CONTRACT NO. 92-344
FINAL REPORT
JANUARY 1997

Development of Predictive Capabilities for Intermedia Transfer Factors for Toxic Air Pollutants

CALIFORNIA ENVIRONMENTAL PROTECTION AGENCY

AIR RESOURCES BOARD
Research Division

DEVELOPMENT OF PREDICTIVE CAPABILITIES FOR INTERMEDIA TRANSFER FACTORS FOR TOXIC AIR POLLUTANTS

Final Report

Contract No. 92-344

Prepared for:

California Air Resources Board
Research Division
2020 L Street
Sacramento, California 95814

Prepared by:

Yoram Cohen
Department of Chemical Engineering
School of Engineering and Applied Science
University of California, Los Angeles

Arthur M. Winer
Environmental Science and Engineering Program
School of Public Health
University of California, Los Angeles

Researchers
Robert Van de Water
Francis Pan
Rajeev Vohra
Lee Zhou
Lizette Hernandez

January 1997

DISCLAIMER

ACKNOWLEDGMENTS

This project was made possible with funding from the California Air Resources Board (Contract No. 92-344). We are grateful for the helpful discussions, participation and review comments of Ralph Propper (Contract Manager), Janette Brooks and Narcisco Gonzales of the Air Resources Board and Drs. Melanie Marti and Robert Blaisedell of the Office of Environmental Health Hazard Assessment. We also appreciate the help of Kim Gurney who helped in various stages of the execution of this project.

This report was submitted in fulfillment of Contract No. 92-344 “Intermedia transfer Factors for Air Toxics Air Pollutants: Development of Predictive Capabilities” by the University of California, Los Angeles under the sponsorship of the California Air Resources Board. Work Was Completed as of July 15, 1996.

ABSTRACT

A user-friendly software package was developed for the compilation and prediction of intermedia transfer factors for air toxics in support of the California Air Resources Board (ARB) multipathway exposure assessment methodology. The intermedia transport factor predictor (ITFP) software consists of three main components. The first is a chemical property database (CHEMBASE) which contains environmentally relevant physicochemical properties, compiled and critically evaluated from various literature sources, for selected air toxics. The second component is a chemical property predictor (CPP) which contains various methods to estimate a selection of physicochemical parameters for different chemical classes. The CPP is based, in part, on chemical-class specific correlations developed specifically for the ITFP software. Finally, the third component is an intermedia transport parameter predictor (ITPP) which is capable of estimating parameters such as dry deposition velocity, wet scavenging coefficients for chemical in the particle-bound and gaseous forms, chemical water/air mass transfer coefficients, and half-life for chemical volatilization from the soil. The ITPP includes both literature-based algorithms and new algorithms developed specifically for the ITFP. The ITFP is modular in its construction and it can be expanded to include additional intermedia transport parameters and chemical property estimation modules.

