reasonable correspondence between predicted and measured values. Considering the limitations inherent in the present model and the margin of error associated with sampling and modelling of such a highly variable system, the results suggest that the models developed here can adequately simulate concentrations in these aquatic systems and can be used for other chemicals.

4.2 Presentation of environmental fate results

The details of environmental fate, transport and behavior of modelled chemicals in both the lakes are described through results of model simulations. The results of steady-state calculations are presented in the segment mass balance figures (Figures 4.1, 4.2, 4.4, 4.5, 4.7 and 4.8). The overall mass balances are shown in Figure 4.3, 4.6 and 4.9.

4.2.1 Nainital Lake

Pb and Cu

The segment mass balance for Pb and Cu are shown in Figure 4.1 and 4.2 respectively. The behaviour and transport of these chemicals in the lake are similar as both have similar physical-chemical properties. Because of high particle-water partition coefficient ($K_p$) values, combined with high deposition rate in the lake, the $D$ value for sediment deposition is very large; their behaviour is, therefore, very much dominated by the tendency to deposit with suspended particulate matter that finally sinks to the bottom of the lake. The chemical's equivalences in water and in sediment are similar while $Z$ values for bulk sediment ($Z_{ST}$) is considerably higher than $Z$ value for bulk water ($Z_{WT}$), rendering high concentrations in sediments.
Figure 4.1: Mass Balance for Pb transport (rates in kg/year)

Figure 4.2: Mass Balance for Cu transport (rates in kg/year)
The majority of the lead enters in segment 1 (north basin) through direct discharges (79%) and non-point sources such as municipal/ anthropogenous discharges and surface run off from the catchment (19%). The contribution from atmospheric deposition is not significant (0.1 to 0.3%) in any of the segments. Sediment burial is the dominant removal process which accounts for 78% of the total input in this segment. The remaining 22% is advected down to segment 2. Segment 1, which receives the largest amount of chemical loadings, acts as a reservoir for about 43% of total lead discharged to the lake and has the highest concentrations in water and sediment. Segment 2 also receives most of its inputs from direct discharges (58%). The remainder comes from municipal/surface run offs (10%), inflow from adjacent segments (31%). Burial is again the dominant removal process in this segment responsible for 56% of total input. Almost 44% is removed via advective transport to adjacent segments. Segment 3 receives significantly large inputs of lead (69%) from advective transport of segment 2, followed by direct discharges (31%). Approximately 52% of incoming lead left the lake by the outflow to downstream Balia River. Loss via burial accounts for only 45%. This segment has the lowest chemical loadings and consequently, it has lowest concentrations in water and sediment.

For Copper, D values for all the removal processes are of comparable magnitude to those for lead. Therefore, percent removal by each process and the fate results for Cu are very much the same as discussed above for Pb. The slight differences in some processes are due to difference in Kp values for Cu.

The overall mass balance are shown in Figure 4.3 (a) and (b). The results suggest that approximately 935 kg lead and 165 kg copper enter the lake Nainital annually. A major portion comes from direct discharges of small scale industries and laboratories around the lake. Almost 85% of the chemicals are buried into the deeper layer of sediments and the remainder 15% leaves the lake by the outflow to the downstream river. There were no losses via volatilization or degrading reactions. Owing to their high Kp values and the high deposition rates, majority of the chemicals are present in the sediment. Consequently, the residence time in sediment, which is calculated as the ratios of amount in
Figure 4.3: Overall Mass Balance for (a) Pb and (b) Cu transport (rates in kg/year)
each compartment (kg) to the input into each compartment (kg/year), is relatively much longer (about 785 days) than the residence time in water (about 165 days). The overall residence time is approximately 3.70 years (1350 days). The results of sensitivity analysis indicates that with declining emissions, the water column will clear of chemicals rapidly due to large sediment deposition fluxes as long as there is no substantial resuspension. The results suggest that Nainital Lake acts as a major reservoir for these metals. Similar implication has been indicated in a recent investigation by Das et al. (1994) who analyzed core sediment samples and assessed the sources of metal contamination in the lake. Their studies indicated that the lake sediment is a common sink for a large part of anthropogenically derived heavy metals due to high sediment accumulation rate. This situation is also very similar to that of another famous Himalayan lake (Dal Lake) in Kashmir region of India where high levels of heavy metals have been recorded in water and sediments as a result of anthropogenic activities and dumping of garbage/municipal wastes including some industrial discharges (Govardhan, 1989).

4.2.2 Rihand Reservoir

HCHs

The physical-chemical properties of the two isomers of hexachlorocyclohexane are alike and thus their environmental fate in the aquatic environment, as shown in Figure 4.4 and 4.5, are similar. Relatively high Henry's law constants of HCHs results in removal by evaporation and subsequent long range transport. Due to their hydrophobic character, the Z values for sediment solids and water particles are much higher than Z value for water (\(Z_{w}\)). The fugacities of HCHs in water and in sediment are comparable and since \(Z_{ST}\) is larger than \(Z_{WT}\), the concentration of the chemical in bulk sediment (i.e. \(Z_{ST}f_{S}\)) is expected to be significantly higher than its concentration in water (i.e. \(Z_{WT}f_{w}\)).

Environmental pathways of HCHs are generally similar in all the segments except that some removal processes are slightly more significant (in terms of kg/year) in segment 2, which has largest in area. Most of the chemical introduced into segment 1 enters via riverin inflow which accounts for 94% of the total input (Figure 4.4 and 4.5). The other sources of loading
Figure 4.4: Mass Balance for lindane (γHCH) transport (rates in kg/year)

Figure 4.5: Mass Balance for αHCH transport (rates in kg/year)
are the atmosphere and inflow from adjacent segments. The inter-segment D values for water and water particles are large as evidenced by the prominent rate of chemical transport by advection. About 50-60% of the chemical is advected down to adjacent segments. The D value for water transformation has the highest magnitude amongst the intra-segment transport for both chemicals thus it is also an important removal process. About 33-40% of the chemical input is removed via degradation reaction in each water column. Despite the chemicals' high affinities for sediment solids, the D values for deposition and water-sediment transfer are much smaller than the D value for advection and water transformation, and only 4-5% of the total input enter the sediment of each compartment. For chemical present in sediment, a substantial amount (70-80%) re-enters the water column via sediment resuspension or sediment-water diffusion while only a small fraction (6 to 15%) is buried and transformed by reactions. The D value for water-air diffusion is relatively low, therefore, volatilization removes only 1.3-3.4% of the total input from each segment. Volatilization rates are slightly higher for α-HCH since its Henry's law constant is little greater than that of γ-HCH. Segment 1 has the lowest concentration of HCH as it receives comparatively a small fraction of chemical loading (5%) from backflow. The increase in area of segment 2 and a subsequent increase in intra-segment D values results in slightly more significant removal by water transformation (40%), water to sediment transfer (5%) and volatilization (2-3.5%). Segment 3, being an industrial discharge zone, has the highest chemical loadings mainly from point source. Consequently, it has the highest concentrations as well as amounts of HCHs in both water and sediment, accommodating up to 73% of the chemicals in the system. Despite having the lowest D value for water and water particles outflow in segment 3 amongst inter-segment D values, the advective transport to downstream river is relatively quite high due to the largest fugacity in this segment and hence the downstream Rihand river is subjected to a considerable source of contamination.

The overall mass balance for γ and α-HCH (Figure 4.6 (a) and (b) respectively) suggest that there is a total annual input of 7660 kg lindane and 8150 kg α-HCH to Rihand reservoir, of which 85% originates from direct industrial discharges and the remaining 15% from riverine inflow. Advective transport is the dominant removal process, accounting for approximately
Figure 4.8: Overall Mass Balance for lindane (a) and αHCH (b) transport (rates in kg/year)
54% of the total input. Loss via reactions in water and sediment together is also quite significant, removing about 43% of chemicals. The remaining 3-5% is lost mostly by volatilization, and very little is buried into bottom sediments. Owing to their hydrophobic nature, high water particle concentration and large water volume, a majority of HCHs are present in the water column. Consequently, the residence time in water is relatively long (about 150 days). Due to the much smaller volume of sediment combined with fast chemical removal from it through reactions, resuspension and burial, a relatively much lower proportion of chemical is within the sediment. Therefore, the residence time of about 91 days in sediment is relatively short. The overall residence time of HCHs in the reservoir is estimated to be about 159 days.

**PAHs**

The BaP and BbF mass balances for Riband reservoir are illustrated in Figure 4.7 and 4.8 respectively. Both chemicals demonstrate similar environmental behaviour as expected from their similar structure and hence their properties. Because of the high K_{OW}'s, their behavior is dominated by a strong tendency to deposit with aerosol and suspended aquatic matter that finally sinks to the bottom of the reservoir. The chemical's fugacities in water and in sediment are again similar while Z values for bulk water (Z_{WT}) are considerably smaller than Z values for bulk sediment (Z_{ST}), causing high concentrations in sediment. In contrast to HCHs, PAHs have various point source loadings into each segment due to industrial emissions from power plants, aluminum smelters and carbon black producers etc. However, direct discharges in segment 3 are considerably higher than in other segments because the large number of chemical industries are located in this region. BbF levels, being slightly higher than BaP in emitted effluents, results in comparatively higher point source emissions.

The atmosphere appears to be an important source of PAH loadings for all segments. There is a significant deposition from the atmosphere in segment 1, accounting for almost 90% of total loadings. The remainder comes from river input (2.2%), direct emissions (1.8%), and inflow from adjacent segment (5.2%). It should be noted that part of the river-transported PAHs may have been originally atmospheric in origin, deposition of them in the catchment area
Figure 4.7: Mass Balance for BaP transport (rates in kg/year)

Figure 4.8: Mass Balance for BbF transport (rates in kg/year)
of the reservoir would precede eventual leaching to the marine environment. Sediment burial is the dominant removal process. About 70% of chemical input is eventually buried. Advection of dissolved and particulate PAHs into downstream segments is also quite significant, representing about 40% of chemical input. This is likely a reflection of the chemical’s hydrophobic nature and its high affinity for sediment and water particles. Water and sediment transformation accounts for 10-13% and 8% respectively. Segment 1, being relatively smaller in volume and receiving lowest amount of loadings amongst other segments, accommodates only 15% of the total amount of PAHs present in Rihand. Consequently, the PAH concentration in water and sediment are lowest in this segment.

Segment 2 also receives the majority of its input from atmospheric deposition (70%). The advective transport from adjacent segments is also significantly large representing about 27% input. The contribution from point source discharge and river input are almost insignificant. The segment 3 i.e. north-west sector of the reservoir which is the discharge zone of Hindalco, Hi-tech Carbon, Kanoria Chemicals and a power plant, has relatively large contributions from direct emissions, accounting for approximately 42-50% of total loadings. About 30% is via atmospheric deposition and the remaining 22 to 26% from advective transport from segment 2. Burial is again the dominant removal process in these segments, responsible for almost 57-67% of total input. Water transformation is approximately 7-15% while sediment transformation is relatively higher in segment 3, accounting for about 24% removal. Significantly large advective transport (21-26%) of PAHs from segment 3 is a major source of pollution to downstream Rihand river. However, segment 3 which receives the largest amount of chemical loadings acts as a reservoir for about 50% of total PAHs and has the highest amount as well as concentrations both in water and sediment.

Overall mass balances for BaP and BbF are depicted in Figure 4.9 (a) and (b) which indicate that approximately 887 kg BaP and 1055 kg BbF enter into the reservoir on an annual basis. A major portion (67 to 73%) is contributed from atmospheric deposition. A closer inspection shows that major atmospheric deposition processes are wet and dry deposition of aerosol-associated PAHs. Emission from point source discharges are approximately 26 to 31%
Figure 4.9: Overall Mass Balance for (a) BaP and (b) BbF transport (rates in kg/year)
while river input contributions are almost insignificant. The net flux of 611 kg BaP and 801 kg BbF between water and surface sediments is also downwards and major processes are deposition and resuspension. Almost 50% of the PAHs are buried into the deeper layer of sediments and a significant amount (33-37%) is transformed by reactions, particularly in sediment compartment. Removal by degradation reactions is specifically important in segment 3 where most of the chemical is present. Almost 12 to 15% of chemicals are advected downstream to Rihand river as PAHs sorbed to water particles are transported downstream by the high current at the dam. However, there is no net removal by evaporation mainly because of low volatility and high concentration of PAHs in air. The overall pattern of PAHs transport in the Rihand ecosystem is thus a downward flux from the atmosphere to the water and to the surface sediment, and finally to the deep sediment. This implies that Rihand reservoir acts as a sink for PAHs; this situation is very similar to those of the St. Lawrence River (Pham et al., 1993) and the Saguenay Fjord system (Lun, 1995) in Quebec as well as Hamilton harbor (Diamond and Mackay, 1993) in Ontario, where high release of PAHs related to intense industrial activities along the shores, have contributed to the contamination of sediments and deterioration of water quality.

The models described above successfully outline the general behaviour of selected chemicals in Indian aquatic systems by identifying the major environmental pathways. When judging the accuracy and precision of the simulation it is important to bear in mind the simplifications and assumptions made by the model such as assuming the steady-state conditions and ignoring the spatial and temporal variability in the system. Assumption of homogeneity in the entire system is also far from reality. There is also a considerable approximation implied in assuming a constant emission of a chemical from a point source discharge which could be highly variable with time.

4.3 Data availability and model applications

Models are useful as regulatory tools which enable loadings to be translated into corresponding ecosystem concentrations. However, there are several other advantages of using such a model beyond obtaining a comprehensive picture of the behavior of these persistent
chemicals in the lakes. These are indicated in the following three situations that are generally encountered in actual practice.

(1) All data available

Though it is rare, there are situations where all the information needed for the modelling purposes is available, i.e. good emission and concentration data are available. These data are not just estimates but are actual measurements from periodic monitoring and sampling. In this case modelling results would not only aim for assessing the model validity i.e. agreement between modelled and measured concentrations, but also raise some question or doubt about suspected measured data or vice versa. It may be necessary to repeat or perform some more experimental measurements in situations where there is a large discrepancy between estimated and measured data. Moreover, the model would give insight into various transport processes that subsequently determines which area should be studied further or examined in more detail during monitoring programs. This is analogous to the model used for understanding HCH behavior in Rihand reservoir.

(2) Emission data - not completely available

Information on direct releases are non-existent in most cases. Sometimes even the exact sources are also not known. Estimation of exact loadings then becomes an extremely difficult task. However, an estimate can be made which is based on some loading assessment; for example, calculation of the discharge rate using production data of various industries and the emission factors. This case has already been discussed in the previous section while examining PAHs behavior in Rihand. Despite knowing the number of sources of PAHs into the reservoir, there was no clear cut information on effluent flow rates or the chemical concentration in the discharges so that some estimation of total discharge could be made. The loadings were, therefore, calculated from available data on production and emission factors. The estimated concentration levels are then compared with the reported values of concentration in each phase. In case of disagreement between these, there could be a need to reexamine the production data from the industries or even identify the exact sources and possibly quantify them.
(3) No data available

Having no information on either emissions or concentration is also very common. In such situations, model simulations can be made based on illustrative loadings (e.g. total loadings of 1000 kg/year) and hence the resulting concentrations can be estimated. In future, if emissions or concentrations are experimentally measured, actual concentrations/or emissions can be predicted by extrapolation or interpolation and can be similarly applied to other chemicals. This has been discussed in the following section and illustrated by the examples.

4.4 Novel and simple approaches for estimating concentrations in aquatic systems

Two simple approaches are suggested:

(1) A loading-concentration model

The model results show that there is a distinct chemical-specific relationship between the total loadings and prevailing steady-state concentrations. Since the equations inherent in the model are linear, this overall relationship is linear. The model was run for both lakes for all chemicals for illustrative total inputs (atmospheric, effluents, river inflow) of 1000 kg/year. The concentrations in water and sediments were calculated and are presented in Table 4.3. This table can be used to deduce the potential benefits of reducing emissions. For example the current emissions of lindane to Rihand reservoir are 6500 kg/year and yield a concentration of 0.12 to 0.82 µg/L in water and 1.57 to 16.1 ng/g in sediment. The data in Table 4.3, if proportioned to 6500 kg/year give values of 0.39 µg/L in water and 10.5 ng/g in sediment, which is in satisfactory agreement with the concentrations predicted by the QWASI model. If it is decided that a desirable objective for lindane water concentration in the reservoir is 0.10 µg/L which is the Indian standard for potable water, the emissions would have to be reduced to about 1666 kg/year. It is also interesting to note that concentrations in water and sediment (Table 4.3) increase from dichlorobenzene to hexachlorobenzene i.e. from less to more hydrophobic compounds.

These calculations involve no knowledge of the details of the model, but they do use the results of the model. This may be valuable for regulatory agencies.
Table 4.3: Steady-state concentrations resulting from input of 1000 kg/year

<table>
<thead>
<tr>
<th>Substances</th>
<th>Lake Water concentration (μg/L)</th>
<th>Lake Sediment concentration (ng/g)</th>
<th>Rihand Water concentration (μg/L)</th>
<th>Resevoir Sediment concentration (ng/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>lead</td>
<td>1.16</td>
<td>247000</td>
<td>0.003</td>
<td>753</td>
</tr>
<tr>
<td>copper</td>
<td>1.09</td>
<td>248000</td>
<td>0.002</td>
<td>754</td>
</tr>
<tr>
<td>1,4-dichlorobenzene</td>
<td>1.52</td>
<td>192</td>
<td>0.013</td>
<td>0.12</td>
</tr>
<tr>
<td>1,2,3,5-tetrachlorobenzene</td>
<td>1.85</td>
<td>5530</td>
<td>0.018</td>
<td>8.95</td>
</tr>
<tr>
<td>pentachlorobenzene</td>
<td>1.87</td>
<td>14800</td>
<td>0.019</td>
<td>27.5</td>
</tr>
<tr>
<td>hexachlorobenzene</td>
<td>1.81</td>
<td>71100</td>
<td>0.021</td>
<td>159</td>
</tr>
<tr>
<td>lindane (γ-HCH)</td>
<td>7.38</td>
<td>2350</td>
<td>0.060</td>
<td>1.63</td>
</tr>
<tr>
<td>α-HCH</td>
<td>7.03</td>
<td>2500</td>
<td>0.060</td>
<td>1.96</td>
</tr>
<tr>
<td>benzo(a)pyrene</td>
<td>1.81</td>
<td>11000</td>
<td>0.019</td>
<td>158</td>
</tr>
<tr>
<td>benzo(b)fluoranthene</td>
<td>1.27</td>
<td>12700</td>
<td>0.017</td>
<td>187</td>
</tr>
</tbody>
</table>
(2) A second simple model applicable to many chemicals

The success of the QWASI model suggests that it may be feasible to derive a very simple "first order" or "screening" model which could be applied to a variety of chemicals with minimal data requirements. This model is derived using the fugacity approach but can be applied using conventional partition coefficients. The derivation follows.

The overall results show that generally fugacity in sediment is higher than in water by a factor of 2. If, however, it is assumed that the sediment and water reach equal fugacities (f), the overall mass balance equation is:

\[ E = f \sum D = f (D_r + D_x + D_T + D_w + D_s + D_b) \]  \hspace{1cm} (1)

where the D values are defined earlier in Table 2.2. Substituting \( C_W Z_W \) for \( f \) and the equations in Table 2.2 for D values, it can be shown that:

\[ E = C_W (k_v A + G_X + G_T K_{PW} + 0.7 V_w / \tau_w + 0.7 V_w \phi_S K_{SW} / \tau_S + U_B A \phi_S K_{SW}) \]  \hspace{1cm} (2)

where

- \( E \) = emission rate (g/h)
- \( C_W \) = concentration in water (g/m³)
- \( k_v \) = water side evaporation mass transfer coefficient (m/h) and is given by
  \[ 1 / k_v = 1 / k_w + 1 / K_{AW} k_A \]
- \( k_w \) and \( k_A \) are the water and air side mass transfer coefficients and \( K_{AW} \) is the air-water partition coefficient.
- \( A \) = lake surface area (m²)
- \( G_X \) = flow rate of water from the lake (m³/h) = \( V_w / \tau_R \) where \( \tau_R \) is the water residence time (h)
- \( V_w \) is the water volume (m³)
- \( G_T \) = flow rate of particles from the lake (m³/h) and can be estimated from \( G_X \) and the particle concentration in the outflow water
- \( \tau_w \) and \( \tau_S \) = transformation half lives in water and sediment (h) respectively
\[ U_b = \text{burial velocity of the bulk sediment (m/h)} \]
\[ \phi_S = \text{volume fraction of solids in the sediment} \]
\[ K_{SW} = \text{sediment-water partition coefficient} \]

From the above equation, \( C_W \) can be calculated, followed by \( C_S \) as \( C_W K_{SW} \). Most of these quantities are fairly readily available. The chemical-specific quantities are \( K_{AW} \), \( K_{PW} \), \( K_{SW} \), \( \tau_W \) and \( \tau_S \), for which estimation methods are available (e.g. Lyman et al., 1982).

