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An Assessment of Two Screening Models

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PREDICTION OF CHEMICAL PARTITIONING IN THE ENVIRONMENT

An Assessment of Two Screening Models

FINAL DRAFT REPORT

by

Warren J. Lyman

Arthur D. Little, Inc.

for the

U.S. Environmental Protection Agency

Office of Water Regulations and Standards

Monitoring and Data Support Division

Washington, D.C. 20460

Task Manager: Charles Delos

Project Officer: Michael Slimak

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FOREWORD

Effective regulatory action for toxic chemicals requires an understanding of the human and environmental risks associated with the manufacture, use, and disposal of the chemical. Determining the origins of risks requires an understanding of the behavior the chemical in traversing the environment. Such behavior includes the chemical's tendency to undergo biological or chemical degradation, and its tendency to partition between phases.

The intent of this work was to explore facile methods for predicting the partitioning between air, water, soil, sediment, and biota, under both equilibrium and steady state (nonequilibrium) conditions. As performed for the 114 organic compounds on the EPA water programs list of 129 priority pollutants, partitioning estimates can suggest the environmental media most subject to contamination by each compound, and thereby assist in guiding investigative and analytical efforts into productive directions.

Charles G. Delos, Task Manager
Water Quality Analysis Branch
Monitoring and Data Support Division (WH-553)
Office of Water Regulations and Standards

ABSTRACT

This report provides an assessment of two screening models that may be used to predict environmental partitioning, and the importance of certain degradation and transport pathways, for organic chemicals. These models may play an important role in environmental fate assessments, in the initial steps of risk assessments for new or existing chemicals, and in the planning of laboratory and field tests with such chemicals.

The models studies were: (1) a fugacity-based model by Donald Mackay which provides different levels of sophistication for a variety of situations; and (2) a partitioning model by W. Brock Neely based on data from a model ecosystem. Both models are easy to use, require a minimum of input data, and are capable of solution with a hand calculator. Model outputs for both include predictions of the precent of the chemical in the air, water and soil compartments. Other outputs may also be obtained, the Mackay model being much more flexible in this regard.

This report describes each model, provides detailed instructions for their use, shows the results of sample calculations for several chemicals, and provides a comparison of monitoring data and predicted values for a few cases.

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I. INTRODUCTION

A. Background

As an initial step in hazard or risk assessments for toxic chemicals, and in the planning of laboratory and field tests with such chemicals, it is important to understand the likely transport and fate of the chemical. Which environmental compartment (air, water, soils, sediments, biota) will be most affected? Which transport and degradation pathways (photolysis, hydrolysis, volatilization, etc.) will be most important? Rough guesses can sometimes be made by simple inspection of the chemical's properties and reaction rate data - if such are available - or by the use of mathematical models which seek to yield defensible and quantitative estimates. Unfortunately, realistic chemical fate models usually require extensive input information (not always available) and a computer for solving the lengthly calculations.

A simple, initial estimate of environmental partitioning, fate and transport is thus desired; one involving an approach with minimal input data requirements and capable of solution with a hand calculator. Such approaches have been proposed by Mackay (1979) and Neely (1978a, b), amongst others. It was the primary objective of this study to investigate these two approaches and to determine their applicability to the general need described above. Table 1 provides summary information on the models studied.

B. Mackay's Fugacity Approach

Fugacity* is a thermodynamic property of a chemical. It is related to chemical potential but is easier to use in practical applications. Fugacity has units of pressure (e.g., atm.) and is sometimes thought of as a "corrected pressure" or "escaping tendency" of a chemical from a phase. Three further points (Mackay, op. cit.):

* From the Latin *fuga*, meaning flight or escape.

TABLE 1

Summary Information on the Models Studied

	Neely's Method	Mackay's Model		
		Level I	Level II	Level III
PROCESSES MODELED	• Partitioning in model ecosystem	• Equilibrium partitioning	• Steady-state partitioning • Degradation • Flux of chemical into model environment • Advection out of model environment	• Steady-state partitioning • Degradation • Flux of chemical into any subcompartment • Advection out of model environment • Inter-compartmental transfers
CHEMICAL-SPECIFIC INPUTS REQUIRED[a]	H, S (4 compartment)	M, MW, H, K_{oc}, BCF (6 compartments)[b]	MW, H, K_{oc}, I, k_{xi} (4 compartments)[b]	MW, H, K_{oc}, I_i, k_{xi}, D_{ij} (4 compartments)[b]
OUTPUTS[a]	% in Air, Water and Soil; half-life for clearance from fish	M_i, C_i	M_i, C_i, R_i, τ, $M(=\Sigma M_i)$	M_i, C_i, R_i, τ, $M(=\Sigma M_i)$

a. Section VII provides definitions for the symbols used in this report. For many organic chemicals all of the input chemical properties required (S, H, K_{oc}, k_x, D) can be estimated.

b. Additional compartments may be modeled if desired. Additional parameters will be required in some cases.

1) Fugacity is linearly proportional to concentration (at least at the low concentrations of anthropogenic chemicals usually found in the environment).

2) For two phases in contact, the tendency is for a chemical to move out of the phase where it has the higher fugacity value into the other phase.

3) When the chemical's fugacity in the two phases is the same, the distribution of the chemical between the two phases is the equilibrium distribution.

As is always the case with thermodynamic considerations, an approach that only considers fugacity cannot tell us how quickly a chemical is (or should be) approaching equilibrium between two phases, just in which direction equilibrium lies. There are two general areas in which the approach can contribute to a better understanding of the fate and transport of toxic substances. First, if concentration data are available for a pollutant in several phases, these concentration data can be converted to fugacities and the fugacity levels compared. Second, the approach may be used to predict environmental levels (at equilibrium) for a new compound which is being marketed for the first time, or for an old chemical for which there are significant data gaps in the ambient monitoring file.

A four-tiered approach is suggested by Mackay. We report here on investigations of the first three levels of calculations.

Level I considers the equilibrium partitioning of an organic chemical in a static model environment with specified subcompartments (e.g., air, water, soil, biota). No degradation or transport is allowed. The calculations require that the subcompartments be roughly described (volumes, sediment and biota "concentrations," temperature, etc.) and that the amount of the chemical in the model environment be specified. A relatively small number of chemical-specific parameters are also required.

These parameters are used to calculate a "fugacity capacity constant," Z, which is related to fugacity, f, and compartment concentration, C, by the formula C = Zf.

Level II allows a steady-state input of the chemical into the model environment, advection out of the model environment, and degradation by any process for which a first-order degradation rate constant can be obtained. Compartmental concentrations, removal rates and an overall lifetime of the chemical (in the model environment) are calculated, again using the basic fugacity approach.

Level III improves upon the previous levels by allowing a steady-state input of the chemical into any subcompartment and non-instantaneous intercompartment transfers (e.g., volatilization). All other features of the Level I and II calculations are kept and the same outputs calculated.

Level IV (not investigated in this study) is concerned with non-steady-state distributions in the environment. The calculations would generally require a computer.

C. Neely's Approach

The Neely work (Neely, 1978 a, b) is based upon laboratory data from a model environment into which small amounts of various chemicals were placed. After a suitable waiting period, the concentration in each major compartment - air, water, soil - was measured. The half-life for clearanc from fish is also obtained from laboratory data.

Using such data for ten chemicals exhibiting a wide range of solubilities and vapor pressures, four regression equations were derived allowing predictions of partitioning and fish clearance rates for other chemicals. These predictions are intended to be used in a screening process and are not expected to provide defensible quantitative estimates of chemical partitioning.

D. Study Objectives

The primary objective of the study was to investigate the Neely and Mackay models to assess the ease of use and usefulness for estimating the partitioning, transport and fate of organic chemicals in the environment. A secondary objective was to use the Mackay Level I approach to predict the partitioning of most - if not all - of the organic priority pollutants. Other secondary objectives were to compare the Neely and Level I Mackay approaches, to investigate the sensitivity of the model to various input parameters, and to compare model outputs (predicted environmental concentrations) with monitoring data for a selected group of chemicals.

E. Report Contents

Section II - Provides conclusions drawn from this study.

Section III - Describes Mackay's Level I approach. All necessary equations and step-by-step instructions for their use are provided. Calculations are shown for all organic priority pollutants.

Section IV - Describes Neely's approach. All necessary equations are given. Calculations are shown for 20 organic chemicals and the results compared with the Level I (Mackay) predictions.

Section V - Describes Mackay's Level II approach. All necessary equations and step-by-step instructions for their use are provided. Calculations are shown for a test set of 24 chemicals. Comparisons with monitoring data are made for 8 chemicals.

Section VI - Describes Mackay's Level III approach. All necessary equations and step-by-step instructions for their use are provided. Sample calcualtions, including a sensitivity analysis for two parameters, are provided for one chemical.

Section VII - Provides a listing of the symbols used in this report.

Section VIII - References.

II. CONCLUSIONS

1. All of the models studied are easy to use, require a minimum of input data (much of them estimable), and are capable of solution with a hand calculator. All are essentially limited to use with single-component organic chemicals, i.e., they cannot be used for complex mixtures, solutions, salts, polymers or inorganic compounds.

2. Both the Mackay (Level I) and the Neely models fulfill the need for a simple, easy to use environmental partitioning model. The Neely approach is somewhat easier to use and requires fewer input parameters. It can, however, yield mathematically incorrect results (e.g., percents <0 or >100 for partitioning) which, while unsettling, can be overlooked if they are used only for screening purposes. The Mackay Level I model is a more rigorous approach with a significant amount of flexibility with regard to the type of environment to be considered. The subcompartments and their accessible volumes must be described, if concentrations in specific compartments are to be calculated. Accessible volumes of the subcompartments do not need to be defined if only concentration ratios (e.g., concentration in air/concentration in water) are to be calculated.

3. If the analyst is only interested in calculating concentration ratios between pairs of subcompartments or the percent (mass) in any subcompartment, the Level I Mackay calculation should be used. (The Level I and Level II methods give identical results for these calculations.) Accessible volumes in each subcompartment do not have to be specified for the former calculation (concentration ratios) but do for the latter (percent distribution of mass).

4. Both the Level I and Level II Mackay calculations give results for an environment which has attained equilibrium partitioning. The nature of this partitioning is most simply calculated with the Level I model; the relative importance of various degradation processes can only be assessed with the Level II (or III) model. The Level II model

thus requires that degradation rate constants (e.g., for hydrolysis, biodegradation, photolysis) be known or estimated.

5. The Level III Mackay model allows the analyst to obtain the absolute (or relative) concentrations in various subcompartments under non-equilibrium conditions. For these calculations it is necessary for the important intercompartmental transfer processes to be described in a set mathematical format. At present, only volatilization from water can be included in a rigorous manner; transfer coefficients for other intercompartmental transfer processes must be guessed. This is considered to be a significant limitation of the Level III approach. Just how closely the Level III outputs resemble those from Levels I and II appears to depend primarily on how the input load is distributed between the media (air, land, water) and on the selected intercompartmental transfer coefficients. The results of Level I, II and III calculations for one chemical (trichloroethylene) are compared on page VI-12; the output shown there indicates the range of answers that may be obtained with various Level III inputs.

6. These models make no attempt to describe the fate and transport of a chemical in a well-defined, realistic environment. Both essentially consider a generalized box environment containing air, water, soil and biota (plus other compartments, if desired, in the Mackay model) and equilibrium or steady-state partitioning. The models should primarily be considered as screening models to determine what future studies are likely to be important for a particular chemical.

7. In spite of the limitations mentioned in (6) above, there will always be a temptation to use some of these models as predictive tools for specific locations. The Mackay Level II and III models incorporate a sufficient degree of realism--at least with regard to chemical degradation and transport--that the calculated environmental concentrations might be taken as realistic predictions in some cases.

8. If the Mackay model is to be used as a predictive model for a specific location, then some special care must be taken in the description of the model environment so that it approximates the actual environment. This poses some problems since the Mackay model does not, as currently formulated, allow for different portions of a subcompartment to contain different concentrations of a chemical; all portions of that subcompartment are taken to be equally accessible to the partitioning chemical. A related problem is the size or accessible volume of a subcompartment in relation to the lifetime or mobility of the pollutant in that subcompartment. It is unrealistic, for example, to stipulate a 10 km height for the air compartment for a chemical which is released at ground level and has an atmospheric lifetime of only a few hours (e.g., due to rapid photolysis). For such a chemical a 1 km height would be more appropriate.

A comparison of calculated concentrations (Level II) with monitoring data is given in Section V-G for eight chemicals. The comparison showed that wide discrepancies may frequently be seen, especially for surface water concentrations. These discrepancies may be due to the combined effects of: (1) a bias towards more polluted media in monitoring programs; (2) problems in obtaining meaningful averages from reported data; and (3) a bias in the sample calculations of this report towards less polluted areas. None of these possible reasons reflects any fundamental flaw in the model used.

III. LEVEL I MACKAY CALCULATIONS

A. Basic Assumptions

The basic assumptions of the Level I calculations are as follows:

- All of the environmental subcompartments (air, water, soil, etc.) are at equilibrium, and there is no net flux of the subcompartment material (air, water, soil, etc.) into or out of any subcompartment or the compartment as a whole.

- The chemical is at equilibrium in the environmental compartment, and there is no net transport of the chemical between any subcompartments, and no net flux into or out of the compartment as a whole.

- No chemical or biological degradation of the chemical takes place.

In addition to the above, there are a number of assumptions (or estimates of various parameters) that are associated with a particular set of calculations. One such set of assumptions is related to the size, accessible volumes, and nature of the various subcompartments selected for study. Details on the compartment-related parameters selected for use in the Level I calculations are given in the following subsection. The specific numbers used were selected somewhat subjectively and are not to be considered representative of all environments. Key assumptions associated with the values selected include the following:

- The accessible volume in the air compartment encompasses the air up to the top of the troposphere ($\sim$ 10 km). (This is too large for highly reactive chemicals and too small for very stable chemicals; e.g., the fluorocarbons.)

- Deep soils and deep ocean waters are not considered to be accessible to the chemical. (This will hold for chemicals with modest half-lives.)

The Level I calculations require a value for the total amount of the chemical in the environmental compartment if a real attempt is being made to predict actual environmental concentrations. Obtaining such a value would require either (1) extensive monitoring data on the chemical, or (2) detailed information on emission rates, transport pathways (and rates) and degradation rates. The time requirements for such a data compilation or evaluation effort are significant, and thus we have selected a route which, while only allowing the calculation of relative amounts and concentrations of the chemical in each subcompartment, is rapid and still allows important conclusions to be drawn:

- The total amount of each chemical in the selected compartment is 100 moles.

B. Description of the Model Environment *

Figure 1 provides a schematic diagram of the selected model environment. The subcompartments selected here for study are:

1. Air
2. Surface waters
3. Suspended sediments
4. Bottom sediments
5. Aquatic biota
6. Soils

There is no reason that fewer or more subcompartments could not be used by other users of this method. The specific compartment-related parameters used in our calculations are detailed below; subscripts on any symbol refer to the subcompartments identified above.

* A listing of the symbols used in this (and subsequent) sections is given in Section VII.

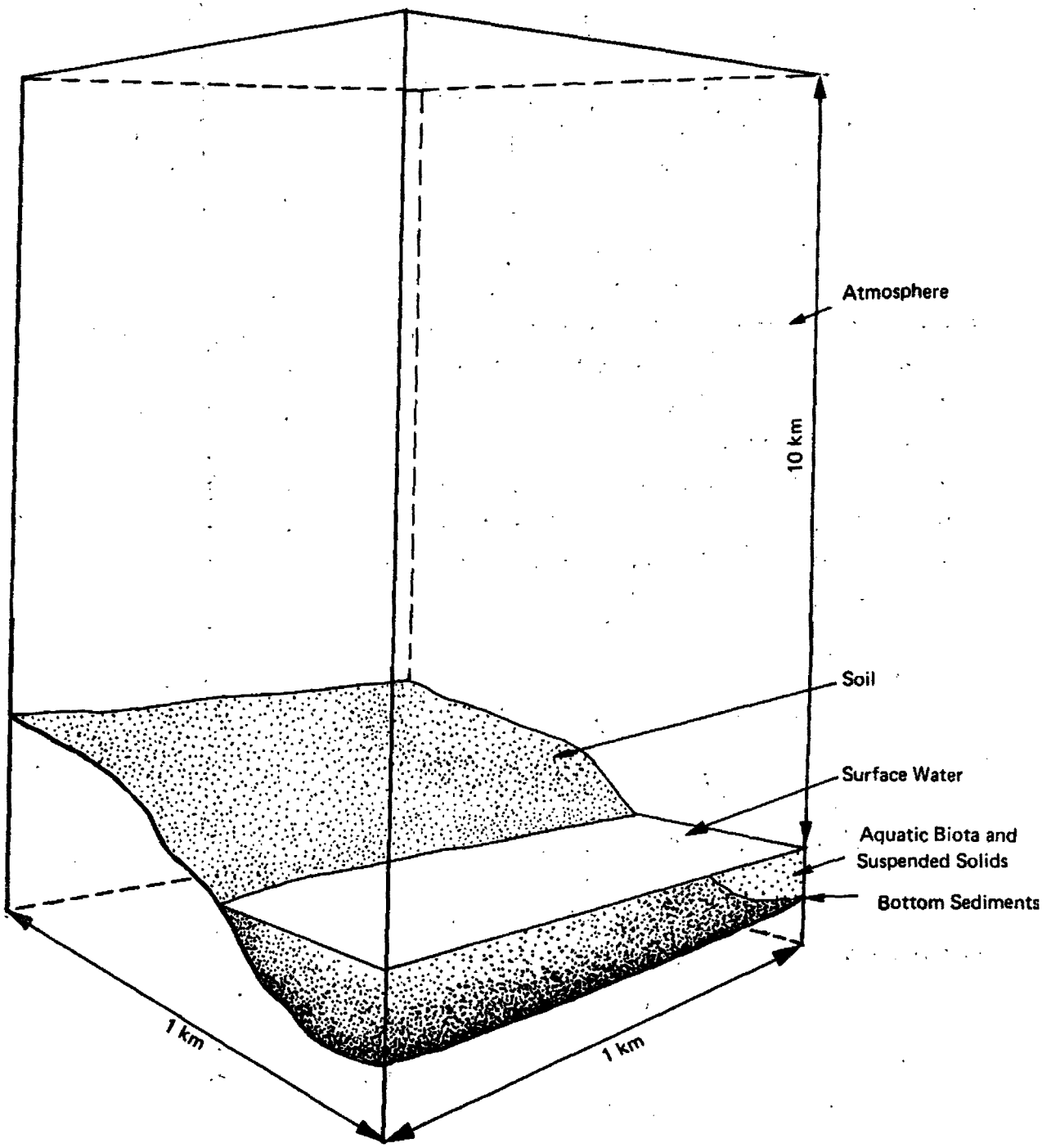

FIGURE 1 SCHEMATIC OF ENVIRONMENTAL COMPARTMENT SELECTED FOR ESTIMATION OF EQUILIBRIUM PARTITIONING OF ORGANIC CHEMICALS

Note: Diagram is not to scale. Dimensions and accessible volumes of each subcompartment given in the text.

1) Accessible Volumes (V_i). The volumes of each subcompartment that were considered accessible to all chemicals are as follows:

Air: V_1 = 1 km x 1 km x 10 km(high) = 10^{10} m^3

Surface water: V_2 = 1 km x 0.05 km x 3 km(deep) = 1.5 x 10^5 m^3

Suspended sediments*: $V_3 = V_2$ = 1.5 x 10^5 m^3

Bottom sediments*: V_4 = 1 km x 0.05 km x 10 cm(deep) = 5 x 10^3 m^3

Aquatic biota*: $V_5 = V_2$ = 1.5 x 10^5 m^3

Soils: V_6 = 1 km x 0.95 km x 15 cm(deep) = 1.4 x 10^5 m^3

2) "Concentration" of Suspended and Bottom Sediments and Soil (c_{s_i}). Within the accessible volumes for subcompartments 3, 4, and 6, some of the volume is taken up by water or air. The sediments or soil may thus be considered to exist at a certain "concentration" within these volumes. The selected concentrations are:

Suspended sediments : c_{s_3} = 10 g/m^3

Bottom sediments : c_{s_4} = 2 x 10^6 g/m^3

Soils : c_{s_6} = 2 x 10^6 g/m^3

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*Initially the accessible volume for suspended sediments and aquatic biota are taken to be the same as for the surface waters. A correction factor is applied later that accounts for the fact that suspended sediments and aquatic biota take up only a fraction of the surface water volume. A similar correction factor is applied for bottom sediments.

3) Organic Carbon Content of Sediments and Soils $(oc)_i$. Since we have selected to use soil and sediment adsorption coefficients, K_{oc}, which are based upon the organic carbon content, (oc), of the soil, this content must be specified. Values of (oc) vary widely in nature with the range of 0.1% - 20% encompassing most values. The following values have been used for our Level I calculations:

Suspended and bottom sediments : $(oc)_3 = (oc)_4 = 10\%$

Soils : $(oc)_6 = 2\%$

4) "Concentration" of Biota in Water (B). The volume fraction of biota in the surface waters is taken to be 5×10^{-5} m^3/m^3. If the density is assumed to be 1 g/cm^3, the "concentration" is 5×10^{-5} g/g. Mackay, in his original discussion of the biotic subcompartment, required one additional parameter, y, the fraction of the aquatic biota that could be considered equivalent to octanol. This was done so that the octanol/water partition coefficient (K_{ow}) could be used in place of the bioconcentration factor (BCF) in assessing the uptake of the chemical by biota. (Values of log K_{ow} and log BCF can be related by linear regression equations). We have decided to write our basic equation in terms of BCF rather than y x K_{ow}, since it better describes what is implied in the term and shows explicitly how (or where) a measured value of BCF may be used. In numerous cases, however, it will be necessary to use values of BCF that have been estimated via K_{ow} or some other parameter.

5) Temperature (T). A temperature of 20°C (293K) was selected for the Level I calculations. The temperature is only used directly in one part of the calculations (the Z factor for the air subcompartment), but it is an indirect factor for the other chemical-specific parameters (e.g., solubility, vapor pressure) which are a function of temperature. It should be noted that many of the chemical-specific parameter values used here were derived at temperatures other than 20°C, usually 25°C or some other value near room temperature. No correc-

tions were applied for the Level I calculations, since the results would not be significantly affected by such small temperature changes.

C. Chemical-Specific Parameters Required

For the Level I calculations, the following chemical-specific input parameters are required:

- Henry's Law constant, H
- Soil and sediment adsorption coefficient, K_{oc}
- Bioconcentration factor for aquatic life, BCF
- Molecular weight, MW

Values of H, K_{oc}, BCF and MW were taken, when available, from a draft report by SRI, International. Although not explicitly stated in this draft report, it should be understood that a large fraction of the listed values are estimates and may be in error by one of the order of magnitude or more. Values of H are usually taken as the ratio of the chemical's vapor pressure (P_{vp}) to its water solubility (S). Values of H for 21 chemicals were not given in the SRI report and were estimated by A. D. Little. The values we estimated, and the values of P_{vp} and S from which the values of H were derived, are listed in Table 2. P_{vp} values were estimated using a modified Watson correlation which requires a measured or estimated value of the boiling point. Most of the S values were estimated using a measured or estimated value of the octanol/water partition coefficient (K_{ow}) and one or more suitable regression equations relating log S to log K_{ow}; the values of S for the two halomethanes were derived from a fragment constant approach.*

*Details of the estimation methods used are provided in two draft chapters (Ch. 2: Solubility in Water, by W. Lyman; and Ch. 14: Vapor Pressure, by C. Grain) which are part of a chemical-property estimation methods handbook currently being prepared by A. D. Little under contract to the U.S. Army. The report will be available in 1981.