TABLE OF CONTENTS

List of Figures

Appendix B

List of Tables

<u>Appendix B</u>

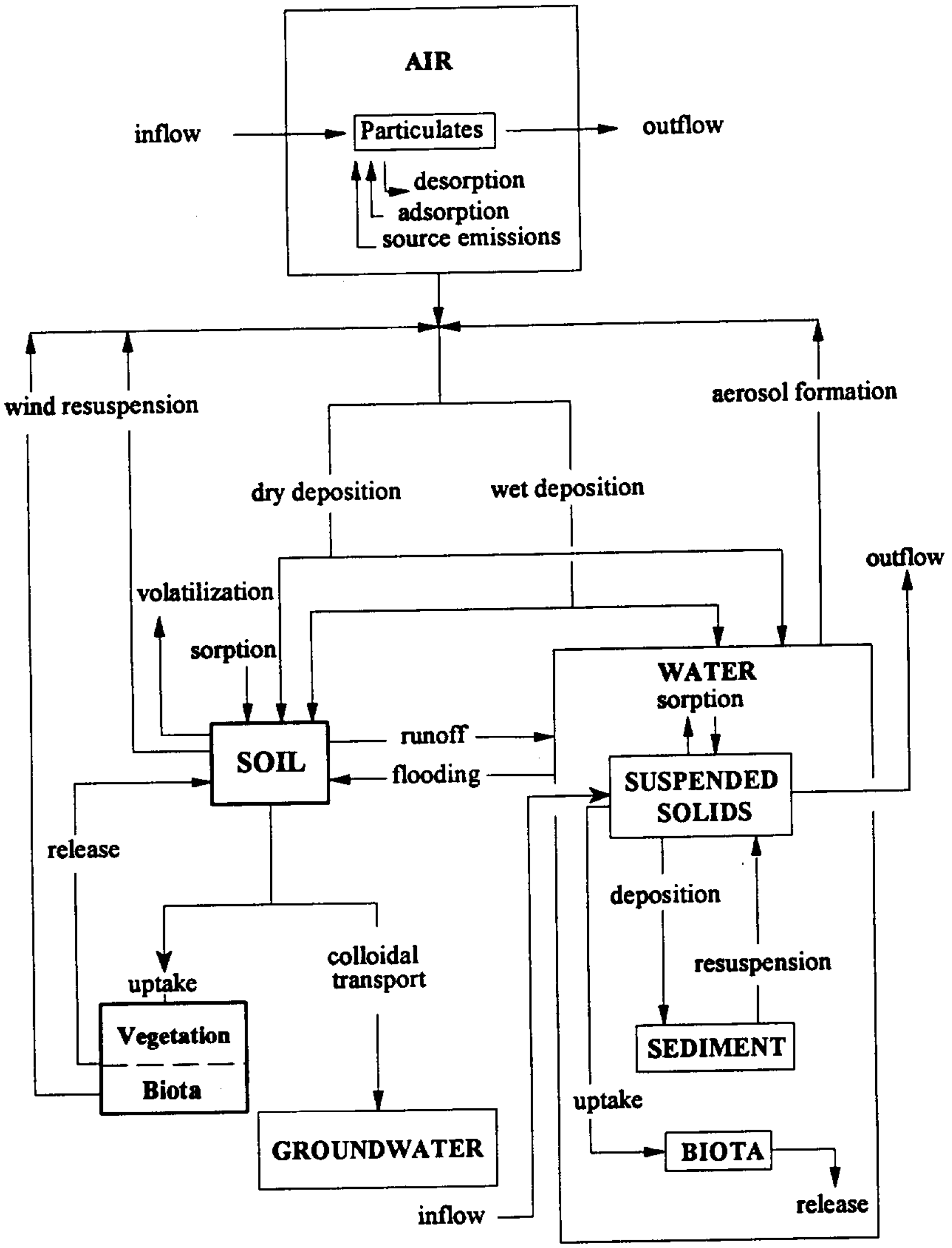
1. INTRODUCTION

In recent years the management of air toxics has been steadily shifting towards integrated multimedia approaches (Chow and Connor, 1993; ARB/DHS, 1992; SCAQMD, 1988; CAPCOA, 1990, 1992; National Research Council, 1991; Cohen, 1986b; Draggan et al., 1987; and references therein). An integrated multimedia approach is logical since pollutants which are released to the environment as the result of a variety of human-related activities (air emissions and/or direct discharge to surface water, etc.) move across environmental boundaries and are therefore found in most media. Clearly, the development of rational risk reduction strategies, designed to minimize the adverse effects of air toxics emissions on human and ecological receptors, requires a clear understanding of the sources of pollutants and their pathways to the receptors of concern. The movement of pollutants among the various environmental media occurs via a variety of intermedia transport processes as illustrated in Figure 1.1 (Cohen and Clay, 1994).

The evaluation of exposure of human and other ecological receptors to air toxics requires that the various intermedia chemical transport pathways among the environmental media with which the receptor is in contact be appropriately identified. Estimates for the rates of contaminant intake by the receptors via the various exposure pathways can be obtained using a variety of methods as described in a number of references (National Academy of Sciences, 1991, SCAQMD, 1988; ARB/DHS, 1992; CAPCOA, 1990,1992; Air & Waste Management Association, 1989). Such an analysis requires knowledge of the multimedia distribution of the air toxics of interest. Extensive review of various approaches to determining multimedia distribution of air toxics have been presented in the literature, and there is a growing list of studies which have focused on multimedia analysis of the distribution of pollutants in the environment (Onishi et al., 1990; Cohen, 1986a, 1987; Allen et al., 1989).