To test this simple model it was programmed in GW BASIC and run for both lakes with inputs of 1000 kg/year i.e. 114 g/h. The results obtained for all chemicals in both lakes are compared with the QWASI model results in Figure 4.10. The plots of log \( C_W \) and log \( C_S \) for simple vs. QWASI exhibit good linearity with correlation coefficients of 0.99 and 0.98 respectively. The mean deviations in log \( C_W \) and log \( C_S \) are 0.09 and 0.20 units, corresponding to a factor of 1.23 and 1.58 respectively. The use of this simple model in estimating loading reductions can be explained again with the example of lindane in Rihand Reservoir. The current emission of 6500 kg lindane /year to the reservoir yield a water concentration of 0.12 to 0.82 \( \mu \text{g/L} \). The data for this model, if proportioned to 6500 kg/year gives value of 0.40 \( \mu \text{g/L} \) in water, which is in satisfactory agreement with the concentrations predicted by the QWASI model. Again, if the desirable objective for lindane water concentration in the reservoir is 0.10 \( \mu \text{g/L} \), the emission would have to be reduced to 1625 kg/year. It is suggested that this simple model be used for screening purposes to give a rapid mass balance estimate of concentrations in water and sediment and to explore the benefits of loading reductions.

4.5 Implications for better management of emissions

The models suggest that water quality in these aquatic systems is primarily controlled by the current contaminants input. Since the persistence of the chemicals in the system is relatively short, it seems likely that present contamination is the result of quite recent discharges. Changes in chemical loadings, not surprisingly, greatly influence the water and sediment concentrations. The results of the sensitivity analysis indicate that doubling the point source loadings almost doubles the concentrations while halving the loadings reduces the water and
Figure 4.10: Logarithm of (a) water and (b) sediment concentration for Simple vs. QWASI models
sediment concentrations to almost half of the current values. This suggests priorities for contaminant control measures. It is, of course, possible that some of the sediment is actively mixed by storms, dredging and shipping activities, exposing deeper and more contaminated sediments to the water column. If the sediment is left relatively undisturbed, water quality should respond fairly rapidly to any changes in inputs.

4.5.1 Remedial Strategies

The remedial action should be directed to (1) reduce current loadings (2) dredge or isolate the sediments in case of high contaminant concentration in local areas (3) leave the sediment undisturbed, if possible enhance burial. It is beyond the scope of this thesis to suggest remedial strategies in detail, but some examples are given below for Rihand Reservoir to illustrate the approaches which could be taken.

(1) The results suggest that the principal contamination source of HCHs are land based, mainly the discharges of liquid effluents from the pesticide plant, which should be the primary target for control to improve the water quality.

(2) For PAHs, majority of chemical enters via atmospheric deposition of PAHs bearing particulates. Therefore, the efforts should be directed to minimize the air emissions that are generated during combustion of coal in power plants. If possible, use of anthracite coal should be preferred to reduce high molecular weight PAHs.

(3) Industries located in north-west sector of the reservoir such as aluminum, chlore-alkali, carbon black plan etc. are identified as major sources of air borne as well as land based PAHs. Thus, efforts should be made to reduce and control the emissions from these plants.

(4) A redesign or replacement of appropriate process technology should be considered where ever it is possible; for example, in case of aluminum plants, prebake anode technology generates far less PAHs than the Söderberg anode process and similarly, the use of fluidized-bed boilers allows less generation of particulates and PAHs in thermal power plants.
5. CONCLUSIONS

(1) The octanol-water partition coefficients ($K_{OW}$) and their temperature dependence over the range 5 to 45 °C have been determined for selected chlorobenzenes with greater accuracy than previously.

(2) The values of log $K_{OW}$ at 25 °C range from 3.23 for 1,4-dichlorobenzene to 5.46 for hexachlorobenzene; the enthalpy of phase change ranges from 17 kJ/mol for 1,4-dichlorobenzene to 24 kJ/mol for hexachlorobenzene.

(3) Tricaprylin appears to be a better surrogate for lipids than 1-octanol. It is a triglyceride and, therefore, similar to fish and other lipids. The mutual solubilities of tricaprylin and water are less than for the 1-octanol/water system. In addition, tricaprylin has a lower vapor pressure than octanol. The odor associated with 1-octanol is not a problem in case of tricaprylin.

(4) The values of log $K_{TW}$ at 25 °C range from 3.56 for 1,2-dichlorobenzene to 5.59 for hexachlorobenzene; the enthalpy of phase change ranges from 9.7 kJ/mol for 1,2-dichlorobenzene to 16 kJ/mol for hexachlorobenzene.

(5) Tricaprylin is superior to triolein as a lipid surrogate. The tricaprylin-water partition coefficients for the chlorobenzenes are similar to the literature values reported for the triolein/water system. However, tricaprylin is easier to purify than triolein and because of its lower molar mass, passes easily through gas chromatographic columns, unlike triolein.

(6) The water quality mass balance models were developed and successfully applied for lead, copper, lindane, $\alpha$-HCH, benzo(a)pyrene, and benzo(b)fluoranthene in two Indian lakes.
(7) Model results were partially validated and environmental fate, transport, and behaviour of the chemicals have been described through results of model simulations. This improved the understanding of the chemicals fate in the Indian lakes, for which some remedial strategies are suggested.

(8) Two other simple and novel modelling approaches were developed; these simple models may be used for screening purposes to give rapid mass balance estimates of water and sediment concentrations as well as to explore the benefits of loading reductions.
6. RECOMMENDATIONS

(1) The octanol-water partition coefficients (K_{OW}) and their temperature dependence should be determined for other class of compounds. This will contribute to the existing data base on temperature dependence and can be important to more accurate modelling of the fate and behaviour of these chemicals.

(2) In case of tricaprylin, the results should be further evaluated and clarified with more compounds and intensive experimental work that would permit more critical analyses of the linearity in plots of log K_{TW} vs. log K_{OW}.

(3) Further studies are required to determine the relationship between log K_{TW} and (lipid-based) BCF and examine whether the correlation of log BCF with log K_{OW} will be statistically different from that of log BCF with log K_{TW}.

(4) Studies should also be conducted to measure the solubility of chlorobenzenes in tricaprylin so that values of the ratio of chemical solubility in tricaprylin to solubility in water can be compared with the actually determined tricaprylin-water partition coefficients from this study.

(5) Tricaprylin-air partition coefficients (K_{TA}) should also be measured and compared to recently available octanol-air partition coefficients (K_{OA}).

(6) Investigations on the suitability of other lipid surrogate such as methyl esters derived from triglycerides should also be the subject of future studies.

(7) The water quality models should be further applied and validated for more chemicals in some other tropical lakes and rivers such as Bhopal Lake, Hussainsagar Lake, lakes of Jaipur and the Ganges River.
(8) The unsteady-state model should also be developed to examine the effects of temporal and spatial variations in parameters such as chemical loadings, hydrological and limnological conditions, and seasonal changes in the lake.
7. REFERENCES


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Appendices

Appendix A: Computer program listing of QWASI and Simple models for Rihand Reservoir and Nainital Lake.

Appendix B: Calibration plots and calculations for octanol-water and tricaprylin-water partition coefficients.

Appendix C: Sensitivity Analysis
Appendix A: Program listing of QWASI model for Rihand Reservoir

5 REM QMULT : MULTI-PURPOSE QWASI MODEL FOR UP TO 9 SEGMENTS
7 REM application to Rihand Reservoir
10 REM PART 1 SET COMPUTING VARIABLES
20 DIM HS(20),Y(20,9),D(10,10),P$ (20),DP(12,12)
30 REM Nomenclature Conventions
40 LPRINT CHR$(15)
50 WIDTH "lptl:",160
55 N=3 'Number of segments
60 REM Define segment names
70 NS(1)="South basin"
80 NS(2)="Middle basin"
90 NS(3)="North-west basin"
100 NS(4)="Fourth section"
110 NS(5)="Fifth section"
120 NS(6)="Sixth section"
130 NS(7)="Seventh section"
140 NS(8)="Eighth section"
150 NS(9)="Ninth section"
160 REM
170 REM Identify processes
180 PS(1)="Sediment burl"
190 PS(2)="Sediment trnf"
200 PS(3)="Sediment resn"
210 PS(4)="Sedt-watr difn"
220 PS(5)="Sedt depn"
230 PS(6)="Water transf"
240 PS(7)="Water-air dif"
250 PS(8)="Atmos depson"
260 PS(9)="(Rain diss)"
270 PS(10)="(Wet pt depn)"
280 PS(11)="(Dry pt depn)"
290 REM PART 2 DIMENSIONS AND PROPERTIES OF THE AQUATIC SYSTEM
300 REM Segment Dimensions
309 REM AW(I) is water area m2
310 AW(1)=148800000# : AW(2)=199900000# : AW(3)=116300000# : AW(4)=8000000!
329 REM HW(I) is water depth m
330 HW(1)=20 : HW(2)=22 : HW(3)=25 : HW(4)=10
340 HW(5)=15 : HW(6)=10 : HW(7)=10 : HW(8)=10 : HW(9)=10
349 REM HS(I) is sediment depth m
350 HS(1)=.02 : HS(2)=.02 : HS(3)=.02 : HS(4)=.022
360 HS(5)=.03 : HS(6)=.011 : HS(7)=.03 : HS(8)=.01 : HS(9)=.01
370 FOR I = 1 TO N
380 AS(I)=AW(I) 'Sediment areas m2
390 VW(I)=AW(I)*HW(I) 'Water volumes m3
400 VS(I)=AS(I)*HS(I) 'Active sediment volumes m3
410 NEXT I
415 RAIN=.2 'rain rate m/year
420 REM Phase densities (kg/L or g/cm3)
430 DENW=1: DENQ=1.5
440 DENP(1)=1.8: DENP(2)=2: DENP(3)=21: DENP(4)=21
450 DENP(5)=2: DENP(6)=2: DENP(7)=21: 'Suspended particles
460 DENP(8)=2: DENP(9)=2
470 DENS(1)=1.8: DENS(2)=2: DENS(3)=21: DENS(4)=21
480 DENS(5)=2: DENS(6)=2: DENS(7)=2 'Sediment solids
485 DENS(8)=2: DENS(9)=2
490 ORGP(1)=.1: ORGP(2)=.1: ORGP(3)=.15: ORGP(4)=.2
500 ORGP(5)=.2: ORGP(6)=.2: ORGP(7)=.2
501 ORGP(8)=.2: ORGP(9)=.2: 'Organic content of particles
510 ORGS(1) = .07: ORGS(2) = .08: ORGS(3) = .1: ORGS(4) = .1
520 ORGS(5) = .1: ORGS(6) = .1: ORGS(7) = .1
521 ORGS(8) = .2: ORGS(9) = .2: 'Organic content of sediment

530 REM Particle Concentrations
540 VFQ = 1.1E-10: 'Vol Fraction of Aerosols
541 CPF = VFQ * DENQ * 10^-12 'Concentration Aerosols, ug/m3
550 VFS(1) = .07: VFS(2) = .07: VFS(3) = .07: VFS(4) = .07: VFS(5) = .07: VFS(6) = .07: VFS(7) = .07: VFS(8) = .07: VFS(9) = .07 'Volume fraction of sediment solids
570 CSP(1) = 95: CSP(2) = 82: CSP(3) = 19: CSP(4) = 51: CSP(5) = 5: CSP(6) = 5: CSP(7) = 5: CSP(8) = 5: CSP(9) = 5 'Suspended solids concentration in water g/m3 or mg/L
590 FOR I = 1 TO N+1
600 VFP(I) = CSP(I) / (DENP(I)*10^6) 'Vol fraction of suspended particles
620 GH(I) = RAIN*AW(I) / 365 / 24 'Rain rates m3/h from rate in m/year
630 GI(I) = 0: GX(I) = 0
640 NEXT I
660 FOR I = 1 TO N+1
670 FOR J = 1 TO N+1
680 GW(I, J) = 0: GP(I, J) = 0
690 NEXT J
700 NEXT I
705 REM Water inflow rates by rivers and runoff m3/h
710 GI(1) = 5650000: GI(2) = 11800: GI(3) = 1100
720 GI(4) = 0: GI(5) = 0: GI(6) = 0
722 GI(7) = 0: GI(8) = 0: GI(9) = 0
725 GI(7) = 500000: GI(8) = 400000: GI(9) = 1000000
730 REM Set water exchange rates m3/h
740 GW(2, 1) = 1*GI(1): GW(3, 2) = 1*(GI(1) + GI(2)): GW(4, 3) = 0*(GI(1) + GI(2) + GI(3))
760 GW(1, 2) = GI(1) + GW(2, 1)
780 GW(2, 3) = GI(2) + GW(1, 2) + GW(3, 2) - GW(2, 1)
790 GW(3, 4) = GI(3) + GW(2, 3) + GW(4, 3) - GW(3, 2)
800 GW(4, 5) = GI(4) + GW(3, 4) + GW(5, 4) - GW(4, 3)
810 GW(5, 6) = GI(5) + GW(4, 5) + GW(6, 5) - GW(5, 4)
820 GW(6, 7) = GI(6) + GW(5, 6) + GW(7, 6) - GW(6, 5)
821 GW(7, 8) = GI(7) + GW(6, 7) + GW(8, 7) - GW(7, 6)
822 GW(8, 9) = GI(8) + GW(7, 8) + GW(9, 8) - GW(8, 7)
830 REM Suspended Particle Flows (g/h)
840 FOR I = 1 TO N+1
850 FOR J = 1 TO N+1
860 GP(I, J) = GW(I, J) * VFP(I) 'Particle flows m3/h
870 NEXT J
880 NEXT I
890 REM Suspended Particle Fluxes g/m2/year
900 DEP(I) = 15: DEP(2) = 13: DEP(3) = 10
910 DEP(4) = DEP(3): DEP(5) = 5: 'Particle deposition rates g/m2/day
915 DEP(7) = 5: DEP(8) = 5: DEP(9) = 5 'Particle deposition rates g/m2/day
920 RES(I) = 1.2: RES(2) = 6: RES(3) = 2
925 RES(4) = RES(3): RES(6) = 2
930 RES(7) = 2: RES(8) = 2: RES(9) = 2 'Particle resuspension rates g/m2/day
940 BUR(I) = 6.5: BUR(2) = 4.7: BUR(3) = 2.5:
945 BUR(4) = BUR(3): BUR(5) = 2
950 BUR(7) = 2: BUR(8) = 2: BUR(9) = 2 'Particle burial rates g/m2/day
960 FOR I = 1 TO N
970 GD(I) = DEP(I) * AS(I) / 24 / DENP(I) * 1000000
980 GR(I) = RES(I) * AS(I) / 24 / DENS(I) * 1000000
990 GB(I) = BUR(I) * AS(I) / 24 / DENS(I) * 1000000
1000 NEXT I
1010 REM Atmospheric Deposition (m3/h)
1020 Q = 2000000 'Scavenging ratio
1030 VDEP=10 'Dry deposition velocity m/h
1040 FOR I = 1 TO N
1050 GC(I)=GM(I)*VFQ*Q
1060 GQ(I)=VDEP*AW(I)*VFQ
1070 GQT(I)=GQ(I)+GC(I)
1080 NEXT I
1090 REM PART 3 INPUT OF CHEMICAL PROPERTIES
1100 PRINT "There are two methods of entering chemical properties:
1110 PRINT "Method P is to enter physical chemical properties 
1120 PRINT "Method K is to enter partition coefficients 
1130 PRINT "Specify a chemical by entering one of the following:"
1140 PRINT "A chemical to be user-specified by method P: 1" 
1150 PRINT "A chemical to be user-specified by method K: 2"
1160 PRINT "A chemical previously specified: 3"
1170 PRINT "A chemical from the following list:"
1180 PRINT "Lead (K) 4, Copper (K) 5, Dichlorobenzene (P) 6, Tetrachlorobenzene (P) 7, Pentachlorobenzene (P) 8, Lindane (P) 10, Benzopyrene (P) 11, alpha-BCfI (P) 12, Benzofluoranthene (P) 13.
1190 INPUT QQ
1200 ON QQ GOTO 1220, 1520, 1910, 1630, 1635, 1320, 1325, 1330, 1335, 1336, 1337, 1338, 1339
1210 PRINT "INPUT CHEMICAL PROPERTIES ANY PREVIOUS VALUES IN PARENTHESES ( )
1220 PRINT "CHEMICAL NAME (preferably in CAPITALS):" INPUT CS
1230 PRINT "TEMPERATURE deg C (in; TC; )": INPUT TC
1240 PRINT "MELTING POINT deg C (for liquids input system temp above):" "TM; "": INPUT TM
1250 PRINT "MOLECULAR WEIGHT g/mol ("; WM; "): INPUT WM
1260 PRINT "WATER SOLUBILITY g/m3 ("; SOLY; "): INPUT SOLY
1270 PRINT "VAPOR PRESSURE Pa ("; VP; "): INPUT VP
1280 PRINT "LOG OCTANOL-WATER PARTITION COEFFICIENT KOW ("; LKOW; "): INPUT LKOW
1290 PRINT "DEGRADATION HALF LIFE IN SEDIMENT hours ("; TDS; "): INPUT TDS
1300 PRINT "DEGRADATION HALF LIFE IN WATER hours ("; TDW; "): INPUT TDW : GOTO 1340
1380 CS$="BENZO(b)FLUORANTHENE" : WM=252.32 : SOLY=.0015 : VP=1.5E-07 : LKOW=6.5 : TDS=350 : 000 : TDW=120000 : TC=25 : TM=168 : GOTO 1340
1390 REM chemical is specified by method P: PRINT " "
1350 'Adjust chemical properties
1360 TK = TC + 273 'temperature in degrees Kelvin
1370 TMX=TM+273
1380 R = 8.314 'gas constant
1390 FRAT=EXP(6.79*(1-TMX/TK))
1400 VPL=VP/FRAT 'subcooled liquid vapor pressure
1410 SOLM = SOLY/WM 'solubility (mol/m^3)
1420 H = VP/SOLM 'Henry's Law constant (Pa m^3/mol)
1430 KOW = 10^-LKOW 'octanol-water partition coefficient
1440 KDAS=H/RTK
1450 KDFW=.05*KOW
1460 KDQA=60000000/VPL
1465 KDQW=KDQA*KDAW
1470 FOR I=1 TO N+1
1480 KFPW(I)=.41*KOW*ORGP(I)
1490 KPSW(I)=.41*KOW*ORGS(I)
1500 NEXT I
1510 GOTO 1680
1520 PRINT "INPUT CHEMICAL PROPERTIES, ANY PREVIOUS VALUES IN PARENTHESES ( )"
1530 PRINT "CHEMICAL NAME (preferably in CAPITALS) (";CS;"): INPUT CS
1540 PRINT "TEMPERATURE deg C (";TC;"): INPUT TC
1550 PRINT "MOLECULAR WEIGHT g/mol (";WM;"): INPUT WM
1560 PRINT "PARTITION COEFFICIENTS ARE COMMON TO ALL SEGMENTS"
1570 PRINT "SEDIMENT-WATER PARTITION COEFFICIENT KPSW L/kg (";KPSW;"): INPUT KPSW"
1580 PRINT "PARTICLE-WATER PARTITION COEFFICIENT KPPW L/kg (";KPPW;"): INPUT KPPW"
1590 PRINT "AEROSOL-WATER PARTITION COEFFICIENT KDQW dimless (";KDQW;"): INPUT KDQW"
1600 PRINT "FISH-WATER PARTITION COEFFICIENT KDPW dimless (";KDPW;"): INPUT KDPW"
1610 PRINT "DEGRADATION HALF LIFE IN SEDIMENT hours (";TDS;"): INPUT TDS
1620 PRINT "DEGRADATION HALF LIFE IN WATER hours (";TDW;"): INPUT TDW : GOTO 1680
1630 CS="lead";WM=207 ;KDAW=1E-11;KPSWC=333000 ;KPPWC=668000 ;KDPW=9 ;KDQW=100
01;TDS=1E+11;TDW=1E+11;TC=15 ;KDQA=1E-11; GOTO 1640
1635 CS="Copper";WM=63.6 ;KDAW=1E-11;KPSWC=333000 ;KPPWC=1336000 ;KDPW=9 ;KDQW=100
01;TDS=1E+11;TDW=1E+11;TC=15 ;KDQA=1E-11; GOTO 1640
1640 FOR I=1 TO N+1
1650 KPSW(I)=KPSW
1660 KPPW(I)=KPPW
1670 NEXT I
1680 REM Calculate dimensionless partition coefficients
1690 TK=TC+273
1700 FOR I=1 TO N+1
1710 KDPW(I)=KPPW(I)*DENP(I)
1720 KDSW(I)=KPSW(I)*DENS(I)
1730 NEXT I
1740 PRINT "Reaction rate constants (h^-1)"
1750 KS = .693/TDS "sediment reaction rate constant
1760 KW = .693/TDW "water reaction rate constant
1770 REM PART 4 CALCULATION OF Z AND D VALUES AND RESPONSE TIMES
1780 REM Calculate equivalent Z values
1790 ZW = 1 "Z for water
1800 ZA = KDAW "Z for air
1810 ZF = KDFW "Z for fish
1820 ZQ = KDQW*ZW "Z for aerosol particles
1830 FOR I=1 TO N+1
1840 ZP(I) = KDPW(I) "Z for water particles
1850 ZS(I) = KDSW(I) "Z for sediment particles
1860 ZST(I)=ZW*(1-VFPS(I))+ZS(I)*VFPS(I) 'Z for bulk sediment
1870 ZWT(I) = ZW*(1-VFP(I))+ZP(I)*VFP(I) 'Z for bulk water
1880 NEXT I
1890 ZAT = ZA*(1-VFQ)+VFQ*ZQ 'Z for bulk air
1900 FRQ=VFQ*ZQ/(VFQ*ZQ+(1-VFQ)*ZA) 'Fraction of chemical on aerosol
1910 'Mass Transfer Coefficients (m/h)
1920 KVA = 1! 'volatilization: air side
1930 KW = .01 'volatilization: water side
1940 KV = KDAW/(KDAW/KV+1/KVA) 'overall water side
1950 KT = .0002 'sediment-water diffusion
1960 REM Calculation of process D values DP(J,I) and response times
1962 REM Subscript J refers to the process eg burial
1964 REM Subscript I refers to the segment  
1970 FOR I=1 TO N  
1980 DP(1,I) = GB(I) * ZS(I)  ' burial  
1990 DP(2,I) = VS(I) * ZST(I) * KS  ' sediment transformation  
2000 DP(3,I) = GR(I) * ZS(I)  ' sediment resuspension  
2010 DP(4,I) = KT * AS(I) * ZW  ' sediment-water diffusion  
2020 DP(5,I) = GD(I) * ZP(I)  ' sediment deposition  
2030 DP(6,I) = VW(I) * ZWT(I) * KW  ' water transformation  
2040 DP(7,I) = KV * AW(I) * ZW  ' volatilization  
2050 DP(9,I) = GH(I) * ZW  ' rain dissolution  
2060 DP(10,I) = GC(I) * ZQ  ' wet particle deposition  
2070 DP(11,I) = GGQ(I) * ZQ  ' dry particle deposition  
2080 DP(8,I)=DP(9,I)+DP(10,I)+DP(11,I)  
2090 NEXT I  
2100 FOR I = 1 TO N+1  
2110 FOR J = 1 TO N+1  
2120 DJ(I,J)=GW(I,J)*ZW  ' water flow  
2130 DQ(I,J)=GP(I,J)*ZP(I)  ' particle flow  
2140 D(I,J)=DJ(I,J)+DQ(I,J)  ' total flow  
2150 NEXT J  
2160 NEXT I  
2270 ' Calculate response times in years  
2280 FOR I=1 TO N  
2290 TYS(1,I)=VS(I)*ZST(I)/DP(1,I)/8760  
2300 TYS(2,I)=VS(I)*ZST(I)/DP(2,I)/8760  
2310 TYS(3,I)=VS(I)*ZST(I)/DP(3,I)/8760:TYS(3,I)=VW(I)*ZWT(I)/DP(3,I)/8760  
2320 TYS(4,I)=VS(I)*ZST(I)/DP(4,I)/8760:TYS(4,I)=VW(I)*ZWT(I)/DP(4,I)/8760  
2330 TYS(5,I)=VS(I)*ZST(I)/DP(5,I)/8760:TYS(5,I)=VW(I)*ZWT(I)/DP(5,I)/8760  
2340 TYS(6,I)=VW(I)*ZWT(I)/DP(6,I)/8760  
2345 IF DP(7,I)=0 GOTO 2360  
2350 TYS(7,I)=VW(I)*ZWT(I)/DP(7,I)/8760  
2360 TYS(8,I)=VW(I)*ZWT(I)/DP(8,I)/8760  
2370 NEXT I  
2380 REM PART 5 INPUT CHEMICAL QUANTITIES DATA  
2390 PRINT "INPUT CHEMICAL QUANTITIES, ANY PREVIOUS VALUES IN PARENTHESES ( )  
2400 PRINT "A chemical to be user-specified 1"  
2410 PRINT "Specify chemical quantities by entering one of the following"  
2420 PRINT "Chemical quantities as previously specified 2"  
2430 PRINT "Quantities specified for a chemical from the following list "  
2440 PRINT "Lead 3 ,Copper 4 ,Dichlorobenzene 5 ,Tetrachlorobenzene 6 ,Penta chlorobenzene 7 ,Hexachlorobenzene 8 ,Lindane 9 ,Benzopyrene 10 ,alph-HCH 11 ,Benzofluoranthene 12.  
2450 INPUT QQQ  
2460 ON QQQ GOTO 2600,2680,2480,2520,2535,2550,2565,2580,2592,2596,2600,2604  
2470 REM Discharge data  CIG(i) is concn in rivers g/m3,EPK(i) is kg/year point source  
2480 EPK(1)=450 :EPK(2)=250:EPK(3)=80 :EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)=1 :EPK(9)=2 'Point source discharges kg/year,Lead data  
2490 CIG(1)=.05 :CIG(2)=.05 :CIG(3)=.05 :CIG(4)=.0004:CIG(5)=0:CIG(6)=.0003 :CIG(7)=.001:CIG(8)=.003:CIG(9)=.0004' Concentrations in river inputs g/m3  
2500 CAN=.84 'Air concn ng/m3 go to 2680  
2510 GOTO 2680  
2520 EPK(1)=40 :EPK(2)=15 :EPK(3)=7 :EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)=1 :EPK(9)=2 'Point source discharges kg/year,Copper data  
2525 CIG(1)=.05:CIG(2)=.05 :CIG(3)=.05 :CIG(4)=.0004:CIG(5)=0:CIG(6)=.0003:CIG(7)=.001:CIG(8)=.003:CIG(9)=.0004' Concentrations in river inputs g/m3  
2530 CAN=.76 'Air concn ng/m3 go to 2680  
2531 GOTO 2680  
2535 EPK(1)=450 :EPK(2)=250:EPK(3)=80 :EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)=1 :EPK(9)=2 'Point source discharges kg/year,DicB data  
2540 CIG(1)=.05 :CIG(2)=.05 :CIG(3)=.05 :CIG(4)=.0004:CIG(5)=0:CIG(6)=.0003
<table>
<thead>
<tr>
<th>Concentrations in river inputs g/m³</th>
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<td>'Air concn ng/m³ go to 2680</td>
<td>GOTO 2680</td>
<td>EPK(1)=450</td>
<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, TetracB data</td>
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<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, HexaCB data</td>
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<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, Lindane data</td>
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<tr>
<td>CAN=.3</td>
<td>'Air concn ng/m³ go to 2680</td>
<td>GOTO 2680</td>
<td>EPK(1)=450</td>
<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, alpha-HCH data</td>
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<tr>
<td>CAN=.5</td>
<td>'Air concn ng/m³ go to 2680</td>
<td>GOTO 2680</td>
<td>EPK(1)=450</td>
<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, Benzo(a)pyrene data</td>
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</tr>
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<td>CAN=.84</td>
<td>'Air concn ng/m³ go to 2680</td>
<td>GOTO 2680</td>
<td>EPK(1)=450</td>
<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, Benzo(b)fluoranthene data</td>
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<td>GOTO 2680</td>
<td>EPK(1)=450</td>
<td>EPK(2)=250:EPK(3)=80:EPK(4)=1:EPK(5)=0:EPK(6)=31:EPK(7)=0</td>
<td>EP K(8)=1:EPK(9)=2 'Point source discharges kg/year, Benzo(c)fluoranthene data</td>
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</table>