Table 2

Estimates of S, P_{vp} and H for Selected Chemicals[a]

No.[b]	Chemical	Mol. Wt.	S (mg/L)	P_{vp} (mm Hg)	H (atm-m^3/mole)
14.	Endosulfan sulfate	422.9	100	3.3×10^{-8}	1.8×10^{-10}
16.	Endrin aldehyde	381	0.1[c]	1.3×10^{-7}	6.5×10^{-7}
18.	Heptachlor epoxide	389.2	(0.350)	1.0×10^{-7}	1.5×10^{-7}
20.	TCDD	322	(0.0002)	6.1×10^{-7}	1.3×10^{-3}
29.	2-Chloronaphthalene	162.6	2.8	1.6×10^{-2}	1.2×10^{-3}
33.	Methane, chlorodibromo	208.3	4,600	(15)	8.9×10^{-4}
34.	Methane, dichlorobromo	163.8	6,000	(50)	1.8×10^{-3}
60.	Ether, 4-bromophenyl phenyl	249.1	380	(1.5×10^{-3})	1.3×10^{-6}
62.	Bis(2-chloroethoxy) methane	173.1	(8.1×10^{4})	1.1×10^{-1}	3.1×10^{-7}
81.	Phenol, 4-nitro	139.1	(1.6×10^{4})	3.2×10^{-6}	3.7×10^{-7}
83.	Phenol, 2,4-dimethyl	122.2	(4,200)	(6.2×10^{-2})	2.4×10^{-6}
84.	m-Cresol, p-chloro	142.6	(3850)	7.1×10^{-3}	3.5×10^{-7}
85.	o-Cresol, 4,6-dinitro	198.1	950	7.3×10^{-5}	2.0×10^{-8}
89.	Phthalate, di-N-octyl	391	(3.0)	3.3×10^{-5}	5.7×10^{-6}
91.	Phthalate, Butyl benzyl	312	(2.9)	8.6×10^{-6}[d]	1.2×10^{-11}
108.	Nitrosamine, dimethyl	74.1	4.9×10^{5}	2.7×10^{0}	5.4×10^{-6}
109.	Nitrosamine, diphenyl	198.2	26	1.4×10^{-5}	1.4×10^{-7}
110.	Nitrosamine, di-N-propyl	130.2	(9900)	1.6×10^{-3}	2.8×10^{-8}
111.	Benzidine	184.2	890	6.8×10^{-7}	1.8×10^{-10}
112.	Benzidine, 3,3'-dichloro	253.1	(4)	2.9×10^{-7}	2.4×10^{-8}
113.	Hydrazine, 1,2-diphenyl	184.2	30	9.2×10^{-5}	7.4×10^{-7}

a. The values of S and P_{vp} in parentheses are from the draft SRI, International, report. The other values of S and P_{vp} are estimates,

Table 2 footnotes (continued)

a temperature of ~20°C, by Arthur D. Little, Inc. Values of H are derived from the S and P_{vp} values as follows:

$$H \left(\frac{atm \cdot m^3}{mole}\right) = \frac{P_{vp} \text{ (mm Hg)} \cdot MW \text{ (g/mole)}}{S \text{ (mg/L)} \cdot 760}$$

b. No. = index number of chemical used in subsequent listing of all organic priority pollutants.

c. This value is an "educated guess"; it is more uncertain than other estimates.

d. This is a measured value from Gledhill et al. (1980).

The values of H, K_{OC}, BCF, and MW used for all of the priority pollutants are provided in Table 3. This table also provides the calculated fugacity (f), which is the first parameter calculated in the Level I approach described in the following subsection.

The total mass (M) of each chemical in the environmental compartment is taken as 100 moles for the Level I calculations. (See subsection A above for rationale.)

D. Level I Equations

The basic tenet of the Mackay approach is that, at equilibrium, the fugacity of the chemical is the same in all subcompartments; i.e.,

$$f_1 = f_2 = f_3 = f_4 = f_5 = f_6 \ (= f) \qquad (1)$$

This fugacity, which has the units of pressure (atm), can be regarded as the chemical's "escaping tendency" or "corrected pressure" within a phase.

A second major tenet is that f is proportional to the chemical's concentration (C), at least at the low concentrations of anthropogenic chemicals usually found in the environment. Mackay uses the symbol Z for the proportionality constant:

$$C = Zf \qquad (2)$$

With C in mol/m^3 and f in atm, Z will have units of $mol/m^3 atm$.

The value of Z depends upon both the nature of the chemical and the environment it is in. It is also a function of temperature and pressure. Mackay gives the following equations for the calculation of Z in each subcompartment; the basis for these equations is discussed more fully in his paper (op cit.):

1. Air:

$$Z_1 = 1/RT = 41.6 \text{ at } 20^{\circ}C \quad (3)$$

(R = gas constant = 8.2×10^{-5} m^3atm/mol. deg.)

(T = temperature, K)

2. Surface Water:

$$Z_2 = 1/H \ (= S/P_{vp}) \quad (4)$$

3. Suspended sediments*:

$$Z_3 = 10^{-6} K_{p_3} c_{s_3} / H \quad (5)$$

(K_p = soil adsorption coefficient)

or $$Z_3 = 10^{-8} (oc)_3 K_{oc} c_{s_3} / H \quad (6)$$

($K_{oc} = 100 \cdot K_p/(oc)$)

((oc) = % organic carbon in soil or sediment)

4. Bottom sediments*:

$$Z_4 = 10^{-6} K_{p_4} c_{s_4} / H \quad (7)$$

or

$$Z_4 = 10^{-8} (oc)_4 K_{oc} c_{s_4} / H \quad (8)$$

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*Eqs. 5, 7, 9, and 11 are given by Mackay (op cit.). Eqs. 6, 8, and 12 (which involves the use of K_{oc} in place of K_p and Eq. 10 which uses BCF in place of y . K_{ow}) have been used in the calculations here.

5. Aquatic Biota*:

$$Z_5 = B \cdot y \cdot K_{ow}/H \tag{9}$$

or

$$Z_5 = B \cdot BCF/H \tag{10}$$

6. Soils:

$$Z_6 = 10^{-6} K_{p_6} c_{s_6}/H \tag{11}$$

or

$$Z_6 = 10^{-8} (oc)_6 K_{oc} c_{s_6}/H \tag{12}$$

With the above Z-factors, the fugacity is given by

$$f = M/\sum_{i=1}^{6} (V_i Z_i) \tag{13}$$

where M is the total amount of the chemical in the compartment, the Z_i values are obtained from Eqs. 3 to 12, and the V_i values are the accessible volumes of each of the six subcompartments, as described in subsection B-1 above. When the selected values of V_i and Eqs. 3, 4, 6, 8, 10 and 12 are substituted into Eq. 13, the result is:

$$\begin{aligned} f = M/(&4.16 \times 10^{11} + 1.5 \times 10^{5}/H + 1.5 \times 10^{-3}(oc)_3 K_{oc} c_{s_3}/H \\ &+ 0.5 \times 10^{-4}(oc)_4 K_{oc} c_{s_4}/H + 1.5 \times 10^{5} B\,(BCF)/H \\ &+ 1.4 \times 10^{-3} (oc)_6 K_{oc} c_{s_6}/H) \end{aligned} \tag{14}$$

Then, with the selected values of (oc), c_s and B (see subsection B above), Eq. 14 becomes:

$$\begin{aligned} f = MH/(&4.16 \times 10^{11} H + 1.5 \times 10^{5} + 0.15 K_{oc} + 10^{3} K_{oc} \\ &+ 7.5(BCF) + 5.6 \times 10^{3} K_{oc}) \end{aligned} \tag{15}$$

which may be reduced to:

$$f = MH/(4.16 \times 10^{11}H + 1.5 \times 10^{5} + 6.6 \times 10^{3}K_{oc} + 7.5(BCF)) \quad (16)$$

Equation 16 was then evaluated for all of the organic priority pollutants using the values of H, K_{oc} and BCF from Table 3; M was taken as 100 moles for each chemical. The calculated f values are also given in Table 3; they range from about 10^{-10} to 10^{-18} atm.

It should be noted that, for certain classes of chemicals, just one term in the denominator of Eq. 16 may be important. Values of H (range $\sim 10^{-7}$ to 1), K_{oc} (range $\sim$ 1 to 10^{6}) and BCF (range $\sim$ 1 to 10^{6}) vary greatly. For chemicals with relatively low K_{oc} and BCF values and relatively high H valuess (i.e., hydrophylic, volatile chemicals), the first term in the denominator will dominate and Eq. 16 reduces to:

$$f = M/4.16 \times 10^{11} \quad (17)$$

which is equal to 2.4×10^{-10} atm with M = 100 moles. Approximately 50 percent of the chemicals listed in Table 3 have f values of $\sim 2 \times 10^{-10}$ because of this combination of factors.

Two other points are worth noting. First, the calculated f values are directly proportional to M, the total mass of the chemical in the compartment. The values of f in Table 3 are for M = 100 moles. An adjustment of f for any other value of M is thus a straightforward ratio calculation. For example, to obtain f for M = 10 moles, the values of f in Table 3 would be divided by 10 (100/10 = 10).

Second, both K_{oc} and BCF are measures of hydrophobicity in that they represent the ratio of the chemical's concentration in some organic medium (soil, biota) to that in water. A more general measure of hydrophobicity is K_{ow}, the octanol/water partition coefficient. Two fairly general regression equations relating K_{ow} to K_{oc} and BCF are*:

*Eq. 18 from Kenaga, E.E., and C.A.I. Goring (1980).
Eq. 19 from Veith et al. (1979).

$$\log K_{oc} = 0.544 \log K_{ow} + 1.377 \quad (18)$$

and

$$\log BCF = 0.76 \log K_{ow} - 0.23 \quad (19)$$

With these relationships, Eq. 16 may be written with only two chemical-specific parameters, H and K_{ow}:

$$f = MH/(4.16\times10^{11}H+1.5\times10^{5}+1.6\times10^{5}(K_{ow})^{0.544}+4.4(K_{ow})^{0.76}) \quad (20)$$

This equation thus expresses f in terms of two, obviously important, partition coefficients: an air/water partition coefficient (H) and an organics/water partition coefficient (K_{ow}). These two coefficients are not independent variables, since both depend on the hydrophilicity (e.g, solubility) of the chemical.

Once values of f have been calculated, the mass of the chemical in each subcompartment, M_i, is obtained from

$$M_i = f\ V_i\ Z_i \text{ moles} \quad (21)$$

Since in our own case $\sum M_i = 100$ moles, the individual values of M_i are equivalent to the percent of the chemical in each subcompartment. The calculated values of M_i (M_1 = mass in air, M_2 = mass in surface water, etc.) are shown in Table 4.

Once the M_i values have been obtained, the concentration of the chemical in each subcompartment, C_i, is obtained from

$$C_i = Z_i f \text{ mol/m}^3 \quad (22)$$

or

$$C_i = M_i/V_i \text{ mol/m}^3 \quad (23)$$

The units of C_i from Eqs. 22 and 23 are moles per cubic meter of the environment; i.e., moles per m^3 of air for C_1, moles per m^3 of water for C_2, C_3, and C_5, moles per m^3 of bottom sediments for C_4,

and moles per m^3 of soil for C_6. Concentrations of chemicals in the environment are more commonly expressed on a volume per volume basis for the air compartment and on a weight per weight (or weight per volume) basis for the other subcompartments. Conversion to these more common units requires the use of the c_s values for soils and sediments, the B value for biota, and the molecular weight (MW) of the compound. For the environmental compartment chosen, the equations for calculating concentrations, C_i', in the more common units are:

$$C_1' = 2.4\ M_1 \text{ ppt (vol/vol)} * \quad (24)$$

$$C_2' = (MW)M_2/0.15 \text{ ppt (wt/wt)} \quad (25)$$

$$C_3' = (MW)M_3/1.5 \times 10^{-6} \text{ ppt (wt/wt)} \quad (26)$$

$$C_4' = (MW)M_4 \times 10^{2} \text{ ppt (wt/wt)} \quad (27)$$

$$C_5' = (MW)M_5/7.5 \times 10^{-6} \text{ ppt (wt/wt)} \quad (28)$$

$$C_6' = (MW)M_6/0.28 \text{ ppt (wt/wt)} \quad (29)$$

Equations 24 to 29 were used to calculate subcompartment concentrations for each of the organic priority pollutants. The results are provided in Table 5. Again, it should be pointed out that these calculated concentrations are based upon an assumed total load (M) of 100 moles of each chemical in the total compartment. But again, the C_i' values are directly proportional to M so that adjustments may easily be made for different estimates of M. The values of C_3' and C_4' are equal, since we have assumed that the organic carbon content of the suspended and bottom sediments is the same (10%).

If only concentration ratios between two subcompartments are to be calculated, just the fugacity coefficients (Z) need to be calculated. The ratio of concentrations in subcompartments i and j (cf. Eq. 22) is simply: $c_i/c_j = Z_i/Z_j$.

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*If units of wt/vol are desired for air, use
$c_1'' = M_1(MW)/10\ ng/m^3$

Step-by-Step Instructions

(1) For the pollutant of interest, obtain MW, H, K_{oc}, BCF and M (mass of chemical in model environment). H may be estimated from $MW \cdot P_{vp}/(S \cdot 760)$ where P_{vp} is the vapor pressure (mm Hg) and S is the solubility (mg/L); H will be in the correct units desired here ($atm\ m^3/mol$).

(2) For the model environment, select the desired values for the accessible volumes of each subcompartment, V_i (m^3), the concentration of soil and sediments in their respective subcompartments, c_s (g/m^3), the organic carbon content of these soils and sediments, oc (%), the volume fraction of biota in the surface waters, B, and the temperature, T (K).

(3) For the subcompartments of interest, calculate the fugacity coefficients, Z_i ($mol\ m^3/atm$), from equations 3, 4, 6, 8, 10 and 12 (or 3, 4, 5, 7, 9 and 11 if the original Mackay approach is to be used).

(4) Calculate the chemical's fugacity using equation 13. (If equation set 3, 4, 6, 8, 10 and 12 is used for the Z_i values, and the accessible volumes (V_i) are the same as were selected for the model environment used here, then equation 14 may be used to calculate f. If, in addition, the values of (oc), c_s and B are the same as in the model environment selected here, then equation 16 may be used to calculate f.)

(5) Calculate the mass, M_i (mol), of the chemical in each subcompartment using equation 21.

(6) Calculate the concentration, C_i (mol/m^3), of the chemical in each subcompartment using either equation 22 or 23. Note that these concentration units are mass per cubic meter of environment. Equations 24-29 allow concentrations, C_i', to be calculated and

expressed in more conventional units (ppt by volume for air and ppt by weight for the other compartments).

TABLE 3

Chemical-Specific Input Parameters[a] for
Level I Approach, and Calculated Fugacity (f)

No.	Name	MW	H	K_{oc}	BCF	f
	I. Pesticides					
1.	Acrolein	56.06	5.66×10^{-5}	.563	0.17	2.39×10^{-10}
2.	Aldrin	365.	1.7×10^{-4}	1.10×10^{5}	3.29×10^{4}	2.13×10^{-11}
3.	α-BHC	291.	6.0×10^{-6}	4.27×10^{3}	1.28×10^{3}	1.95×10^{-11}
4.	β-BHC	291.	4.5×10^{-7}	4.27×10^{3}	1.28×10^{3}	1.58×10^{-12}
5.	γ-BHC (Lindane)	291.	8.16×10^{-6}	4.27×10^{3}	1.28×10^{3}	2.57×10^{-11}
6.	δ-BHC	291.	2.07×10^{-7}	4.27×10^{3}	1.28×10^{3}	7.28×10^{-13}
7.	Chlordane	406.	9.4×10^{-5}	1.66×10^{5}	4.98×10^{4}	8.28×10^{-12}
8.	DDD	320.	2.15×10^{-8}	8.92×10^{5}	2.67×10^{5}	3.65×10^{-16}
9.	DDE	318.	6.79×10^{-5}	5.02×10^{6}	1.50×10^{6}	2.05×10^{-13}
10.	DDT	354.5	1.58×10^{-5}	4.47×10^{6}	1.34×10^{6}	5.35×10^{-14}
11.	Dieldrin	381.	4.57×10^{-10}	1.91×10^{3}	572.	3.58×10^{-15}
12.	α-Endosulfan	406.9	1.0×10^{-5}	0.0126	0.00378	2.32×10^{-10}
13.	β-Endosulfan	406.9	1.91×10^{-5}	0.0126	0.00378	2.36×10^{-10}
14.	Endosulfan Sulfate	422.9	1.8×10^{-10}	0.0276	0.00827	1.20×10^{-13}
15.	Endrin	381.	4.0×10^{-7}	1.91×10^{3}	572.	3.09×10^{-12}