Field monitoring the multimedia distribution of the numerous air toxics in the environment is a difficult task which requires a formidable expense. Thus, various models have been proposed for the purpose of determining the multimedia human exposure to air toxics and subsequent pollutant intake (ARB/DHS, 1992; CAPCOA, 1992; SCAQMD, 1988; and references therein). Multimedia models require a range of chemical-specific and region-specific input parameters that pertain to the estimation of chemical flux across various environmental phase boundaries (e.g., air/water, air vegetation. Air/soil, water/biota) and accumulation in the various environmental

Figure 1.1 Major Intermedia Transport Pathways in a Multimedia System



media (air, water, soil, water, biota, etc.). The intermedia transport parameters and environmental partition coefficients are usually termed intermedia transfer factors (ITFs). The ITFs required in multimedia analysis of chemical transport and fate and exposure analysis have been described in detail in a number of references (ARB, 1994; ARB/DHS, 1992; CAPCOA, 1992; Cohen and Clay, 1994; Cohen and Van de Water, 1994; Cohen et al, 1990; Onishi et al., 1990; DTSC, 1993; SCAQMD, 1988; and references therein).

Given the large number of chemicals for which exposure analysis and risk assessment may be needed, a systematic determination of each chemical's ITFs through laboratory or field experiments would place an economically unacceptable burden on industry and regulatory authorities. Moreover, such an approach would not be feasible in any realistic time frame. It is also important to note that even for the most studied compounds, there is a serious lack of experimental data for various ITF values (ARB, 1994; section 4.4). As an alternative, various estimation methods which are based on available theory, experimental data and appropriate correlations have been proposed in the literature to predict the values of ITFs of newly discovered or previously studied chemicals. In selecting and/or developing ITF estimation methods for regulatory applications it is imperative that practical and convenient algorithms are utilized that require minimum user input of model parameters. Thus, the motivation for this project was to provide a flexible and user-friendly software with integrated ITF estimator and a physicochemical property database. This software tool can be used in conjunction with existing exposure and risk assessment models used by the California Environmental Protection Agency (CalEPA). The software is modular and it is designed to allow for future expansion of the chemical data base and the addition of modules of interest to CalEPA.

2. RELATIONSHIP TO CAPCOA AND OBJECTIVES

2.1 Utilization of the ITFP by Cal/EPA

The process of multimedia assessment of human health risk is now deeply rooted in Cal/EPA's regulations for air toxics. However, given the numerous chemicals that are listed as air toxics, the need for chemical-specific intermedia transfer factors is overwhelming and obtaining comprehensive experimental data for all compounds of interest is not feasible in any realistic time frame. Consequently, there is an urgent need to develop acceptable tools that will allow the estimation of intermedia transfer factors and thereby supplement and enhance the utility of current Cal/EPA models and guidelines for multipathway exposure and risk analysis for air toxics.

For example, the Cal/EPA's CAPCOA model (CAPCOA, 1992) and the CalTox model (DTSC, 1993) accept default values for various intermedia transfer parameters selected to provide for conservative estimates of health risks. However, there is a need for an auxiliary intermedia transport factor predictor (ITFP) module that will allow for estimation of "chemical-specific" and "region-specific" ITF values, in the absence of experimental data. These scenario-specific ITF values will especially help in Cal/EPA's health risk analyses to determine if the default values are indeed reasonable for specific cases. Another example is the recent experience with the ITFP by Cal/EPA's Office of Environmental Health Hazard Assessment (OEHHA). In this case, air/particle partition coefficients were calculated in order to determine which chemicals would be considered in multipathway analysis in OEHHA's Technical Support Document for Exposure and Stochastic Analysis. In addition, OEHHA staff consulted the CHEMBASE component of the ITFP as a source for fish bioconcentration factors, Kow values, and soil half lives for chemicals. The information on fate and transport assisted OEHHA in developing scientific criteria for inclusion or exclusion of chemical for multipathway analysis. In general, the ITFP could serve to estimate physicochemical and transport parameters for chemicals for which limited information is available

2.2 Objectives

In order to develop the Intermedia Transfer Factor Predictor (ITFP) a number of key objectives were set after consultation with the Air Resources Board (ARB) and the Office of Environmental Health Hazard Assessment (OEHHA). The project objectives are listed below.