**Note:** The text appears to be a part of a program or script, possibly related to chemical concentration calculations. It includes variables such as `CAN`, `EPK`, `CGI`, and `EPK(9)`, and seems to be structured in a way typical of a programming language, likely for environmental or chemical data analysis.
\[ \text{EPG} (I) = \text{EPK} (I) \times 1000 / 8760 \text{ g/h point} \]

\[ \text{ETG} (I) = \text{EWG} (I) + \text{EPG} (I) \text{ 'total g/h} \]

\[ \text{ET} (I) = \text{ETG} (I) / \text{WM} \text{ 'total mol/h} \]

\[ \text{ETK} (I) = \text{ETG} (I) \times 8760 / 1000 \text{ 'total kg/year} \]

\[ \text{ETG} (I) = \text{EWG} (I) + \text{EPG} (I) \text{ 'total g/h} \]

\[ \text{ET} (I) = \text{ETG} (I) / \text{WX} \text{ 'total mol/h} \]

\[ \text{ETK} (I) = \text{BT} (I) \times 8760 / 1000 \text{ 'total kg/year} \]

\[ \text{NEXT} I \]

\[ \text{FOR} I = 1 \text{ TO } 9 \]

\[ \text{DT} (I) = 1 \]

\[ \text{NEXT} I \text{ inserted dummy dt values to avoid division by zero} \]

\[ \text{FOR} I = 1 \text{ TO } N \]

\[ \text{I} (I) = \text{ET} (I) + (\text{DP}(7, I) + \text{DP}(8, I)) \times \text{FA} \]

\[ \text{DB} (I) = \text{DP}(1, I) + \text{DP}(2, I) + \text{DP}(3, I) + \text{DP}(4, I) \]

\[ \text{NEXT} I \]

\[ \text{LPRINT} " " \]

\[ \text{PRINT " Input printing requirements ; zero for 'No', 1 for 'Yes'"} \]

\[ \text{PRINT " Physical-chemical properties, and Z values"} \]

\[ \text{INPUT P1} \]

\[ \text{PRINT " Chemical quantity data"} \]

\[ \text{INPUT P2} \]

\[ \text{PRINT " Segment dimensions, properties, D values and response times"} \]

\[ \text{INPUT P3} \]

\[ \text{IF SEL=2 GOTO 3080} \]

\[ \text{PRINT " Concentrations, amounts and process rates"} \]

\[ \text{INPUT P4} \]

\[ \text{PRINT " Individual segment mass balances"} \]

\[ \text{INPUT P5} \]

\[ \text{PRINT " "} \]

\[ \text{LPRINT} \]

\[ \text{REM PART 6 PRINT OUT SYSTEM DESCRIPTION} \]

\[ \text{IF P1=0 GOTO 3610} \]

\[ \text{PRINT " Physical-chemical and Partitioning Properties of "} \]

\[ \text{PRINT " "} \]

\[ \text{LPRINT USER " Temperature (deg C)"} \]

\[ \text{\# \# \; TC} \]

\[ \text{LPRINT USER " Temperature (deg K)"} \]

\[ \text{\# \# \; TK} \]

\[ \text{LPRINT USER " Gas constant (J/mol K)"} \]

\[ \text{\# \# \; R} \]

\[ \text{LPRINT USER " Molecular mass (g/mol)"} \]

\[ \text{\# \# \; WM} \]

\[ \text{LPRINT USER " Melting point (deg C) (system temp. for liquids)"} \]

\[ \text{\# \# \; FM} \]

\[ \text{LPRINT USER " Solubility (g/m^3)"} \]

\[ \text{\# \# \# \# \; SLY} \]

\[ \text{LPRINT USER " Solubility (mol/m^3)"} \]

\[ \text{\# \# \# \# \; SOLM} \]

\[ \text{LPRINT USER " Vapour pressure (Pa)"} \]

\[ \text{\# \# \# \# \; VP} \]

\[ \text{LPRINT USER " Subcooled liquid vapour pressure (Pa)"} \]

\[ \text{\# \# \# \# \; VPL} \]

\[ \text{LPRINT USER " Fugacity ratio"} \]

\[ \text{\# \# \# \# \; FRAT} \]

\[ \text{LPRINT USER " Henry's Law constant (Pa m^3/mol)"} \]

\[ \text{\# \# \# \# \; H} \]

\[ \text{LPRINT USER " Log octanol-water partition coefficient"} \]

\[ \text{\# \# \; LKOW} \]
3230 LPRINT USING " Octanol-water partition coefficient | ##.##^*
3240 LPRINT USING " Air-water partition coefficient (dimensionless) | ##.##^*
3250 LPRINT USING " Aerosol-air partition coefficient (dimensionless) | ##.##^*
3260 LPRINT USING " Fish-water partition coefficient (dimensionless) | ##.##^*
3270 LPRINT USING " Water reaction half life (hours) | ##.##^*
3280 LPRINT USING " Sediment reaction half life (hours) | ##.##^*
3290 LPRINT "----------------------------------------------------------"
3300 LPRINT ""
3310 LPRINT " Z Values common to all segments "
3320 LPRINT "----------------------------------------------------------"
3330 LPRINT USING " Z for air | ##.##^* ;ZD
3340 LPRINT USING " Z for aerosols | ##.##^* ;ZQ
3350 LPRINT USING " Z for bulk air | ##.##^* ;ZAT
3360 LPRINT USING " Z for water | ##.##^* ;ZW
3370 LPRINT USING " Z for fish with 5% lipid at equilibrium | ##.##^* ;ZF
3380 LPRINT "----------------------------------------------------------"
3390 LPRINT ""
3400 HS(1)=" Z for water particles |
3410 HS(2)=" Z for sediment solids |
3420 HS(3)=" Z for bulk water |
3430 HS(4)=" Z for bulk sediment |
3440 HS(5)=" Part-water ptn coef (L/kg) |
3450 HS(6)=" Sedt-water ptn coef (L/kg) |
3460 FOR I=1 TO N
3470 Y(I,I)=ZP(I);Y(2,I)=ZS(I);Y(3,I)=ZW(I);Y(4,I)=ZT(I);Y(5,I)=KPPW(I);Y(6,I)
3480 NEXT I
3490 LPRINT " Z Values which are segment specific (Pa.m3/mol) "
3500 LPRINT " Property Segment No 1 2 3 4 5 6 7 8 9"
3510 LPRINT "----------------------------------------------------------"
3520 FOR J=1 TO 6
3530 LPRINT HS(J);
3540 FOR I=1 TO N
3550 LPRINT USING "##.##^* ;Y(J,I);"
3560 NEXT I
3570 LPRINT ""
3580 NEXT J
3590 LPRINT "----------------------------------------------------------"
3600 LPRINT ""
3610 IF P2=0 GOTO 4020
3620 LPRINT " Chemical quantity data"
3630 LPRINT "----------------------------------------------------------"
3640 LPRINT USING " Air concn ng/m3 | ##.##^* ;CAN
3650 LPRINT USING " Air concn mol/m3 | ##.##^* ;CA
3660 LPRINT USING " Fractn on aerosols | ##.##^* ;FRQ
3670 LPRINT USING " Air equivalence | ##.##^* ;FA
3720 LPRINT "----------------------------------------------------------"
3730 LPRINT ""
3740 HS(1)=" Point sources kg/year |
3750 HS(2)=" Inflow river conc g/m3 or mg/L |
3760 HS(3)=" Inflow in rivers g/h |
3770 HS(4)=" Inflow in rivers kg/year "
3780 HS(5)=" Total input kg/year "
3790 HS(6)=" Inflow in rivers mol/h "
3800 HS(7)=" Point sources mol/h "
3810 HS(8)=" Total input mol/h "
3820 FOR I = 1 TO N
3830 Y(1,I)=GPI(I):Y(2,I)=CGI(I):Y(3,I)=EWI(I):Y(4,I)=EWK(I)
3840 Y(5,I)=ETK(I):Y(6,I)=EW(I):Y(7,I)=EP(I):Y(8,I)=ET(I)
3850 NEXT I
3860 LPRINT " Discharges Segment No 1 2 3 4 5 6 7 8 9 * "
3870 LPRINT " "
3880 FOR J= 1 TO 4
3890 LPRINT HS(J);
3900 FOR I=1 TO N
3910 LPRINT USING "####.#### " ;Y(J,I);
3920 NEXT I
3930 LPRINT " 
3940 NEXT J
3950 LPRINT " "
3960 LPRINT " 
3970 LPRINT " "
3980 LPRINT USING " # # # #### " ;ETT
3990 LPRINT USING " # # # #### " ;ETG
4000 LPRINT USING " # # # #### " ;ETKT
4010 LPRINT " "
4020 IF P3=0 GOTO 6040
4030 REM Print out segment properties
4040 FOR I=1 TO N
4050 Y(I,I)=GPI(I):Y(I,2)=CGI(I):Y(I,3)=EWI(I):Y(I,4)=EWK(I)
4060 Y(I,5)=ETK(I):Y(I,6)=EW(I):Y(I,7)=EP(I):Y(I,8)=ET(I)
4070 Y(I,9)=ETT(I):Y(I,10)=ETG(I):Y(I,11)=ETKT(I)
4080 LPRINT " "
4090 NEXT I
4100 HS(1)=" Frn OC in water particles "
4110 HS(2)=" Frn OC in sediment particles "
4120 HS(3)=" Den particles wrt (g/cm^3) "
4130 HS(4)=" Den sur sed parts (g/cm^3) "
4140 HS(5)=" Vol frn water particles "
4150 HS(6)=" Conc water part (mg/L) "
4160 HS(7)=" Vol frn sol in sediment "
4170 HS(8)=" Water area (m^2) "
4180 HS(9)=" Sediment area (m^2) "
4190 HS(10)=" Water volume (m^3) "
4200 HS(11)=" Sediment volume (m^3) "
4210 HS(12)=" Mean water depth (m) "
4220 HS(13)=" Mean active sed depth (m) "
4230 HS(14)=" Rain rate (m^3/h) "
4240 HS(15)=" Water inflow rate (m^3/h) "
4250 LPRINT " Segment properties "
4260 LPRINT " Property Segment No 1 2 3 4 5 6 7 8 9 "
4270 LPRINT " "
4280 LPRINT " "
4290 FOR J= 1 TO 15
4300 LPRINT HS(J);
4310 FOR I=1 TO N
```
4320 LPRINT USING ".##";Y(J,I);
4330 NEXT I
4340 LPRINT ";
4350 NEXT J
4360 LPRINT "--------------------------------------------------
4370 LPRINT "Inter-segment water exchanges m3/h and D values"
4380 LPRINT "Source Destination"
4390 LPRINT 1 2 3 4 5
4400 LPRINT 6 7 8 9
4410 LPRINT "--------------------------------------------------
4420 FOR I=1 TO N
4430 LPRINT USING ";##";G(I,J);
4440 FOR J=1 TO N
4450 LPRINT USING ";##.##";GW(I,J);
4460 NEXT J
4470 LPRINT ";
4480 NEXT I
4490 LPRINT "--------------------------------------------------
4500 LPRINT "Inter-segment particle exchanges (m3/h)
4510 LPRINT "Source Destination"
4520 LPRINT 1 2 3 4 5
4530 LPRINT 6 7 8 9
4540 LPRINT "--------------------------------------------------
4550 FOR I=1 TO N
4560 LPRINT USING ";##";G(I,J);
4570 FOR J=1 TO N
4580 LPRINT USING ";##.##";GP(I,J);
4590 NEXT J
4600 LPRINT ";
4610 NEXT I
4630 LPRINT "--------------------------------------------------
4640 LPRINT "Inter-segment particle exchange D values"
4660 LPRINT "Source Destination"
4670 LPRINT 1 2 3 4 5
4680 LPRINT 6 7 8 9
4690 FOR I=1 TO N
4700 LPRINT USING ";##";G(I,J);
4710 FOR J=1 TO N
4720 LPRINT USING ";##.##";GW(I,J);
4730 NEXT J
4740 LPRINT ";
4750 NEXT I
4770 LPRINT "--------------------------------------------------
4830 LPRINT "Inter-segment D values (total)
4840 LPRINT "Source Destination"
4850 LPRINT 1 2 3 4 5
4860 LPRINT 6 7 8 9
4880 LPRINT "--------------------------------------------------
```
4870 FOR I=1 TO N+1
4880 LPRINT USING "##|I;
4890 FOR J=1 TO N+1
4900 LPRINT USING "##.##.##";D(I,J);
4910 NEXT J
4920 LPRINT "  
4930 NEXT I
4940 LPRINT "----------------------------------