No.	Name	MW	H	K_{oc}	BCF	f
16.	Endrin Aldehyde	381.	6.5×10^{-7}	759.	228.	1.20×10^{-11}
17.	Heptachlor	373.5	3.95×10^{-3}	1.41×10^{4}	4.24	2.27×10^{-10}
18.	Heptachlor Epoxide	389.2	1.5×10^{-7}	246.	73.7	8.17×10^{-12}
19.	Isophorone	138.2	5.75×10^{-6}	100.	30.0	1.80×10^{-10}
20.	TCDD (2,3,7,8-Tetrachlorodibenzo-p-dioxin)	322.	1.3×10^{-3}	3.80×10^{6}	1.14×10^{6}	5.07×10^{-12}
21.	Toxaphene	414.	0.21	1.1×10^{3}	330.	2.40×10^{-10}
II.	PCB's and Related Compounds					
22.	PCB-1016 (Arochlor 1016)	257.9	3.3×10^{-4}	2.1×10^{5}	6.3×10^{4}	2.17×10^{-11}
23.	PCB-1221 (Arochlor 1221)	200.7	1.2×10^{-4}	6.6×10^{3}	2.0×10^{3}	1.28×10^{-10}
24.	PCB-1232 (Arochlor 1232)	232.2	8.6×10^{-4}	880.	264.	2.36×10^{-10}
25.	PCB-1242 (Arochlor 1242)	266.5	1.98×10^{-3}	7.2×10^{3}	2.1×10^{3}	2.27×10^{-10}
26.	PCB-1248 (Arochlor 1248)	299.5	3.6×10^{-3}	3.2×10^{5}	9.5×10^{4}	9.97×10^{-11}
27.	PCB-1254 (Arochlor 1254)	328.4	2.6×10^{-3}	6.1×10^{5}	1.8×10^{5}	5.09×10^{-11}
28.	PCB-1260 (Arochlor 1260)	375.7	0.74	7.7×10^{6}	2.3×10^{6}	2.06×10^{-10}
29.	2-Chloronaphthalene	162.6	1.2×10^{-3}	5.5×10^{3}	1.68×10^{3}	2.24×10^{-10}
III.	Halogenated Aliphatics					
30.	Methane, Bromo- (Methylbromide)	94.94	0.197	6.77	2.03	2.40×10^{-10}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
31.	Methane, Chloro- (Methylchloride)	50.49	0.04	4.9	1.47	2.40×10^{-10}
32.	Methane, Dichloro- (Methylene chloride)	84.94	2.98×10^{-3}	10.0	3.00	2.40×10^{-10}
33.	Methane, Chlorodibromo-	208.29	8.9×10^{-4}	95.6	28.7	2.40×10^{-10}
34.	Methane, Dichlorobromo-	163.83	1.8×10^{-3}	69.2	20.8	2.40×10^{-10}
35.	Methane, Tribromo- (Bromoform)	252.75	5.44×10^{-4}	132.	39.6	2.39×10^{-10}
36.	Methane, Trichloro- (Chloroform)	119.38	2.88×10^{-3}	50.2	15.4	2.40×10^{-10}
37.	Methane, Tetrachloro- (Carbon tetrachloride)	153.82	2.32×10^{-2}	502.	150	2.40×10^{-10}
38.	Methane, Trichlorofluoro-	137.4	0.11	182.	54.6	2.40×10^{-10}
39.	Methane, Dichlorodifluoro-	120.91	2.98	66.1	19.8	2.40×10^{-10}
40.	Ethane, Chloro-	64.52	1.48×10^{-2}	17.0	5.10	2.40×10^{-10}
41.	Ethane, 1,1-Dichloro-	98.96	4.26×10^{-3}	34.7	10.4	2.40×10^{-10}
42.	Ethane, 1,2-Dichloro-	98.98	9.14×10^{-4}	16.6	4.98	2.40×10^{-10}
43.	Ethane, 1,1,1-Trichloro-	133.41	3.0×10^{-2}	174.	52.2	2.40×10^{-10}
44.	Ethane, 1,1,2-Trichloro-	133.41	7.42×10^{-4}	64.6	19.4	2.40×10^{-10}
45.	Ethane, 1,1,2,2-Tetrachloro-	167.85	3.80×10^{-4}	251	75.4	2.38×10^{-10}
46.	Ethane, Hexachloro-	236.74	2.49×10^{-3}	2.29×10^{4}	6.88×10^{3}	2.10×10^{-10}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
47.	Ethene, Chloro- (Vinyl chloride)	62.5	198.	9.34	2.80	2.40×10^{-10}
48.	Ethene, 1,1-Dichloro-	96.94	0.160	38.0	11.4	2.40×10^{-10}
49.	Ethene, Trans-dichloro-	96.94	6.9×10^{-2}	9.56	2.87	2.40×10^{-10}
50.	Ethene, Trichloro-	131.39	9.10×10^{-3}	38.0	11.4	2.40×10^{-10}
51.	Ethene, Tetrachloro-	165.83	2.0×10^{-2}	360.	100.	2.40×10^{-10}
52.	Propane, 1,2-Dichloro-	112.99	2.31×10^{-3}	57.6	17.3	2.40×10^{-10}
53.	Propene, 1,3-Dichloro-	110.98	1.33×10^{-3}	29.5	8.86	2.40×10^{-10}
54.	Butadiene, Hexachloro-	260.79	2.56×10^{-2}	1.00×10^{3}	300.	2.40×10^{-10}
55.	Cyclopentadiene, Hexachloro-	272.77	1.61×10^{-2}	1.05×10^{3}	314.	2.40×10^{-10}
IV.	Ethers					
56.	Ether, Bis(2-chloromethyl)-	115.	2.1×10^{-4}	1.32	0.396	2.40×10^{-10}
57.	Ether, Bis(chloroethyl)-	143.	1.3×10^{-5}	15.9	4.76	2.30×10^{-10}
58.	Ether, Bis(2-chloroisopropyl)-	171.1	1.1×10^{-4}	69.2	20.8	2.37×10^{-10}
59.	Ether, 2-chloroethyl vinyl-	106.6	2.50×10^{-7}	7.59	2.28	8.22×10^{-11}
60.	Ether, 4-Bromophenyl phenyl-	249.11	1.3×10^{-6}	6.61×10^{4}	1.98×10^{4}	2.97×10^{-13}
61.	Ether, 4-Chlorophenyl phenyl-	204.66	2.19×10^{-4}	1.70×10^{4}	1.44×10^{4}	1.07×10^{-10}
62.	Bis(2-chloroethoxy) methane	173.1	3.1×10^{-7}	5.89	1.77	9.75×10^{-11}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
V.	Monocyclic Aromatics (Excluding Phenols, Cresols, Phthalates)					
63.	Benzene	78.12	5.5×10^{-3}	74.2	22.3	2.40×10^{-10}
64.	Benzene, Chloro-	112.56	3.58×10^{-3}	380.	114.	2.40×10^{-10}
65.	Benzene, 1,2-Dichloro-	147.01	1.93×10^{-3}	2.00×10^{3}	599.	2.36×10^{-10}
66.	Benzene, 1,3-Dichloro-	147.01	3.61×10^{-3}	2.00×10^{3}	599.	2.38×10^{-10}
67.	Benzene, 1,4-Dichloro-	147.01	3.1×10^{-3}	2.00×10^{3}	599.	2.38×10^{-10}
68.	Benzene, 1,2,4-Trichloro-	181.45	2.31×10^{-3}	1.02×10^{4}	3.07×10^{3}	2.25×10^{-10}
69.	Benzene, Hexachloro-	284.79	6.79×10^{-4}	1.45×10^{6}	4.34×10^{5}	6.89×10^{-12}
70.	Benzene, Ethyl-	106.16	6.58×10^{-3}	1.20×10^{3}	361.	2.40×10^{-10}
71.	Benzene, Nitro-	123.11	1.31×10^{-5}	40.8	12.2	2.23×10^{-10}
72.	Toluene	92.13	5.17×10^{-3}	339.	102.	2.40×10^{-10}
73.	Toluene, 2,4-Dinitro-	182.14	4.5×10^{-6}	105.	31.4	1.66×10^{-10}
74.	Toluene, 2,6-Dinitro-	182.14	7.9×10^{-6}	105.	31.4	1.91×10^{-10}
VI.	Phenols and Cresols					
75.	Phenol	94.1	4.54×10^{-7}	16.2	4.87	1.02×10^{-10}
76.	Phenol, 2-Chloro-	128.56	1.03×10^{-5}	83.2	25.0	2.07×10^{-10}
77.	Phenol, 2,4-Dichloro-	163.0	2.8×10^{-6}	437.	131.	6.67×10^{-11}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
78.	Phenol, 2,4,6-Trichloro-	197.5	4×10^{-6}	2.24×10^{3}	672.	2.41×10^{-11}
79.	Phenol, Pentachloro-	266.4	2.8×10^{-6}	6.03×10^{4}	1.81×10^{4}	7.01×10^{-13}
80.	Phenol, 2-Nitro-	139.1	7.56×10^{-6}	30.9	9.28	2.16×10^{-10}
81.	Phenol, 4-Nitro-	139.1	3.7×10^{-11}	51.3	15.4	7.57×10^{-15}
82.	Phenol, 2,4-Dinitro-	184.1	6.54×10^{-10}	55.	16.5	1.26×10^{-13}
83.	Phenol, 2,4-Dimethyl	122.2	2.4×10^{-6}	347.	104.	6.98×10^{-11}
84.	m-Cresol, p-Chloro-	142.6	3.5×10^{-7}	381.	114.	1.25×10^{-11}
85.	o-Cresol, 4,6-Dinitro-	198.1	2.0×10^{-8}	276.	82.7	1.01×10^{-12}
VII.	Phthalate Esters					
86.	Phthalate, Dimethyl-	194.2	2.15×10^{-6}	112.	33.7	1.21×10^{-10}
87.	Phthalate, Diethyl-	222.2	1.2×10^{-6}	1.35×10^{3}	405.	1.25×10^{-11}
88.	Phthalate, Di-N-butyl	278.3	4.5×10^{-6}	1.95×10^{5}	5.85×10^{4}	3.50×10^{13}
89.	Phthalate, Di-N-octyl	391.	5.7×10^{-6}	4.08×10^{9}	1.22×10^{9}	2.12×10^{-17}
90.	Phthalate, Bis(2-ethylhexyl)-	391.	3.0×10^{-7}	2.24×10^{9}	6.72×10^{8}	2.03×10^{-18}
91.	Phthalate, Butyl benzly-	312.	1.2×10^{-11}	1.95×10^{5}	5.85×10^{4}	9.32×10^{-19}
VIII.	Polycyclic Aromatic Hydrocarbons					
92.	Acenaphthene	154.2	9.1×10^{-5}	5.25×10^{3}	1.58×10^{3}	1.25×10^{-10}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
93.	Acenaphthylene	152.2	1.45×10^{-3}	2.89×10^{3}	866.	2.33×10^{-10}
94.	Anthracene	178.0	1.28×10^{-3}	1.55×10^{4}	4.65×10^{3}	2.02×10^{-10}
95.	Benzo(a) anthracene	228.3	1.0×10^{-6}	2.24×10^{5}	6.72×10^{4}	6.76×10^{-14}
96.	Benzo(b) fluoranthene	252.3	1.38×10^{-4}	6.31×10^{5}	1.89×10^{5}	3.27×10^{-12}
97.	Benzo(k) fluoranthene	252.3	3.0×10^{-4}	6.31×10^{5}	1.89×10^{5}	6.99×10^{-12}
98.	Benzo(g,h,i) perylene	276.	1.44×10^{-2}	1.78×10^{6}	5.34×10^{5}	8.12×10^{-11}
99.	Benzo(a) pyrene	252.	4.91×10^{-7}	6.31×10^{5}	1.89×10^{5}	1.18×10^{-14}
100.	Chrysene	228.3	1.05×10^{-6}	2.24×10^{5}	6.72×10^{4}	7.10×10^{-14}
101.	Dibenzo(a,h) anthracene	278.4	7.3×10^{-8}	3.24×10^{6}	9.72×10^{5}	3.41×10^{-16}
102.	Fluoranthene	202.3	6.5×10^{-6}	4.37×10^{4}	1.31×10^{4}	2.23×10^{-12}
103.	Fluorene	166.2	1.1×10^{-3}	4.47×10^{3}	1.34×10^{3}	2.26×10^{-10}
104.	Indeno(1,2,3-cd) pyrene	276.3	5.87×10^{-10}	1.78×10^{6}	5.34×10^{5}	5.00×10^{-18}
105.	Naphthalene	128.2	4.6×10^{-4}	1.07×10^{3}	322.	2.32×10^{-10}
106.	Phenanthrene	178.2	2.26×10^{-4}	1.55×10^{3}	4.65×10^{3}	2.16×10^{-10}
107.	Pyrene	202.3	5.1×10^{-6}	4.37×10^{4}	1.31×10^{4}	1.75×10^{-12}
IX.	Nitrosamines and Other Nitrogen-Containing Compounds					
108.	Nitrosamine, Dimethyl- (DMN)	74.1	5.4×10^{-7}	0.12	0.035	1.44×10^{-10}

TABLE 3 (cont.)

No.	Name	MW	H	K_{oc}	BCF	f
109.	Nitrosamine, Diphenyl-	198.2	1.4×10^{-7}	2.69×10^{3}	808.	7.79×10^{-13}
110.	Nitrosamine, Di-N-propyl-	130.2	2.8×10^{-8}	17.0	5.10	1.02×10^{-11}
111.	Benzidine	184.2	1.8×10^{-10}	19.5	5.85	6.46×10^{-14}
112.	Benzidine, 3,3-Dichloro-	253.1	2.4×10^{-8}	525.	157.	6.62×10^{-13}
113.	Hydrazine, 1,2-Diphenyl-	184.2	7.4×10^{-7}	17.8	5.34	1.29×10^{-10}
114.	Acrylonitrile	53.1	70	0.46	0.137	2.40×10^{-10}

a. MW = molecular weight (g/mol); H = Henry's Law constant (atm · m^3/mol); K_{oc} = soil (and sediment) adsorption coefficient based on organic carbon; BCF = bioconcentration factor for aquatic life. f calculated from Eq. 16 with M = 100 moles.

Caution: A large fraction of the H, K_{oc} and BCF values are estimates which may differ from the actual values by one order of magnitude (or more in some cases). The values listed here should not be considered as reliable.

Source: Draft report by SRI, International for values of MW, H, K_{oc}, and BCF except as noted in Table 2.

TABLE 4

Mass (M_i, Moles) of Chemical in Each Subcompartment Using Level I Approach[a]

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
	I. Pesticides						
1.	Acrolein	99.35	6.33×10^{-1}	3.56×10^{-7}	2.38×10^{-3}	5.38×10^{-6}	1.33×10^{-2}
2.	Aldrin	8.87	1.88×10^{-2}	2.07×10^{-3}	13.78	3.10×10^{-2}	77.28
3.	α-BHC	8.09	4.86×10^{-1}	2.08×10^{-3}	13.84	3.11×10^{-2}	77.54
4.	β-BHC	6.56×10^{-1}	5.6×10^{-1}	2.25×10^{-3}	14.97	3.37×10^{-2}	83.82
5.	γ-BHC (Lindane)	10.70	4.73×10^{-1}	2.02×10^{-3}	13.45	3.02×10^{-2}	75.34
6.	δ-BHC	3.03×10^{-1}	5.28×10^{-1}	2.25×10^{-3}	15.02	3.38	84.12
7.	Chlordane	3.44	1.32×10^{-2}	2.19×10^{-3}	14.62	3.29×10^{-2}	81.89
8.	DDD	1.52×10^{-4}	2.55×10^{-3}	2.27×10^{-3}	15.15	3.40×10^{-2}	84.82
9.	DDE	8.51×10^{-2}	4.52×10^{-4}	2.27×10^{-3}	15.13	3.39×10^{-2}	84.74
10.	DDT	2.23×10^{-2}	5.08×10^{-4}	2.27×10^{-3}	15.14	3.40×10^{-2}	84.80
11.	Dieldrin	1.49×10^{-3}	1.18	2.25×10^{-3}	14.97	3.36×10^{-2}	83.82
12.	α-Endosulfan	96.52	3.48	4.39×10^{-8}	2.92×10^{-4}	6.58×10^{-7}	1.64×10^{-3}
13.	β-Endosulfan	98.15	1.85	2.33×10^{-8}	1.56×10^{-4}	3.50×10^{-7}	8.72×10^{-4}
14.	Endosulfan Sulfate	4.98×10^{-2}	99.83	2.76×10^{-6}	1.84×10^{-2}	4.13×10^{-5}	.10
15.	Endrin	1.29	1.16	2.22×10^{-3}	14.78	3.32×10^{-2}	82.74

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
16.	Endrin Aldehyde	5.0	2.8	2.1×10^{-3}	14.0	3.1×10^{-2}	78.3
17.	Heptachlor	94.6	8.6×10^{-3}	1.2×10^{-4}	8.1×10^{-1}	1.8×10^{-6}	4.5
18.	Heptachlor Epoxide	3.4	8.2	2.0×10^{-3}	13.4	5.0×10^{-2}	75.0
19.	Isophorone	74.7	4.7	4.7×10^{-4}	3.1	7.03×10^{-3}	17.5
20.	TCDD (2,3,7,8-Tetrachlorodibenzo-p-dioxin)	2.1	5.9×10^{-4}	2.2×10^{-3}	14.8×10^{1}	3.3×10^{-2}	83.0
21.	Toxaphene	100.	1.7×10^{-4}	1.9×10^{-7}	1.3×10^{-3}	2.8×10^{-6}	7.1×10^{-3}
II.	PCB's and Related Compounds						
22.	PCB-1016 (Arochlor 1016)	9.0	9.8×10^{-3}	2.1×10^{-3}	13.8	3.1×10^{-2}	77.2
23.	PCB-1221 (Arochlor 1221)	53.3	.16	1.1×10^{-3}	7.0	1.6×10^{-2}	39.5
24.	PCB-1232 (Arochlor 1232)	98.4	4.1×10^{-2}	3.6×10^{-5}	.24	5.4×10^{-4}	1.4
25.	PCB-1242 (Arochlor 1242)	94.5	1.7×10^{-2}	1.2×10^{-4}	.83	1.8×10^{-3}	4.6
26.	PCB-1248 (Arochlor 1248)	41.5	4.2×10^{-3}	1.3×10^{-3}	8.9	2.0×10^{-2}	49.6
27.	PCB-1254 (Arochlor 1254)	21.2	2.9×10^{-3}	1.8×10^{-3}	11.9	2.6×10^{-2}	66.9
28.	PCB-1260 (Arochlor 1260)	86.0	4.2×10^{-5}	3.2×10^{-4}	2.1	4.8×10^{-3}	12.0
29.	2-Chloronaphthalene	93.2	2.8×10^{-2}	1.5×10^{-4}	1.0	2.4×10^{-3}	5.7
III.	Halogenated Aliphatics						
30.	Methane, Bromo- (Methylbromide)	100.	1.8×10^{-4}	1.2×10^{-9}	8.3×10^{-6}	1.9×10^{-8}	4.6×10^{-5}

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
31.	Methane, Chloro- (Methylchloride)	100.	9.0×10^{-4}	4.4×10^{-9}	2.9×10^{-5}	6.6×10^{-8}	1.6×10^{-4}
32.	Methane, Dichloro- (Methylene chloride)	100.	1.2×10^{-2}	1.2×10^{-7}	8.1×10^{-4}	1.8×10^{-6}	4.5×10^{-3}
33.	Methane, Chlorodibromo-	99.8	4.0×10^{-2}	3.9×10^{-6}	2.6×10^{-2}	5.8×10^{-5}	.14
34.	Methane, Dichlorobromo-	100.	2.0×10^{-2}	1.4×10^{-6}	9.2×10^{-3}	2.1×10^{-5}	5.2×10^{-2}
35.	Methane, Tribromo- (Bromoform)	99.6	6.6×10^{-2}	8.7×10^{-6}	5.8×10^{-2}	1.3×10^{-4}	.33
36.	Methane, Trichloro- (Chloroform)	100.	1.3×10^{-2}	6.3×10^{-7}	4.2×10^{-3}	9.6×10^{-6}	2.34×10^{-2}
37.	Methane, Tetrachloro- (Carbon tetrachloride)	100.	1.6×10^{-3}	7.8×10^{-7}	5.2×10^{-3}	1.2×10^{-5}	2.9×10^{-2}
38.	Methane, Trichlorofluoro-	100.	3.3×10^{-4}	6.0×10^{-8}	4.0×10^{-4}	8.9×10^{-7}	2.2×10^{-3}
39.	Methane, Dichlorodifluoro-	100.	1.2×10^{-5}	8.0×10^{-10}	5.3×10^{-6}	1.2×10^{-8}	3.0×10^{-5}
40.	Ethane, Chloro-	100.	2.4×10^{-3}	4.1×10^{-8}	2.8×10^{-4}	6.2×10^{-7}	1.5×10^{-3}
41.	Ethane, 1,1-Dichloro-	100.	8.5×10^{-3}	2.9×10^{-7}	2.0×10^{-3}	4.4×10^{-6}	1.1×10^{-2}
42.	Ethane, 1,2-Dichloro-	100.	3.9×10^{-2}	6.5×10^{-7}	4.4×10^{-3}	9.8×10^{-6}	2.4×10^{-2}
43.	Ethane, 1,1,1-Trichloro-	100.	1.2×10^{-3}	2.1×10^{-7}	1.4×10^{-3}	3.1×10^{-6}	7.8×10^{-3}
44.	Ethane, 1,1,2-Trichloro-	99.8	4.9×10^{-2}	3.1×10^{-6}	2.1×10^{-2}	4.7×10^{-5}	.12
45.	Ethane, 1,1,2,2-Tetrachloro-	98.9	9.4×10^{-2}	2.4×10^{-5}	.16	3.5×10^{-4}	.88
46.	Ethane, Hexachloro-	87.3	1.3×10^{-2}	2.9×10^{-4}	1.9	4.3×10^{-3}	10.8

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
47.	Ethene, Chloro- (Vinyl chloride)	100.	1.8×10^{-7}	1.7×10^{-12}	1.1×10^{-8}	2.5×10^{-11}	6.4×10^{-8}
48.	Ethene, 1,1-Dichloro-	100.	2.3×10^{-4}	8.6×10^{-9}	5.7×10^{-5}	1.3×10^{-7}	3.2×10^{-4}
49.	Ethene, Trans-dichloro-	100.	5.23×10^{-4}	5.0×10^{-9}	3.3×10^{-5}	7.5×10^{-8}	1.9×10^{-4}
50.	Ethene, Trichloro-	100.	4.06×10^{-3}	1.5×10^{-7}	1.0×10^{-3}	2.3×10^{-6}	5.6×10^{-3}
51.	Ethene, Tetrachloro-	99.96	1.80×10^{-3}	6.49×10^{-7}	4.33×10^{-3}	9.01×10^{-6}	2.42×10^{-2}
52.	Propane, 1,2-Dichloro-	100.	1.6×10^{-2}	9.0×10^{-7}	6.0×10^{-3}	1.3×10^{-5}	3.4×10^{-2}
53.	Propene, 1,3-Dichloro-	100.	2.7×10^{-2}	8.0×10^{-7}	5.3×10^{-3}	1.2×10^{-5}	3.0×10^{-2}
54.	Butadiene, Hexachloro-	100.	1.4×10^{-3}	1.4×10^{-6}	9.4×10^{-3}	2.1×10^{-5}	5.3×10^{-2}
55.	Cyclopentadiene, Hexachloro-	100.	2.2×10^{-3}	2.3×10^{-6}	1.6×10^{-2}	3.5×10^{-5}	8.8×10^{-2}
IV.	Ethers						
56.	Ether, Bis(2-chloromethyl)-	99.8	.17	2.3×10^{-7}	1.5×10^{-3}	3.4×10^{-6}	8.4×10^{-3}
57.	Ether, Bis(chloroethyl)-	95.6	2.6	4.2×10^{-5}	.28	6.3×10^{-4}	1.6
58.	Ether, Bis(2-chloroisopropyl)-	98.7	.32	2.2×10^{-5}	.15	3.4×10^{-4}	.84
59.	Ether, 2-chloroethyl vinyl-	34.2	49.3	3.7×10^{-4}	2.5	5.6×10^{-3}	14.0
60.	Ether, 4-Bromophenyl phenyl-	.12	3.4×10^{-2}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.7
61.	Ether, 4-Chlorophenyl phenyl-	44.8	7.4×10^{-2}	1.3×10^{-3}	8.4	5.3×10^{-2}	46.8
62.	Bis(2-chloroethoxy) methane	44.8	7.4×10^{-2}	1.3×10^{-3}	8.4	5.3×10^{-2}	46.8

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
V.	Monocyclic Aromatics (Excluding Phenols, Cresols, Phthalates)						
63.	Benzene	100.	6.6×10^{-3}	4.9×10^{-7}	3.2×10^{-3}	7.3×10^{-6}	1.8×10^{-2}
64.	Benzene, Chloro-	99.8	1.0×10^{-2}	3.8×10^{-6}	2.5×10^{-2}	5.7×10^{-5}	.14
65.	Benzene, 1,2-Dichloro-	98.4	1.8×10^{-2}	3.7×10^{-5}	.25	5.5×10^{-4}	1.4
66.	Benzene, 1,3-Dichloro-	99.1	9.9×10^{-3}	2.0×10^{-5}	.13	3.0×10^{-4}	.74
67.	Benzene, 1,4-Dichloro-	99.0	1.2×10^{-2}	2.3×10^{-5}	.15	3.4×10^{-4}	.86
68.	Benzene, 1,2,4-Trichloro-	93.4	1.5×10^{-2}	1.5×10^{-5}	1.0	2.2×10^{-3}	5.6
69.	Benzene, Hexachloro-	2.9	1.5×10^{-3}	2.2×10^{-3}	14.7	3.3×10^{-2}	82.4
70.	Benzene, Ethyl-	99.7	5.5×10^{-3}	6.6×10^{-6}	4.4×10^{-2}	9.9×10^{-5}	.24
71.	Benzene, Nitro-	92.9	2.6	1.0×10^{-4}	.70	1.6×10^{-3}	3.9
72.	Toluene	99.9	7.0×10^{-3}	2.4×10^{-6}	1.6×10^{-2}	3.6×10^{-5}	8.8×10^{-2}
73.	Toluene, 2,4-Dinitro-	68.9	5.5	5.8×10^{-4}	3.9	8.7×10^{-3}	21.7
74.	Toluene, 2,6-Dinitro-	79.6	3.6	3.8×10^{-4}	2.5	5.7×10^{-3}	14.2
VI.	Phenols and Cresols						
75.	Phenol	42.3	33.6	5.4×10^{-4}	3.6	8.2×10^{-3}	20.3
76.	Phenol, 2-Chloro-	86.0	3.0	2.5×10^{-4}	1.7	3.8×10^{-3}	9.3
77.	Phenol, 2,4-Dichloro-	27.7	3.6	1.6×10^{-3}	10.4	2.3×10^{-2}	58.3

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
78.	Phenol, 2,4,6-Trichloro-	10.0	.90	2.0×10^{-3}	13.5	3.0×10^{-2}	75.6
79.	Phenol, Pentachloro-	.29	3.8×10^{-2}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.5
80.	Phenol, 2-Nitro-	89.9	4.3	1.3×10^{-4}	.88	2.0×10^{-3}	4.9
81.	Phenol, 4-Nitro-	3.1×10^{-3}	30.7	1.6×10^{-3}	10.5	2.4×10^{-2}	58.8
82.	Phenol, 2,4-Dinitro-	5.2×10^{-2}	29.2	1.6×10^{-3}	10.7	2.4×10^{-2}	60.0
83.	Phenol, 2,4-Dimethyl	29.0	4.4	1.5×10^{-3}	10.1	2.3×10^{-2}	56.5
84.	m-Cresol, p-Chloro-	5.2	5.3	2.0×10^{-3}	13.6	3.0×10^{-2}	75.9
85.	o-Cresol, 4,6-Dinitro-	.42	7.6	2.1×10^{-3}	13.9	3.1×10^{-2}	78.0
VII.	Phthalate Esters						
86.	Phthalate, Dimethyl-	50.1	8.4	9.4×10^{-4}	6.2	1.4×10^{-2}	35.2
87.	Phthalate, Diethyl-	5.2	1.6	2.1×10^{-3}	14.1	3.2×10^{-2}	79.1
88.	Phthalate, Di-N-butyl	.15	.12	2.3×10^{-3}	15.1	3.4×10^{-2}	84.7
89.	Phthalate, Di-N-octyl	8.8×10^{-6}	5.6×10^{-7}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
90.	Phthalate, Bis(2-ethylhexyl)-	8.4×10^{-7}	1.0×10^{-6}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
91.	Phthalate, Butyl benzly-	3.9×10^{-7}	1.2×10^{-6}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
VIII.	Polycyclic Aromatic Hydrocarbons						
92.	Acenaphthene	52.0	.21	1.1×10^{-3}	7.2	1.6×10^{-2}	40.4

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
93.	Acenaphthylene	96.9	2.4×10^{-2}	7.0×10^{-5}	.46	1.0×10^{-3}	2.6
94.	Anthracene	83.9	2.4×10^{-2}	3.7×10^{-4}	2.4	5.5×10^{-3}	13.7
95.	Benzo(a) anthracene	2.8×10^{-2}	1.0×10^{-2}	2.3×10^{-3}	15.1	3.4×10^{-2}	83.7
96.	Benzo(b) fluoranthene	1.4	3.6×10^{-3}	2.2×10^{-3}	14.9	3.4×10^{-2}	83.7
97.	Benzo(k) fluoranthene	2.9	3.5×10^{-3}	2.2×10^{-3}	14.7	3.3×10^{-2}	82.3
98.	Benzo(g,h,i) perylene	33.8	8.5×10^{-4}	1.5×10^{-3}	10.0	2.3×10^{-2}	56.2
99.	Benzo(a) pyrene	4.9×10^{-3}	3.6×10^{-3}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
100.	Chrysene	3.00×10^{-2}	1.0×10^{-2}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
101.	Dibenzo(a,h) anthracene	1.4×10^{-4}	7.0×10^{-4}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
102.	Fluoranthene	.93	5.1×10^{-2}	2.2×10^{-3}	15.0	3.4×10^{-2}	84.0
103.	Fluorene	93.9	3.1×10^{-2}	1.4×10^{-4}	.92	2.1×10^{-3}	5.1
104.	Indeno(1,2,3-cd) pyrene	2.1×10^{-6}	1.3×10^{-3}	2.3×10^{-3}	15.1	3.4×10^{-2}	84.8
105.	Naphthalene	96.4	7.6×10^{-2}	8.1×10^{-5}	5.4×10^{-1}	1.2×10^{-3}	3.0
106.	Phenanthrene	90.0	.14	2.2×10^{-4}	1.5	3.3×10^{-2}	84.2
107.	Pyrene	.73	5.2×10^{-2}	2.3×10^{-3}	15.0	3.4×10^{-2}	84.2
IX.	Nitrosamines and Other Nitrogen-Containing Compounds						
108.	Nitrosamine, Dimethyl- (DMN)	59.8	40.0	4.8×10^{-6}	3.2×10^{-2}	7.0×10^{-5}	.18

TABLE 4 (cont.)