1. Classify air toxics that are of interest to the ARB and the OEHHA into a number of logical groups. Work with the ARB and OEHHA to derive a suitable classification scheme to be used in constructing the ITFP.

2. Compile and develop as deemed necessary the ITF algorithms that will be included in the ITFP.

3. Develop a physicochemical database for selected chemicals, in consultation with the ARB and OEHHA. This database will be prepared as a dBASE file with a Visual Basic browser.

4. Develop the ITFP software with a user-interface for the windows environment. The user-interface will be developed using Visual Basic for Windows.

5. Test the ITF predictor and debug the software as necessary.

6. Prepare the final version of the ITF predictor and the physicochemical data base. The final report will consist of the above software and the accompanying description of the methodology used to develop CHEMBASE and the ITFP and a description of the software modules.

3. THE ITFP: OVERVIEW AND DEVELOPMENT METHODOLOGY

3.1 What is the ITFP

The intermedia transfer factor predictor (ITFP) is a computer software package for the estimation of environmental chemical partition coefficients and intermedia transfer factors. The ITFP consists of three integrated modules. The first is a chemical data base (CHEMBASE) of carefully selected physicochemical properties and partition coefficients for 102 air toxics. The second module is a chemical property predictor (CPP) designed to estimate the molar volume, solubility, bioconcentration factor, octanol/water partition coefficient and the organic carbon water partition coefficient for selected chemical classes. Finally, the third module is an intermedia transport parameter predictor (ITPP) designed to estimate a selected number of intermedia transport coefficients which are pertinent in multimedia assessment of air toxics. The ITFP is written in Visual Basic for Windows and its three modules are seamlessly integrated. The modular construction of the ITFP provides for easy expansion and the addition of modules and algorithms to both the CPP, ITFP and the expansion of CHEMBASE to include additional chemicals and properties. The ITFP design also provides for interfacing with multimedia models of transport and fate, exposure and risk assessment.

3.2 Methodology

In the first phase of the ITFP development, various toxic chemicals of interest were classified by chemical classes most appropriate for the ITFP. The purpose of the chemical classification was to utilize a smaller set of chemical classes for which chemical class-specific ITF estimation methods could be developed. Therefore, the UCLA ITFP research team with the ARB and OEHHA staff narrowed the list of 400-plus compounds, provided by the ARB, to 52 representative compounds. Subsequently, these chemicals were grouped into convenient chemical classes according to functional groups and chemical structure (see section 4.1).

The chemicals included in CHEMBASE were selected to represent various members of the selected chemical classes (see section 4.1). The chemical parameter fields in CHEMBASE represent the major chemical parameters needed in environmental multimedia assessment models. The physicochemical properties and partition coefficients for these chemicals were selected from numerous references under the selection criteria described in section 4.3.

Chemical class-specific correlations were reviewed and compiled from the literature for the selected CPP parameters. Selected correlations were included in the CPP where appropriate. In addition, chemical class-specific correlations were developed specifically for the CPP using ITF data compiled from the literature. Also, a stand-alone companion biomagnification factor (BMF) module was developed. The BMF module considers the accumulation of toxics in finned fish through a linear food-chain model. The details of the CPP development work and the various CPP correlations are described in section 6.2 and Appendix B.

The ITF parameters which are included in the ITPP were selected based on a review of various environmental multimedia assessment models (Cheng et al., 1995; Cohen and Clay, 1994; CAPCOA, 1992; Mackay, 1991; Cohen et al., 1991; Onishi et al., 1990; SCAQMD, 1988; and references therein). The various ITF algorithms were either compiled from the literature or developed specifically for the ITPP. The selected ITF algorithms were extensively evaluated using the integrated spatial-multimedia-compartmental model (ISMCM) developed at UCLA (Cohen and Clay, 1994; Cohen and Van de Water, 1994; Van de Water, 1995). Both the CPP and the ITPP are designed to utilize chemical-specific information from CHEMBASE or they can be used to predict parameters for a user-specified chemical.