4950 LPRINT "  
4960 LPRINT "  
4970 LPRINT " Sediment-water exchange processes"
4980 LPRINT " Property Segment No 1 2 3 4 5 6 7 8 9"
4990 LPRINT "----------------------------------

5000 HS(1)=" Sediment depn g/m2/day 
5010 HS(2)=" Sediment resn g/m2/day 
5020 HS(3)=" Sediment burl g/m2/day 
5030 HS(4)=" Sediment depn m3/h 
5040 HS(5)=" Sediment resuspn m3/h 
5050 HS(6)=" Sediment burial m3/h 

5060 FOR I = 1 TO N
5070 Y(1,I)=DEP(I):Y(2,I)=RES(I):Y(3,I)=BUR(I)
5080 Y(4,I)=GD(I):Y(5,I)=GR(I):Y(6,I)=GB(I)
5090 NEXT I
5100 FOR J= 1 TO 6
5110 LPRINT HS(J);
5120 FOR I=1 TO N
5130 LPRINT USING "##.##.##";Y(J,I);
5140 NEXT I
5150 LPRINT "  
5160 NEXT J
5170 LPRINT "----------------------------------

5180 LPRINT 
5190 LPRINT " Mass Transfer Coefficients (m/h) "
5200 LPRINT "----------------------------------

5210 LPRINT USING " Volatilization: Air side 
5220 LPRINT USING " Volatilization: Water side 
5230 LPRINT USING " Overall water side 
5240 LPRINT USING " Sediment-water diffusion 

5250 LPRINT "  
5260 LPRINT "  
5270 LPRINT 
5280 LPRINT " Atmospheric Flow and Deposition Parameters "
5290 LPRINT "----------------------------------

5300 LPRINT USING " Deposition velocity (m/h) 
5310 LPRINT USING " Scavenging ratio 
5320 LPRINT USING " Density of aerosols (g/cm3) 
5330 LPRINT USING " Volume fraction aerosol particles 
5340 LPRINT USING " Concentration: aerosol particles (ug/m3) 
5350 LPRINT USING " Rain rate (m/year) 

5360 LPRINT "  
5370 LPRINT "  
5380 LPRINT " D Values for transport and transformation processes"
5390 LPRINT " Process Segmt No 1 2 3 4 5 6 7 8 9"
5400 LPRINT "----------------------------------
5410 FOR J = 1 TO 11
5420 LPRINT P$(J);
5430 FOR I = 1 TO N
5440 LPRINT USING " ######" |";DP(J,I);
5450 NEXT I
5460 LPRINT " |
5470 NEXT J
5480 LPRINT "-----------------------------------------------"

5490 LPRINT " Total D DE(I) |
5500 FOR I = 1 TO N
5510 LPRINT USING " ######" |";DE(I);
5520 NEXT I
5530 LPRINT " |
5540 LPRINT " Total D DT(I) |
5550 FOR I = 1 TO N
5560 LPRINT USING " ######" |";DT(I);
5570 NEXT I
5580 LPRINT " |
5590 LPRINT " Total inpt I(I)|
5600 FOR I = 1 TO N
5610 LPRINT USING " ######" |";I(I);
5620 NEXT I
5630 LPRINT " |
5640 LPRINT "-----------------------------------------------"

5650 LPRINT " Sediment response times ie VZ/D (years) "
5660 LPRINT " Process Segmt No | 1 | 2 | 3 | 4 |
5670 5 | 6 | 7 | 8 | 9 |
5680 LPRINT "-----------------------------------------------"

5690 FOR J = 1 TO 5
5700 LPRINT P$(J);
5710 FOR I = 1 TO N
5720 LPRINT USING " ######" |";TYS(J,I);
5730 NEXT I
5740 LPRINT " |
5750 NEXT J
5760 LPRINT "-----------------------------------------------"

5770 LPRINT " |
5780 LPRINT " Water response times ie VZ/D (years) "
5790 LPRINT " Process Segmt No | 1 | 2 | 3 | 4 |
5800 5 | 6 | 7 | 8 | 9 |
5810 LPRINT "-----------------------------------------------"

5810 FOR J = 3 TO 8
5820 LPRINT P$(J);
5830 FOR I = 1 TO N
5840 LPRINT USING " ######" |";TYW(J,I);
5850 NEXT I
5860 LPRINT " |
5870 NEXT J
5880 LPRINT "-----------------------------------------------"

5900 HS$(1)=" Point sources kg/year |
5910 HS$(2)=" Inflow river conc g/m3 or mg/L |
5920 HS$(3)=" Inflow in rivers g/h |
REM Calculate all fugacities /equivalences
LPRINT " "

FOR I = 1 TO N
  J1=DT(1)
  J2=DT(2)*D(1,2)/DT(1)
  J3=DT(3)*D(2,3)/DT(2)
  J4=DT(4)*D(3,4)/DT(3)
  J5=DT(5)*D(4,5)/DT(4)
  J6=DT(6)*D(5,6)/DT(5)
  J7=DT(7)*D(6,7)/DT(6)
  J8=DT(8)*D(7,8)/DT(7)
  J9=DT(9)*D(8,9)/DT(8)
  IJ1=I(1)
  IJ2=I(2)+IJ1*D(1,2)/J1
  IJ3=I(3)+IJ2*D(2,3)/J2
  IJ4=I(4)+IJ3*D(3,4)/J3
  IJ5=I(5)+IJ4*D(4,5)/J4
  IJ6=I(6)+IJ5*D(5,6)/J5
  IJ7=I(7)+IJ6*D(6,7)/J6
  IJ8=I(8)+IJ7*D(7,8)/J7
  IJ9=I(9)+IJ8*D(8,9)/J8
  FW(9)=IJ9/J9
  FW(8)=(IJ8+FW(9)*D(9,8))/J8
  FW(7)=(IJ7+FW(8)*D(8,7))/J7
  FW(6)=(IJ6+FW(7)*D(7,6))/J6
  FW(5)=(IJ5+FW(6)*D(6,5))/J5
  FW(4)=(IJ4+FW(5)*D(5,4))/J4
  FW(3)=(IJ3+FW(4)*D(4,3))/J3
  FW(2)=(IJ2+FW(3)*D(3,2))/J2
  FW(1)=(IJ1+FW(2)*D(2,1))/J1
FOR I = 1 TO N
  FS(I)=FW(I)*(DP(4,I)+DP(5,I))/(DP(1,I)+DP(2,I)+DP(3,I)+DP(4,I))
  NEXT I
MTT=O:MTTK=O
FOR I = 1 TO N
  CST(I)=FS(I)*ZST(I)
  CSTN(I)=CST(I)*WM*1000000
  MWT(I)=FW(I)*VW(I)*ZWT(I)
  MST(I)=FS(I)*VS(I)*ZST(I)
  MT(I)=MWT(I)+MST(I)
  MTR(I)=MT(I)*WM/1000
  MTT=MTT+MT(I)
  MTTK=MTTK+MTK(I)
NEXT I
REM Calculate process rates
FOR I = 1 TO N
  R(J,I)=FS(I)*DP(J,I):RK(J,I)=R(J,I)*WM*8760/1000
R(Q,I)=(FS(I)-FW(I))*DP(4,I)*WM*8760/1000
RK(4,I)=R(4,I)*WM*8760/1000
FOR J= 5 TO 6
R(J,I)=FW(I)*DP(J,I)*RK(J,I)=R(J,I)*WM*8760/1000
NEXT J
R(7,I)=(FW(I)-FA)+DP(7,I)*RK(7,1)=R(7,1)*WM*8760/1000
R(8,1)=FA*DP(8,1)*RK(8,1)=R(8,1)*WM*8760/1000
RWS(I)=(FW(I)+DP(3,I)+DP(4,I))*RWSK(I)=RWS(I)*WM*8760/1000
RWS(I)=EW(I)*(DP(4,I)+DP(5,I))*RWSK(I)=RWS(I)*WM*8760/1000
NEXT I
FOR I= 1 TO N+1
R(J,I)=FW(I)+RJY(I,J)=RJY(I,J)*WM*8760/1000
NEXT J
NEXT I
FOR I= 1 TO N+1
RI(I)=0;RX(I)=0
FOR J= 1 TO N+1
RX(I)=RX(I)+RJY(I,J)
NEXT J
NEXT I
RXK(I)=RX(I)*WM*8760/1000
RX(I)=RI(I)*WM*8760/1000
NEXT I
REM
FOR P4=0 GOTO 7610
REM Print output
LPRINT "Concentrations and amounts in each segment"
HS(1)="Aquiv in water column"
HS(2)="Aquiv in sediment"
HS(3)="Conc bulk water (mol/m3)"
HS(4)="Conc bulk water (ng/L)"
HS(5)="Conc bulk sed (mol/m3)"
HS(6)="Conc sed solids (ng/g)"
HS(7)="Amt water column (mol)"
HS(8)="Amt water column (kg)"
HS(9)="Amount in sediment (mol)"
HS(10)="Amount in sediment (kg)"
HS(11)="Total amt in segt (mol)"
HS(12)="Total amt in segt (kg)"
FOR I= 1 TO N
Y(1,I)=FW(I);Y(2,I)=FS(I);Y(3,I)=CWT(I);Y(4,I)=CWTN(I);Y(5,I)=CST(I)
Y(6,I)=CSTN(I);Y(7,I)=MWT(I)
Y(8,I)=MWTK(I);Y(9,I)=HST(I);Y(10,I)=MT(I);Y(12,I)=MTK(I)
NEXT I
LPRINT "Property Segment No 1 2 3 4 5 6 7 8 9"
LPRINT "---------------------------------------------"
FOR J= 1 TO 12
LPRINT HS(J);"Y(J,I);"
NEXT I
LPRINT "---------------------------------------------"
LPRINT "Grand total mol ";MTT
REM Print out transport and transformation rates
FOR I = 1 TO N
Y(I,1) = R(I,1)
Y(2,1) = R(2,1)
Y(3,1) = R(3,1)
Y(4,1) = R(4,1)
Y(5,1) = R(5,1)
Y(I,6) = R(I,6)
Y(7,1) = R(7,1)
Y(8,1) = R(8,1)
Y(9,1) = RK(I,1)
Y(10,1) = RK(2,1)
Y(11,1) = RK(3,1)
Y(12,1) = RK(4,1)
Y(13,1) = RK(5,1)
Y(14,1) = RK(6,1)
Y(15,1) = RK(7,1)
Y(16,1) = RK(8,1)
NEXT I

LPRINT " Process rates mol/h"
6 7 8 9

FOR J = 1 TO 8
LPRINT P$(J)
FOR I=1 TO N
LPRINT USING "##.##[^~^]"; Y(J,I)
NEXT I
LPRINT ""
NEXT J

LPRINT " Process rates kg/year"
6 7 8 9

FOR J = 1 TO 8
LPRINT P$(J)
FOR I=1 TO N
LPRINT USING "###.#####|"; Y(J+8,I)
NEXT I
LPRINT ""
NEXT J

LPRINT " Inter-segment transfers mol/h"
LPRINT " Source Destination"
6 7 8 9

FOR I=1 TO N+1
LPRINT USING "##|"; I
FOR J=1 TO N+1
LPRINT USING "##.##[^~^]|"; RJY(I,J)
NEXT J
LPRINT ""
NEXT I

LPRINT " Inter-segment transfers kg/year"
LPRINT " Source Destination"
6 7 8 9
---

7500 LPRINT " "
7510 FOR I=1 TO N+1
7520 LPRINT USING "## | ;I ;
7530 FOR J=1 TO N+1
7540 LPRINT USING "###.#### | ;RJYK(I,J);
7550 NEXT J
7560 LPRINT " 
7570 NEXT I
7580 LPRINT " "
---

7590 LPRINT " 
7600 IF FS=0 GOTO 8100
7610 FOR I=1 TO N
7620 LPRINT
7625 LPRINT CHR$(12)
7628 INPUT "Press any key to continue";QQQ$
7630 LPRINT "Segment No";I," ie ";NS(I);"mol/h kg/year"
7640 LPRINT " 
7650 LPRINT USING "Point source discharges       ###.#### ####
7660 LPRINT USING "River inflow discharges       ###.#### ####
7670 LPRINT USING "Total inflow from adjacent segments ####.#### ####
7680 LPRINT USING "Total outflow to adjacent segments ####.#### ####
7690 LPRINT USING "Atmospheric deposition         ####.#### ####
7700 LPRINT USING "Net diffusive loss to atmosphere ####.#### ####
7710 LPRINT USING "Water transformation         ####.#### ####
7720 LPRINT USING "Water to sediment transfer ####.#### ####
7730 LPRINT USING "Sediment to water transfer ####.#### ####
7740 LPRINT USING "Sediment transformation ####.#### ####
7750 LPRINT USING "Sediment burial            ####.#### ####
7760 LPRINT " 
7770 LPRINT "Details of exchange processes"
7780 RM=FA*DP(9,I):RMK=RM*WM*8760/1000
7790 RC=FA*DP(10,I):RCK=RC*WM*8760/1000
7800 RQ=FA*DP(11,I):RQK=RQ*WM*8760/1000
7810 RNW=DP(7,I)*(FW(I)-FA): RNWK=RNW*WM*8760/1000
7820 RTN=DP(4,I)*(FS(I)-EW(I)): RTNK=RTN*WM*8760/1000
7830 RSWD=DP(4,I)*PS(I): RSWDK=RSWD*WM*8760/1000
7840 RWSD=DP(4,I)*FW(I): RWSDK=RWSD*WM*8760/1000
7850 RA=DP(7,I)*FA: RAK=RA*WM*8760/1000
7860 RV=DP(7,I)*FW(I): RVK=RV*WM*8760/1000
7870 SUMWI=EW(I)+EP(I)+R(8,I)+RI(I)+RWS(I): SUMWIK=SUMWI*WM*8760/1000
7880 SUMX=R(7,I)+R(6,I)+RX(I)+RWS(I): SUMWX=SUMX*WM*8760/1000
7890 SUMSI=RWS(I): SUMSIK=SUMSI*WM*8760/1000
7900 SUMSX=RSW(I)+R(2,I)+R(1,I): SUMSXK=SUMSX*WM*8760/1000
7910 LPRINT USING "Rain dissolution ###.#### ####
7920 LPRINT USING "Wet particle deposition ###.#### ####
7930 LPRINT USING "Water to sediment transfer ####.#### ####
7940 LPRINT USING "Water transformation         ####.#### ####
7950 LPRINT USING "River inflow discharges       ###.#### ####
7960 LPRINT USING "Point source discharges       ###.#### ####
7970 LPRINT " 
---

"Press any key to continue";QQQ$
LPRINT USING "Dry particle deposition" RQ, RQK
LPRINT USING "Absorption" RA, RAK
LPRINT USING "Volatilization" RV, RVK
LPRINT USING "(Net water to air diffusion)" RVN, RVNK
LPRINT USING "Sediment deposition" R(5,I), R(5,I)
LPRINT USING "Sediment resuspension" R(3,I), R(3,I)
LPRINT USING "(Net sediment to water diffusion)" RTN, RTNK
LPRINT USING "Sediment to water diffusion" RSWD, RSWDK
LPRINT USING "Water to sediment diffusion" RWSD, RWSDK
LPRINT USING "Total input to water column" SUMWI, SUMWK
LPRINT USING "Total output from water column" SUMWX, SUMWXK
LPRINT USING "Total input to sediment" SUMSI, SUMSIK
LPRINT USING "Total output from sediment" SUMSX, SUMSXX
LPRINT " "
NEXT I
LPRINT CHRS(12)
END
Program listing of QWASI model for Nainital Lake

5 REM QMULT : MULTI-PURPOSE QWASI MODEL FOR UP TO 9 SEGMENTS

7 REM application to Lake Nainital

10 REM PART 1 SET COMPUTING VARIABLES

20 DIM HS(20),Y(20,9),D(10,10),PS(20),DP(12,12)

30 REM Nomenclature Conventions

40 LPRINT CHR$(15)

50 WIDTH "lpt1:",160

55 N=3 'Number of segments

60 REM Define segment names

70 NS(1)="North basin"

80 NS(2)="Middle basin"

90 NS(3)="South basin"

100 NS(4)="Fourth section"

110 NS(5)="Fifth section"

120 NS(6)="Sixth section"

130 NS(7)="Seventh section"

140 NS(8)="Eighth section"

150 NS(9)="Ninth section"

160 REM

170 REM Identify processes

180 PS(1)="Sediment burr"

190 PS(2)="Sediment trnf"

200 PS(3)="Sediment resn"

210 PS(4)="Sedt-watr difn"

220 PS(5)="Sedt depn"

230 PS(6)="Water transp"

240 PS(7)="Water-air dif"

250 PS(8)="Atmos depson"

260 PS(9)="(Rain diss)"

270 PS(10)="(Wet pt depn)"

280 PS(11)="(Dry pt depn)"

290 REM PART 2 DIMENSIONS AND PROPERTIES OF THE AQUATIC SYSTEM

300 REM Segment Dimensions

309 REM AW(I) is water area m2

310 AW(1)=150000! : AW(2)=155000! : AW(3)=155000! : AW(4)=8000000!


329 REM HW(I) is water depth m

330 HW(1)=18 : HW(2)=18 : HW(3)=18 : HW(4)=10

340 HW(5)=15 : HW(6)=10 : HW(7)=20 : HW(8)=10 : HW(9)=10

349 REM HS(I) is sediment depth m

350 HS(1)=.02 : HS(2)=.02 : HS(3)=.02 : HS(4)=.022

360 HS(5)=.03 : HS(6)=.0111 : HS(7)=.03 : HS(8)=.01 : HS(9)=.01

370 FOR I = 1 TO N

380 AS(I)=AW(I) 'Sediment areas m2

390 VW(I)=AW(I)*HW(I) 'Water volumes m3

400 VS(I)=AS(I)*HS(I) 'Active sediment volumes m3

410 NEXT I

415 RAIN=.3 'rain rate m/year

420 REM Phase densities (kg/L or g/cm3)

430 DENW=1: DENQ=1.5 'Water and aerosols

440 DEMP(1)=2: DEMP(2)=2: DEMP(3)=2: DEMP(4)=2:

450 DEMP(5)=2: DEMP(6)=2: DEMP(7)=2: Suspended particles

460 DEMP(8)=2: DEMP(9)=2

470 DENS(1)=2: DENS(2)=2: DENS(3)=2: DENS(4)=2:

480 DENS(5)=2: DENS(6)=2: DENS(7)=2: Sediment solids

485 DENS(8)=2: DENS(9)=2

490 ORGP(1)=.2: ORGP(2)=.2: ORGP(3)=.2: ORGP(4)=.2

500 ORGP(5)=.2: ORGP(6)=.2: ORGP(7)=.2
501 ORGP(8)=.2: ORGP(9)=.2: 'Organic content of particles
510 ORGS(1)=.2: ORGS(2)=.2: ORGS(3)=.2: ORGS(4)=.1
520 ORGS(5)=.1: ORGS(6)=.1: ORGS(7)=.1
521 ORGS(8)=.2: ORGS(9)=.2: 'Organic content of sediment
530 REM Particle Concentrations
540 VFQ=4.4E-11: 'Vol Fraction of Aerosols
541 CFQ=VFQ*DENQ*10^12: 'Concentration Aerosols, ug/m3
550 VFS(1)=.07: VFS(2)=.07: VFS(3)=.07: VFS(4)=.07: VFS(5)=.07: VFS(6)=.07: VFS(7)=.07: VFS(8)=.07: VFS(9)=.07: 'Vol fraction of sediment solids
570 CSP(1)=25: CSP(2)=30: CSP(3)=40: CSP(4)=50: CSP(5)=50: CSP(6)=50: CSP(7)=50: CSP(8)=50: CSP(9)=50: 'Suspended solids concentration in water g/m3 or mg/L
590 FOR I = 1 TO N+1
600 VFP(I)=CSP(I)/(DENP(I)*10^12): 'particle flows m3/h
640 NEXT I
660 FOR I = 1 TO N+1
670 FOR J=1 TO N+1
680 GW(I,J)=0: GP(I,J)=0
690 NEXT J
700 NEXT I
705 REM Water inflow rates by rivers and runoff m3/h
710 GI(1)=250: GI(2)=100: GI(3)=0
720 GI(4)=0: GI(5)=0: GI(6)=0
722 GI(7)=0: GI(8)=0: GI(9)=0
725 GI(7)=500000: GI(8)=400000: GI(9)=1000001
730 REM Set water exchange rates m3/h
740 GW(2,1)=.05*GI(1): GW(3,2)=.05*(GI(1)+GI(2)): GW(4,3)=0*(GI(1)+GI(2)+GI(3))
760 GW(1,2)=GI(1)+GW(2,1)
780 GW(2,3)=GI(2)+GW(1,2)+GW(3,2)-GW(2,1)
790 GW(3,4)=GI(3)+GW(2,3)+GW(4,3)-GW(3,2)
800 GW(4,5)=GI(4)+GW(3,4)+GW(5,4)-GW(4,3)
810 GW(5,6)=GI(5)+GW(4,5)+GW(6,5)-GW(5,4)
820 GW(6,7)=GI(6)+GW(5,6)+GW(7,6)-GW(6,5)
821 GW(7,8)=GI(7)+GW(6,7)+GW(8,7)-GW(7,6)
822 GW(8,9)=GI(8)+GW(7,8)+GW(9,8)-GW(8,7)
830 REM Suspended Particle Flows (g/h)
840 FOR I=1 TO N+1
850 FOR J=1 TO N+1
860 GP(I,J)=GW(I,J)*VFP(I): 'particle flows m3/h
870 NEXT J
880 NEXT I
890 REM Suspended Particle Fluxes g/m2/year
900 DEP(1)=5.5: DEP(2)=5: DEP(3)=5: DEP(4)=DEP(3): DEP(5)=5: 'Particle deposition rates g/m2/day
910 DEP(7)=5: DEP(8)=5: DEP(9)=5: 'Particle deposition rates g/m2/day
920 RES(1)=1: RES(2)=2: RES(3)=2: RES(4)=RES(3): RES(6)=2
930 RES(7)=2: RES(8)=2: RES(9)=2: 'Particle resuspension rates g/m2/day
940 BUR(1)=2.5: BUR(2)=1.8: BUR(3)=1.3: BUR(4)=BUR(3): BUR(6)=2
950 BUR(7)=2: BUR(8)=2: BUR(9)=2: 'Particle burial rates g/m2/day
960 FOR I=1 TO N
970 GD(I)=DEP(I)*AS(I)/24/DENP(I)/10000000000:
980 GR(I)=RES(I)*AS(I)/24/DENS(I)/10000000000:
990 GB(I)=BUR(I)*AS(I)/24/DENS(I)/10000000000:
1000 NEXT I
1010 REM Atmospheric Deposition (m3/h)
Qo = 200000! 'Scavenging ratio
VDEP = 10 'Dry deposition velocity m/h