No.	Name	M_1	M_2	M_3	M_4	M_5	M_6
109.	Nitrosamine, Diphenyl-	.32	.83	2.2×10^{-3}	15.0	3.4×10^{-2}	83.8
110.	Nitrosamine, Di-N-propyl-	4.3	54.8	9.3×10^{-4}	6.2	1.4×10^{-2}	34.8
111.	Benzidine	2.7×10^{-2}	53.8	1.0×10^{-3}	7.0	1.6×10^{-2}	39.2
112.	Benzidine, 3,3-Dichloro-	.28	4.1	2.2×10^{-3}	14.5	3.2×10^{-2}	81.1
113.	Hydrazine, 1,2-Diphenyl-	53.5	26.1	4.6×10^{-4}	3.1	7.0×10^{-3}	17.3
114.	Acrylonitrile	100.	5.2×10^{-7}	2.7×10^{-13}	1.6×10^{-9}	3.5×10^{-12}	8.8×10^{-9}

a. Calculated from Eq. 21 with M = 100 moles. Thus, the individual M_i values (in moles) are equivalent to the percent in each subcompartment. The subscripts on M identify the environmental subcompartments as follows:

1. Air
2. Surface water
3. Suspended sediments
4. Bottom sediments
5. Aquatic biota
6. Soils

TABLE 5

Calculated Concentrations (ppt) of Chemicals in Each Subcompartment Using Level I Approach[a]

No. Name	C_1'[b]	C_2'	C_3' and C_4'	C_5'	C_6'
I. Pesticides					
1. Acrolein	240.	240.	13.	40.	2.7
2. Aldrin	210.	46.	5.0×10^5	1.5×10^6	1.0×10^5
3. α-BHC	19.	940.	4.0×10^5	1.2×10^6	8.1×10^4
4. β-BHC	1.6	1000.	4.4×10^5	1.3×10^6	8.7×10^4
5. γ-BHC (Lindane)	26.	920.	3.9×10^5	1.2×10^6	7.8×10^4
6. δ-BHC	7.3×10^{-1}	1000.	4.4×10^5	1.3×10^6	8.7×10^4
7. Chlordane	8.3	36.	5.9×10^5	1.8×10^6	1.2×10^5
8. DDD	3.6×10^{-4}	5.4	4.8×10^5	1.5×10^6	9.7×10^4
9. DDE	.20	.96	4.8×10^5	1.4×10^6	9.6×10^4
10. DDT	5.3×10^{-2}	1.2	5.4×10^5	1.6×10^6	1.1×10^5
11. Dieldrin	3.6×10^{-3}	3000.	5.7×10^5	1.7×10^6	1.1×10^5
12. α-Endosulfan	230.	940.	12.	36.	2.4
13. β-Endosulfan	240.	5000.	6.3	19.	1.3
14. Endosulfan Sulfate	.12	2.8×10^5	780.	2300.	160.
15. Endrin	3.1	3000.	5.6×10^5	1.7×10^6	1.1×10^5

TABLE 5 (cont.)

No.	Name	C_1' [b]	C_2'	C_3' and C_4'	C_5'	C_6'
16.	Endrin Aldehyde	12.	7000.	5.3×10^5	1.6×10^6	1.1×10^5
17.	Heptachlor	230.	220.	3.0×10^4	91.	6.1×10^3
18.	Heptachlor Epoxide	8.2	2.1×10^4	5.2×10^5	1.6×10^6	1.0×10^5
19.	Isophorone	180.	4.3×10^3	4.3×10^4	1.3×10^5	8.6×10^3
20.	TCDD (2,3,7,8-Tetrachlorodibenzo-p-dioxin)	5.1	1.3	4.8×10^5	1.4×10^6	9.5×10^4
21.	Toxaphene	240.	.47	52.	160.	10.
II.	PCB's and Related Compounds					
22.	PCB-1016 (Arochlor 1016)	220.	17.	3.6×10^5	1.1×10^6	7.1×10^4
23.	PCB-1221 (Arochlor 1221)	130.	210.	1.4×10^5	4.3×10^5	2.8×10^4
24.	PCB-1232 (Arochlor 1232)	240.	64.	5600.	1.7×10^4	1100.
25.	PCB-1242 (Arochlor 1242)	230.	31.	2.2×10^4	6.4×10^4	4.4×10^3
26.	PCB-1248 (Arochlor 1248)	100.	8.3	2.7×10^5	7.9×10^5	5.3×10^4
27.	PCB-1254 (Arochlor 1254)	51.	6.4	3.9×10^5	1.2×10^6	7.8×10^4
28.	PCB-1260 (Arochlor 1260)	210.	.10	8.1×10^4	2.4×10^5	1.6×10^4
29.	2-Chloronaphthalene	220.	30.	1.7×10^4	5.1×10^4	3000.
III.	Halogenated Aliphatics					
30.	Methane, Bromo- (Methylbromide)	240.	.12	7.8×10^{-2}	24	1.6×10^{-2}

TABLE 5 (cont.)

No.	Name	$C_1^{\prime}$ [b]	$C_2^{\prime}$	$C_3^{\prime}$ and $C_4^{\prime}$	$C_5^{\prime}$	$C_6^{\prime}$
31.	Methane, Chloro- (Methylchloride)	240.	.30	.15	.45	3.0×10^{-2}
32.	Methane, Dichloro- (Methylene chloride)	240.	6.9	6.9	21.	1.4
33.	Methane, Chlorodibromo-	240.	56.	540.	1600.	110.
34.	Methane, Dichlorobromo-	240.	22.	150.	450.	30.
35.	Methane, Tribromo- (Bromoform)	240.	110.	1500.	4400.	290.
36.	Methane, Trichloro- (Chloroform)	240.	10.	50.	150.	10.
37.	Methane, Tetrachloro- (Carbon tetrachloride)	240.	1.6	80.	240.	16.
38.	Methane, Trichlorofluoro-	240.	.30	5.5	16.	1.1
39.	Methane, Dichlorodifluoro-	240.	9.8×10^{-3}	6.4×10^{-2}	.19	1.3×10^{-2}
40.	Ethane, Chloro-	240.	1.0	1.8	5.3	.36
41.	Ethane, 1,1-Dichloro-	240.	5.6	19.	58.	3.9
42.	Ethane, 1,2-Dichloro-	240.	26.	43.	130.	8.6
43.	Ethane, 1,1,1-Trichloro-	240.	1.1	19.	56.	3.7
44.	Ethane, 1,1,2-Trichloro-	240.	43.	280.	840.	56.
45.	Ethane, 1,1,2,2-Tetrachloro-	240.	110.	260.	7900.	530.
46.	Ethane, Hexachloro-	210.	20.	4.6×10^{4}	1.4×10^{5}	9.1×10^{3}

TABLE 5 (cont.)

No.	Name	C_1' [b]	C_2'	C_3' and C_4'	C_5'	C_6'
47.	Ethene, Chloro- (Vinyl chloride)	240.	7.6×10^{-5}	7.1×10^{-5}	2.1×10^{-4}	1.4×10^{-5}
48.	Ethene, 1,1-Dichloro-	240.	.15	.55	1.7	.11
49.	Ethene, Trans-dichloro-	240.	.34	.32	.97	6.5×10^{-2}
50.	Ethene, Trichloro-	240.	3.5	13.	40.	2.6
51.	Ethene, Tetrachloro-	240.	2.00	72.	200.	14.
52.	Propane, 1,2-Dichloro-	240.	12.	68.	200.	14.
53.	Propene, 1,3-Dichloro-	240.	20.	59.	180.	12.
54.	Butadiene, Hexachloro-	240.	2.4	240.	730.	49.
55.	Cyclopentadiene, Hexachloro-	240.	4.1	430.	1300.	85.
IV.	Ethers					
56.	Ether, Bis(2-chloromethyl)-	240.	130.	17.	52.	3.5
57.	Ether, Bis(chloroethyl)-	230.	2500.	4000.	1.2×10^4	800.
58.	Ether, Bis(2-chloroisopropyl)-	240.	370.	2600.	7700.	510.
59.	Ether, 2-chloroethyl vinyl-	82.	3.5×10^4	2.7×10^4	8.0×10^4	5.3×10^3
60.	Ether, 4-Bromophenyl phenyl-	.30	57.	3.8×10^5	1.1×10^6	7.5×10^4
61.	Ether, 4-Chlorophenyl phenyl-	100.	100.	1.7×10^5	1.4×10^6	3.4×10^4
62.	Bis(2-chloroethoxy) methane	97.	5.4×10^4	3.2×10^4	9.6×10^4	6400.

TABLE 5 (cont.)

No.	Name	C_1' [b]	C_2'	C_3' and C_4'	C_5'	C_6'
V.	Monocyclic Aromatics (Excluding Phenols, Cresols, Phthalates)					
63.	Benzene	240.	3.4	25.	76.	5.1
64.	Benzene, Chloro-	240.	7.5	290.	860.	57.
65.	Benzene, 1,2-Dichloro-	240.	18.	3600.	1.1×10^4	720.
66.	Benzene, 1,3-Dichloro-	240.	9.7	1900.	5800.	390.
67.	Benzene, 1,4-Dichloro-	240.	11.	2300.	6800.	450.
68.	Benzene, 1,2,4-Trichloro-	220.	18.	1.8×10^4	5.4×10^4	3600.
69.	Benzene, Hexachloro-	6.9	2.9	4.2×10^5	1.3×10^6	8.4×10^4
70.	Benzene, Ethyl-	240.	3.9	460.	1400.	93.
71.	Benzene, Nitro-	220.	2100.	8600.	2.6×10^4	1700.
72.	Toluene	240.	4.3	150.	440.	29.
73.	Toluene, 2,4-Dinitro-	170.	6700.	7.0×10^4	2.1×10^5	1.4×10^4
74.	Toluene, 2,6-Dinitro-	190.	4400.	4.6×10^4	1.4×10^5	9300
VI.	Phenols and Cresols					
75.	Phenol	100.	2.1×10^4	3.4×10^4	1.0×10^5	6.8×10^3
76.	Phenol, 2-Chloro-	210.	2600.	2.1×10^4	6.4×10^4	4300.
77.	Phenol, 2,4-Dichloro-	67.	3900.	1.7×10^5	5.1×10^5	3.4×10^4

TABLE 5 (cont.)

No.	Name	C_1' [b]	C_2'	C_3' and C_4'	C_5'	C_6'
78.	Phenol, 2,4,6-Trichloro-	24.	1200.	2.7×10^5	8.0×10^5	5.3×10^4
79.	Phenol, Pentachloro-	.70	67.	4.0×10^5	1.2×10^6	8.0×10^4
80.	Phenol, 2-Nitro-	220.	4000.	1.2×10^4	3.7×10^4	2500.
81.	Phenol, 4-Nitro-	7.6×10^{-3}	2.8×10^4	1.5×10^5	4.4×10^5	2.9×10^4
82.	Phenol, 2,4-Dinitro-	.13	3.6×10^4	2.0×10^5	5.9×10^5	3.9×10^4
83.	Phenol, 2,4-Dimethyl	70.	3600.	1.2×10^5	3.7×10^5	2.5×10^4
84.	m-Cresol, p-Chloro-	12.	5000.	1.9×10^5	5.8×10^5	3.9×10^4
85.	o-Cresol, 4,6-Dinitro-	1.0	1.0×10^4	2.8×10^5	8.3×10^5	5.5×10^4
VII.	Phthalate Esters					
86.	Phthalate, Dimethyl-	120.	1.1×10^4	1.2×10^5	3.7×10^5	2.4×10^4
87.	Phthalate, Diethyl-	13.	2300.	3.2×10^5	9.4×10^5	6.3×10^4
88.	Phthalate, Di-N-butyl	.35	22.	4.2×10^5	1.3×10^6	8.4×10^4
89.	Phthalate, Di-N-octyl	2.1×10^{-5}	1.5×10^{-3}	5.9×10^5	1.8×10^6	1.2×10^5
90.	Phthalate, Bis(2-ethylhexyl)-	2.0×10^{-6}	2.6×10^{-3}	5.9×10^5	1.8×10^6	1.2×10^5
91.	Phthalate, Butyl benzly-	9.3×10^{-7}	24.	4.7×10^5	1.4×10^6	9.5×10^4
VIII.	Polycyclic Aromatic Hydrocarbons					
92.	Acenaphthene	130.	210.	1.1×10^5	3.4×10^5	2.2×10^4

TABLE 5 (cont.)

No.	Name	C_1^{b}	C_2	C_3 and C_4	C_5	C_6
93.	Acenaphthylene	230.	250.	7100.	2.1×10^4	1400.
94.	Anthracene	200.	28.	4.3×10^4	1.3×10^5	8700.
95.	Benzo(a) anthracene	6.7×10^{-2}	15.	3.5×10^5	1.0×10^6	6.9×10^4
96.	Benzo(b) fluoranthene	3.3	6.0	3.8×10^5	1.1×10^6	7.5×10^4
97.	Benzo(k) fluoranthene	7.0	5.9	3.7×10^5	1.1×10^6	7.4×10^4
98.	Benzo(g,h,i) perylene	81.0	1.6	2.8×10^5	8.3×10^5	5.5×10^4
99.	Benzo(a) pyrene	1.2×10^{-2}	6.0	3.8×10^5	$1,1 \times 10^6$	7.6×10^4
100.	Chrysene	7.1×10^{-2}	15.	3.5×10^5	1.0×10^6	6.9×10^4
101.	Dibenzo(a,h) anthracene	3.4×10^{-4}	13.	4.2×10^5	4.2×10^5	8.4×10^4
102.	Fluoranthene	2.2	69.	3.0×10^5	9.1×10^5	6.1×10^4
103.	Fluorene	230.	34.	1.5×10^4	4.6×10^4	3.0×10^3
104.	Indeno(1,2,3-cd) pyrene	5.0×10^{-6}	2.4	4.2×10^5	4.2×10^5	8.4×10^4
105.	Naphthalene	230.	65.	6.9×10^3	2.1×10^4	1.4×10^3
106.	Phenanthrene	220.	170.	2.6×10^4	7.9×10^5	5.3×10^3
107.	Pyrene	1.8	70.	3.0×10^5	9.1×10^5	6.1×10^4
IX.	Nitrosamines and Other Nitrogen-Containing Compounds					
108.	Nitrosamine, Dimethyl- (DMN)	140.	2.0×10^4	240.	690.	47.

TABLE 5 (cont.)

No.	Name	C_1' [b]	C_2'	C_3' and C_4'	C_5'	C_6'
109.	Nitrosamine, Diphenyl-	.78	1100.	3.0×10^{5}	8.9×10^{5}	5.9×10^{4}
110.	Nitrosamine, Di-N-propyl-	10.	4.8×10^{4}	8.1×10^{4}	2.4×10^{5}	1.6×10^{4}
111.	Benzidine	6.4×10^{-2}	6.6×10^{4}	1.3×10^{5}	3.9×10^{5}	2.6×10^{4}
112.	Benzidine, 3,3-Dichloro-	.66	7000.	3.7×10^{5}	1.1×10^{6}	7.3×10^{4}
113.	Hydrazine, 1,2-Diphenyl-	130.	3.2×10^{4}	5.7×10^{4}	1.7×10^{5}	1.1×10^{4}
114.	Acrylonitrile	240.	1.8×10^{-4}	8.4×10^{-6}	2.5×10^{-5}	1.7×10^{-6}

a. Calculated from Eqs. 24-29. C_1' is in units of ppt (vol/vol); all other values are in units of ppt (wt/wt). Calculations assume 100 moles of the chemical are contained within the total environmental compartment. The subscripts on C identify the environmental subcompartments as follows:

1. Air
2. Surface water
3. Suspended sediments
4. Bottom sediments
5. Aquatic biota
6. Soils

Note that concentration ratios are independent of the total mass in the environment and the volumes of the individual subcompartments.

b. To convert air concentrations to ng/m^3, multiply the value of C_1, given here by MW/24.

IV. CALCULATIONS USING NEELY'S APPROACH

A. Basis for Approach

Researchers at the Dow Chemical Co. (Midland, MI) have investigated the distribution of a number of chemicals after placement in a simulated aquatic/terrestrial ecosystem (Neely, 1978a, 1978b). A scenario (Blau and Neeley, 1975; Neely and Blau, 1977) was used involving the introduction of 0.15 g/hr of the test chemical into the ecosystem for a 30-day period (Neely, 1978c). This was followed by a 30-day clearance period. The percent of the test chemical in air, water and soil was determined after the first 30-day period. The half-life for clearance from fish was determined during the 30-day clearance period. A brief description of the ecosystem used in these tests is shown in Table 6.

The test set of chemicals used, along with their relevant properties, are shown in Table 7. The percent of each chemical found in water, soil, and air - and the fish clearance rate - are shown in Table 8.

Four regression equations were found to describe the results of these tests in a statistically significant manner. They are:

$$\% \text{ in Air} = -0.247(1/H) + 7.9 \log S + 100.6 \quad (30)$$

$$\% \text{ in Water} = 0.054(1/H) + 1.32 \quad (31)$$

$$\% \text{ in Soil} = 0.194(1/H) - 7.65 \log S - 1.93 \quad (32)$$

$$\log t_{1/2} = 0.0027(1/H) - 0.282 \log S + 1.08 \quad (33)$$

where H = Henry's Law Constant = P_{vp}/S

S = water solubility (mM/L)*

P_{vp} = vapor pressure (mm Hg)

$t_{1/2}$ = half-life for clearance from fish in ecosystem (hr)

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* To convert values of S from mg/L (e.g., the values in Table 6) to mM/L, divide by the molecular weight.

Table 6

Description of the Model Ecosystem Used by Neely

Parameter	Values
Volume of Water	3.6×10^8 cm^3
Average depth of water	89 cm
Total weight of soil	1.5×10^7 g[a.]
% organic matter in soil	0.13%
Total weight of fish	8,580g
Weight of average fish	15g
Rate of chemical addition	0.15 g/hr
Duration of chemical addition	30 days
Clearance period	30 days

a. This is based on a conversion factor of 3.7 g of soil per cm^2 for a 2.5 cm layer.

Source: Neely (1978c)

Table 7

Properties of a Series of Chemicals Tested in the Simulated Aquatic Ecosystem

	Molecular Weight	Vapor Pressure (mm Hg)	Water Solubility (ppm)
Toluene	92	30	470
p-Dichlorobenzene	147	1	79
Trichlorobenzene	180	0.5	30
Hexachlorobenzene	285	10^{-5}	0.035
Diphenyl	154	9.7×10^{-3}	7.5
Trichlorobiphenyl	256	1.5×10^{-3}	0.05
Tetrachlorobiphenyl	291	4.9×10^{-4}	0.05
Pentachlorobiphenyl	325	7.7×10^{-5}	0.01
DDT	350	10^{-7}	1.2×10^{-3}
Perchloroethylene	166	14	150

Source: Neely (1978a).

Table 8

Distribution of the Chemicals Shown in Table 7 in the Various Compartments of the Simulated Ecosystem

Chemical	Water, %	Soil, %	Air, %	$t_{1/2}$ from fish[a], h
Toluene	0.9 (1.33)[b]	0.4 (∿0)	98.6 (∿100)	10 (7.6)
p-Dichlorobenzene	1.24 (1.31)	1.28 (0.24)	97.5 (98)	15 (14)
Trichlorobenzene	1.33 (1.34)	2.06 (4.09)	96 (94)	17 (20)
Hexachlorobenzene	3.57 (1.98)	39.4 (31)	56 (68)	162 (164)
Diphenyl	2.27 (1.59)	5.4 (9)	92.2 (89)	27 (29)
Trichlorobiphenyl	1.38 (1.33)	15.2 (26)	83 (71)	96 (134)
Tetrachlorobiphenyl	1.5 (1.34)	17 (27)	81 (71)	104 (139)
Pentachlorobiphenyl	1.5 (1.34)	21 (33)	77 (65)	229 (226)
DDT	1.26 (3.17)	67.5 (46.5)	28 (49)	915 (517)
Perchloroethylene	1 (1.32)	1 (∿0)	98 (100)	14 (12)

a. This is the time for clearance from the fish in the simulated aquatic ecosystem once addition of chemical was terminated.

b. The numbers in parenthesis were estimated from the regression equations.

Source: Neely (1978a)

Table 8 shows the predicted percentages (and $t_{1/2}$ values) for the test set of chemicals used by Dow.