4. CHEMBASE

4.1 Chemical Classes

CHEMBASE contains a selection of air toxics which represent a number of different chemical classes. These chemical classes which are shown in Table 4.1 were selected after reviewing a representative list of air toxics as discussed in section 3.2. This is not a comprehensive selection of all of the chemical classes appropriate for airtoxics; however, it is a selection of sufficient interest and it provides a basis for future expansion of CHEMBASE. The specific chemicals and physicochemical parameters included in CHEMBASE are given in Tables 4.2 and 4.3, respectively.

4.2 Selection of CHEMBASE Chemicals and Database Parameters

CHEMBASE chemicals were selected though consultation with the ARB and OEHHA to represent the various chemical classes shown in Table 4.1. The chemicals included in CHEMBASE are listed in Table 4.2. CHEMBASE includes physicochemical parameters and partition coefficients for the seven air toxics which were critically evaluated by the authors in a previous UCLA/ARB study (ARB, 1994) and the fifteen chemicals compiled by McKone et al. (1993). These previous ARB studies have identified major physicochemical parameters that are useful in multimedia analyses of chemical transport and fate and exposure. Accordingly, CHEMBASE parameters were selected to provide the major parameters necessary for multimedia analysis. There are twenty four major physicochemical parameters and partition coefficients fields (see Table 4.2) for each chemical in CHEMBASE. In addition CHEMBASE contains a number of calculated fields which allow the user to estimate the vapor pressure at different temperatures and to estimate media partition coefficients for a set of default media properties.

Table 4.1

Chemical Classes Included in CHEMBASE

Aldehyde	Aromatic ester
Chlorinated Alkane	Aromatic ether
Brominated Alkane	Hydrazine
Chlorinated Alkene	Ketone
Alkene oxide	Nitrile
Chlorinated alkyl ether	Nitroamine
Benzene/Alkylated Benzene	Chlorinated pesticide
Chlorinated aromatic	biphenyl
Chlorobenzene	Phenol
Nitrobenzene	Alkylated Phenols
Aromatic amine	Chlorophenol
chlorinated dibenzofuran	Polycyclic aromatic
Chlorinated dioxin	Polychlorinated Biphenyl