FOR I = 1 TO N
GC(I) = GM(I) * VFQ * Q
VDEP * AW(I) * VFQ
GQT(I) = GQ(I) + GC(I)

NEXT I

REM PART 3 INPUT OF CHEMICAL PROPERTIES
PRINT "There are two methods of entering chemical properties:"
PRINT "Method P is to enter physical chemical properties"
PRINT "Method K is to enter partition coefficients"
PRINT "A chemical to be user-specified by method P 1"
PRINT "A chemical to be user-specified by method K 2"
PRINT "A chemical previously specified 3"
PRINT "A chemical from the following list 4"
PRINT "Lead (K) 4 , Copper (K) 5 , Dichlorobenzene (P) 6 , Tetrachlorobenzene (P) 7 , Pentachlorobenzene (P) 8 , Hexachlorobenzene (P) 9 , Lindane (P) 10 , Benzofluoranthene (P) 11 , alpha-HCB (P) 12 , Benzofluoranthene (P) 13 ,
INPUT QQ
ON QQ GOTO 1220, 1520, 1310, 1320, 1325, 1330, 1335, 1340, 1345, 1350, 1355, 1360, 1365, 1370, 1380, 1390, 1400, 1410, 1420, 1430, 1440
CS = "BENZO(b)FLUORANTHENE" : WM = 252.32 : SOLY = .0015 : VP = 1.5E-07 : LKOW = 6.5 : TDS = 350000 : TDW = 120000 : TC = 25 : TM = 168 : GOTO 1340
REM chemical is specified by method P:PRINT ""
REM 'Adjust chemical properties
TK = TC + 273 'temperature in degrees Kelvin
TMK = TK + 273
R = 8.314 'gas constant
FRAT = EXP(6.79 * (1 - TKM/TK))
VPL = VP / FRAT 'subcooled liquid vapor pressure
SOLM = SOLY / WM 'solubility (mol/m^3)
H = VP / SOLM 'Henry's Law constant (Pa m^3/mol)
KOW = 10 * LKOW 'octanol-water partition coefficient
KDAH = H / RK
1450  KDFW=.05*KOW
1460  KDQA=60000001/VPL
1465  KDQW=KDQA*KDAW
1470  FOR I=1 TO N+1
1480  KPPW(I)=.41*KOW*ORGP(I)
1490  KPSW(I)=.41*KOW*ORGS(I)
1500  NEXT I
1510  GOTO 1680
1520  PRINT "INPUT CHEMICAL PROPERTIES, ANY PREVIOUS VALUES IN PARENTHESES ( )"
1530  PRINT "CHEMICAL NAME (preferably in CAPITALS) (";CS");": INPUT CS
1540  PRINT "TEMPERATURE deg C (";TC");": INPUT TC
1550  PRINT "MOLECULAR WEIGHT g/mol (";WM");": INPUT WM
1560  PRINT "PARTITION COEFFICIENTS ARE COMMON TO ALL SEGMENTS"
1570  PRINT "SEDIMENT-WATER PARTITION COEFFICIENT KPSW L/kg (";KPSW");": INPUT KPSW
1580  PRINT "PARTICLE-WATER PARTITION COEFFICIENT KPPW L/kg (";KPPW");": INPUT KPPW
1590  PRINT "AEROSOL-WATER PARTITION COEFFICIENT KDQW dim'less (";KDQW");": INPUT KDQW
1600  PRINT "FISH-WATER PARTITION COEFFICIENT KDFW dim'less (";KDFW");": INPUT KDFW
1610  PRINT "DEGRADATION HALF LIFE IN SEDIMENT hours (";TDS");": INPUT TDS
1620  PRINT "DEGRADATION HALF LIFE IN WATER hours (";TDW");": INPUT TDW : GOTO 1680
1630  CS="Lead"; WM=207 ; KDAW=1E-11; KPSWC=3330001; KPPWC=6680001; KDQW=10001; TDS=1E+11;TDW=1E+11; TC=25: KDQA=1E-11: GOTO 1640
1635  CS="Copper"; WM=63.6; KDAW=1E-11; KPSWC=3330001; KPPWC=13360001: KDQW=10001; TDS=1E+11; TDW=1E+11; TC=25: KDQA=1E-11: GOTO 1640
1640  FOR I= 1 TO N+1
1650  KPSW(I)=KPSWC
1660  KPPW(I)=KPPWC
1670  NEXT I
1680  REM Calculate dimensionless partition coefficients
1690  TK=TC+273
1700  FOR I=1 TO N+1
1710  KDFW(I)=KPPW(I)*DENP(I)
1720  KDSW(I)=KPSW(I)*DENS(I)
1730  NEXT I
1740  'Reaction rate constants (h^-1)
1750  KS = .693/TDS  'sediment reaction rate constant
1760  KW = .693/TDW  'water reaction rate constant
1770  REM PART 4 CALCULATION OF Z AND D VALUES AND RESPONSE TIMES
1780  REM Calculate equivalent Z values
1790  ZW = 1  'Z for water
1800  ZA = KDAW  'Z for air
1810  ZF = KDFW  'Z for fish
1820  ZQ = KDQW*ZW  'Z for aerosol particles
1830  FOR I= 1 TO N+1
1840  ZP(I) = KDFW(I)  'Z for water particles
1850  ZS(I) = KDSW(I)  'Z for sediment particles
1860  ZST(I)=ZW*(1-VFP(I))+ZS(I)*VFS(I)  'Z for bulk sediment
1870  ZWT(I) = ZW*(1-VFP(I))+ZP(I)*VFP(I)  'Z for bulk water
1880  NEXT I
1890  ZAT = ZA*(1-VFQ) + VFQ * ZQ  'Z for bulk air
1900  PRO=VFQ*ZQ/(VFQ*ZQ+(1-VFQ)*ZA)  'Fraction of chemical on aerosol
1910  'Mass Transfer Coefficients (m/h)
1920  KVA = 11  'volatilization: air side
1930  KVW = .01  'volatilization: water side
1940  KV = KDAW/(KDAW/KV + 1/KVA)  'overall water side
1950  KT = .0002  'sediment-water diffusion
1960  REM Calculation of process D values DP(J,I) and response times
1962 REM Subscript J refers to the process e.g. burial
1964 REM Subscript I refers to the segment
1970 FOR I=1 TO N
1980 DP(1,I) = GB(I) * ZS(I) 'burial
1990 DP(2,I) = VS(I) * ZST(I) * KS 'sediment transformation
2000 DP(3,I) = GR(I) * ZS(I) 'sediment resuspension
2010 DP(4,I) = KT * AS(I) * ZW 'sediment-water diffusion
2020 DP(5,I) = GD(I) * ZP(I) 'sediment deposition
2030 DP(6,I) = VW(I) * ZST(I) * KS 'sediment transformation
2040 DP(7,I) = KV * AW(I) * ZW 'volatilization
2050 DP(9,I) = GM(I) * ZW 'sediment-water diffusion
2060 DP(10,I) = GC(I) * ZQ 'wet particle deposition
2070 DP(11,I) = GQ(f) * ZQ 'dry particle deposition
2080 DP(8,I)=DP(9,I)+DP(10,I)+DP(11,I)
2090 NEXT I
2100 FOR I = 1 TO N+1
2110 FOR J = 1 TO N+1
2120 DJ(I,J)=GW(I,J)*ZW 'water flow
2130 DY(I,J)=GP(I,J)*ZP(I) 'particle flow
2140 D(I,J)=DJ(I,J)+DY(I,J) 'total flow
2150 NEXT J
2160 NEXT I
2170 'Calculate response times in years
2180 FOR I=1 TO N
2190 TYS(1,I)=VS(I)*ZST(I)/DP(1,I)/8760
2200 TYS(2,I)=VS(I)*ZST(I)/DP(2,I)/8760
2210 TYS(3,I)=VS(I)*ZST(I)/DP(3,I)/8760:TYW(3,I)=VW(I)*ZWT(I)/DP(3,I)/8760
2220 TYS(4,I)=VS(I)*ZST(I)/DP(4,I)/8760:TYW(4,I)=VW(I)*ZWT(I)/DP(4,I)/8760
2230 TYS(5,I)=VS(I)*ZST(I)/DP(5,I)/8760:TYW(5,I)=VW(I)*ZWT(I)/DP(5,I)/8760
2240 TYS(6,I)=VS(I)*ZST(I)/DP(6,I)/8760:TYW(6,I)=VW(I)*ZWT(I)/DP(6,I)/8760
2250 TYS(7,I)=VS(I)*ZST(I)/DP(7,I)/8760:TYW(7,I)=VW(I)*ZWT(I)/DP(7,I)/8760
2260 TYS(8,I)=VS(I)*ZST(I)/DP(8,I)/8760:TYW(8,I)=VW(I)*ZWT(I)/DP(8,I)/8760
2270 TYS(9,I)=VS(I)*ZST(I)/DP(9,I)/8760:TYW(9,I)=VW(I)*ZWT(I)/DP(9,I)/8760
2280 TYS(10,I)=VS(I)*ZST(I)/DP(10,I)/8760:TYW(10,I)=VW(I)*ZWT(I)/DP(10,I)/8760
2290 TYS(11,I)=VS(I)*ZST(I)/DP(11,I)/8760:TYW(11,I)=VW(I)*ZWT(I)/DP(11,I)/8760
2295 TYS(12,I)=VS(I)*ZST(I)/DP(12,I)/8760:TYW(12,I)=VW(I)*ZWT(I)/DP(12,I)/8760
2300 TYS(13,I)=VS(I)*ZST(I)/DP(13,I)/8760:TYW(13,I)=VW(I)*ZWT(I)/DP(13,I)/8760
2305 TYS(14,I)=VS(I)*ZST(I)/DP(14,I)/8760:TYW(14,I)=VW(I)*ZWT(I)/DP(14,I)/8760
2310 TYS(15,I)=VS(I)*ZST(I)/DP(15,I)/8760:TYW(15,I)=VW(I)*ZWT(I)/DP(15,I)/8760
2315 TYS(16,I)=VS(I)*ZST(I)/DP(16,I)/8760:TYW(16,I)=VW(I)*ZWT(I)/DP(16,I)/8760
2320 TYS(17,I)=VS(I)*ZST(I)/DP(17,I)/8760:TYW(17,I)=VW(I)*ZWT(I)/DP(17,I)/8760
2325 TYS(18,I)=VS(I)*ZST(I)/DP(18,I)/8760:TYW(18,I)=VW(I)*ZWT(I)/DP(18,I)/8760
2330 TYS(19,I)=VS(I)*ZST(I)/DP(19,I)/8760:TYW(19,I)=VW(I)*ZWT(I)/DP(19,I)/8760
2335 TYS(20,I)=VS(I)*ZST(I)/DP(20,I)/8760:TYW(20,I)=VW(I)*ZWT(I)/DP(20,I)/8760
2340 TYS(21,I)=VS(I)*ZST(I)/DP(21,I)/8760:TYW(21,I)=VW(I)*ZWT(I)/DP(21,I)/8760
2345 IF DP(7,I)=0 GOTO 2360
2350 TYW(7,I)=VW(I)*ZWT(I)/DP(7,I)/8760
2355 TYW(8,I)=VW(I)*ZWT(I)/DP(8,I)/8760
2360 TYW(9,I)=VW(I)*ZWT(I)/DP(9,I)/8760
2365 TYW(10,I)=VW(I)*ZWT(I)/DP(10,I)/8760
2370 NEXT I
2380 REM PART 5 INPUT CHEMICAL QUANTITIES DATA
2390 PRINT "INPUT CHEMICAL QUANTITIES, ANY PREVIOUS VALUES IN PARENTHESES ( )"
2400 PRINT "Specify chemical quantities by entering one of the following"
2410 PRINT "A chemical to be user-specified 1"
2420 PRINT "Chemical quantities as previously specified 2"
2430 PRINT "Quantities specified for a chemical from the following list "
2440 PRINT "Lead 3 ,Copper 4 ,Dichlorobenzene 5 ,Tetrachlorobenzene 6 ,Penta chlorobenzene 7 ,Hexachlorobenzene 8 ,Lindane 9 ,Benzopyrene 10, alph-HCH 11, Benzofluoranthene 12."
2450 INPUT QQQ
2460 ON QQQ GOTO 2600,2680,2480,2520,2535,2550,2565,2580,2592,2596,2600,2604
2470 REM Discharge data CGI(i) is concn in rivers g/m3 ,EPK(i) is kg/year point discharge
2480 EPK(1)=450:EPK(2)=250:EPK(3)=80 :EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)=1
2490 EPK(9)=2 'Point source discharges kg/year,Lead data
2495 CGI(1)=.05:CGI(2)=.05 : CGI(3)=.05 : CGI(4)=.002: CGI(5)=0.0003:CGI(7)=0:CGI(8)=0.003:CGI(9)=0.0004 ' Concentrations in river inputs g/m3
2500 CAN=+.84 'Air concn ng/m3 go to 2680
2510 GOTO 2680
2520 EPK(1)=100:EPK(2)=40 :EPK(3)=20 :EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)
2525 CGI(1)=.001 :CGI(2)=.001 : CGI(3)=.001 :CGI(4)=.0001:CGI(6)=.00003:CGI(7)=0
2530 CAN=+.76 'Air concn ng/m3 go to 2680
2535 EPK(1)=0:EPK(2)=0 :EPK(3)=1000: EPK(5)=0:EPK(6)=31:EPK(7)=0 : EPK(8)
2540 EPK(9)=2 'Point source discharges kg/year,DiCB data
Concentrations in river inputs g/m³

Concentrations in river inputs g/m³

Point source discharges kg/year, TetraCB data

Point source discharges kg/year, PentaCB data

Point source discharges kg/year, HexaCB data

Point source discharges kg/year, Lindane data

Point source discharges kg/year, alpha-HCH data

Point source discharges kg/year, Benzo(b)fluoranthene data

Concentrations in river inputs g/m³

Air concn ng/m³ go to 2680

CONCNS (ng/µm³) IN ATMOSPHERE (";CAN;"): INPUT CAN

ETCT=0:ETT=0:ETKT=0

FA=CA/ZAT 'air fugacity

EW(I)=EWG(I)/WM 'mol/h water

EW(I)=EWG(I)/WM 'mol/h water
2740 EWK(I)=EWG(I)*8760/1000 'kg/year water
2750 EPG(I)=EPG(I)*1000/8760 'g/h point
2760 EP(I)=EPG(I)/WM 'mol/h point
2770 ETG(I)=EWG(I)+EPG(I) 'total g/h
2780 ET(I)=ETG(I)/WM 'total mol/h
2790 ETK(I)=ETG(I)*8760/1000 'total kg/year
2800 EGTG=ETG(I)+ETG(I) 'grand total g/h
2810 ETT=ETT+ET(I) 'grand total mol/h
2820 ETKT=ETKT+ETK(I) 'grand total kg/year
2830 NEXT I
2840 FOR I=1 TO 9
2841 DT(I)=1 'inserted dummy dt values to avoid division by zero
2860 FOR I = 1 TO N
2870 I(I)=ET(I)+(DP(7,I)+DP(8,I))*FPA
2880 DF(I)=DP(4,I)+DP(5,I)+DP(6,I)+DP(7,I)-(DP(3,I)+DP(4,I))*(DP(4,I)+DP(5,I))/(DP(1,I)+DP(2,I)+DP(3,I)+DP(4,I))
2900 NEXT I
2910 LPRINT " "
2920 PRINT "Input printing requirements ; zero for 'No',1 for 'Yes'
2930 PRINT "Physical-chemical properties, and Z values 
2940 INPUT P1
2950 PRINT "Chemical quantity data 
2960 INPUT P2
2970 PRINT "Segment dimensions, properties, D values and response times"
2980 INPUT P3
3010 IF SEL=2 GOTO 3080
3020 PRINT "Concentrations, amounts and process rates"
3030 INPUT P4
3040 PRINT "Individual segment mass balances"
3050 INPUT P5
3060 LPRINT
3070 REM  PART 6 PRINT OUT SYSTEM DESCRIPTION
3080 IF P1=0 GOTO 3610
3090 LPRINT "Physical-chemical and Partitioning Properties of ";CS$ 
3100 LPRINT "-----------------------------------------------"
3110 LPRINT USING "| Temperature (deg C) | #
3120 LPRINT USING "| Temperature (deg K) | ##
3130 LPRINT USING "| Gas constant (J/mol K) | ###
3140 LPRINT USING "| Molecular mass (g/mol) | ####
3150 LPRINT USING "| Melting point (deg C) (system temp. for liquids) | ####
3160 LPRINT USING "| Solubility (g/m^3) | ####
3170 LPRINT USING "| Solubility (mol/m^3) | ####
3180 LPRINT USING "| Vapour pressure (Pa) | ####
3190 LPRINT USING "| Subcooled liquid vapour pressure (Pa) | ####
3200 LPRINT USING "| Fugacity ratio | ####
3210 LPRINT USING "| Henry's Law constant (Pa m^3/mol) | ####
3220 LPRINT USING "| Log octanol-water partition coefficient | #
Octanol-water partition coefficient |  
Air-water partition coefficient (dimensionless) |  
Aerosol-air partition coefficient (dimensionless) |  
Fish-water partition coefficient (dimensionless) |  
Water reaction half life (hours) |  
Sediment reaction half life (hours) |  
Octanol-water partition coefficient  |  
Air-water partition coefficient (dimensionless)  |  
Aerosol-air partition coefficient (dimensionless)  |  
Fish-water partition coefficient (dimensionless)  |  
Water reaction half life (hours)  |  
Sediment reaction half life (hours)  

---

**Z Values common to all segments**

Z for air  |  ;ZA  
Z for aerosols  |  ;ZQ  
Z for bulk air  |  ;ZAT  
Z for water  |  ;ZW  
Z for fish with 5% lipid at equilibrium  |  ;ZF  

---

**Values which are segment specific (Pa.m³/mol)**

<table>
<thead>
<tr>
<th>Property Segment No</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part-water ptn coef (L/kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment-water ptn coef (L/kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

```
FOR I = 1 TO N
Y(I,I) = ZP(I);Y(2,I) = ZS(I);Y(3,I) = ZWT(I);Y(4,I) = ZST(I);Y(5,I) = KPSW(I);Y(6,I) = KPSW(I)
NEXT I
```

---

```
FOR J = 1 TO 6
LPRINT HS(J);
FOR I = 1 TO N
LPRINT USING "##.###"|";Y(J,I);
NEXT I
LPRINT " 
NEXT J
```

---

```
FOR J = 1 TO 6
LPRINT HS(J);
FOR I = 1 TO N
LPRINT USING "##.###"|";Y(J,I);
NEXT I
LPRINT " 
NEXT J
```

---

```
IF P2 = 0 GOTO 4020
```

---

```
LPRINT " Chemical quantity data"
```

---

```
LPRINT " Air concn ng/m³ | ##.###"|";CAN
LPRINT " Air concn mol/m³ | ##.###"|";CA
LPRINT " Fractn on aerosols | ##.###"|";FRQ
LPRINT " Air equivalence | ##.###"|";FA
```