It should be pointed out that the use of Equations 30 to 33 were not intended by Neely to provide the user with quantitative predictions of environmental concentrations that would be an end in themselves. These regression equations were proposed as part of a decision tree (Neeley, 1978a) which can lead the user to a decision on what, if any, additional environmental tests should be carried out on a chemical of concern. The percent values calculated are simply used to rank a chemical with regard to its potential as an air, water, soil, and/or aquatic biota pollutant. The decision tree proposed by Neely (1978a) included the following cut-off points:

Compartment	If	Tests to be Conducted
Air	>90%	Photodegradation; model impact on stratosphere
Water	>2%	Degradation (chemical and biological) in water
Soil	>4%	Degradation (chemical and biological) in soils
Fish	$t_{1/2}$ >100 hrs.	Bioconcentration factors in aquatic biota; metabolic degradation/elimination.

The decision tree also involves considerations of the use pattern (e.g., confined vs dispersive) of the chemical and its physical form (polymers are given a low ranking).

A final comment on Equations 30-33 is required. This set of equations has been normalized so that the sum of the percentages in air, water and soil should sum to approximately 100% for any chemical. While it is recognized that, in reality, the percent in any one compartment cannot be >100 or <0%, the regression equations may yield values outside these values for some chemicals. This is to be expected due to a combina-

tion of experimental errors and the inability of the relatively-simple regression equations to explain all of the variability in the measured data.

B. Sample Calculations

The test set of compounds selected for use is shown in Table 9 along with the input data required for each chemical. These input data were obtained from a draft report by SRI, International (Menlo Park, CA). The test set consists of twenty chemicals representing a variety of chemical classes.

Equations 30 to 33 were applied to each of the test chemicals. The results are shown in Table 10. Underneath the calculated values for % in air, water and soil are the corresponding values (M_1, M_2 and M_6, respectively) from the Level I fugacity calculations (Table 4).

The results of the Neely approach shown in Table 10 are somewhat disturbing if attention is focused on the unrealistic percentages associated with some chemicals. Percentages <0% or >100% were associated with nearly one-half of the test set (9 out of 20 chemicals). The "Total %" value is unrealistic for only one chemical, 2,4-dinitrophenol.

If, however, the numbers in Table 10 are only used - as described in A above - to decide if additional tests are required, then the results are meaningful for essentially the whole test set. The chemicals that exceed the cut-off points associated with Neely's decision tree are listed below.

(Text continues on page IV-12)

Table 9

Chemicals and Input Data Used with Neely's Equations

No. Name	MW (g)	P_{vp} (mm Hg)	S (mg/L)	1/H (mm Hg·m^3/mole)
I. Pesticides				
2. Aldrin	365	6×10^{-6}	.017	7.76
5. γ-BHC (Lindane)	291	1.6×10^{-4}	7.52	161.51
17. Heptachlor	373.5	3.0×10^{-4}	0.056	.50
II. PCB's and Related Compounds				
23. PCB-1221 (Arochlor 1221)	200.7	6.7×10^{-3}	15	11.2
24. PCB-1260 (Arochlor 1260)	375.7	4.05×10^{-5}	.0027	1.77×10^{-1}
III. Halogenated Aliphatics				
32. Methane, Dichloro- (Methylene chloride)	84.94	362.4	20,000	6.50×10^{-1}
48. Ethene, 1,1-Dichloro	96.94	591	400	6.98×10^{-3}
54. Butadiene, Hexachloro	260.79	0.15	2	5.1×10^{-2}
IV. Ethers				
56. Ether, Bis(2-chloromethyl)-	115	30	2.2×10^{4}	6.38
61. Ether, 4-chlorophenyl phenyl-	204.66	2.7×10^{-3}	3.3	5.97
V. Monocylic Aromatics (Excluding Phenols, Cresols, Phthalates)				
67. Benzene, 1,4-Dichloro	147.01	1.18	79	4.55×10^{-1}
73. Toluene, 2,4-Dinitro	182.14	5.1×10^{-3}	270	290.7

Table 9 (continued)

No. Name	MW (g)	P_{vp} (mm Hg)	S (mg/L)	1/H (mm Hg·, ^{3}/mole)
VI Phenols and Cresols				
77. Phenol, 2,4-Dichloro-	163	5.9×10^{-2}	4.6×10^{3}	478.3
82. Phenol, 2,4-Dinitro-	184.1	1.49×10^{-5}	5.6×10^{3}	$2.04 \times 10^{+6}$
VII. Phthalate Esters				
87. Phthalate, Diethyl-	222.2	3.5×10^{-3}	896	1.15×10^{3}
90. Phthalate, Bis(2-Ethylhexyl)-	391	2×10^{-7}	0.4	5.12×10^{3}
VIII. Polycylic Aromatic Hydrocarbons				
93. Acenaphthylene	152.2	2.9×10^{-2}	3.93	.89
99. Benzo(a)pyrene	252	5.6×10^{-9}	3.8×10^{-3}	2.69×10^{3}
105. Naphthalene	128.2	8.7×10^{-2}	31.7	2.84
IX. Nitrosamines and Other Nitrogen-Containing Compounds				
114. Acrylonitrile	53.1	100	7.9×10^{4}	14.88

Table 10

Results of Calculations Using the Neely Approach[a]

No. Name	% in Air	% in Water	% in Soil	Total %	$t_{1/2}$ (hrs.)
I. Pesticides					
2. Aldrin	64.5 (8.87)[a]	1.7 (0.02)[a]	32.7 (77.3)[a]	98.9	210.2
5. Y -BHC (Lindane)	48.2 (10.7)	10.0 (10.47)	41.5 (75.3)	99.7	92.0
17. Heptachlor	70.3 (94.6)	1.3 (0.009)	27.4 (4.5)	99.0	144.4
II. PCB's and Related Compounds					
23, PCB-1221 (Arochlor) 1221	88.9 (53.3)	1.9 (0.16)	8.9 (39.5)	99.7	26.8
28. PCB-1260 (Arochlor) 1260	59.9 (86.0)	1.4 (4×10^{-5})	37.5 (12.0)	98.7	339.6
III. Halogenated Aliphatics					
32. Methane, Dichloro- (methylene chloride)	119.2 (~100)	1.4 (0.01)	-19.9 (4×10^{-3})	100.6	2.6
48. Ethene,1,1-Dichloro-	105.5 (~100)	1.3 (2×10^{-4})	-6.6 (3×10^{-4})	100.0	8.1
54. Butadiene, Hexachloro	83.9 (~100)	1.3 (0.001)	14.3 (.05)	99.5	47.5

Table 10 (continued)

No. Name	% in Air	% in Water	% in Soil	Total %	$t_{1/2}$ (hrs.)
IV. Ethers					
56. Ether, Bis (2-Chloromethyl)	117.1 (99.8)	1.7 (0.17)	-18.1 (0.008)	100.6	2.8
61. Ether, 4-Chlorophenyl Phenyl-	85.0 (44.8)	1.6 (7.4×10^{-2})	12.9 (46.8)	99.5	40.0
V. Monocylic Aromatics (Excluding Phenols, Cresols, Phthalates)					
67. Benzene, 1,4-Dichloro-	98.4 (99.0)	1.3 (0.01)	.22 (0.86)	99.9	14.4
73. Toluene, 2,4-Dinitro-	30.2 (68.9)	17.0 (5.5)	53.2 (21.7)	100.3	65.5
VI. Phenols and Cresols					
77. Phenol, 2,4-Dichloro-	-6.1 (27.7)	27.1 (3.6)	79.8 (58.3)	100.8	91.7
82. Phenol, 2,4-Dinitro-	-5.0×10^{5} (0.05)	1.1×10^{5} (29.2)	4.0×10^{5} (60.0)	2.14×10^{3}	$>9.9 \times 10^{99}$
VII. Phthalate Esters					
87. Phthalate, Diethyl-	-179.2 (5.2)	63.5 (1.6)	216.9 (79.1)	101.3	1.0×10^{4}
90. Phthalate, Bis(2-ethylhexyl)	-1190 (8×10^{-7})	277.5 (1×10^{-6})	1010 (84.8)	104.4	5.4×10^{15}

Table 10 (continued)

	% in Air	% in Water	% in Soil	Total %	$t_{1/2}$ (hrs.)
VIII. Polycyclic Aromatic Hydrocarbons					
93. Acenaphthylene	87.8 (96.9)	1.4 (0.02)	10.4 (2.6)	99.6	33.9
99. Benzo(a)pyrene	~600 (0.005)	147 (0.004)	557 (84.8)	101.5	5.1×10^{9}
105. Naphthalene	95.1 (96.4)	1.5 (0.08)	3.3 (3.0)	99.8	18.1
IX Nitrosamines and Other Nitrogen Containing Compounds					
114. Acrylonitrile	122.0 (100)	2.1 (5×10^{-7})	~23.3 (9×10^{-9})	100.8	1.68

a. Vales in parenthesis are the corresponding results (M_1, M_2 and M_6) from the Level I fugacity calculations (Table 3).

Air Pollutants (% in Air >90%)	Water Pollutants (% in Water >2%)
Methane, dichloro	γ-BHC
Ethene, 1,1-dichloro-	Toluene, 2,4-dinitro-
Ether, Bis(2-chloromethyl)-	Phenol, 2,4-dichloro-
Benzene, 1,4-dichloro	Phenol, 2,4-dinitro-
Naphthalene	Phthalate, diethyl-
Acrylonitrile	Phthalate, Bis(2-ethylhexyl)
	Benzo(a)pyrene
	Acrylonitrile

Soil Pollutants (% in Soil >4%)	Fish Pollutants ($t_{1/2}$ >100h)
Aldrin	Aldrin
γ-BHC	Heptachlor
Heptachlor	PCB-1260
PCB-1221	Phenol, 2,4-dinitro(?)
PCB-1260	Phthalate, diethyl-
Butadiene, hexachloro-	Phthalate, Bis(2-ethylhexyl)
Ether, 4-chlorophenyl phenyl-	Benzo(a)pyrene
Toluene, 2,4-dinitro-	
Phenol, 2,4-dichloro-	
Phenol, 2,4-dinitro-	
Phthalate, diethyl-	
Phthalate, Bis(2-ethylhexyl)	
Acenaphthylene	
Benzo(a)pyrene	

All of the assignments as air, water, and/or soil pollutants appear reasonable in connection with the results of the Level I fugacity calculations, and the known (or estimated) properties of these chemicals.

V. LEVEL II MACKAY CALCULATIONS

A. Basic Assumptions/Model Output

The Level II calculations go beyond the Level I equilibrium calculations by allowing:

1) Degradation (by first-order kinetics only) in each subcompartment;

2) A net flux of the chemical into the total compartment; and

3) Removal of the chemical from a subcompartment by advection, e.g., transport in the air or water.

The Level II calculations do not consider rates of intercompartmental transport via such pathways as runoff, washout or volatilization. Equilibrium partitioning between the subcompartments (a dynamic steady state) is allowed. All other aspects of the basic model, including the concept of accessible volumes for a chemical in each subcompartment, still remain.

The Level II calculations provide as output estimates of the following:

1) The mass, M_i (mol), of the pollutant in each subcompartment;

2) The concentration, C_i (mol/m^3) or C_i' (ppt), of the pollutant in each subcompartment;

3) The rate of removal of the pollutant from each subcompartment, R_i (mol/yr), due to the combined action of degradation and advection; and

4) The mean residence time, τ (yr), for the pollutant in the model environment.

B. Description of the Model Environment

The Level II calculations were, with one exception, carried out for the same model environment used with the Level I calculations. (See Section III-B.) The exception involves the elimination of the Suspended Sediments and Biota subcompartments. Their elimination does not materially affect the predicted concentrations for the remaining subcompartments (air, water, sediments, soil) since their accessible volumes are small. Elimination of the two subcompartments simplifies the calculations but does not prohibit the model from estimating pollutant concentrations in these subcompartments from the estimated concentration in water.

As noted above, the Level II calculations can account for advection, i.e., the net loss of a chemical due to transport in air, water or sediment. The rate of loss due to advection must be calculated with some assumed fluid transport velocities (e.g., air speed, current speed) for the appropriate subcompartment. Examples of Level II calculations with and without advection were provided in Subsection E below. The additional Level II calculations reported in Subsection F have all assumed that no advection losses take place.

C. Chemical-Specific Parameters Required

For the level II calculations described below, the following chemical-specific input parameters are required:

1) Henry's Law constant, H (atm m^3/mol);

2) Soil and sediment adsorption coefficient, K_{oc};

3) Molecular weight, MW (g/mol)

4) First-order rate constants, k (yr^{-1}), for all important chemical, photochemical or biological degradation pathways, by subcompartment; and

5) The rate of input of the chemical into the total compartment, I (mol/yr).

The bioconcentration factor for aquatic life, BCF, would have been required if the Biota subcompartment had been kept in the model.

Values of H, K_{oc} and MW were taken, when available, from a draft report by SRI, International. Gaps were filled with estimates by Arthur D. Little, Inc. Values of these parameters for the organic priority pollutants were previously listed. (See Table 3.)

For the sample Level II calculations described below, a subset of 24 chemicals from the full list of organic priority pollutants was selected. Most of these chemicals have been (or are currently) the subject of Risk Assessment studies by Arthur D. Little, Inc. for the Environmental Protection Agency. The list of selected chemicals is given in Table 11.

Table 11 also gives the values of the degradation rate constants used for each chemical. These values are mostly order-of-magnitude estimates based upon data and discussions by Callahan et al. (1979), Tabak (1980) and unpublished material prepared by SRI, International; in risk assessment documents currently being prepared by Arthur D. Little, Inc.; and in other miscellaneous sources. These values, while considered reasonable, are for example purposes only. The shake-flask

TABLE 11

First-Order Rate Constants (k, Years^{-1}) Used in Level II Calculations[a]

No.	Compound	Biodegradation[b]	Photolysis[c] Air	Photolysis[c] Water	Hydrolysis	Oxidation
	Pesticides					
7.	Chlordane	0.03	18	4.2	0.1	0
11.	Dieldrin	0.2	4.2	4.2	0.2	0
17.	Heptachlor	0.1	4.2	4.2	260	0
20.	TCDD	0.03	51	4.2	0	0
	PCBs and Related Compounds					
29.	2-Chloronaphthalene	3	0.1	0.1	0	0.1
	Halogenated Aliphatics					
36.	Chloroform	1	3	0	0.6	0
39.	Dichlorodifluoromethane	0	0.02	0	0	0
42.	1,2-Dichloroethane	0.01	10	0	0	0
43.	1,1,1-Trichloroethane	0.07	3	0	1.4	0
47.	Chloroethene	0	1000	0	0.07	0
50.	Trichloroethylene	1	63	0	0.8	2.8
	Halogenated Ethers					
56.	Bis(2-chloromethyl)ether	0	26	0	10^5	0
57.	Bis(2-chloroethyl)ether	3	1500	0	1	0
	Monocyclic Aromatics					
63.	Benzene	2	1000	0	0	0
65.	1,2-Dichlorobenzene	2	84	0	0	0
68.	1,2,4-Trichlorobenzene	2	250	0	0	0
72.	Toluene	3	400	0	0	0
	Phenols and Cresols					
75.	Phenol	3	2000	63	0	63
77.	2,4-Dichlorophenol	3	0	0	0	0
79.	Pentachlorophenol	0.7	18	14	0	0
81.	4-Nitrophenol	3	0	84	0	0
	Phthalate Esters					
90.	Bis(2-ethylhexyl)phthalate	0.4	0	0	10^{-4}	0
	Polycyclic Aromatic Hydrocarbons					
95.	Benzo[a]anthracene	0.5	250	1900	0	160
105.	Naphthalene	3	0	250	0	8.4

a. The values given for rate constants are mostly order-of-magnitude estimates based upon data and discussions by Callahan, et al. (1979), Tabak (1980), unpublished material prepared by SRI International, risk assessment documents currently being prepared by Arthur D. Little, Inc., and other miscellaneous sources. These values, while considered to be reasonable, are for example purposes only.

b. Biodegradation rate constants were, in many cases, taken to be about one twentieth of the rate measured in seeded tests.

c. Photolysis is taken here to include any light-induced reaction, including reaction with hydroxyl radicals in the atmosphere.

biodegradation data of Tabak (1980) were especially useful in selecting biodegradation rate constants. In many cases, a first-order degradation rate was taken to be 0.05 times the initial rate measured in these seeded tests.

As shown in Table 12, certain degradation rate constants were assumed to be applicable to two or more subcompartments. Thus, the biodegradation rate constant (k_B) for a chemical was always assumed to be applicable to the surface water, sediment and soil subcompartments. Similarly, the rate of hydrolysis (k_H) was assumed to be the same in these three subcompartments, while the rate of oxidation in water (k_O) was cut in half for the sediment and soil subcompartments. Biodegradation hydrolysis and oxidation (excluding light-induced free-radical oxidation) were not allowed in the air subcompartment. Light-induced degradation was limited to the air and surface water subcompartments.

The estimated flux of each chemical into the model environment, I (mol/yr), was derived whenever possible from emissions estimates provided in the risk analysis documents (being prepared by Arthur D. Little, Inc.), from preliminary estimates provided by Acurex, Inc., or from other in-house reports. If these reports provided an estimate of the total annual losses to the environment (to air, water and land) in the U.S., that figure (in kg/yr) was divided by the area of the 48 contiguous states (7.86×10^6 km^2) to obtain a flux - in $kg/km^2 \cdot yr$ - for our model environment which has a surface area of 1 km^2. Dividing this flux by the molecular weight (kg/mol) provides the value of I in the desired units (mol/yr). No emissions estimates were available for 5 of the 24 compounds in the test set; reasonable default values were selected for these chemicals. The values of I for each test chemical is provided below with the discussion in Section F.

TABLE 12

Scheme for Assignment of Rate Constants for Level II Calculations

Phase	Degradation Process				
		Photodegradation			
	Biodegradation	Air	Water	Hydrolysis	Oxidation
Air	0	k_{P_a}	0	0	0
Surface Water	k_B	0	k_{P_w}	k_H	k_O
Sediment	k_B	0	0	k_H	$0.5k_O$
Soil	k_B	0	0	k_H	$0.5k_O$

D. Level II Equations

The basic tenets of the fugacity approach used for Level I (see Section III) are also valid for the Level II calculations. Most of the parameters used were previously defined along with the Level I description. A summary list is provided below:

subscript i = compartment identifier (For sample calculations given here: 1 = air, 2 = surface water, 3 = sediments, 4 = soil)

C_i = pollutant concentration (mol/m^3)

C_i' = pollutant concentration (ppt in v/v for air and w/w for water, sediments and soil)

c_{s_i} = "concentration" of sediments or soil in their respective subcompartments (g/m^3)

f = pollutant's fugacity (atm)

H = Henry's Law constant ($atm\ m^3/mol$)

I = flux of pollutant into model environment (mol/yr)

$k(\ )$ = first order rate constant for degradation; k_B for biodegradation, k_H for hydrolysis, etc. (yr^{-1})

K_i = overall first-order degradation constant for each subcompartment (yr^{-1}). Obtained from sum of individual $k_{(\ )}$ values and - if desired - advection rate constants.

K_{oc} = soil or sediment adsorption coefficient based on organic carbon content

M_i = mass of pollutant in each subcompartment (mol)

MW = pollutant's molecular weight (g/mol)

$(oc)_i$ = organic carbon content of sediments or soil

R = gas constant

R_i = rate of removal of pollutant in each subcompartment (mol/yr)

T = temperature (K)

τ = mean residence time of pollutant in model environment (yr)

V_i = accessible volume of each subcompartment (m^3)

Z_i = fugacity coefficient of pollutant in each subcompartment (mol/m^3 atm)

A good narrative discussion of the Level II calculations is provided in the original article by Mackay (1979). The detailed instructions provided below follow his basic instructions with few modifications.

Step-by-Step Instructions

(1) For the pollutant of interest, obtain MW, H, K_{oc}, I and $k_{(\ )}$ (the individual degradation rate constants). [It is helpful to set up a matrix, such as the one shown in Table 12, for listing the selected values of $k_{(\ )}$ for each subcompartment.]

(2) For the model environment, determine the desired values of V_i, c_{s_i} and $(oc)_i$. [The values used here for the test set are shown

in Table 13.]

(3) Determine, for each subcompartment, the total first-order rate constant for degradation (plus advection if desired) by summing the appropriate $k_{(\ )}$ values:

$$K_i = \sum_j k_{(\ )_j} \tag{34}$$

[The summations used for our test set are shown in Table 13.] All $k_{(\ )}$ values, and thus K_i, must be in units of yr^{-1}.

(4) Determine, for each subcompartment, the value of the fugacity coefficient, Z_i (mol/m^3), using the equations given previously for the Level I calculations: equations 3, 4, 8 and 12 [in Section III] for the air, water, sediments and soil subcompartments, respectively. [These equations are also provided in Table 13.]

(5) Calculate the fugacity of the pollutant, f (atm), from:

$$f = I/\sum_i V_i Z_i K_i \tag{35}$$

(6) Calculate the mass of the pollutant in each subcompartment, M_i, from:

$$M_i = f Z_i V_i \tag{36}$$

and then calculate the total amount of the pollutant in the model environment from $\sum_i M_i$.

(7) Calculate the concentration of the pollutant in each subcompartment with:

$$C_i \ (mol/m^3) = Z_i f = M_i/V_i \tag{37}$$

TABLE 13

Summary of Compartment-Specific Equations and Parameters for Level II Calculations

i	Phase	$K_i(yr^{-1})$	$V_i(m^3)$	$Z_i(mol/m^3\ atm)$	$C_i'(ppt)$
1	Air	k_{P_a}	10^{10}	1/RT(=41.6 at 20°C)	$2.4M_1$ (v/v)[c]
2	Surface Water	$k_B = k_{P_w} + k_H + k_0$	1.5×10^5	1/H	(MW)M_2/0.15 (w/w)[d]
3	Sediments	$k_B + k_H + 0.5k_0$	5×10^3	$10^{-8}(oc)_3 K_{oc} c_{s_3}$/H (=0.2$K_{oc}$/H)[a]	(MW)M_3·100 (w/w)
4	Soil	$k_B + k_H + 0.5k_0$	1.4×10^5	$10^{-8}(oc)_4 K_{oc} c_{s_4}$/H (=0.04$K_{oc}$/H)[b]	(MW)M_4/0.28 (w/w)

a. Assumes $(oc)_3 = 10\%$, $c_{s_3} = 2 \times 10^6\ g/m^3$

b. Assumes $(oc)_4 = 2\%$, $c_{s_4} = 2 \times 10^6\ g/m^3$

c. (v/v) = volume to volume ratio

d. (w/w) = weight to weight ratio

If concentrations, C_i', in units of ppt (v/v for air and w/w for the other subcompartments) are desired, the equations given previously for the Level I calculations may be used: equations 24, 25, 27, and 29 [in Section III] for the air, water, sediment and soil subcompartments, respectively. [These equations are also provided in Table 13.]

(8) Calculate the rate of removal of the pollutant from each subcompartment from:

$$R_i \text{ (mol/yr)} = V_i C_i K_i = f\ V_i Z_i K_i \qquad (38)$$

(9) Calculate the average residence time of the pollutant in the model environment from:

$$\tau \text{ (yr)} = \sum_i M_i / I \qquad (39)$$

E. Level II Calculations, with Advection, for One Chemical

Level II calculations, with the consideration of advection, were carried out for tetrachloroethylene. The simple four-compartment model described above was used. The first-order rate constants used are shown in Table 14 and Table 15 shows some of the intermediate parameters that must be calculated; values are shown for two cases: with and without advection.