Table 4.2

LIST OF CHEMBASE CHEMICALS

CHEM_NAME	CAS_NUMBER	CHEM_TYPE	CH_FORMULA
1,1-Dichloroethene	75-35-4	Chlorinated Alkene	C2H2Cl2
1,2-Dichloroethane	107-06-2	Chlorinated Alkane	C2H4Cl2
1,2-Dichloropropane	78-87-5	Chlorinated Alkane	C3H6Cl2
1,2- Diphenylhydrazine	122-66-7	Hydrazine	C12H12N2
1,3-Butadiene	106-99-0	Alkene	C4H6
1,3-Dinitrobenzene	99-65-0	Nitrobenzene	C6H4N2O4
1,4- Dichlorobenzene	106-46-7	Chlorobenzene	C6H4Cl2
1,4-Dioxane	123-91-1	Ether	C4H8O2
2,4- Dinitrotoluene	121-14-2	Nitrobenzene	C7H6N2O4
2,6- Dinitrotoluene	606-20-2	Nitrobenzene	C7H6N2O4
3,3- Dichlorobenzidine	91-94-1	Chlorinated Benzidine	C12H10Cl2N2
1,1,1- Trichloroethane	71-55-6	Chlorinated Alkane	C2H3Cl3
1,1,2- Trichloroethane	79-00-5	Chlorinated Alkane	C2H3Cl3
1,3,5-Trinitrobenzene	99-35-4	Nitrobenzene	C6H3N3O6
2,4,6- Trichlorophenol	88-06-2	Chlorophenol	C6H3Cl3O
2,4,6-Trinitrotoluene	118-96-7	Nitrobenzene	C7H5N3O6
1,1,2,2- Tetrachloroethane	79-34-5	Chlorinated Alkane	C2H2Cl4
2,3,7,8 -Tetra(CDF)	51207-31-9	Chlorinated Dibenzofuran	C6H2Cl2OC6H2Cl2
2,3,7,8-TCDD	1746-01-6	Chlorinated Dioxin	C12H4Cl4O2
2,3,4,7,8 - Penta(CDF)	51207-31-4	Chlorinated Dibenzofuran	C6H2Cl2OC6HCl3
1,2,3,4,7,8 - Hexa(CDF)	70658-26-9	Chlorinated Dibenzofuran	C6H2Cl2OC6Cl4
1,2,3,4,7,8 - Hexachloro DPD	39227-26-8	Chlorinated Dioxin	Cl2C6H2OC6Cl4
1,2,3,4,6,7,8 - Hepta(CDF)	67462-39-4	Chlorinated Dibenzofuran	C6HCl3OC6Cl4
1,2,3,4,6,7,8 - Heptachloro DPD	35822-46-9	Chlorinated Dioxin	Cl3C6HO2C6Cl4
1,2,3,4,7,8,9 - Hepta(CDF)	55673-89-7	Chlorinated Dibenzofuran	C6HCl3OC6Cl4
Acenaphthene	83-32-9	Polycyclic Aromatic	C12H10
Acenaphthylene	208-96-8	Polycyclic Aromatic	C12H8
Acrolein	107-02-8	Aldehyde/Alkene	C3H4O
Acrylonitrile	107-13-1	Nitrile/Alkene	C3H3N
Aldrin	309-00-2	Chlorinated Pesticide	C12H8Cl6
Ammonia (anhydrous)	7664-41-7	Ammonia	NH3
Anthracene	120-12-7	Polycyclic Aromatic	C14H10
Aroclor 1016 (PCB)	12674-11-2	Polychlorinated Biphenyl	PCB
Aroclor 1221 (PCB)	11104-28-2	Polychlorinated Biphenyl	PCB
Aroclor 1232 (PCB)	11141-16-5	Polychlorinated Biphenyl	PCB
Aroclor 1242 (PCB)	53469-21-9	Polychlorinated Biphenyl	PCB
Aroclor 1248 (PCB)	12672-29-6	Polychlorinated Biphenyl	PCB
Aroclor 1254 (PCB)	11097-69-1	Polychlorinated Biphenyl	PCB
Aroclor 1260 (PCB)	11096-82-5	Polychlorinated Biphenyl	PCB
Benzene	71-43-2	Benzene/Alkylated Benzene	C6H6
Benzidine	92-87-5	Aromatic Amine	C12H12N2
Benzo(a)anthracene	56-55-3	Polycyclic Aromatic	C18H12
Benzo(a)pyrene	50-32-8	Polycyclic Aromatic	C20H12
Benzo(b)fluoranthene	205-99-2	Polycyclic Aromatic	C22H12