---

```
HS(1) =" Point sources kg/year "
HS(2) =" Inflow river conc g/m³ or mg/L "
```
3760 HS(3)=" Inflow in rivers g/h"
3770 HS(4)=" Inflow in rivers kg/year"
3780 HS(5)=" Total input kg/year"
3790 HS(6)=" Inflow in rivers mol/h"
3800 HS(7)=" Point sources mol/h"
3810 HS(8)=" Total input mol/h"
3820 FOR I = 1 TO N
3830 Y(I,1)=EPK(I):Y(2,I)=CGI(I):Y(3,I)=EWG(I):Y(4,I)=EWK(I)
3840 Y(5,I)=ETK(I):Y(6,I)=EW(I):Y(7,I)=EP(I):Y(8,I)=ET(I)
3850 NEXT I
3860 LPRINT " Discharges Segment No 1 2 3 4 5 6 7 8 9"
3870 LPRINT "-------0-0-------0----------0"
4310 FOR I=1 TO N
4320 LPRINT USING "##.##^## ";Y(J,I);
4330 NEXT I
4340 LPRINT "*
4350 NEXT J
4360 LPRINT "--------------------------------------------------------------------------------------"  
4370 LPRINT "*
4380 LPRINT "Inter-segment water exchanges m3/h and D values"
4390 LPRINT " Source  Destination  "
4400 LPRINT "  1  2  3  4  5  6  7  8  9*"
4410 LPRINT "--------------------------------------------------------------------------------------"  
4420 FOR I=1 TO N
4430 LPRINT USING "|  ##|  ";I;
4440 FOR J=1 TO N
4450 LPRINT USING "|  ##|  ";GW(I,J);
4460 NEXT J
4470 LPRINT "*
4480 NEXT I
4490 LPRINT "--------------------------------------------------------------------------------------"  
4500 LPRINT "*
4510 LPRINT " Inter-segment particle exchanges (m3/h)  "
4520 LPRINT " Source  Destination  "
4530 LPRINT "  1  2  3  4  5  6  7  8  9*"
4540 LPRINT "--------------------------------------------------------------------------------------"  
4550 FOR I=1 TO N
4560 LPRINT USING "|  ##|  ";I;
4570 FOR J=1 TO N
4580 LPRINT USING "|  ##|  ";GP(I,J);
4590 NEXT J
4600 LPRINT "*
4610 NEXT I
4620 LPRINT "--------------------------------------------------------------------------------------"  
4640 LPRINT "*
4650 LPRINT " Inter-segment particle exchange D values  "
4660 LPRINT " Source  Destination  "
4670 LPRINT "  1  2  3  4  5  6  7  8  9*"
4680 LPRINT "--------------------------------------------------------------------------------------"  
4690 FOR I=1 TO N
4700 LPRINT USING "|  ##|  ";I;
4710 FOR J=1 TO N
4720 LPRINT USING "|  ##|  ";DY(I,J);
4730 NEXT J
4740 LPRINT "*
4750 NEXT I
4770 LPRINT "--------------------------------------------------------------------------------------"  
4780 LPRINT
4830 LPRINT " Inter-segment D values (total)  "
4840 LPRINT " Source  Destination  "
4850 LPRINT "  1  2  3  4  5  6  7  8  9*"
FOR I = 1 TO N
FOR J = 1 TO N
LPRINT USING "## |";I;
LPRINT USING "## |";D(I,J);
NEXT J
NEXT I
LPRINT ""
LPRINT "Sediment-water exchange processes"
LPRINT "Property Segment No 1 2 3 4 5 6 7 8 9"
LPRINT ""
HS(1)="Sediment depn g/m2/day"
HS(2)="Sediment resn g/m2/day"
HS(3)="Sediment burl g/m2/day"
HS(4)="Sediment depn m3/h"
HS(5)="Sediment resuspn m3/h"
HS(6)="Sediment burial m3/h"
FOR I = 1 TO N
Y(I,1) = DEP(I); Y(2,1) = RES(I); Y(3,1) = BUR(I)
Y(4,1) = GD(I); Y(5,1) = GR(I); Y(6,1) = GB(I)
NEXT I
LPRINT HS(J);
FOR I = 1 TO N
LPRINT USING "## |";Y(J,1);
NEXT I
LPRINT ""
LPRINT "Mass Transfer Coefficients (m/h)"
LPRINT "Volatilization: Air side "
LPRINT "Volatilization: Water side "
LPRINT "Overall water side "
LPRINT "Sediment-water diffusion"
LPRINT "Deposition velocity (m/h)"
LPRINT "Scavenging ratio "
LPRINT "Density of aerosols (g/cm3)"
LPRINT "Volume fraction aerosol particles"
LPRINT "Concentration: aerosol particles (ug/m3)"
LPRINT "Rain rate (m/year)"
LPRINT "D Values for transport and transformation processes"
LPRINT "Process Segmt No 1 2 3 4 5 6 7 8 9"
5400 LPRINT "-----------------------------------------------"
5410 FOR J = 1 TO 11
5420 LPRINT P$(J);
5430 FOR I = 1 TO N
5440 LPRINT USING "##.#^##;DP(J,I);
5450 NEXT I
5460 LPRINT ""
5470 NEXT J
5480 LPRINT "-----------------------------------------------"
5490 LPRINT "| Total D DE(I) | "
5500 FOR I = 1 TO N
5510 LPRINT USING "##.#^##;DE(I);
5520 NEXT I
5530 LPRINT ""
5540 LPRINT "| Total D DT(I) | ";
5550 FOR I = 1 TO N
5560 LPRINT USING "##.#^##;DT(I);
5570 NEXT I
5580 LPRINT ""
5590 LPRINT "| Total inpt I(I)| ";
5600 FOR I = 1 TO N
5610 LPRINT USING "##.#^##;I(I);
5620 NEXT I
5630 LPRINT ""
5640 LPRINT "-----------------------------------------------"
5650 LPRINT "Sediment response times ie VZ/D (years) "
5660 LPRINT "Process Segmt No 1 2 3 4"
5670 LPRINT " 5 6 7 8 9"
5680 LPRINT "-----------------------------------------------"
5690 FOR J = 1 TO 5
5700 LPRINT P$(J);
5710 FOR I = 1 TO N
5720 LPRINT USING "##.#^##;TYS(J,I);
5730 NEXT I
5740 LPRINT ""
5750 NEXT J
5760 LPRINT "-----------------------------------------------"
5770 LPRINT "Water response times ie VZ/D (years) "
5780 LPRINT "Process Segmt No 1 2 3 4"
5790 LPRINT " 5 6 7 8 9"
5800 LPRINT "-----------------------------------------------"
5810 FOR J = 3 TO 8
5820 LPRINT P$(J);
5830 FOR I = 1 TO N
5840 LPRINT USING "##.#^##;TYW(J,I);
5850 NEXT I
5860 LPRINT ""
5870 NEXT J
5880 LPRINT "-----------------------------------------------"
5900 H$(1)="Point sources kg/year"
5910 H$(2)="Inflow river conc g/m3 or mg/L"
5920 H$3=H3
5930 H$4=H4
5940 H$5=H5
5950 H$6=H6
5960 H$7=H7
5970 H$8=H8
5980 FOR I = 1 TO N
5990 Y(1,I)=EPK(I):Y(2,I)=CGI(I):Y(3,I)=EWG(I):Y(4,I)=EWK(I)
6000 Y(5,I)=ETK(I):Y(6,I)=EW(I):Y(7,I)=EP(I):Y(8,I)=ET(I)
6010 NEXT I
6020 \* Calculate all fugacities /equivalences
6030 J1=DT(1)
6040 J2=DT(2)-D(2,1)*D(1,2)/DT(1)
6050 J3=DT(3)-D(3,2)*D(2,3)/DT(2)
6060 J4=DT(4)-D(4,3)*D(3,4)/DT(3)
6070 J5=DT(5)-D(5,4)*D(4,5)/DT(4)
6080 J6=DT(6)-D(6,5)*D(5,6)/DT(5)
6090 J7=DT(7)-D(7,6)*D(6,7)/DT(6)
6100 J8=DT(8)-D(8,7)*D(7,8)/DT(7)
6110 J9=DT(9)-D(9,8)*D(8,9)/DT(8)
6120 IJ1=I(1)
6130 IJ2=I(2)+IJ1*D(1,2)/J1
6140 IJ3=I(3)+IJ2*D(2,3)/J2
6150 IJ4=I(4)+IJ3*D(3,4)/J3
6160 IJ5=I(5)+IJ4*D(4,5)/J4
6170 IJ6=I(6)+IJ5*D(5,6)/J5
6180 IJ7=I(7)+IJ6*D(6,7)/J6
6190 IJ8=I(8)+IJ7*D(7,8)/J7
6200 IJ9=I(9)+IJ8*D(8,9)/J8
6210 IJ9=I(9)+IJ8*D(8,9)/J8
6220 FW(9)=IJ9/J9
6230 FW(8)=(IJ8+FW(9)*D(9,8))/J8
6240 FW(7)=(IJ7+FW(8)*D(8,7))/J7
6250 FW(6)=(IJ6+FW(7)*D(7,6))/J6
6260 FW(5)=(IJ5+FW(6)*D(6,5))/J5
6270 FW(4)=(IJ4+FW(5)*D(5,4))/J4
6280 FW(3)=(IJ3+FW(4)*D(4,3))/J3
6290 FW(2)=(IJ2+FW(3)*D(3,2))/J2
6300 FW(1)=(IJ1+FW(2)*D(2,1))/J1
6310 FOR I = 1 TO N
6320 FS(I)=FW(I)*(DP(4,I)+DP(5,I))/(DP(1,I)+DP(2,I)+DP(3,I)+DP(4,I))
6330 NEXT I
6340 MTT=0:MTTK=0
6350 FOR I = 1 TO N
6360 CWT(I)=FW(I)*ZWT(I)
6370 CSTN(I)=CWT(I)*WM*1000000
6380 CSTN(I)=CSTN(I)*WM*1000/DENS(I)
6390 MWT(I)=FW(I)*VW(I)*ZWT(I)
6400 MWT(I)=MWT(I)*WM/1000
6410 MSTR(I)=MSTR(I)*WM/1000
6420 MT(I)=MSTR(I)+MST(I)
6430 NEXT I
6440 REM Calculate process rates
6450 FOR I = 1 TO N
6460 FOR J = 1 TO 3
6470 \*
R(J,I) = FS(I) * DP(J,I) : RK(J,I) = R(J,I) * WM*8760/1000
FOR J = 5 TO 6
R(J,I) = FW(I) * DP(J,I) : RK(J,I) = R(J,I) * WM*8760/1000
NEXT J
R(I,J) = (FS(I) - FW(I)) * DP(Q,I) : RK(I,J) = R(I,J) * WM*8760/1000 FOR J = 5 TO 6
R(J,I) = PW(I) * DP(J,I) : RK(J,I) = R(J,I) * WM*8760/1000 NEXT J
R(7,I) = (FW(I) - FA) * DP(7,I) : RK(7,I) = R(7,I) * WM*8760/1000
R(8,I) = FA * DP(8,I) : RK(8,I) = R(8,I) * WM*8760/1000
RSW(I) = FS(I) * DP(3,I) + DP(4,I)) : RSW(I) = RSW(I) * WM*8760/1000
RWS(I) = FW(I) * (DP(4,I) + DP(5,I)) : RWS(I) = RWS(I) * WM*8760/1000 NEXT I
FOR I = 1 TO N+1
FOR J = 1 TO N+1
R(JY(I,J) = D(I,J) * EW(I) : R(JYK(I,J) = EWY(I,J) * WM*8760/1000
NEXT J
NEXT I
FOR I = 1 TO N+1
RX(I) = RX(I) + WY(I,J)
RI(I) = RI(I) + R(I,J)
RXK(I) = RX(I) * WM*8760/1000
RIR(I) = RI(I) * WM*8760/1000
NEXT I
LPRINT "Concentrations and amounts in each segment"
H$(1) = "Aquiv in water column"
H$(2) = "Aquiv in sediment"
H$(3) = "Conc bulk water (mol/m3)"
H$(4) = "Conc bulk water (ng/L)"
H$(5) = "Conc bulk sed (mol/m3)"
H$(6) = "Conc sed solids (ng/g)"
H$(7) = "Amt water column (mol)"
H$(8) = "Amt water column (kg)"
H$(9) = "Amount in sediment (mol)"
H$(10) = "Amount in sediment (kg)"
H$(11) = "Total amt in segt (mol)"
H$(12) = "Total amt in segt (kg)"
FOR I = 1 TO N
Y(I,1) = FW(I) : Y(2,I) = FS(I) : Y(3,I) = CWT(I) : Y(4,I) = CWTN(I) : Y(5,I) = CST(I)
Y(6,I) = CWTN(I) : Y(7,I) = MWT(I)
Y(8,I) = MSTN(I) : Y(9,I) = MST(I) : Y(10,I) = MTK(I) : Y(11,I) = MT(I) : Y(12,I) = MTK(I)
NEXT I
LPRINT "Property Segment No 1 2 3 4 5 6 7 8 9"
LPRINT "-----------------------------------------------
LPRINT "------------------------------
LPRINT "------------------------------
LPRINT "------------------------------
LPRINT "------------------------------
LPRINT "------------------------------"
REM Print out transport and transformation rates
FOR I=1 TO N
   Y(6,I)=R(6,I):Y(7,I)=R(7,I):Y(8,I)=R(8,I)
NEXT I

LPRINT "Process rates mol/h"
FOR J=1 TO 8
   LPRINT P(J);
FOR I=1 TO N
   LPRINT USING "##.##~~~" ;Y(J,I);
NEXT I
NEXT J

LPRINT "Process rates kg/year"
FOR J=1 TO 8
   LPRINT P(J);
FOR I=1 TO N
   LPRINT USING "##.##~~~" ;Y(J+8,I);
NEXT I
NEXT J

LPRINT "Inter-segment transfers mol/h"
LPRINT "Source Destination"
LPRINT 1 2 3 4 5
LPRINT 6 7 8 9

LPRINT "Inter-segment transfers kg/year"
LPRINT "Source Destination"
LPRINT 1 2 3 4 5
7500 LPRINT "-------------------------------------------------------------------------------"
7510 FOR I=1 TO N+1
7520 LPRINT USING "|    |;I ;
7530 FOR J=1 TO N+1
7540 LPRINT USING "|I;RJYK(I,J);
7550 NEXT J
7560 LPRINT " -
7570 NEXT I
7580 LPRINT "-------------------------------------------------------------------------------"
7590 LPRINT " -
7600 IF P5=0 GOTO 8100
7610 FOR I=1 TO N
7620 LPRINT
7625 LPRINT CHR$(12)
7628 INPUT "Press any key to continue";QQQ$ 7630 LPRINT "Segment No";I;" ie";NS(I)";mol/h kg/year"
7640 LPRINT " -
7650 LPRINT USING "Point source discharges "###.### #####
7660 LPRINT USING "River inflow discharges "###.### #####
7670 LPRINT USING "Total inflow from adjacent segments "###.### #####
7680 LPRINT USING "Total outflow to adjacent segments "###.### #####
7690 LPRINT USING "Atmospheric deposition "###.### #####
7700 LPRINT USING "Net diffusive loss to atmosphere "###.### #####
7710 LPRINT USING "Water transformation "###.### #####
7720 LPRINT USING "Water to sediment transfer "###.### #####
7730 LPRINT USING "Sediment to water transfer "###.### #####
7740 LPRINT USING "Sediment transformation "###.### #####
7750 LPRINT USING "Sediment burial "###.### #####
7760 LPRINT " -
7770 LPRINT "Details of exchange processes"
7780 RM=FA*DP(9,I):RMK=RM*WM*8760/1000
7790 RC=FA*DP(10,I):RCK=RC*WM*8760/1000
7800 RQ=FA*DP(11,I):RQK=RQ*WM*8760/1000
7810 RVN=DP(7,I)*FW(I)-PA):RVNK=RVN*WM*8760/1000
7820 RTN=DP(4,I)*PS(I)-FW(I)):RTNK=RTN*WM*8760/1000
7830 RSWD=DP(4,I)*PS(I):RWSDK=RWSD*WM*8760/1000
7840 RWSD=DP(4,I)*FW(I):RWSDK=RWSD*WM*8760/1000
7850 RA=DP(7,I)*FA:RAK=RA*WM*8760/1000
7860 RV=DP(7,I)*FW(I):RVK=RV*WM*8760/1000
7870 SUMWI=EW(I)+EP(I)+R(8,I)+RI(I)+RSW(I):SUMWI=SUMWI*WM*8760/1000
7880 SUMWX=R(7,I)+R(6,I)+RX(I)+RWS(I):SUMWX=SUMWX*WM*8760/1000
7890 SUMSI=RSW(I):SUMSI=SUMSI*WM*8760/1000
7900 SUMSX=RSW(I)+R(2,I)+R(I,1):SUMSX=SUMSX*WM*8760/1000
7910 LPRINT USING "Rain dissolution "###.### #####
7920 LPRINT USING "Wet particle deposition "###.### #####
7930 ";R, RMK
7930 LPRINT USING "Dry particle deposition
7940 LPRINT USING "Absorption
7950 LPRINT USING "Volatileization
7960 LPRINT USING " (Net water to air diffusion)
7970 LPRINT USING "Sediment deposition
7980 LPRINT USING "Sediment resuspension
7990 LPRINT USING " (Net sediment to water diffusion)
8000 LPRINT USING "Sediment to water diffusion
8010 LPRINT USING "Water to sediment diffusion
8020 LPRINT
8030 LPRINT USING "Total input to water column
8040 LPRINT USING "Total output from water column
8050 LPRINT
8060 LPRINT USING "Total input to sediment
8070 LPRINT USING "Total output from sediment
8080 LPRINT " 
8090 NEXT I
8095 LPRINT CHR$(12)
8100 END
5 REM A SIMPLE MODEL APPLICABLE TO MANY CHEMICALS
10 LPRINT CHR$(15)
15 WIDTH "lpt1:" , 160
30 LPRINT CHR$(15)
40 WIDTH "lpt1:" , 160
50 REM DIMENSIONS AND PROPERTIES OF THE AQUATIC SYSTEM
60 A=4.642E+08 ' Lake surface area m2
70 HW=23 ' Water depth m3
80 HS=.03 ' Sediment depth m
90 VW*A*HW ' Water volumes m3
100 VS*A*HS ' Sediment volume m3
110 DEMP=2 : 'Suspended particles density kg/L
120 DENS=2 : 'Suspended solids density kg/L
130 ORGP=.12: 'organic content of particles
140 ORGS=.1: 'organic content of sediment
150 FS=.07: 'Volume fraction sediment solids
160 UB=1.48E-06: 'Particle burial velocity of bulk sedt. m/h
170 FP=.00003: 'Volume fraction of suspended particles in outflow
180 GX=5400001: 'Flow rate of water from lake m3/h
185 GP=GX*FP
190 REM INPUT OF CHEMICAL PROPERTIES
200 PRINT "Lead 1 , Copper 2 , Dichlorobenzene 3 , Tetrachlorobenzene 4 , Pentachlorobenzene 5 , Hexachlorobenzene 6 , Lindane 7 , BenzoPyrene 8 , alpha-HCH 9 , Benzo(a)pyrene 10 ."
210 INPUT QQ
220 ON QQ GOTO 230,240,250,260,270,280,290,300,310,320,
270 CS="PENTACHLOROBENZENE":WM=250.3:KDAA=0.354:VP=0.889:KPD=5.06:TDS=17000:TDM=10000:TC=25:TM=86:GOTO 340
280 CS="HEXACHLOROBENZENE":WM=284.8:KDAA=0.0782:VP=0.0023:KPD=5.6:TDS=550001:TDM=500001:TC=25:TM=230:GOTO 340
330 KOW=10*KPD 'octanol-water partition coefficient
340 KPW=.41*KOW*ORGP*DEMP
360 KSW=.41*KOW*ORGS*DENS
370 'Mass Transfer Coefficients (m/h)
380 KA=11 'volatilization: air side
390 KW=.01 'volatilization: water side
400 KV=KDAA/(KDAA/KW+1/KA) 'overall water side
410 I=114 : 'Total emission g/h
415 REM REMOVAL FLOW RATES AND PERCENTAGE REMOVAL OF EACH
420 XV=KV*A
430 XX=GX
440 XP=GP*KP
450 XW=.7*VW/TDW
460 XS=.7*VS*FS*KSW/TDS
470 XB=UB*A*FS*KSW
480 XT=XV+XX+XP+XW+XS+XB
490 PXV=XV*100/XT
500 PXX=XX*100/XT
510 PXP=XP*100/XT
520 PXW=XW*100/XT
530 PXS=XS*100/XT
540 PXB=XB*100/XT
550 CW=(I/XT)*1000 "CONC. IN WATER microgram/L"
560 CS=(CW*KSW)/DENS "CONC. IN SEDIMENT microgram/gram"
570 PRINT,USING "Concentration in water ";CW
580 PRINT,USING "Concentration in sediment ";CS
590 PRINT,USING "VOLATILIZATION RATE:PERCENT ";XV, PXV
600 PRINT,USING "WATER FLOW RATE, PERCENT ";XX, PXX
610 PRINT,USING "PARTICLE FLOW RATE, PERCENT ";XP, PXP
620 PRINT,USING "WATER TRANSFORMATION, PERCENT ";XW, PXW
630 PRINT,USING "SEDT. TRANSFORMATION, PERCENT ";XS, PXS
640 PRINT,USING "SEDIMENT BURIAL, PERCENT ";XB, PXB
650 END
5 REM A SIMPLE MODEL APPLICABLE TO MANY CHEMICALS

10 LPRINT CHR$(15)
15 WIDTH "lpt1":160
30 LPRINT CHR$(15)
40 WIDTH "lpt1":160

50 REM DIMENSIONS AND PROPERTIES OF THE AQUATIC SYSTEM
60 A=4600000: 'Lake surface area m^2
70 HW=18: 'Water depth m
80 HS=.03: 'Sediment depth m
90 VW=A*HW: 'Water volumes m^3
100 VS=A*HS: 'Sediment volumes m^3

110 DENP=2: 'Suspended particles density kg/L
120 DENS=2: 'Suspended solids density kg/L
130 ORGP=.2: 'Organic content of particles
140 ORGS=.2: 'Organic content of sediment
150 FS=.07: 'Volume fraction sediment solids
160 UB=5.2E-07: 'Particle burial velocity of bulk sedt. m/h
170 FP=.00001: 'Volume fraction of sus particles in outflow
180 GX=350: 'Flow rate of water from lake m^3/h
185 GP=GX*FP

190 REM INPUT OF CHEMICAL PROPERTIES
200 PRINT "Lead 1, Copper 2, Dichlorobenzene 3, Tetrachlorobenzene
4, Pentachlorobenzene 5, Hexachlorobenzene 6, Lindane 7, BenzoPyrene 8
, alpha-HCH 9, Benzofluoranthene 10."