For the case with advection it was assumed that: (1) the air compartment was constantly swept with a wind whose velocity was 16 km/hr; (2) the water compartment was a river, 50m wide, 3m deep, with a current of 3.2 km/hr. In both cases a steady-state input of 200 mol/yr was assumed.

The final results of the Level II calculations are shown in Table 16. The calculated values for "total removal rate" ($V_i C_i K_i$) show that

TABLE 14

First-Order Rate Constants for Tetrachloroethylene (Years^{-1})[a]

Phase	Biodegradation	Photolysis[b]	Hydrolysis	Oxidation	Advection	Total
1a. Tetrachloroethylene (no advection)						
Air	0	50.6	0	0	0	50.6
Water	1	1	0.1	1	0	3.1
Sediment	1	0	0.1	0.5	0	1.6
Soil	1	0	0.1	0.5	0	1.6
1b. Tetrachloroethylene (with advection)						
Air	0	50.6	0	0	1.04×10^5	1.04×10^5
Water	1	1	0.1	1	2.80×10^4	2.80×10^4
Sediment	1	0	0.1	0.5	0	1.6
Soil	1	0	0.1	0.5	0	1.6

a. The values given here for the rate constants are mostly order-of-magnitude estimates based upon data and discussions from Callahan et al. (1979) and - to a much lesser extent - a few other sources. These values, while considered to be reasonable, are for example purposes only.

b. Photolysis is taken here to include any light-induced reaction, including reaction with hydroxyl radicals in the atmosphere.

TABLE 15

Level II Calculations for Tetrachloroethylene - Intermediate Parameters[a]

Phase	Z_i $\left(\frac{mol}{m^3 \cdot atm}\right)$	V_i (m^3)	K_i (yr^{-1})	$Z_i V_i K_i$ $\left(\frac{mol}{atm \cdot yr}\right)$
Air	41.6	10^{10}	50.6 $(1.04 \times 10^5)^a$	2.10×10^{13} $(4.33 \times 10^{16})^a$
Water	50	1.5×10^5	3.1 $(2.80 \times 10^4)^a$	2.33×10^7 $(2.10 \times 10^{11})^a$
Sediment	3600	5×10^3	1.6	2.88×10^7
Soil	720	1.4×10^5	1.6	1.62×10^8 $\Sigma = 2.10 \times 10^{13}$ $(= 4.33 \times 10^{16})^a$

a. For K_i and $Z_i V_i K_i$, two values are given. The top number is for the case involving no advection. The bottom number, in parenthesis, involves advection associated with the air and water subcompartments.

TABLE 16

Final Results of Level II Calculations for Tetrachloroethylene[a,b,c]

Phase	M_i (mol)	C_i' (ppt)	$V_i C_i K_i$ (mol/yr)
Air	3.96 (1.9×10^{-3})	9.5 (4.6×10^{-3})	200 (200)
Water	7.1×10^{-5} (3.5×10^{-8})	7.9×10^{-2} (3.8×10^{-5})	2.2×10^{-4} (9.7×10^{-4})
Sediment	1.7×10^{-4} (8.3×10^{-8})	2.8 (1.4×10^{-3})	2.7×10^{-4} (1.4×10^{-7})
Soil	9.6×10^{-4} (4.7×10^{-7}) $\Sigma = 3.96$ (3.1×10^{-3})	0.57 (2.8×10^{-4})	1.5×10^{-3} (7.4×10^{-7})

a. M_i = mass of chemical in each subcompartment;
C_i' = concentration of chemical in each subcompartment. Units are (vol/vol) for air and (wt/wt) for other subcompartments.
$V_i C_i K_i$ = total removal rate from subcompartment.

b. Two values are given for each parameter. The top number is for the case involving no advection. The bottom number, in parenthesis, involves advection associated with the air and water subcompartments.

c. Steady-state input (I) of 200 moles/yr assumed in both cases.

degradation in the atmosphere is, by far, the most important fate pathway for this chemical.

F. Level II Calculations for Test Set (No Advection)

Level II calculations were carried out for the test set of 24 chemicals listed in Table 11. This table also shows the values of the degradation rate constants used. No advection out of the model environment was allowed.

The results of the calculations are given in Table 17. This table also provides the values for the other chemical-specific input parameters required (MW, H, K_{oc}, I) and the values of some of the intermediate parameters (f, K_i, Z_i, and $V_i Z_i K_i$). It should be noted that the primary outputs - M_i, C_i' and R_i - are all directly proportional to the input flux, I. Thus, adjustment of the primary outputs is easy if a different value of I is selected.

Some of the model outputs, in particular the values of τ (residence time) and C_i' (subcompartment concentrations), are displayed in Figures 2-5 so that the relative position of the various chemicals can be seen. Predicted values of τ are seen (Fig. 2) to vary over five orders of magnitude, from 50 years for dichlorodifluoromethane (a stratospheric pollutant) to 0.25d for bis(2-chloroethyl)ether. When model calculations for specific chemicals are being run this residence time should be considered as an important factor in setting the accessible volumes (V_i) of each subcompartment. If, for example, a preliminary calculation shows $\tau \leq$ 1d and degradation in the atmosphere is important (i.e., R_1 is large in comparison with R_2, R_3 and R_4), then the accessible volume for the air compartment (V_1) should probably be reduced in a second (revised) calculation. A height of 1 km (rather than the 10 km used for the test set here) would be more appropriate.

(Text continues on page V-26)

TABLE 17

Results of Level II Calculations for Test Set

7. Chlordane

Inputs MW = 406 H = 9.4×10^{-5} atm m^3/mol
K_{oc} = 1.66×10^{5} I = 3.1 mol/yr

Outputs

f = 3.43×10^{-13} atm ΣM_i = 4.14 mol τ = 1.3 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	18	18.1	0.13	0.13
Z_i =	41.6	1.06×10^{4}	3.53×10^{8}	7.06×10^{7}
$V_iZ_iK_i$ =	7.49×10^{12}	2.88×10^{10}	2.30×10^{11}	1.28×10^{12}
M_i =	0.143	5.45×10^{-4}	0.606	3.39
C_i =	0.343	1.48	2.46×10^{4}	4.92×10^{3}
R_i =	2.57	9.88×10^{-3}	7.89×10^{-2}	0.439

11. Dieldrin

Inputs MW = 381 H = $4.57 \times 10_2^{-10}$ atm m^3/mol
K_{oc} = 1.91×10^{3} I = 3.3×10^{-2} mol/yr

Outputs

f = 2.63×10^{-18} atm ΣM_i = 7.35×10^{-2} mol τ = 2.2 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	4.2	4.6	0.4	0.4
Z_i =	41.6	2.19×10^{9}	8.36×10^{11}	1.67×10^{11}
$V_iZ_iK_i$ =	1.75×10^{12}	1.51×10^{15}	1.67×10^{15}	9.35×10^{15}
M_i =	1.10×10^{-6}	8.65×10^{-4}	1.10×10^{-2}	6.16×10^{-2}
C_i =	2.64×10^{-6}	2.20	419	83.8
R_i =	4.60×10^{-6}	3.97×10^{-3}	4.39×10^{-3}	2.46×10^{-2}

17. Heptachlor

Inputs MW = 373.5 H = 3.95×10^{-3} atm m^3/mol
K_{oc} = 1.41×10^{4} I = 0.31 mol/yr

Outputs

f = 3.93×10^{-14} atm ΣM_i = 0.0172 mol τ = 5.5×10^{-2} yr (= 20d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	4.2	264	260	260
Z_i =	41.6	253	7.14×10^{5}	1.43×10^{5}
$V_iZ_iK_i$ =	1.75×10^{12}	1.00×10^{10}	9.28×10^{11}	5.20×10^{12}
M_i =	1.63×10^{-2}	1.49×10^{-6}	1.40×10^{-4}	7.87×10^{-4}
C_i =	3.91×10^{-2}	3.71×10^{-3}	5.23	1.05
R_i =	6.88×10^{-2}	3.93×10^{-4}	3.65×10^{-2}	0.204

20. TCDD

Inputs MW = 322 H = 1.3×10^{-3} atm m^3/mol
K_{oc} = 3.80×10^{6} I = 5.1×10^{-7} mol/yr

Outputs

f = 2.34×10^{-20} atm ΣM_i = 4.61×10^{-7} mol τ = 0.90 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	51	4.23	0.03	0.03
Z_i =	41.6	769	5.85×10^{8}	1.17×10^{8}
$V_iZ_iK_i$ =	2.12×10^{13}	4.88×10^{8}	8.78×10^{10}	4.91×10^{11}
M_i =	9.73×10^{-9}	2.70×10^{-12}	6.84×10^{-8}	3.83×10^{-7}
C_i =	2.34×10^{-8}	5.80×10^{-9}	2.20×10^{-3}	4.41×10^{-4}
R_i =	4.96×10^{-7}	1.14×10^{-11}	2.06×10^{-9}	1.15×10^{-8}

TABLE 17 (cont.)

29. 2-Chloronaphthalene

Inputs MW = 162.6 H = 1.2×10^{-3} atm m^3/mol
K_{oc} 5.5×10^3 I = 2.3×10^{-2} mol/yr

Outputs

f = 1.72×10^{-13} atm ΣM_i = 7.66×10^{-2} mol τ = 3.3 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0.1	3.2	3.05	3.05
Z_i =	41.6	833	9.17×10^5	1.83×10^5
$V_iZ_iK_i$ =	4.16×10^{10}	4.00×10^8	1.40×10^{10}	7.81×10^{10}
M_i =	7.14×10^{-2}	2.14×10^{-5}	7.86×10^{-4}	4.39×10^{-3}
C_i' =	0.171	2.32×10^{-2}	12.8	2.55
R_i =	7.16×10^{-3}	6.88×10^{-5}	2.41×10^{-3}	1.34×10^{-2}

39. Dichlorodifluoromethane

Inputs MW = 120.9 H = 2.98 atm m^3/mol
K_{oc} = 66.1 I = 100 mol/yr

Outputs

f = 1.20×10^{-8} atm ΣM_i = 5010 mol τ = 50 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0.02	0	0	0
Z_i =	41.6	0.336	4.44	0.887
$V_iZ_iK_i$ =	8.3×10^9	0	0	0
M_i =	5010	6.07×10^{-4}	2.68×10^{-4}	1.50×10^{-3}
C_i' =	1.20×10^4	0.489	3.24	0.646
R_i =	99.6	0	0	0

36. Chloroform

Inputs MW = 119.4 H = 2.88×10^{-3} atm m^3/mol
K_{oc} = 50.2 I = 21 mol/yr

Outputs

f = 1.68×10^{-11} atm ΣM_i = 6.99 mol τ = 0.33 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	3	1.6	1.6	1.6
Z_i =	41.6	347	3.49×10^3	697
$V_iZ_iK_i$ =	1.25×10^{12}	8.33×10^7	2.79×10^7	1.56×10^8
M_i =	6.99	8.74×10^{-4}	2.93×10^{-4}	1.64×10^{-3}
C_i' =	16.8	0.696	3.50	0.699
R_i =	21.0	1.40×10^{-3}	4.69×10^{-4}	2.62×10^{-3}

42. 1,2-Dichloroethane

Inputs MW = 99.0 H = 9.14×10^{-4} atm m^3/mol
K_{oc} = 16.6 I = 86 mol/yr

Outputs

f = 2.07×10^{-11} atm ΣM_i = 8.60 mol τ = 0.10 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	10	0.01	0.01	0.01
Z_i =	41.6	1.09×10^3	3.63×10^3	7.26×10^2
$V_iZ_iK_i$ =	4.16×10^{12}	1.64×10^6	1.82×10^5	1.02×10^6
M_i =	8.60	3.38×10^{-3}	3.75×10^{-4}	2.10×10^{-3}
C_i' =	20.6	2.23	3.71	0.743
R_i =	86.1	3.40×10^{-5}	3.77×10^{-6}	2.11×10^{-5}

43. 1,1,1-Trichloroethane

Inputs MW = 133.4 H = 3.0×10^{-2} atm m^3/mol
K_{oc} 174 I = 240 mol/yr

Outputs

f = 1.92×10^{-10} atm ΣM_i = 79.9 mol τ = 0.33 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	3	1.47	1.47	1.47
Z_i =	41.6	33.3	1.16×10^{3}	232
$V_iZ_iK_i$ =	1.25×10^{12}	7.34×10^{6}	8.53×10^{6}	4.78×10^{7}
M_i =	79.9	9.59×10^{-4}	1.11×10^{-3}	6.24×10^{-3}
C_i' =	192	0.853	14.8	2.97
R_i =	240	1.41×10^{-3}	1.64×10^{-3}	9.18×10^{-3}

47. Chloroethene

Inputs MW = 62.5 H = 198 atm m^3/mol
K_{oc} 9.34 I = 200 mol/yr

Outputs

f = 4.81×10^{-13} atm ΣM_i = 0.200 mol τ = 1.0×10^{-3} yr (= 0.36d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	1000	0.07	0.07	0.07
Z_i =	41.6	5.05×10^{-3}	9.43×10^{-3}	1.89×10^{-3}
$V_iZ_iK_i$ =	4.16×10^{14}	53.0	3.30	18.5
M_i =	0.200	3.64×10^{-10}	2.27×10^{-11}	1.27×10^{-10}
C_i' =	0.480	1.52×10^{-7}	1.42×10^{-7}	2.84×10^{-8}
R_i =	200	2.55×10^{-11}	1.59×10^{-12}	8.90×10^{-12}

50. Trichloroethylene

Inputs MW = 131.4 H = 9.10×10^{-3} atm m^3/mol
K_{oc} = 38.0 I = 97 mol/yr

Outputs

f = 3.70×10^{-12} atm ΣM_i = 1.54 mol τ = 1.59×10^{-2} yr (=5.8d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	63	4.6	3.2	3.2
Z_i =	41.6	110	835	167
$V_iZ_iK_i$ =	2.62×10^{13}	7.59×10^{7}	1.34×10^{7}	7.48×10^{7}
M_i =	1.54	6.11×10^{-5}	1.55×10^{-5}	8.66×10^{-5}
C_i' =	3.70	5.35×10^{-2}	0.204	4.06×10^{-2}
R_i =	96.9	2.81×10^{-4}	4.96×10^{-5}	2.77×10^{-4}

56. Bis(2-chloromethyl)ether

Inputs MW = 115 H = 2.1×10^{-4} atm m^3/mol
K_{oc} = 1.32 I = [1.1×10^{-4} mol/yr]

Outputs

f = 1.27×10^{-18} atm ΣM_i = 5.30×10^{-7} mol τ = 4.8×10^{-3} yr (=1.8d

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	26	1×10^{5}	1×10^{5}	1×10^{5}
Z_i =	41.6	4.76×10^{3}	1.26×10^{3}	251
$V_iZ_iK_i$ =	1.08×10^{13}	7.14×10^{13}	6.3×10^{11}	3.51×10^{12}
M_i =	5.30×10^{-7}	9.10×10^{-10}	8.03×10^{-12}	4.48×10^{-11}
C_i' =	1.27×10^{-6}	6.98×10^{-7}	9.24×10^{-8}	1.84×10^{-8}
R_i =	1.37×10^{-5}	9.07×10^{-5}	8.00×10^{-7}	4.46×10^{-6}

TABLE 17 (cont.)

57. Bis(2-chloroethyl)ether

Inputs MW = 143 H = 1.3×10^{-5} atm m^3/mol
K_{oc} 15.9 I = [8.9×10^{-4} mol/yr]

Outputs

f = 1.43×10^{-18} atm ΣM_i = 6.21×10^{-7} mol τ = 7.0×10^{-4} yr (=0.25d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	1500	4	4	4
Z_i =	41.6	7.69×10^4	2.45×10^5	4.89×10^4
$V_iZ_iK_i$ =	6.24×10^{14}	4.61×10^{10}	4.90×10^9	2.74×10^{10}
M_i =	5.93×10^{-7}	1.64×10^{-8}	1.75×10^{-9}	9.76×10^{-9}
C_i' =	1.42×10^{-6}	1.56×10^{-5}	2.50×10^{-5}	4.99×10^{-6}
R_i =	8.92×10^{-4}	6.59×10^{-8}	7.01×10^{-9}	3.92×10^{-8}

65. 1,2-Dichlorobenzene

Inputs MW = 147.0 H = 1.93×10^{-3} atm m^3/mol
K_{oc} 2.00×10^3 I = 5.9×10^{-3} mol/yr

Outputs

f = 1.69×10^{-16} atm ΣM_i = 7.03×10^{-5} τ = 1.2×10^{-2} yr (=4.3d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	84	2	2	2
Z_i =	41.6	518	2.07×10^5	4.14×10^4
$V_iZ_iK_i$ =	3.49×10^{13}	1.55×10^8	2.07×10^9	1.16×10^{10}
M_i =	7.03×10^{-5}	1.31×10^{-9}	1.75×10^{-7}	9.80×10^{-7}
C_i' =	1.69×10^{-4}	1.28×10^{-6}	2.57×10^{-3}	5.14×10^{-4}
R_i =	5.90×10^{-3}	2.62×10^{-8}	3.50×10^{-7}	1.96×10^{-6}

63. Benzene

Inputs MW = 78.1 H = 5.5×10^{-3} atm m^3/mol
K_{oc} = 74.2 I = 860 mol/yr

Outputs

f = 2.07×10^{-12} atm ΣM_i = 0.86 mol τ = 1.0×10^{-3} yr (=0.36d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	1000	2	2	2
Z_i =	41.6	182	2.70×10^3	540
$V_iZ_iK_i$ =	4.16×10^{14}	5.46×10^7	2.7×10^7	1.51×10^8
M_i =	0.860	5.64×10^{-5}	2.79×10^{-5}	1.56×10^{-4}
C_i' =	2.06	2.94×10^{-2}	0.218	4.36×10^{-2}
R_i =	860	1.13×10^{-4}	5.59×10^{-5}	3.13×10^{-4}

68. 1,2,4-Trichlorobenzene

Inputs MW = 181.4 H = 2.31×10^{-3} atm m^3/mol
K_{oc} = 1.02×10^4 I = 10 mol/yr

Outputs

f = 9.62×10^{-14} atm ΣM_i = 4.28×10^{-2} mol τ = 4.3×10^{-3} yr (=1.6d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	250	2	2	2
Z_i =	41.6	433	8.83×10^5	1.77×10^5
$V_iZ_iK_i$ =	1.04×10^{14}	1.30×10^8	8.83×10^9	4.94×10^{10}
M_i =	4.00×10^{-2}	6.24×10^{-6}	4.24×10^{-4}	2.38×10^{-3}
C_i' =	9.6×10^{-2}	7.55×10^{-3}	7.69	1.54
R_i =	10.0	1.25×10^{-5}	8.49×10^{-4}	4.75×10^{-3}

72. Toluene

Inputs MW = 92.1 H = 5.17×10^{-3} atm m^3/mol
K_{oc} = 339 I = 5.9 mol/yr

Outputs

f = 3.55×10^{-14} atm ΣM_i = 1.48×10^{-2} mol τ = 2.5×10^{-3} yr (=0.92d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	400	3	3	3
Z_i =	41.6	193	1.31×10^{4}	2.62×10^{3}
$V_i Z_i K_i$ =	1.66×10^{14}	8.68×10^{7}	1.96×10^{8}	1.10×10^{9}
M_i =	1.48×10^{-2}	1.03×10^{-6}	2.33×10^{-6}	1.30×10^{-5}
C_i' =	3.55×10^{-2}	6.32×10^{-4}	2.15×10^{-2}	4.29×10^{-3}
R_i =	5.89	3.08×10^{-6}	6.96×10^{-6}	3.90×10^{-5}

75. Phenol

Inputs MW = 94.1 H = 4.54×10^{-7} atm m^3/mol
K_{oc} = 16.2 I = 26 mol/yr

Outputs

f = 2.94×10^{-14} atm ΣM_i = 2.89×10^{-2} mol τ = 1.1×10^{-3} yr (=0.40d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	2000	129	35	35
Z_i =	41.6	2.20×10^{6}	7.14×10^{6}	1.43×10^{6}
$V_i Z_i K_i$ =	8.32×10^{14}	4.26×10^{13}	1.25×10^{12}	6.99×10^{12}
M_i =	1.22×10^{-2}	9.72×10^{-3}	1.05×10^{-3}	5.90×10^{-3}
C_i' =	2.93×10^{-2}	6.10	9.88	1.98
R_i =	24.5	1.25	3.68×10^{-2}	0.206

77. 2,4-Dichlorophenol

Inputs MW = 163 H = 2.8×10^{-6} atm m^3/mol
K_{oc} = 437 I = 3.4×10^{-2} mol/yr

Outputs

f = 1.05×10^{-14} atm ΣM_i = 1.57×10^{-2} mol τ = 0.46 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0	3	3	3
Z_i =	41.6	3.57×10^{5}	3.12×10^{7}	6.24×10^{6}
$V_i Z_i K_i$ =	0	1.61×10^{11}	4.68×10^{11}	2.62×10^{12}
M_i =	4.35×10^{-3}	5.60×10^{-4}	1.63×10^{-3}	9.14×10^{-3}
C_i' =	1.04×10^{-2}	0.608	26.6	5.32
R_i =	0	1.69×10^{-3}	4.91×10^{-3}	2.75×10^{-2}

79. Pentachlorophenol

Inputs MW = 266.4 H = 2.8×10^{-6} atm m^3/mol
K_{oc} = 6.03×10^{4} I = 0.72 mol/yr

Outputs

f = 6.68×10^{-15} atm ΣM_i = 0.952 mol τ = 1.3 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	18	14.7	0.7	0.7
Z_i =	41.6	3.57×10^{5}	4.31×10^{9}	8.61×10^{8}
$V_i Z_i K_i$ =	7.49×10^{12}	7.87×10^{11}	1.51×10^{13}	8.44×10^{13}
M_i =	2.78×10^{-3}	3.58×10^{-4}	0.144	0.805
C_i' =	6.67×10^{-3}	0.636	3.84×10^{3}	766
R_i =	5.00×10^{-2}	5.26×10^{-3}	0.101	0.564

TABLE 17 (cont.)

81. 4-Nitrophenol

Inputs MW = 139.1 H = 3.7×10^{-11}
K_{oc} = 51.3 I = [0.91 mol/yr]

Outputs

f = 2.40×10^{-18} atm ΣM_i = 3.17×10^{-2} mol τ = 3.5×10^{-2} yr (=13d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0	87	3	3
Z_i =	41.6	2.70×10^{10}	2.77×10^{11}	5.55×10^{10}
$V_iZ_iK_i$ =	0	3.52×10^{17}	4.16×10^{15}	2.33×10^{16}
M_i =	9.99×10^{-7}	9.72×10^{-3}	3.32×10^{-3}	1.87×10^{-2}
C_i =	2.40×10^{-6}	9.01	46.2	9.27
R_i =	0	0.845	9.98×10^{-3}	5.59×10^{-2}

90. Bis(2-ethylhexyl)phthalate

Inputs MW = 391 H = 3.0×10^{-7} atm m^3/mol
K_{oc} = 2.24×10^{9} I = 55 mol/yr

Outputs

f = 2.80×10^{-18} atm ΣM_i = 138 τ = 2.5 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0	0.4	0.4	0.4
Z_i =	41.6	3.33×10^{6}	1.49×10^{15}	2.99×10^{14}
$V_iZ_iK_i$ =	0	2.00×10^{11}	2.98×10^{18}	1.67×10^{19}
M_i =	1.16×10^{-6}	1.40×10^{-6}	20.8	117
C_i =	2.78×10^{-6}	3.65×10^{-3}	8.13×10^{5}	1.6×10^{5}
R_i =	0	5.60×10^{-7}	8.34	46.8

95. Benzo[a]anthracene

Inputs MW = 228.3 H = 1.0×10^{-6}
K_{oc} = 2.24×10^{5} I = [5.57×10^{-3} mol/y]

Outputs

f = 4.68×10^{-20} atm ΣM_i = 6.92×10^{-5} mol τ = 1.2×10^{-2} yr (=4.5d)

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	250	2060	80.5	80.5
Z_i =	41.6	1.00×10^{6}	4.48×10^{10}	8.96×10^{9}
$V_iZ_iK_i$ =	1.04×10^{14}	3.09×10^{14}	1.80×10^{16}	1.01×10^{17}
M_i =	1.95×10^{-8}	7.02×10^{-9}	1.05×10^{-5}	5.87×10^{-5}
C_i =	4.68×10^{-8}	1.07×10^{-5}	0.240	4.79×10^{-2}
R_i =	4.87×10^{-6}	1.45×10^{-5}	8.42×10^{-4}	4.73×10^{-3}

105. Naphthalene

Inputs MW = 128.2 H = 4.6×10^{-4} atm m^3/mol
K_{oc} = 1.07×10^{3} I = [9.92 mol/yr]

Outputs

f = 5.07×10^{-11} ΣM_i = 21.9 mol τ = 2.2 yr

i =	1 Air	2 Water	3 Sediment	4 Soil
K_i =	0	261	7.2	7.2
Z_i =	41.6	2.17×10^{3}	4.65×10^{5}	9.30×10^{4}
$V_iZ_iK_i$ =	0	8.50×10^{10}	1.67×10^{10}	9.38×10^{10}
M_i =	21.1	1.65×10^{-2}	0.118	0.661
C_i =	50.6	14.1	1.51×10^{3}	302
R_i =	0	4.31	0.847	4.76

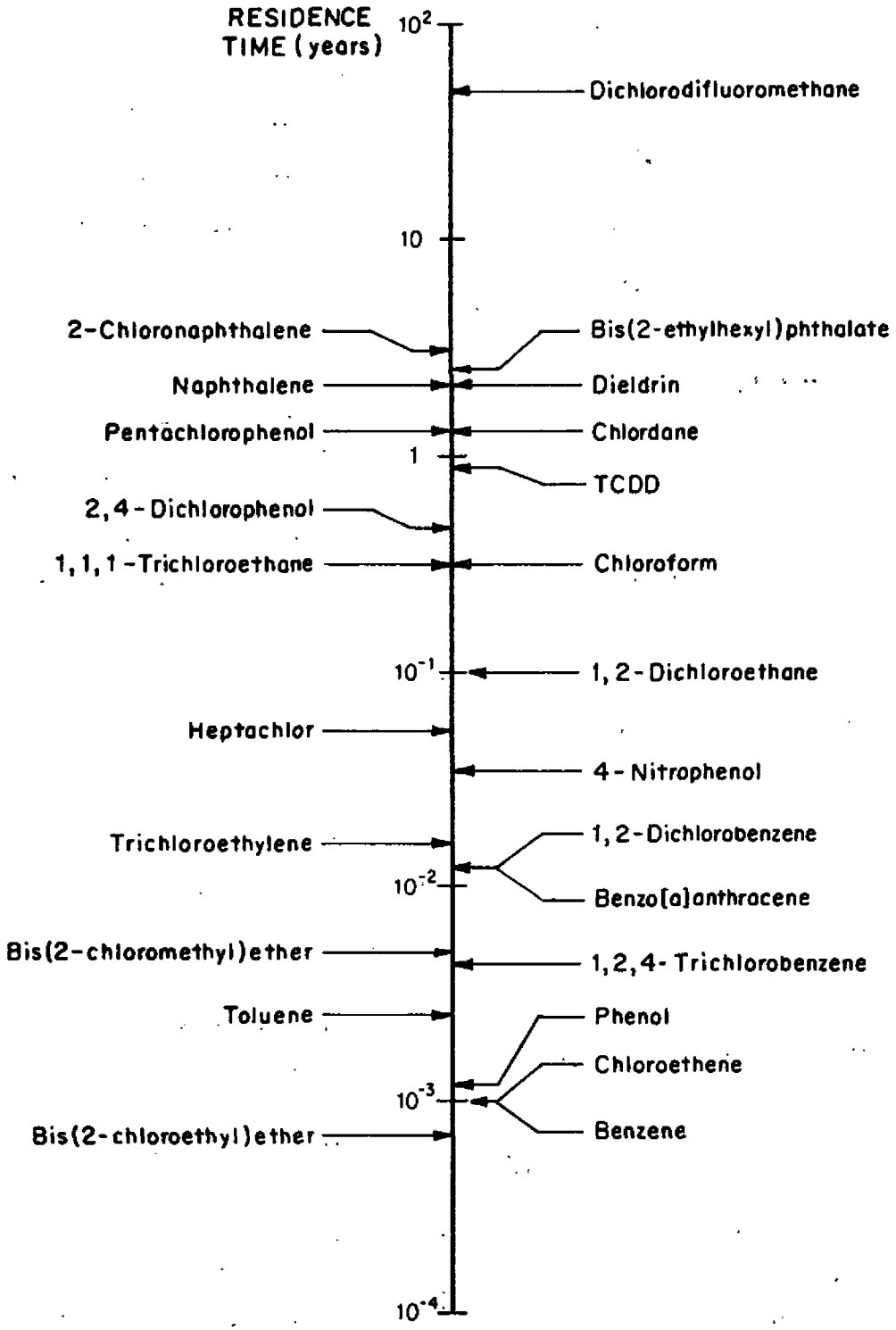


FIGURE 2. ESTIMATED RESIDENCE TIME IN COMPARTMENT FROM LEVEL II CALCULATIONS (No Advection).

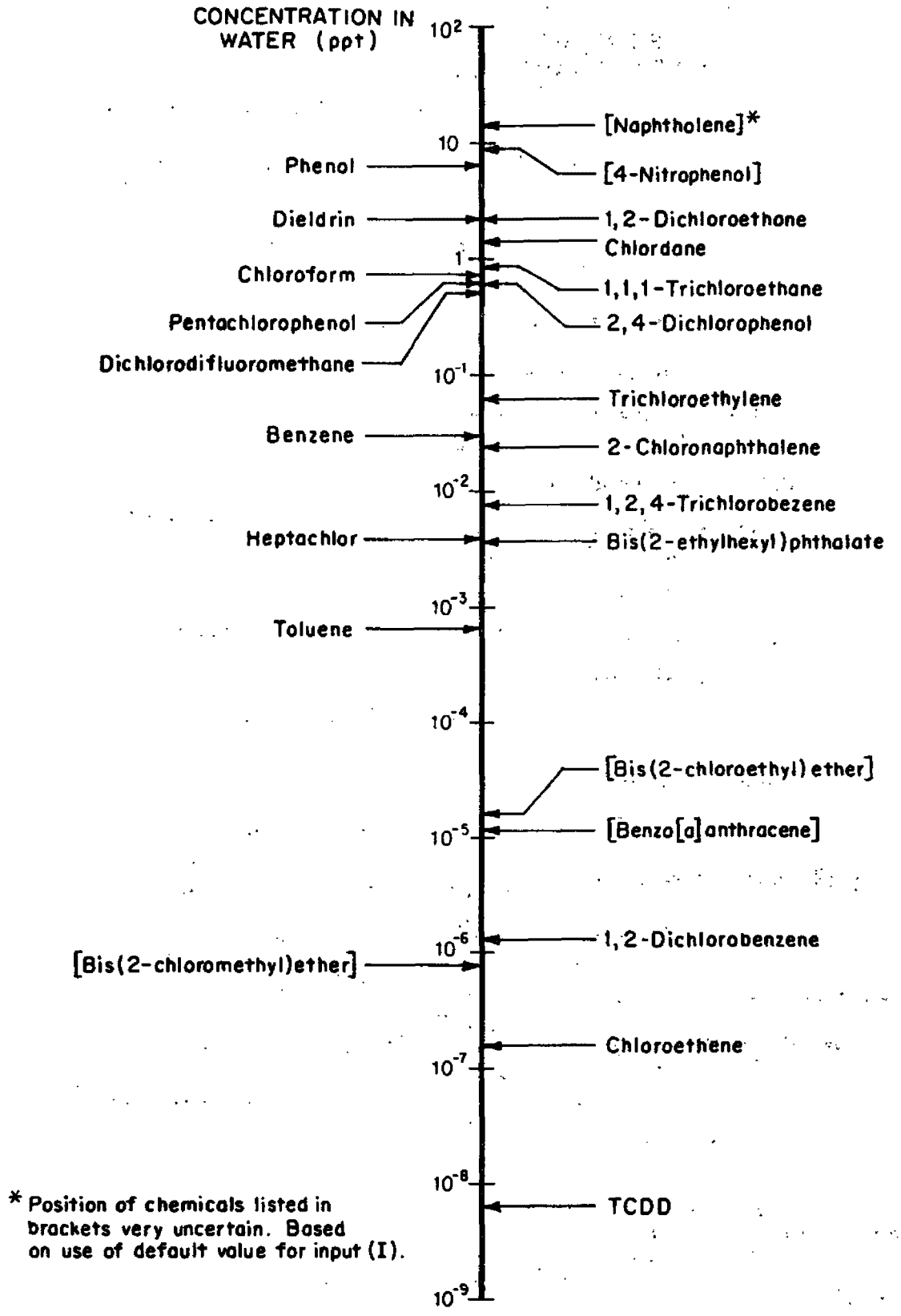


FIGURE 3. ESTIMATED CONCENTRATION IN WATER COMPARTMENT FROM LEVEL II CALCULATIONS (No Advection).

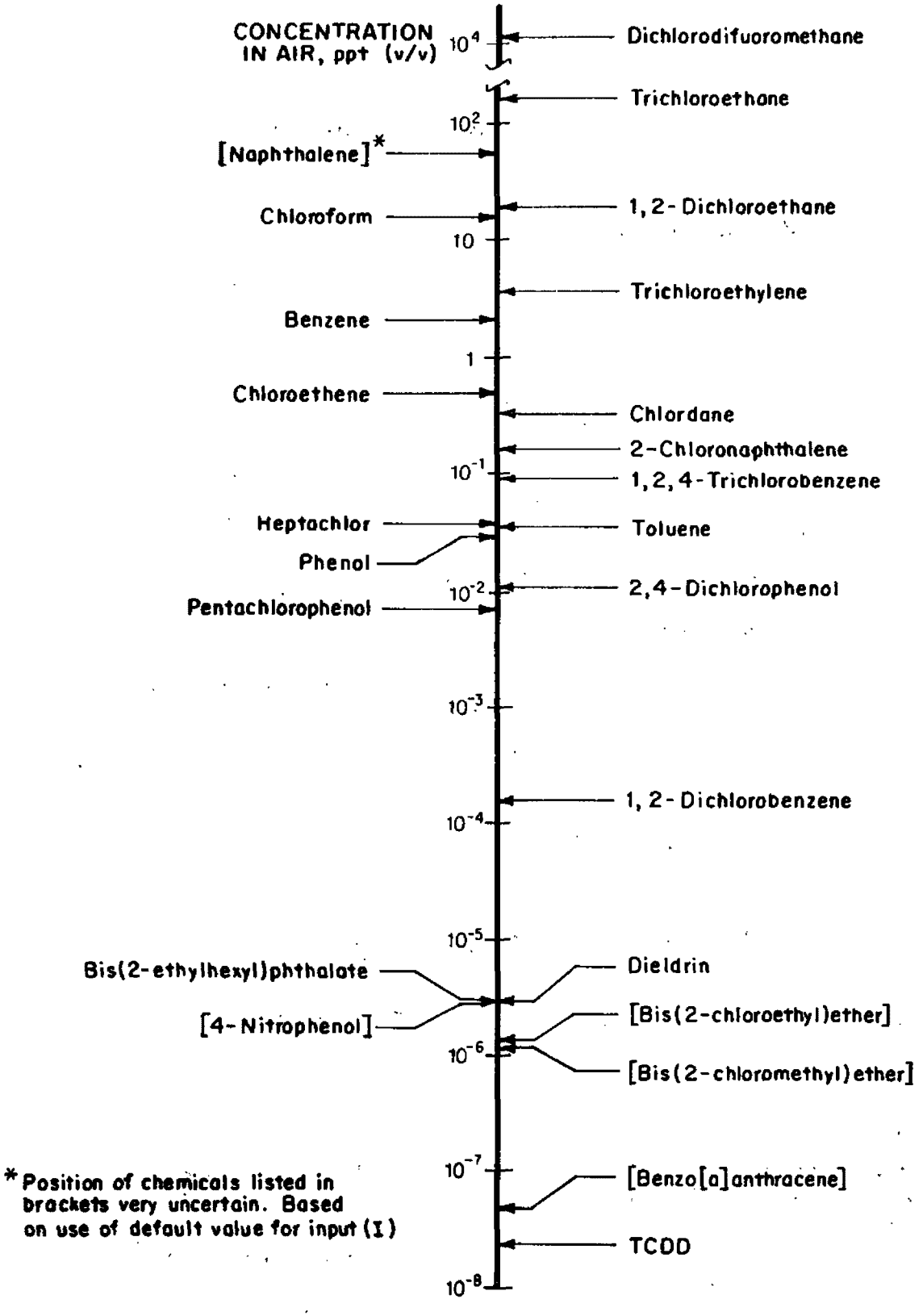


FIGURE 4. ESTIMATED CONCENTRATION IN AIR COMPARTMENT FROM LEVEL II CALCULATIONS (No Advection).

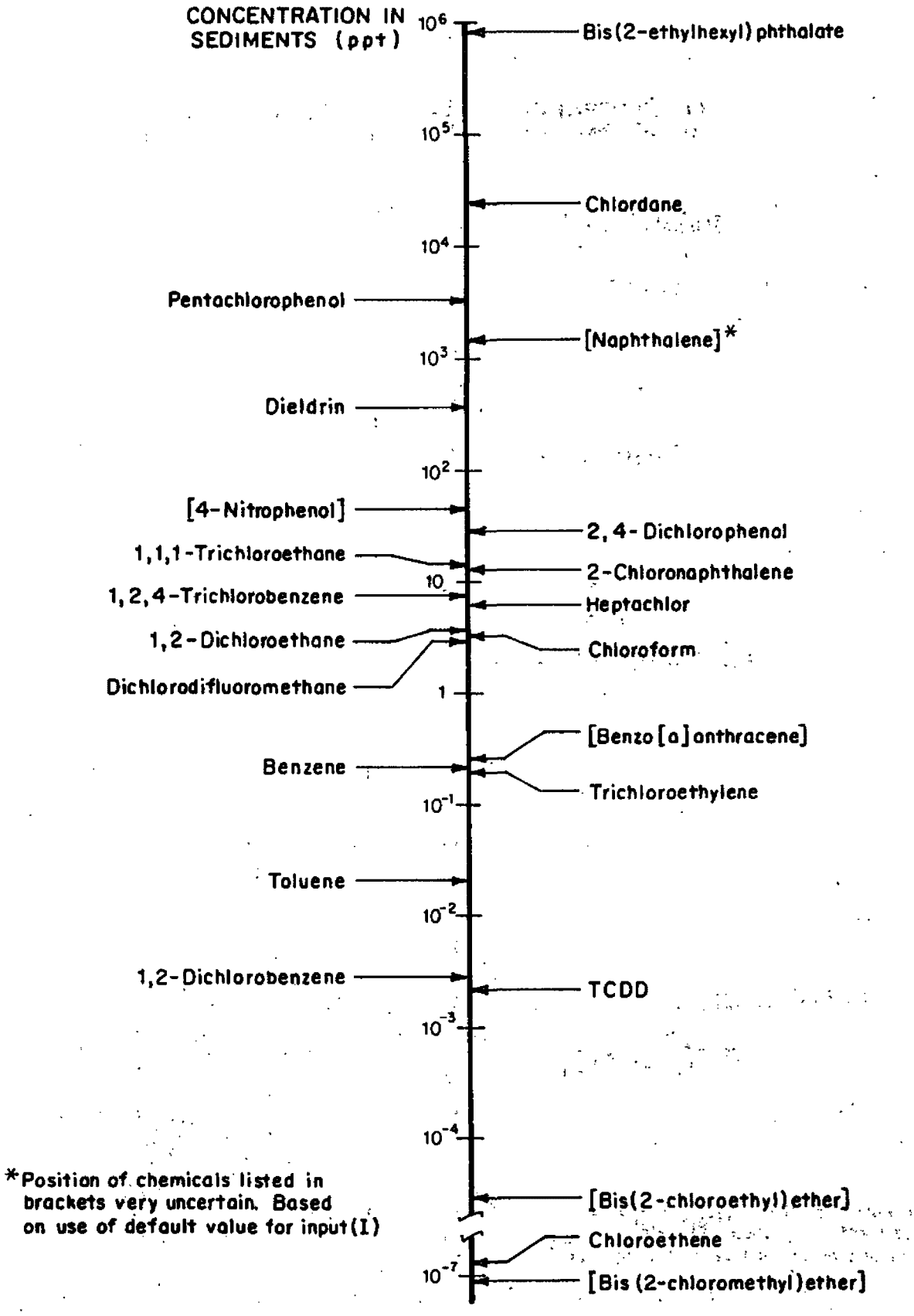


FIGURE 5. ESTIMATED CONCENTRATION IN SEDIMENT COMPARTMENT FROM LEVEL II CALCULATIONS (No Advection).

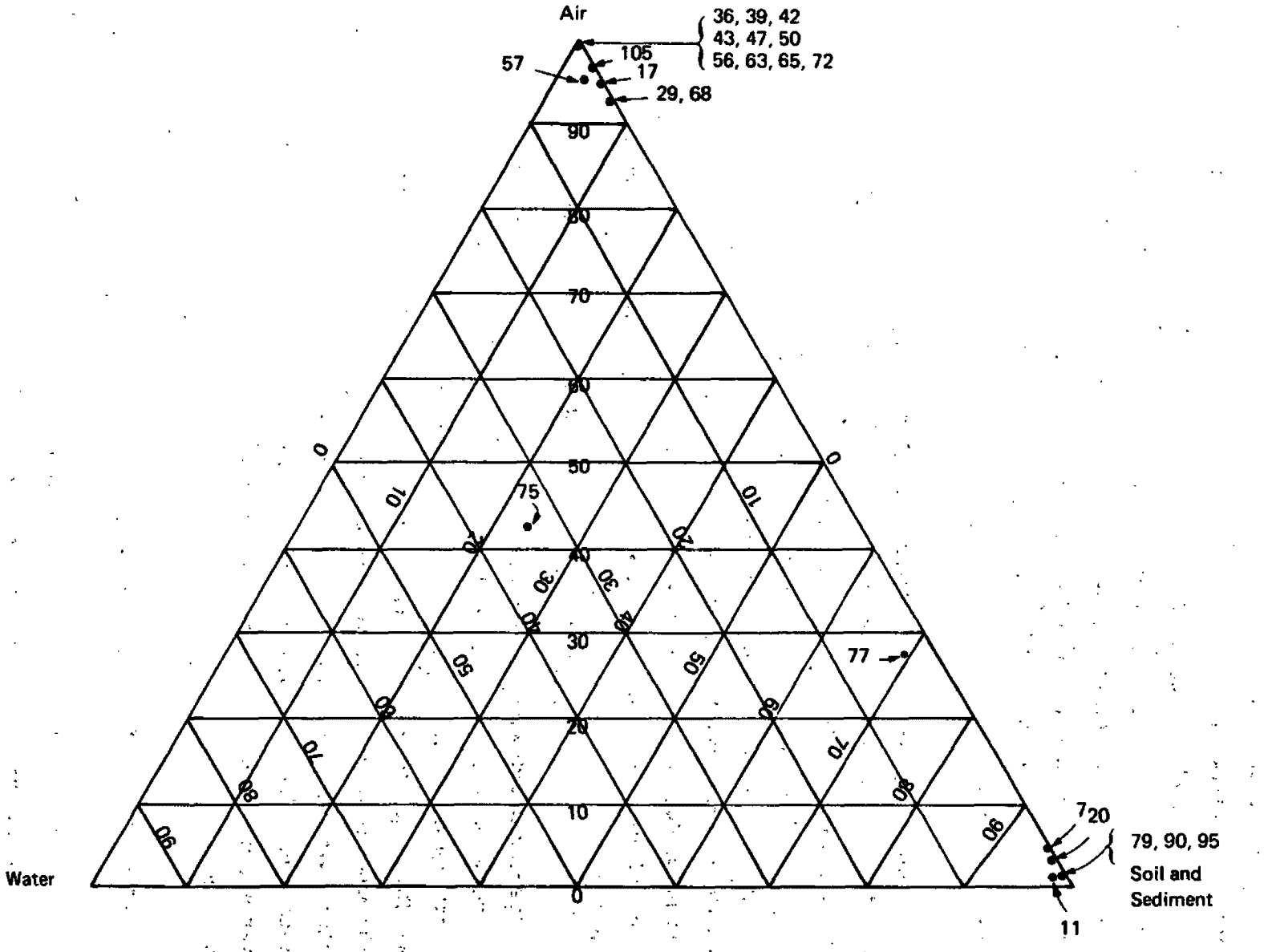
Predicted water compartment concentrations (Fig. 3) range over 10 orders of magnitude while those for air (Fig. 4) and sediments (Fig. 5) range over 12 and 14 orders of magnitude, respectively. Predicted soil concentrations are one fifth of the predicted sediment concentrations and thus the soil concentration ranking would appear as shown in Figure 5. The extremely high value of C_3' shown for bis(2-ethylhexyl)phthalate in Figure 5 results from the high (probably excessively so) value of K_{oc} used (2.2×10^9).

An alternate manner of presenting the predicted environmental concentrations is shown in Figure 6. This figure plots - for each chemical - predicted values of M_1 (mass in air), M_2 (mass in surface water), and $M_3 + M_4$ (total of mass in soil and sediments), expressed as a percent of the total mass in the model environment. This figure dramatizes the (predicted) tendency of most of the selected priority pollutants to reside primarily in the air compartment or the soil/sediment compartments. Only phenol (#75) has an appreciable mass (~34%) residing in the water compartment.