210 INPUT QQ
220 ON QQ GOTO 230,240,250,260,270,280,290,300,310,320,
240 CS="Copper":WM=63.6:KDAW=1E-11:KFW=333000!:KSW=1336000!:KDFW=9:KDW=1000!:TDS=1E+11:TDW=1E+11:TC=25:GOTO 380
290 CS="LINDANE(gamma-HCH)":WM=290.85:SOLY=7.3:KDAW=.000117:KSW=3.7:TDS=170:00:TDW=6000:TC=25:TM=112.5:GOTO 340
320 CS="BENZO(b)FLUORANTHENE":WM=252.32:KDAW=.000102:KSW=6.5:TDS=35000!:TDW=12000:TC=25:TM=168:GOTO 340
340 KOW=10*LKOW
350 KFW=.41*KOW*ORGP*DENP
360 KSW=.41*KOW*ORGS*DENS
370 'Mass Transfer Coefficients (m/h)
380 KA = 1: 'volatilization: air side
390 KW = .01: 'volatilization: water side
400 KV = KDAW/(KDAW/KW + 1/KA): 'overall water side
410 I=114: 'Total emission g/h

415 REM REMOVAL FLOW RATES AND PERCENTAGE REMOVAL OF EACH
420 KV*KV*A
430 XX=GX
440 XP=GP*KFW
450 KW=.7*VW/TDW
460 XS=(.7*VS*FS*KSW)/TDS
470 XB=UB*A*FS*KSW
480 XT=XV+XX+XP+XW+XS+XB
490 PXV=XV*100/XT
500 PXX=XX*100/XT
510 PXP=XP*100/XT
520 PXW=XW*100/XT
530 PXS=XS*100/XT
540 PXB=XB*100/XT
550 CW=(I/XT)*1000  'CONC. IN WATER microgram/L
560 CS=(CW*KSW)/DENS ; 'CONC. IN SEDIMENT microgram/gram
570 PRINT, USING "Concentration in water  #######.###"; CW
580 PRINT, USING "Concentration in sediment  #######.###"; CS
590 PRINT, USING "VOLATILIZATION RATE: PERCENT  #######.###"; XV, PXV
600 PRINT, USING "WATER FLOW RATE, PERCENT  #######.###"; XX, PXX
610 PRINT, USING "PARTICLE FLOW RATE, PERCENT  #######.###"; XP, PXP
620 PRINT, USING "WATER TRANSFORMATION, PERCENT  #######.###"; XW, PXW
630 PRINT, USING "SEDIMENT TRANSFORMATION, PERCENT  #######.###"; XS, PXS
640 PRINT, USING "SEDIMENT BURIAL, PERCENT  #######.###"; XB, PXB
650 END
### Output of QWASI program (lindane in Rihand Reservoir)

#### Physical-chemical and Partitioning Properties of LINDANE (gamma-HCH)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (deg C)</td>
<td>25</td>
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<tr>
<td>Temperature (deg K)</td>
<td>298</td>
</tr>
<tr>
<td>Gas constant (J/mol K)</td>
<td>8.314</td>
</tr>
<tr>
<td>Molecular mass (g/mol)</td>
<td>291</td>
</tr>
<tr>
<td>Melting point (deg C) (system temp. for liquids)</td>
<td>113</td>
</tr>
<tr>
<td>Solubility (g/m³)</td>
<td>7.30E+00</td>
</tr>
<tr>
<td>Solubility (mol/m³)</td>
<td>2.51E-02</td>
</tr>
<tr>
<td>Vapour pressure (Pa)</td>
<td>7.30E-03</td>
</tr>
<tr>
<td>Subcooled liquid vapour pressure (Pa)</td>
<td>5.36E-02</td>
</tr>
<tr>
<td>Fugacity ratio</td>
<td>1.36E-01</td>
</tr>
<tr>
<td>Henry's Law constant (Pa m⁻³/mol)</td>
<td>2.91E-01</td>
</tr>
<tr>
<td>Log octanol-water partition coefficient</td>
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<tr>
<td>Octanol-water partition coefficient</td>
<td>5.01E+03</td>
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<tr>
<td>Air-water partition coefficient (dimensionless)</td>
<td>1.17E-04</td>
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<tr>
<td>Aerosol-air partition coefficient (dimensionless)</td>
<td>1.12E+08</td>
</tr>
<tr>
<td>Fish-water partition coefficient (dimensionless)</td>
<td>2.51E+02</td>
</tr>
<tr>
<td>Water reaction half life (hours)</td>
<td>6.00E+03</td>
</tr>
<tr>
<td>Sediment reaction half life (hours)</td>
<td>1.70E+04</td>
</tr>
</tbody>
</table>

#### Z Values common to all segments

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Z for air</td>
<td>1.17E-04</td>
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<tr>
<td>Z for aerosols</td>
<td>1.31E+04</td>
</tr>
<tr>
<td>Z for bulk air</td>
<td>1.19E-04</td>
</tr>
<tr>
<td>Z for water</td>
<td>1.00E+00</td>
</tr>
<tr>
<td>Z for fish with 5% lipid at equilibrium</td>
<td>2.51E+02</td>
</tr>
</tbody>
</table>

#### Z Values which are segment specific (Pa.m³/mol)

<table>
<thead>
<tr>
<th>Property</th>
<th>Segment No 1</th>
<th>Segment No 2</th>
<th>Segment No 3</th>
<th>Segment No 4</th>
<th>Segment No 5</th>
<th>Segment No 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z for water particles</td>
<td>3.70E+02</td>
<td>4.11E+02</td>
<td>6.16E+02</td>
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<tr>
<td>Z for sediment solids</td>
<td>2.59E+02</td>
<td>3.29E+02</td>
<td>4.11E+02</td>
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<td></td>
<td></td>
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<tr>
<td>Z for bulk water</td>
<td>1.02E+00</td>
<td>1.02E+00</td>
<td>1.01E+00</td>
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<td></td>
<td></td>
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<tr>
<td>Z for bulk sediment</td>
<td>1.91E+01</td>
<td>2.39E+01</td>
<td>2.97E+01</td>
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<td></td>
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<tr>
<td>Part-water ptn coef (L/kg)</td>
<td>2.05E+02</td>
<td>2.05E+02</td>
<td>3.08E+02</td>
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<tr>
<td>Sedt-water ptn coef (L/kg)</td>
<td>1.44E+02</td>
<td>1.64E+02</td>
<td>2.05E+02</td>
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</table>

#### Chemical quantity data

<table>
<thead>
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<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Air concn ng/m³</td>
<td>3.00E-01</td>
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<tr>
<td>Air concn mol/m³</td>
<td>1.03E-12</td>
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<tr>
<td>Fractn on aerosols</td>
<td>1.22E-02</td>
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<tr>
<td>Air equivalence</td>
<td>8.66E-09</td>
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#### Discharges

<table>
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<tr>
<th>Property</th>
<th>Segment No 1</th>
<th>Segment No 2</th>
<th>Segment No 3</th>
<th>Segment No 4</th>
<th>Segment No 5</th>
<th>Segment No 6</th>
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</thead>
<tbody>
<tr>
<td>Point sources kg/year</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>6.50E+03</td>
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<tr>
<td>Inflow river conc g/m³ or mg/L</td>
<td>2.00E-04</td>
<td>1.50E-03</td>
<td>1.50E-03</td>
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<tr>
<td>Inflow in rivers g/h</td>
<td>1.13E+02</td>
<td>1.77E+01</td>
<td>1.65E+00</td>
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<tr>
<td>Inflow in rivers kg/year</td>
<td>9.90E+02</td>
<td>1.55E+02</td>
<td>1.45E+01</td>
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### Segment properties

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<tr>
<td>Frn OC in water particles</td>
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<td>1.00E-01</td>
<td>1.00E-01</td>
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<tr>
<td>Frn OC in sedmt particles</td>
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<td>7.00E-02</td>
<td>8.00E-02</td>
<td>1.00E-01</td>
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<tr>
<td>Den particles wtr (g/cm³)</td>
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<td>1.80E+00</td>
<td>2.00E+00</td>
<td>2.00E+00</td>
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<tr>
<td>Den sur sed parts (g/cm³)</td>
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<td>1.80E+00</td>
<td>2.00E+00</td>
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<td>Vol frn water particles</td>
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<td>Conc water part (mg/L)</td>
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<td>9.60E+01</td>
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<td>Vol frn sol in sediment</td>
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<td>7.00E-02</td>
<td>7.00E-02</td>
<td>7.00E-02</td>
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<tr>
<td>Water area (m²)</td>
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<td>1.49E+08</td>
<td>2.00E+08</td>
<td>1.16E+08</td>
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<tr>
<td>Sediment area (m²)</td>
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<td>1.49E+08</td>
<td>2.00E+08</td>
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<tr>
<td>Water volume (m³)</td>
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<td>4.40E+09</td>
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<td>Sediment volume (m³)</td>
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<td>2.98E+06</td>
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<td>Mean water depth (m)</td>
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<td>Mean active sed depth (m)</td>
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<td>2.00E-02</td>
<td>2.00E-02</td>
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<tr>
<td>Rain rate (m³/h)</td>
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<td>3.40E+03</td>
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<td>Water inflow rate (m³/h)</td>
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### Inter-segment water exchanges m³/h and D values

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### Inter-segment particle exchanges (m³/h)

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<tr>
<td>3</td>
<td>1</td>
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### Inter-segment particle exchange D values

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<tbody>
<tr>
<td>1</td>
<td>2</td>
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### Inter-segment D values (total)

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### Sediment-water exchange processes

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### Mass Transfer Coefficients (m/h)

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### D Values for transport and transformation processes

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### Sediment response times ie VZ/D (years)

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### Concentrations and Amounts in Each Segment

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Grand total mol 11492.87
Grand total kg 3342.701

### Process Rates

**mol/h**

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**kg/year**

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### Inter-segment transfers \( \text{mol/h} \)

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### Inter-segment transfers \( \text{kg/year} \)

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Details of exchange processes

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<td>(Net sediment to water diffusion)</td>
<td>0.003082</td>
<td>7.852</td>
</tr>
<tr>
<td>Sediment to water diffusion</td>
<td>0.015165</td>
<td>38.638</td>
</tr>
<tr>
<td>Water to sediment diffusion</td>
<td>0.012083</td>
<td>30.786</td>
</tr>
</tbody>
</table>

Total input to water column   0.426323  1086.206
Total output from water column | 0.426323  | 1086.206 |

Total input to sediment 0.019842  50.555
Total output from sediment 0.019842  50.555
## Details of Exchange Processes

<table>
<thead>
<tr>
<th>Process</th>
<th>mol/h</th>
<th>kg/year</th>
</tr>
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<tbody>
<tr>
<td>Rain dissolution</td>
<td>0.000040</td>
<td>0.101</td>
</tr>
<tr>
<td>Wet particle deposition</td>
<td>0.000011</td>
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<tr>
<td>Dry particle deposition</td>
<td>0.000025</td>
<td>0.064</td>
</tr>
<tr>
<td>Absorption</td>
<td>0.000201</td>
<td>0.513</td>
</tr>
<tr>
<td>Volatilization</td>
<td>0.008900</td>
<td>22.675</td>
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<tr>
<td>(Net water to air diffusion)</td>
<td>0.008698</td>
<td>22.162</td>
</tr>
<tr>
<td>Sediment deposition</td>
<td>0.008537</td>
<td>21.752</td>
</tr>
<tr>
<td>Sediment resuspension</td>
<td>0.000384</td>
<td>0.977</td>
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<td>(Net sediment to water diffusion)</td>
<td>0.003327</td>
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<tr>
<td>Sediment to water diffusion</td>
<td>0.018667</td>
<td>47.561</td>
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<tr>
<td>Water to sediment diffusion</td>
<td>0.015340</td>
<td>39.085</td>
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</table>

| Total input to water column                  | 0.500255 | 1274.574 |
| Total output from water column               | 0.500255 | 1274.574 |

| Total input to sediment                      | 0.023878 | 60.837 |
| Total output from sediment                   | 0.023878 | 60.837 |
Segment No 3 is North-west basin

<table>
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<th>Description</th>
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<th>kg/year</th>
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<tr>
<td>Point source discharges</td>
<td>2.551175</td>
<td>6500.000</td>
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<td>River inflow discharges</td>
<td>0.005673</td>
<td>14.454</td>
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<tr>
<td>Total inflow from adjacent segments</td>
<td>0.247503</td>
<td>630.600</td>
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<tr>
<td>Total outflow to adjacent segments</td>
<td>1.795621</td>
<td>4574.966</td>
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<tr>
<td>Atmospheric deposition</td>
<td>0.000044</td>
<td>0.113</td>
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<tr>
<td>Net diffusive loss to atmosphere</td>
<td>0.037785</td>
<td>96.270</td>
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<tr>
<td>Water transformation</td>
<td>0.948729</td>
<td>2417.215</td>
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<tr>
<td>Water to sediment transfer</td>
<td>0.107283</td>
<td>273.340</td>
</tr>
<tr>
<td>Sediment to water transfer</td>
<td>0.087496</td>
<td>222.925</td>
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<td>Sediment transformation</td>
<td>0.010503</td>
<td>26.759</td>
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<tr>
<td>Sediment burial</td>
<td>0.009285</td>
<td>23.656</td>
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Details of exchange processes

<table>
<thead>
<tr>
<th>Description</th>
<th>mol/h</th>
<th>kg/year</th>
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<tbody>
<tr>
<td>Rain dissolution</td>
<td>0.000023</td>
<td>0.059</td>
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<tr>
<td>Wet particle deposition</td>
<td>0.000007</td>
<td>0.017</td>
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<tr>
<td>Dry particle deposition</td>
<td>0.000015</td>
<td>0.037</td>
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<tr>
<td>Absorption</td>
<td>0.000117</td>
<td>0.298</td>
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<tr>
<td>Volatilization</td>
<td>0.037902</td>
<td>96.568</td>
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<tr>
<td>(Net water to air diffusion)</td>
<td>0.037785</td>
<td>96.270</td>
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<td>Sediment deposition</td>
<td>0.041952</td>
<td>106.887</td>
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<td>Sediment resuspension</td>
<td>0.000743</td>
<td>1.892</td>
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<tr>
<td>(Net sediment to water diffusion)</td>
<td>0.021422</td>
<td>54.580</td>
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<tr>
<td>Sediment to water diffusion</td>
<td>0.086753</td>
<td>221.033</td>
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<tr>
<td>Water to sediment diffusion</td>
<td>0.065331</td>
<td>166.453</td>
</tr>
</tbody>
</table>

Total input to water column                       | 2.891891 | 7368.093 |
Total output from water column                     | 2.889418 | 7361.791 |

Total input to sediment                            | 0.107283 | 273.340 |
Total output from sediment                          | 0.107283 | 273.340 |
Output of QWASI program (BaP in Rihand Reservoir)

Physical-chemical and Partitioning Properties of BENZO(a)PYRENE

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Temperature (deg C)</td>
<td>25</td>
</tr>
<tr>
<td>Temperature (deg K)</td>
<td>298</td>
</tr>
<tr>
<td>Gas constant (J/mol K)</td>
<td>8.314</td>
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<tr>
<td>Molecular mass (g/mol)</td>
<td>252</td>
</tr>
<tr>
<td>Melting point (deg C)</td>
<td>175</td>
</tr>
<tr>
<td>Solubility (g/m³)</td>
<td>2.00E-03</td>
</tr>
<tr>
<td>Solubility (mol/m³)</td>
<td>7.93E-06</td>
</tr>
<tr>
<td>Vapour pressure (Pa)</td>
<td>1.50E-07</td>
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<tr>
<td>Subcooled liquid vapour pressure (Pa)</td>
<td>4.58E-06</td>
</tr>
<tr>
<td>Fugacity ratio</td>
<td>3.28E-02</td>
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<tr>
<td>Henry’s Law constant (Pa m⁻³/mol)</td>
<td>1.89E-02</td>
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<tr>
<td>Log octanol-water partition coefficient</td>
<td>6.04</td>
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<tr>
<td>Octanol-water partition coefficient</td>
<td>1.10E+06</td>
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<tr>
<td>Air -water partition coefficient (dimensionless)</td>
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<tr>
<td>Aerosol-air partition coefficient (dimensionless)</td>
<td>1.31E+12</td>
</tr>
<tr>
<td>Fish-water partition coefficient (dimensionless)</td>
<td>5.48E+04</td>
</tr>
<tr>
<td>Water reaction half life (hours)</td>
<td>1.00E+04</td>
</tr>
<tr>
<td>Sediment reaction half life (hours)</td>
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</table>

Z Values common to all segments

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z for air</td>
<td>7.64E-06</td>
</tr>
<tr>
<td>Z for aerosols</td>
<td>1.00E+07</td>
</tr>
<tr>
<td>Z for bulk air</td>
<td>1.11E-03</td>
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<tr>
<td>Z for water</td>
<td>1.00E+00</td>
</tr>
<tr>
<td>Z for fish with 5% lipid at equilibrium</td>
<td>5.48E+04</td>
</tr>
</tbody>
</table>

Z Values which are segment specific (Pa.m³/mol)

<table>
<thead>
<tr>
<th>Property</th>
<th>Segment No 1</th>
<th>Segment No 2</th>
<th>Segment No 3</th>
<th>Segment No 4</th>
<th>Segment No 5</th>
<th>Segment No 6</th>
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</thead>
<tbody>
<tr>
<td>Z for water particles</td>
<td>8.09E+04</td>
<td>8.99E+04</td>
<td>1.35E+05</td>
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<tr>
<td>Z for sediment solids</td>
<td>5.66E+04</td>
<td>7.19E+04</td>
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<tr>
<td>Z for bulk water</td>
<td>5.32E+00</td>
<td>4.64E+00</td>
<td>2.28E+00</td>
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<td></td>
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<tr>
<td>Z for bulk sediment</td>
<td>3.97E+03</td>
<td>5.04E+03</td>
<td>6.29E+03</td>
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<td></td>
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<tr>
<td>Part-water ptn coef(L/kg)</td>
<td>4.50E+04</td>
<td>4.50E+04</td>
<td>6.74E+04</td>
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<tr>
<td>Sedt-water ptn coef(L/kg)</td>
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<td>3.60E+04</td>
<td>4.50E+04</td>
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Chemical quantity data

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<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Air concn ng/m³</td>
<td>1.10E+01</td>
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<tr>
<td>Air concn mol/m³</td>
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<tr>
<td>Fractn on aerosols</td>
<td>9.93E-01</td>
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<tr>
<td>Air equivalence</td>
<td>3.93E-08</td>
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Discharges

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<tr>
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<th>Segment No 1</th>
<th>Segment No 2</th>
<th>Segment No 3</th>
<th>Segment No 4</th>
<th>Segment No 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point sources kg/year</td>
<td>4.30E+00</td>
<td>5.40E+00</td>
<td>2.18E+02</td>
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<td></td>
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<tr>
<td>Inflow river conc g/m³ or mg/L</td>
<td>1.00E-06</td>
<td>5.00E-05</td>
<td>9.00E-05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inflow in rivers g/h</td>
<td>5.65E-01</td>
<td>5.90E-01</td>
<td>9.90E-02</td>
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<tr>
<td>Inflow in rivers kg/year</td>
<td>4.95E+00</td>
<td>5.17E+00</td>
<td>8.67E-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Grand total mol/h
- 1.08E-01

### Grand total g/h
- 2.72E+01

### Grand total kg/year
- 2.39E+02

#### Segment properties

<table>
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<th>Segment No</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
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<tr>
<td>Frn OC in water particles</td>
<td>1.00E-01</td>
</tr>
<tr>
<td>Frn OC in solid particles</td>
<td>7.00E-02</td>
</tr>
<tr>
<td>Den particles wtr (g/cm³)</td>
<td>1.80E+00</td>
</tr>
<tr>
<td>Den sur sed parts (g/cm³)</td>
<td>1.80E+00</td>
</tr>
<tr>
<td>Vol frn water particles</td>
<td>5.33E-05</td>
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<tr>
<td>Conc water part (mg/L)</td>
<td>9.60E+01</td>
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<tr>
<td>Vol frn sol in sediment</td>
<td>7.00E-02</td>
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<tr>
<td>Water area (m²)</td>
<td>1.49E+08</td>
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<tr>
<td>Sediment area (m²)</td>
<td>1.49E+08</td>
</tr>
<tr>
<td>Water volume (m³)</td>
<td>2.98E+09</td>
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<tr>
<td>Sediment volume (m³)</td>
<td>2.98E+06</td>
</tr>
<tr>
<td>Mean water depth (m)</td>
<td>2.00E+01</td>
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<tr>
<td>Mean active sed depth (m)</td>
<td>2.00E-02</td>
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<tr>
<td>Rain rate (m³/h)</td>
<td>5.40E+03</td>
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<tr>
<td>Water inflow rate (m³/h)</td>
<td>5.65E+05</td>
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#### Inter-segment water exchanges m³/h and D values

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<tr>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00E+00</td>
<td>6.22E+05</td>
<td>0.00E+00</td>
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<td></td>
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</tr>
<tr>
<td>2</td>
<td>5.65E+04</td>
<td>0.00E+00</td>
<td>6.34E+05</td>
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<tr>
<td>3</td>
<td>0.00E+00</td>
<td>5.77E+04</td>
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#### Inter-segment particle exchanges (m³/h)

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<th>5</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00E+00</td>
<td>3.31E+01</td>
<td>0.00E+00</td>
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<tr>
<td>2</td>
<td>2.29E+00</td>
<td>0.00E+00</td>
<td>2.57E+01</td>
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<tr>
<td>3</td>
<td>5.48E+01</td>
<td>0.00E+00</td>
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#### Inter-segment particle exchange D values

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<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00E+00</td>
<td>2.68E+06</td>
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</tr>
<tr>
<td>2</td>
<td>2.68E+05</td>
<td>0.00E+00</td>
<td>2.31E+06</td>
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<tr>
<td>3</td>
<td>0.00E+00</td>
<td>7.39E+04</td>
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#### Inter-segment D values (total)

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<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00E+00</td>
<td>3.30E+06</td>
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<tr>
<td>2</td>
<td>2.62E+05</td>
<td>0.00E+00</td>
<td>2.94E+06</td>
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</table>
### Sediment-water exchange processes

<table>
<thead>
<tr>
<th>Property</th>
<th>Segment No</th>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sediment depn g/m²/day</td>
<td>1.50E+01</td>
<td>1.30E+01</td>
<td>1.00E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment resn g/m²/day</td>
<td>1.20E+00</td>
<td>6.00E-01</td>
<td>2.00E-01</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Sediment burl g/m²/day</td>
<td>6.50E+00</td>
<td>4.70E+00</td>
<td>2.50E+00</td>
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</tr>
<tr>
<td>Sediment depn m³/h</td>
<td>5.17E+01</td>
<td>5.41E+01</td>
<td>2.42E+01</td>
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<tr>
<td>Sediment respn m³/h</td>
<td>4.13E+00</td>
<td>2.50E+00</td>
<td>4.85E-01</td>
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<tr>
<td>Sediment burial m³/h</td>
<td>2.24E+01</td>
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<td>6.06E+00</td>
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### Mass Transfer Coefficients (m/h)

<table>
<thead>
<tr>
<th>Process</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volatilization:</td>
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</tr>
<tr>
<td>Air side</td>
<td>1.00E+00</td>
</tr>
<tr>
<td>Water side</td>
<td>1.00E-02</td>
</tr>
<tr>
<td>Overall water side</td>
<td>7.63E-06</td>
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<tr>
<td>Sediment-water diffusion</td>
<td>2.00E-04</td>
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</tbody>
</table>

### Atmospheric Flow and Deposition Parameters

<table>
<thead>
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<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
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<td>Deposition velocity (m/h)</td>
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<tr>
<td>Scavenging ratio</td>
<td>2.00E+05</td>
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<tr>
<td>Density of aerosols (g/cm³)</td>
<td>1.50E+00</td>
</tr>
<tr>
<td>Volume fraction aerosol particles</td>
<td>1.10E-10</td>
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<tr>
<td>Concentration: aerosol particles (ug/m³)</td>
<td>1.65E+02</td>
</tr>
<tr>
<td>Rain rate (m/year)</td>
<td>2.00E-01</td>
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### D Values for transport and transformation processes

<table>
<thead>
<tr>
<th>Process</th>
<th>Segmt No</th>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sediment burl</td>
<td>1.27E+06</td>
<td>1.41E+06</td>
<td>5.45E+05</td>
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<td></td>
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<tr>
<td>Sediment trnf</td>
<td>2.73E+05</td>
<td>4.65E+05</td>
<td>3.38E+05</td>
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<tr>
<td>Sediment resn</td>
<td>2.34E+05</td>
<td>1.80E+05</td>
<td>4.36E+04</td>
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<td></td>
<td></td>
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<tr>
<td>Sedt-watr difn</td>
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<td>4.00E+04</td>
<td>2.33E+04</td>
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<tr>
<td>Sedt depn</td>
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### Sediment response times ie VZ/D (years)

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### Water response times in $VZ/D$ (years)

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### Concentrations and amounts in each segment

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**Grand total mol** 4580.316
**Grand total kg** 1155.705

### Process rates mol/h

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### Process rates kg/year

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### Inter-segment transfers mol/h

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### Inter-segment transfers kg/year

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Segment No 1 is South basin

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Details of exchange processes

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Total input to water column 0.111357 246.135
Total output from water column 0.111357 246.135

Total input to sediment 0.054469 120.393
Total output from sediment 0.054469 120.393
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Details of exchange processes

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<td>2.373</td>
</tr>
<tr>
<td>Sediment to water diffusion</td>
<td>0.001871</td>
<td>4.135</td>
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<tr>
<td>Water to sediment diffusion</td>
<td>0.000798</td>
<td>1.764</td>
</tr>
</tbody>
</table>

Total input to water column           | 0.190171 | 420.340 |
Total output from water column         | 0.190171 | 420.340 |

Total input to sediment               | 0.097955 | 216.513 |
Total output from sediment             | 0.097955 | 216.513 |
<table>
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<tr>
<th>Segment No 3 is North-west basin</th>
<th>mol/h</th>
<th>kg/year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point source discharges</td>
<td>0.098628</td>
<td>218.000</td>
</tr>
<tr>
<td>River inflow discharges</td>
<td>0.000392</td>
<td>0.867</td>
</tr>
<tr>
<td>Total inflow from adjacent segments</td>
<td>0.058778</td>
<td>129.918</td>
</tr>
<tr>
<td>Total outflow to adjacent segments</td>
<td>0.067468</td>
<td>149.125</td>
</tr>
<tr>
<td>Atmospheric deposition</td>
<td>0.073449</td>
<td>162.345</td>
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<tr>
<td>Net diffusive loss to atmosphere</td>
<td>0.000006</td>
<td>0.014</td>
</tr>
<tr>
<td>Water transformation</td>
<td>0.021388</td>
<td>47.275</td>
</tr>
<tr>
<td>Water to sediment transfer</td>
<td>0.153137</td>
<td>338.482</td>
</tr>
<tr>
<td>Sediment to water transfer</td>
<td>0.010776</td>
<td>23.819</td>
</tr>
<tr>
<td>Sediment transformation</td>
<td>0.054539</td>
<td>120.549</td>
</tr>
<tr>
<td>Sediment burial</td>
<td>0.087822</td>
<td>194.114</td>
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Details of exchange processes

<table>
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<th>Process</th>
<th>mol/h</th>
<th>kg/year</th>
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</thead>
<tbody>
<tr>
<td>Rain dissolution</td>
<td>0.000104</td>
<td>0.231</td>
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<tr>
<td>Wet particle deposition</td>
<td>0.022992</td>
<td>50.820</td>
</tr>
<tr>
<td>Dry particle deposition</td>
<td>0.050352</td>
<td>111.295</td>
</tr>
<tr>
<td>Absorption</td>
<td>0.000035</td>
<td>0.077</td>
</tr>
<tr>
<td>Volatilization</td>
<td>0.000041</td>
<td>0.091</td>
</tr>
<tr>
<td>(Net water to air diffusion)</td>
<td>0.000006</td>
<td>0.014</td>
</tr>
<tr>
<td>Sediment deposition</td>
<td>0.152055</td>
<td>336.090</td>
</tr>
<tr>
<td>Sediment resuspension</td>
<td>0.007026</td>
<td>15.529</td>
</tr>
<tr>
<td>(Net sediment to water diffusion)</td>
<td>0.002668</td>
<td>5.898</td>
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<tr>
<td>Sediment to water diffusion</td>
<td>0.003751</td>
<td>8.290</td>
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<td>Water to sediment diffusion</td>
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<td>Total input to water column</td>
<td>0.242024</td>
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<td>Total output from water column</td>
<td>0.241999</td>
<td>534.897</td>
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<tr>
<td>Total input to sediment</td>
<td>0.153137</td>
<td>338.482</td>
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<tr>
<td>Total output from sediment</td>
<td>0.153137</td>
<td>338.482</td>
</tr>
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</table>
Appendix B: Calibration plots and calculations for partition coefficient measurements

Octanol-water Partition Coefficient
Chemical: 1,2,3,4 Tetrachlorobenzene
Temp: 25°C

<table>
<thead>
<tr>
<th>Conc</th>
<th>Area</th>
<th>Avg. area</th>
<th>STD</th>
<th>Std. + avg</th>
<th>Std. - avg</th>
<th>Final avg.</th>
</tr>
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<tr>
<td>0.19</td>
<td>12358</td>
<td>12477</td>
<td>231.17</td>
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<td>32705.25</td>
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<td></td>
<td>12211</td>
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<tr>
<td></td>
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<tr>
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<td>12600</td>
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<td></td>
<td>0.5</td>
<td>34784</td>
<td>34241.75</td>
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<td>34842.78</td>
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<td></td>
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<td>152980</td>
<td>135903.3</td>
<td>2554.336</td>
<td>135903.3</td>
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<tr>
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<td>Area</td>
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<td>STD</td>
<td>Std. + area</td>
<td>Std. - area</td>
<td>Final area</td>
</tr>
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<tr>
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<td>135903.3</td>
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<tr>
<td>4</td>
<td>244890</td>
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</tbody>
</table>

Data analysis (Aqueous phase)
sample 1

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>14498</td>
<td>0.1625</td>
<td>0.032473</td>
</tr>
<tr>
<td>14580</td>
<td>0.161748</td>
<td>0.032322</td>
</tr>
<tr>
<td>14460</td>
<td>0.163383</td>
<td>0.032849</td>
</tr>
<tr>
<td>Avg. conc.</td>
<td>0.032481</td>
<td></td>
</tr>
<tr>
<td>SD</td>
<td>0.000164</td>
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</tr>
<tr>
<td>Avg + SD</td>
<td>0.032845</td>
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</tr>
<tr>
<td>Avg - SD</td>
<td>0.032322</td>
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</tr>
<tr>
<td>Final avg.</td>
<td>0.032481 (mg/L)</td>
<td></td>
</tr>
</tbody>
</table>

Data analysis (Octanol phase)
sample 1

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>133300</td>
<td>2.109088</td>
<td>947.7394</td>
</tr>
<tr>
<td>134950</td>
<td>2.13274</td>
<td>950.7331</td>
</tr>
<tr>
<td>135890</td>
<td>2.145167</td>
<td>955.3253</td>
</tr>
<tr>
<td>134960</td>
<td>2.132331</td>
<td>956.9539</td>
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<tr>
<td>Avg. conc.</td>
<td>958.1879</td>
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<tr>
<td>SD</td>
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<tr>
<td>Avg + SD</td>
<td>967.173</td>
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<tr>
<td>Avg - SD</td>
<td>949.2029</td>
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</tr>
<tr>
<td>Final avg.</td>
<td>981.8708 (mg/L)</td>
<td></td>
</tr>
</tbody>
</table>

Data analysis (Aqueous phase)
sample 2

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>14038</td>
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</tr>
<tr>
<td>14038</td>
<td>0.156992</td>
<td>0.037448</td>
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<tr>
<td>Avg. conc.</td>
<td>0.037448</td>
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</tr>
<tr>
<td>SD</td>
<td>2.78586</td>
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<td>Avg + SD</td>
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<td>Avg - SD</td>
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<tr>
<td>Final avg.</td>
<td>0.037448 (mg/L)</td>
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</tbody>
</table>

Data analysis (Aqueous phase)
sample 3

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>14287</td>
<td>0.160227</td>
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</tr>
<tr>
<td>14103</td>
<td>0.157065</td>
<td>0.040241</td>
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<tr>
<td>Avg. conc.</td>
<td>0.040789</td>
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<tr>
<td>SD</td>
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</tr>
<tr>
<td>Avg + SD</td>
<td>0.041082</td>
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<tr>
<td>Avg - SD</td>
<td>0.040308</td>
<td></td>
</tr>
<tr>
<td>Final avg.</td>
<td>0.040894 (mg/L)</td>
<td></td>
</tr>
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Data analysis (Octanol phase)
sample 2

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>131330</td>
<td>2.073875</td>
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<tr>
<td>131040</td>
<td>2.069134</td>
<td>931.1101</td>
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<tr>
<td>131830</td>
<td>2.082051</td>
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<tr>
<td>Avg. conc.</td>
<td>933.759</td>
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<tr>
<td>SD</td>
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<tr>
<td>Avg + SD</td>
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<td>Avg - SD</td>
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<tr>
<td>Final avg.</td>
<td>933.759 (mg/L)</td>
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Data analysis (Octanol phase)
sample 3

<table>
<thead>
<tr>
<th>Area</th>
<th>Conc.</th>
<th>Act. conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>132150</td>
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<td>132160</td>
<td>2.067447</td>
<td>939.3512</td>
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<tr>
<td>131840</td>
<td>2.062215</td>
<td>936.9886</td>
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<tr>
<td>Avg. conc.</td>
<td>938.5418</td>
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</tr>
<tr>
<td>SD</td>
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</tr>
<tr>
<td>Avg + SD</td>
<td>939.8805</td>
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<tr>
<td>Avg - SD</td>
<td>937.2031</td>
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</tr>
<tr>
<td>Final avg.</td>
<td>938.5418 (mg/L)</td>
<td></td>
</tr>
</tbody>
</table>

Sample # | Cw | Cw | Kw | log Kw |
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>981.8708</td>
<td>0.032481</td>
<td>29836.82</td>
<td>4.471392</td>
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<tr>
<td>2</td>
<td>933.790</td>
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<td>3</td>
<td>938.5418</td>
<td>0.040894</td>
<td>23063.17</td>
<td>4.382919</td>
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</table>

Avg. log Kw | 4.410241 |
SD  | 0.055843 |
### Calibration curve for PCBs

<table>
<thead>
<tr>
<th>Temp: 25°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration curve for PCBs</td>
</tr>
</tbody>
</table>

#### Calibration Data

<table>
<thead>
<tr>
<th>Sample</th>
<th>Concentration (mg/L)</th>
<th>Area (in²)</th>
<th>R²</th>
<th>MDL (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 1</td>
<td>0.125</td>
<td>0.025</td>
<td>0.025</td>
<td>0.25</td>
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<tr>
<td>Sample 2</td>
<td>0.250</td>
<td>0.250</td>
<td>0.250</td>
<td>0.250</td>
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<tr>
<td>Sample 3</td>
<td>0.500</td>
<td>0.500</td>
<td>0.500</td>
<td>0.500</td>
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</tbody>
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#### Area Analysis

<table>
<thead>
<tr>
<th>Sample</th>
<th>Area (in²)</th>
<th>R²</th>
<th>MDL (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 1</td>
<td>0.125</td>
<td>0.025</td>
<td>0.25</td>
</tr>
<tr>
<td>Sample 2</td>
<td>0.250</td>
<td>0.250</td>
<td>0.250</td>
</tr>
<tr>
<td>Sample 3</td>
<td>0.500</td>
<td>0.500</td>
<td>0.500</td>
</tr>
</tbody>
</table>

#### Results Summary

- **Sample 1**: Area: 0.125 in², R²: 0.25, MDL: 0.25 mg/L
- **Sample 2**: Area: 0.250 in², R²: 0.250, MDL: 0.250 mg/L
- **Sample 3**: Area: 0.500 in², R²: 0.500, MDL: 0.500 mg/L
### Appendix C: Sensitivity Analysis (lindane in Rihand reservoir)

**Table 3.6: Effect of variation in parameter values on water and sediment concentrations**

<table>
<thead>
<tr>
<th>Adjustment</th>
<th>Parameter</th>
<th>Emission rate (kg/year)</th>
<th>Deposition rate (g/m²/year)</th>
<th>Resuspension rate (g/m²/year)</th>
<th>Burial rate (g/m²/year)</th>
<th>Suspended particle concentration (mg/L)</th>
<th>Half-life in water, hours</th>
<th>Half-life in sediment, hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original (x)</td>
<td></td>
<td>6500</td>
<td>10</td>
<td>0.2</td>
<td>2.5</td>
<td>19</td>
<td>6000</td>
<td>17000</td>
</tr>
<tr>
<td>2 x</td>
<td></td>
<td>13000</td>
<td>20</td>
<td>0.4</td>
<td>5</td>
<td>38</td>
<td>12000</td>
<td>34000</td>
</tr>
<tr>
<td>0.5 x</td>
<td></td>
<td>3250</td>
<td>5</td>
<td>0.1</td>
<td>1.25</td>
<td>9.5</td>
<td>3000</td>
<td>8500</td>
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<tr>
<td>Effect on conc. 2 x</td>
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<td>+ 93%</td>
<td>- 0.01%</td>
<td>+ 0%</td>
<td>- 0%</td>
<td>+ 0%</td>
<td>+ 25%</td>
<td>+ 0%</td>
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</tbody>
</table>

in water

<table>
<thead>
<tr>
<th>C_w (µg/L)</th>
<th>0.5 x</th>
<th>- 53%</th>
<th>+ 0%</th>
<th>- 0%</th>
<th>+ 0%</th>
<th>- 0%</th>
<th>- 28%</th>
<th>- 0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effect on conc. 2 x</td>
<td></td>
<td>+ 93%</td>
<td>+ 38%</td>
<td>- 0.01%</td>
<td>- 8%</td>
<td>- 0.01%</td>
<td>+ 26%</td>
<td>+ 5.6%</td>
</tr>
</tbody>
</table>

in sediment

<table>
<thead>
<tr>
<th>C_s (µg/g)</th>
<th>0.5 x</th>
<th>- 53%</th>
<th>- 19%</th>
<th>+ 0.01%</th>
<th>+ 5%</th>
<th>+ 0.01%</th>
<th>- 29%</th>
<th>- 9.3%</th>
</tr>
</thead>
</table>