Predicted values for removal rates, R_i, show that atmospheric degradation (mostly reaction with light-produced hydroxyl radicals) is the most important loss area for 14 of the 24 chemicals. For two chemicals - 2,4-nitrophenol and bis(2-chloromethyl)ether - degradation in the surface water compartment is the most important; and for the remaining 8 test chemicals, the soil compartment was most important for degradation. These results would be altered (perhaps significantly) if different, adjustable, values of V_i were used and if advection was considered.

G. Comparison of Predicted Concentrations with Monitoring Data

The environmental concentrations predicted by the Level II calculations are compared in Table 18 with monitoring data for eight chemicals. In most cases, monitoring data on surface water concentrations (much of



Note: Numbers by each point refer to the compounds listed in Table 11. The percent of the total mass (in the model environment) in each of the three subcompartments is given by the vertical distance from the line opposite the apex with the named subcompartment.

FIGURE 6 PLOT OF DISTRIBUTION PREDICTED BY LEVEL II CALCULATIONS. PERCENT IN AIR, WATER, OR SOIL AND SEDIMENT COMPARTMENT.

TABLE 18

Measured vs Environmental Concentrations for Selected Chemicals[a]

No.	Compound	Approximate Concentration Ratio: Measured/Predicted	
		Air	Water
36.	Chloroform	1-10	10^3-10^4
39.	Dichlorodifluoromethane	10^{-2}-1	10^3-10^5
50.	Trichloroethylene	1-10^2	$10^4(\pm 10^2)$
51.	Tetrachloroethylene	1-10	10^4-10^7
63.	Benzene	10^2-10^3	10^4-10^5
75.	Phenol	--	10^2-10^4
77.	2,4-Dichlorophenol	--	$\sim 10^4$
79.	Pentachlorophenol	--	10^2-10^5

a. Data on measured concentrations were taken from risk assessment documents being prepared by A.D. Little, Inc. Data clearly labeled as representing sites near pollution sources were excluded in an attempt to obtain "background" concentration data. The predicted concentrations were from the Level II (Mackay) calculations.

the data were from STORET) indicate ambient levels that are 10^4 ($\pm$ 10^2) higher than the surface water concentrations predicted by the model. Monitoring data for atmospheric concentrations (five chemicals) indicated ambient concentrations are generally within a factor of 10 to 10^2 of the Level II predictions reported here. Insufficient data were available to make meaningful comparisons for the other chemicals in the test set or for the soil and sediment compartments.

The wide discrepancies seen for the surface water concentrations is thought to be due to the combined effects of:

1) A bias towards the more polluted streams and rivers in monitoring programs; besides having higher than "average" concentrations, chemical pollutants in these waters may have been discharged to the water and not had time to equilibrate with other environmental compartments;

2) Problems in obtaining meaningful "averages" of concentration data from monitoring programs when detection or reporting levels are often not specified, when the concentrations being reported are frequently near these detection limits, and when data management systems (e.g., STORET) use questionable methods (e.g., using either 0 or the detection limit) when averages must be taken from data sets containing numerous "not detected" or "less than X" entries.

3) A bias towards less polluted areas in the method used here to select the inputs, I (mol/yr), for each chemical into the model environment. The use of total U.S. emissions divided by the area of the 48 contiguous states (to yield I in mol/yr km^2 for the model environment whose area was 1 km^2) will significantly underestimate pollutant loadings for chemicals released in the more populated and industrialized sectors of the U.S. which occupy only a relatively small fraction of its surface area.

The discrepancies seen, then, should not be considered a failure on the part of the basic fugacity model, but a result of inadvertent biases in the monitoring data and model parameters used. Both of these biases can presumably be compensated for, if not fully corrected, in future uses of this model.

VI. LEVEL III MACKAY CALCULATIONS

A. Basic Assumptions/Model Output

The Level III calculations go beyond the Level II calculations by allowing:

1) A steady state flux, I_i (mol/yr), of the pollutant into any subcompartment, i;

2) Time-dependent intercompartmental transfers (e.g., volatilization from water) where a steady-state transfer process may be postulated.

Other processes covered in the Level II calculations (e.g., degradation and advection out of the model environment) may still be included.

The subcompartment-specific pollutant loadings (I_i values) will frequently be available from materials balance studies for a pollutant. These studies may provide estimates of (total) discharges to the subcompartments of interest, i.e., air, surface water and land. This model does not, however, simulate point source discharges. Thus, a discharge to land, for example, would imply a discharge to all of the land in the model environment chosen; the Level III calculations will then assume that all of the land is equally contaminated. This will -- at least for discharges to land -- seldom be a good assumption.

The intercompartmental transfers are postulated to occur as a steady-state transfer rate, N (mol/yr), as:

$$N = D_{ij}(f_i - f_j) \qquad (40)$$

where D_{ij} is the transfer coefficient for transfer between subcompartments i and j, and f_i and f_j are the fugacities of the pollutant in subcompartments i and j, respectively. In this treatment, $D_{ij} = D_{ji}$ and values of D must always be positive. The transfer coefficient, D, has units of mol/(yr atm) and will depend upon the pollutants rate of diffusion and the common transfer area between the two subcompartments. Mackay (op.cit.) has shown that for volatilization from water

$$D = K_G a/RT \tag{41}$$

where K_G is the overall gas mass transfer coefficient (m/yr), a is the interfacial area between the surface water and atmosphere (m^2), R is the gas constant and T the temperature.

K_G is a chemical- and environmental-specific parameter which may be estimated from the chemical's Henry's Law constant and molecular weight (Thomas, 1980). For compounds of relatively low molecular weight (<65 g/mol) the equations given by Thomas (op.cit.) may be combined to give the following expression:

$$K_G = 87.6\ [(0.314H + 7.86\text{x}10^{-5})\sqrt{MW}]^{-1} \text{m/yr} \tag{42}$$

where MW is the molecular weight (g/mol), H is Henry's Law constant (atm m^3/mol), and a temperature of 20°C has been assumed. For compounds of high molecular weight (>65 g/mol) the wind and current velocity, and the mean depth of the water body, are also required for the estimation of K_G. The equations given by Thomas, for one set of wind and current velocities and three depths, may be reduced to the following:

- V wind = 5 m/s (∿10 mph), V current = 0.5 m/s (∿1 mph), Depth of water = 1 M:

$$K_G = 87.6\ [(0.120H + 3.77\text{x}10^{-5})\sqrt{MW}]^{-1} \text{ m/yr} \tag{43}$$

- Depth of water = 3 m (velocities as above):

$$K_G = 87.6\ [(0.057H + 3.77x10^{-5})\sqrt{MW}]^{-1}\ m/yr \quad (44)$$

- Depth of water = 10 m (velocities as above):

$$K_G = 87.6\ [(0.025H + 3.77x10^{-5})\sqrt{MW}]^{-1}\ m/yr \quad (45)$$

Other intercompartmental transfer processes which may be important for some pollutants are volatilization from soil, wet and dry deposition (to land and surface waters), adsorption on and desorption from sediments, and uptake and clearance by aquatic biota. Expressions for the respective transfer coefficients for each of these processes can presumably be devised. However, none are presented in the Mackay work (op. cit.). Thus, for the present, the user must make an informed guess for K_G for these other processes.

Implicit in this treatment of intercompartmental transfers is the assumption that the rate of transfer (N in eq.40) is directly proportional to the difference in the chemical's fugacity in the two subcompartments. This will not always be true.

The Level III calculations provide as output estimates of the following:

1) The mass, M_i(mol), and concentration, C_i(mol/m^3) or C_i' (ppt), of the pollutant in each subcompartment.

2) The rate of removal of the pollutant from each subcompartment, R_i(mol/yr), due to the combined action of degradation, advection and intercompartmental transfer; and

3) The mean residence time, τ (yr), for the pollutant in the model environment.

The effect of intercompartmental transfers is also elucidated in the calculational process.

B. Description of the Model Environment

The Level III sample calculation was carried out for the same model environment used for the Level II calculations. (See Section V.) Only the air, water, sediment and soil subcompartments are considered. No advection out of the model environment is considered.

As noted in subsection A above, some exchange coefficients may require compartment-specific information. For volatilization from water, for example, this includes: (1) the air-water interfacial area (5×10^4 m^2 in the model environment used here); and (2) for chemicals with MW>65, the wind and current velocities and the mean depth of the water. For the sample calculations given below we have selected the conditions of equation 44, i.e., a wind velocity of 5 m/s, a water velocity of 0.5 m/s, and a mean water depth of 3 m.

C. Chemical-Specific Parameters Required

For the Level III calculations described below, the following chemical-specific input parameters are required:

1) Henry's Law constant, H (atm m^3/mol);

2) Soil and sediment adsorption coefficient, K_{oc};

3) Molecular Weight, MW (g/mol);

4) First-order rate constants, k (yr^{-1}), for all important chemical, photochemical or biological degradation pathways, by subcompartment;

5) The rate of input of the chemical, I (mol/yr), into each subcompartment; and

6) Transfer coefficients, D (mol yr^{-1} atm^{-1}), for each intercompartmental transfer process (e.g., volatilization) to be modeled. For volitization from water, D will require only H and MW as chemical-specific input parameters.

The bioconcentration factor for aquatic life, BCF, would have been required if the Biota subcompartment had been kept in the Level III calculations.

D. Level III Equations

The basic tenets of the fugacity approach used for the Level I and II calculations (see Sections III and V) are also valid for the Level III calculations. The parameter symbols used below are the same as in the Level I and II calculations.

The Level III calculations go beyond the Level II calculations by allowing a steady-state flux of the chemical, I_i (mol/yr), into any subcompartment i. Intercompartmental transfers are modeled as a flux, D_{ij} $(f_i - f_j)$, as shown in equation 40. Degradation within a compartment is given (see eq. 38 in Section V) by the product $V_i C_i K_i$. At equilibrium the inputs and outputs in each subcompartment must be equal:

$$I_i = V_i C_i K_i + \sum_j D_{ij} (f_i - f_j) \qquad (46)$$

The summation is over all compartments except i and must include terms for each transfer process being considered. Remembering that C = Zf, equation 46 can be reqritten as:

$$I_i = f_i (V_i K_i Z_i + \sum_j D_{ij}) - \sum_j D_{ij} f_i \qquad (47)$$

In practice, equation 47 must be written out for each subcompartment being considered and then the set of simulataneous equations solved for the f_i values. Considering four subcompartments (e.g., air, water, sediments and soil) will thus yield four simultaneous equations to be solved for f_1, f_2, f_3 and f_4. Calcualtions can then be made for M, C, R and τ in a manner similar to that used in the Level II equations.

Step-by-Step Instructions

(1)
(2)
(3)
(4)

Steps (1) through (4) are the same as were given previously for the Level II calculations (see Section V-D)

(5) Calculate $V_i Z_i K_i$ (mol yr^{-1} atm^{-1}) for each subcompartment.

(6) Calculate or select an exchange coefficient, D_{ij}(mol $yr^{-1}atm^{-1}$), for each intercompartmental transfer process of interest, e.g., volatilization from soil and/or water, adsorption, uptake by biota, etc. For volatilization from water, D is given by equation 41; the K_G parameter needed in equation 41 may be evaluated from equation 42, 43, 44 or 45, as appropriate. Values of D for other transfer processes must be assumed; no equations were given by MacKay (op. cit.) for their calculation.

(7) For each subcompartment i, write out the mass balance equation given by equation 47. If there are n subcompartments, there will be n simultaneous equation which must then be solved for the chemical's fugacity in each compartment, f_i(atm).

(8) Calculate the mass of the pollutant in each subcompartment, M_i, from:

$$M_i(\text{mol}) = f_i V_i Z_i \qquad (48)$$

and then calculate the total amount of the pollutant in the model environment from $\Sigma_i M_i$.

(9) Calculate the concentration of the pollutant in each subcompartment with:

$$C_i \text{ (mol/m}^3\text{)} = Z_i f_i = M_i/V_i \qquad (49)$$

Conversion to units of ppt may be made as described previously for the Level II calculations.

(10) The rate of removal of the pollutant from each subcompartment, R_i (mol/yr), is -- by definition -- equal to I_i in the Leval III calculations.

(11) Calculate the average residence time (τ) of the pollutant in the model environment from:

$$\tau \text{ (yr)} = \Sigma_i M_i/\Sigma_i I_i \qquad (50)$$

E. Level III Sample Calculation

A sample Level III calculation is presented for trichloroethylene in a four-compartment model environment identical to the one described for the Level II test set. The values of the input parameters used here, although considered reasonable, should not be considered to be the "best" values (or even defensible in some cases); they were selected primarily to allow the sample calculation to be run.

For trichloroethylene we have used MW = 131.4 g/mol, $H = 9.1 \times 10^{-3}$ atm m^3/mol, $K_{oc} = 38$ and the same degradation rates assumed for the Level II calculations (see Section V, Table 17). The selected values of I_i and (previously) calculated values of $V_i Z_i K_i$ are as shown below.

Compartment Number	Compartment	Input (I_i) mol/yr	$V_i Z_i K_i$
1	Air	48	2.62×10^{13}
2	Surface water	11	7.59×10^{7}
3	Sediment	0	1.34×10^{7}
4	Soil	38	7.48×10^{7}
	Total	97	

The total input (97 mol/yr) is the same as was used in the Level II sample calculations.

This sample calculation considers the following intercompartmental transfer processes:

Process	Transfer Coefficient
Volatilization from water	D_{12} (= D_{21})
Volatilization from soil	D_{14} (= D_{41})
Adsorption on sediments	D_{23} (= D_{32})

Assuming an air speed of 5 m/s, a current speed of 0.5 m/s, and a mean water depth of 3 m, allows calculation of K_G from equation 44:

$$K_G = 87.6\ [(0.057 \times 9.1 \times 10^{-3} + 3.77 \times 10^{-5})\sqrt{131.4}]^{-1}$$

$$= 1.37 \times 10^{4}\ \text{m/yr}$$

When this is substituted in equation 41 (with the interfacial area $a = 5 \times 10^{4}\ m^2$), D_{12} is calculated as:

$$D_{12} = 1.37 \times 10^{4}(5 \times 10^{4})/2.4 \times 15^{2}$$

$$= 2.85 \times 10^{10}\ \text{mol yr}^{-1}\ \text{atm}^{-1}$$

For the initial calculation we will assume $D_{14} = 10^{10}$ mol/(yr atm) and $D_{23} = 10^{12}$ mol/(yr atm). Since the air/sediment, soil/sediment and soil/water compartment pairs have no common interface, we set $D_{13} = D_{31} = 0$, $D_{34} = D_{43} = 0$ and $D_{24} = D_{42} = 0$.

The general form of the four simultaneous equations (based on equation 47) that require solution is:

$$I_1 = (V_1Z_1K_1 + D_{12} + D_{14})f_1 - (D_{12}f_2 + D_{14}f_4) \quad (51)$$

$$I_2 = (V_2Z_2K_2 + D_{12} + D_{23})f_2 - (D_{12}f_1 + D_{23}f_3) \quad (52)$$

$$I_3 = (V_3Z_3K_3 + D_{23})f_3 - (D_{23}f_2) \quad (53)$$

$$I_4 = (V_4Z_4K_4 + D_{14})f_4 - (D_{14}f_1) \quad (54)$$

Substituting in the input values given above gives:

For:

$i = 1 \quad 48 = (2.62 \times 10^{13} + 2.85 \times 10^{19} + 10^{19})f_1 - (2.85 \times 10^{10}f_2 + 10$

$i = 2 \quad 11 = (7.59 \times 10^{7} + 2.85 \times 10^{10} + 10^{12})f_2 - (2.85 \times 10^{10}f_1 + 10^{1}$

$i = 3 \quad 0 = (1.34 \times 10^{7} + 10^{12})f_3 - (10^{12}f_2)$

$i = 4 \quad 38 = (7.48 \times 10^{7} + 10^{10})f_4 - (10^{10}f_1)$

Collecting terms yields:

$$48 = 2.62 \times 10^{13}f_1 - 2.85 \times 10^{10}f_2 - 10^{10}f_4$$

$$11 = -2.85 \times 10^{10}f_1 + 1.03 \times 10^{12}f_2 - 10^{12}f_3$$

$$0 = - 10^{12}f_2 + 10^{12}f_3$$

$$38 = - 10^{10}f_1 + 1.01 \times 10^{10}f_4$$

The solution of this set of simultaneous equations yields:

$$f_1 = 3.67 \times 10^{-12} \text{ atm}$$

$$f_2 = f_3 = 3.70 \times 10^{-10} \text{ atm}$$

$$f_4 = 3.77 \times 10^{-9} \text{ atm}$$

Steps 8 and 9 of the step-by-step instructions (equations 48 and 49) are then used to find the mass (M_i) and concentration (C_i) in each compartment. The results are shown below and the predicted concentrations compared with the Level II output.

	1 Air	2 Water	3 Sediment	4 Soil
M_i (mol) =	1.53	6.1×10^{-3}	1.5×10^{-3}	8.8×10^{-2}
C_i (mol/m) =	1.5×10^{-10}	4.1×10^{-8}	3.1×10^{-7}	6.3×10^{-7}
C_i' (ppt) =	3.7	5.3	20	41
C_i' from Level II (ppt) =	3.7	0.054	0.20	0.041

For this example we also have a total pollutant load in the model environment (ΣM_i) of 1.63 mol and an average residence time (τ) of 0.017 yr (6.1 d). The Level II calculations predicted 1.54 mol and 5.8 d, respectively. The significant differences in the predicted values of C_i for the Level II and III calculations (for the water, sediment and soil compartments) should be noted.

Sensitivity Analysis

The Level III calculations introduce two new parameters: subcompartment-specific inputs (I_i) and intercompartmental transfer coefficients (D_{ij}). The sensitivity of the model outputs to variations in these inputs will depend, in part, on the values of many of the other chemical- and environment-specific inputs. Thus, generalizations are not possible and the user must conduct his/her own sensitivity analyses on a case-by-case basis.

Table 19 presents the results of a (partial) sensitivity analysis for the trichloroethylene calculations described above. This table shows the results of the Level I and II calculations followed by eight Level III cases in which the D_{ij} and I_i values were changed. Case No. 1 (Base Case) is the one described in detail in the text above. In Case Nos. 2-4, values of D_{14} and D_{23} (which had been guessed at for the base case) were varied over three to four orders of magnitude, generally resulting in minor changes in the predicted concentrations. In Case Nos. 5-8, the subcompartment inputs (I_1 - I_4) were varied, but the total input was kept at 97 mol/yr. In Case No. 5, no discharge to water is allowed and the air and soil compartments receive about 60% and 40%, respectively. In Case Nos. 6-8, all of the discharge is to one compartment: the air, soil, and water compartments, respectively. In these latter cases (Nos. 5-8 vs. Base Case) the model output, excepting the air compartment, is seen to be fairly sensitive to the varying I_i inputs.

One general conclusion that might be made from the analysis above is that predicted concentrations for a subcompartment that contains a large percentage of the total mass of the chemical (e.g., air for trichloroethylene) will be fairly insensitive to changes in D_{ij} and I_i variations. The converse statement would be equally valid.

TABLE 19

Sensitivity of Level III Outputs to D_{ij} and I_i Values.
Test Calculations for Trichloroethylene

Case No.	Method of Calculation	Concentration (ppt)[a] in: Air	Water	Sediment	Soil
	Level I[b]	240	3.5	13	2.6
	Level II[c]	3.7	0.054	0.20	0.041
	Level III:[d]				
1	Base[d]	3.7	5.3	20	41
2	$D_{23}=10^9$	3.7	5.5	21	41
3	$D_{14}=10^8$	3.1	5.3	20	24
4	$D_{14}=10^{12}$	3.7	5.7	22	0.45
5	$I_1=59$, $I_2=I_3=0$, $I_4=38$	3.7	0.050	0.19	41
6	$I_1=97$, $I_2=I_3=I_4=0$	3.7	0.050	0.19	0.040
7	$I_1=I_2=I_3=0$, $I_4=97$	3.7	0.050	0.19	100
8	$I_1=0$, $I_2=97$, $I_3=I_4=0$	3.5	46	170	0.038

a. ppt (v/v) for air and ppt (w/w) for other compartments.

b. Level I calculation assumed 100 moles of chemical were in the model environment. No degradation allowed.

c. Level II calculation assumed total input of 97 mol/yr into model environment. Degradation allowed. Mass of chemical in compartment calculated to be 1.54 mol.

d. All Level III calculations assumed total input to model environment was 97 mol/yr. Base case is the example worked out (in detail) in the text where:

TABLE 19 (cont.)

$D_{12} = 2.85 \times 10^{10}$	$I_1 = 48$
$D_{14} = 10^{10}$	$I_2 = 11$
$D_{23} = 10^{12}$	$I_3 = 0$
	$I_4 = 38$

In runs 2 through 8, changes in these input parameters were made as indicated in the second column. For example, in Case No. 4 D_{14} was set at 10^{12}; all other inputs remained as specified above for the base case.

VII. LIST OF SYMBOLS USED

a = Area of common interface between two subcompartments (m^2)

B = Volume fraction of biota in surface waters. (Assumed to be 5×10^{-5} m^3/m^3 in sample Level I calculations.)

BCF = Bioconcentration factor for aquatic life

C = Concentration of chemical (mol/m^3)

C′ = Concentration of chemical (ppt by volume in air and ppt by weight in other compartments)

c_s = Concentration of soil or sediments in soil or sediments compartments, respectively (g/m^3)

D = Transfer coefficient for transfer between subcompartments (mol/yr. atm)

f = Fugacity of chemical (atm)

H = Henry's Law constant (atm m^3/mol) ($\frac{\text{mm Hg}}{\text{mM/L}}$ in Neely's equations)

I = Rate of input of chemical into model environment or a specific subcompartment (mol/yr)

i,j = Used as subscripts to identify subcompartments. See Subscripts below.

K = Overall (or total) first-order degradation rate constant for chemical (yr^{-1})

k = First-order degradation rate constant for chemical (yr^{-1})

K_G = Overall gas mass transfer coefficient for volatilization (m/yr)

K_{oc} = Soil or sediment adsorption coefficient base on organic carbon content

K_{ow} = Octanol water partition coefficient

K_p = Soil adsorption coefficient

M = Mass of chemical (mol)

MW = Molecular weight (g/mol)

N = Steady-state transfer rate for chemical between two subcompartments (mol/yr)

(oc) = Organic carbon content of soil or sediment (%)

P_{vp} = Vapor pressure of chemical (mm Hg)

R = Gas constant (8.2×10^{-5} atm m^3/mol deg)

R_i = Total rate of removal of chemical from subcompartment i (mol/yr)

S = Solubility of chemical (mg/L) (mM/L in Neely's equations)

T = Temperature (K)

$t_{1/2}$ = Half-life for clearance from fish (hr)

τ = Mean residence time of chemical in model environment (yr)

V = Accessible volume of a subcompartment (m^3)

y = Fraction of aquatic biota that can be considered equivalent to octanol

Z = Fuacity coefficient (mol m^3/atm)

Subscripts (i)

i	Level I Calculations	Level II and III Calculations
1	Air	Air
2	Surface water	Surface water
3	Suspended sediments	Bottom sediments
4	Bottom sediments	Soils
5	Aquatic biota	
6	Soils	

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