Benzo(ghi)perylene	191-24-2	Polycyclic Aromatic	C20H12
Benzo(k)fluoranthene	207-08-9	Polycyclic Aromatic	C20H12
Bis(2-chloroethyl) ether (BCEE)	111-44-4	Chlorinated Alkyl Ether	C4H8Cl2O
Bis(chloromethyl) ether	542-88-1	Chlorinated Alkyl Ether	C2H4Cl2O
Bromodichloromethane	75-27-4	Brominated/Chlorinated Alkane	CHBrCl2
Bromoform	75-25-2	Brominated Alkane	CHBr3
Carbon Tetrachloride	56-23-5	Chlorinated Alkane	CCl4
Cellosolve	110-80-5	Alkyl Ether	C4H10O2
Cellosolve Acetate	111-15-9	Ester	C6H12O3
Chlordane	57-74-9	Chlorinated Pesticide	C10H6Cl8
Chlorobenzene	108-90-7	Chlorobenzene	C6H5Cl
Chlorodibromomethane	124-48-1	Brominated/Chlorinated Alkane	CHBr2Cl
Chloroethane	75-00-3	Chlorinated Alkane	C2H5Cl
Chloroform	67-66-3	Chlorinated Alkane	CHCl3
Chloromethane	74-87-3	Chlorinated Alkane	CH3Cl
Chrysene	218-01-9	Polycyclic Aromatic	C18H12
Cis-1,2- dichloroethene	156-59-2	Chlorinated Alkene	C2H2Cl2
DDD	72-54-8	Chlorinated Pesticide	C14H10Cl4
DDE	72-55-9	Chlorinated Pesticide	C14H8Cl4
DDT	50-29-3	Chlorinated Pesticide	C14H9Cl5
Di(2-ethylhexyl)phthalate	117-81-7	Aromatic Ester	C24H38O4
Di-n- butylphthalate	84-74-2	Aromatic Ester	C16H22O4
Dibenz(a,h)anthracene	53-70-3	Polycyclic Aromatic	C22H14
Dieldrin	60-57-1	Chlorinated Pesticide	C12H8Cl6O
Endrin	72-20-8	Chlorinated Pesticide	C12H8Cl6O
Ethylbenzene	100-41-4	Benzene/Alkylated Benzene	C8H10
Ethylene Oxide	75-21-8	Ether	C2H4O
Fluoranthene	206-44-0	Polycyclic Aromatic	C16H10
Fluorene	86-73-7	Polycyclic Aromatic	C13H10
Formaldehyde	50-00-0	Aldehyde	CH2O
Heptachlor	76-44-8	Chlorinated Pesticide	C10H5Cl7
Hexachlorobenzene	118-74-1	Chlorinated Aromatic	C6Cl6
Indeno(1,2,3-cd)pyrene	193-39-5	Polycyclic Aromatic	C22H12
Isophorone	78-59-1	Ketone	C9H14O
Lindane	58-89-9	Chlorinated Pesticide	C6H6Cl6
Mercury	7439-97-6	Metal	Hg
Methyl Chloride	75-09-2	Chlorinated Alkane	CH2Cl2
N-Nitrosodimethylamine	62-75-9	Nitrosamine	C2H6N2O
N-nitrosodiphenylamine	86-30-6	Nitrosamine	C12H10N2O
Naphthalene	91-20-3	Polycyclic Aromatic	C10H8
Nitrobenzene	98-95-3	Nitrobenzene	C6H5NO2
Octachloro - DPD	3268-87-9	Chlorinated Dioxin	Cl4C6O2C6Cl4
Octachlorinated dibenzofuran	39001-02-0	Chlorinated Dibenzofuran	C6Cl4OC6Cl4
Pentachlorophenol	87-86-5	Chlorophenol	C6HCl5O
Phenanthrene	85-01-8	Polycyclic Aromatic	C14H10
Phenol	108-95-2	Phenol	C6H60
Pyrene	129-00-00	Polycyclic Aromatic	C16H10
Tetrachloroethylene	127-18-4	Chlorinated Alkene	C2Cl4
Toluene	108-88-3	Benzene/Alkylated Benzene	C7H8
Toluene-2,4-diisocyanate	584-84-9	Monoaromatic/Isocyanate	C9H6N2O2

Toxaphene	8001-35-2	Chlorinated Pesticide	C10H10Cl8
Trans-1,2- dichloroethene	156-60-5	Chlorinated Alkene	C2H2Cl2
Trichloroethylene	79-01-6	Chlorinated Alkene	C2HCl3
Vinyl Chloride	75-01-4	Chlorinated Alkene	C2H3Cl
Xylene (mixed)	1330-20-7	Benzene/Alkylated Benzene	C8H10
m-Xylene	108-38-3	Benzene/Alkylated Benzene	C8H10
o-Xylene	95-47-6	Benzene/Alkylated Benzene	C8H10
p-Xylene	106-42-3	Benzene/Alkylated Benzene	C8H10

(CDF chlorinated dibenzofuran, DPD dibenzo-p-dioxin, DDT 1,1,1-Trichloro - 2,2 bis(p-chlorophenyl) ethane, DDE 1,1-dichloro-2,2-bis(p-chlorophenyl) ethylene, DDD 1,1 dichloro-2,2-bis(p-chlorophenyl) ethane, TCDD tetrachlorodibenzo-p-dioxin)

Table 4.3
Physicochemical Parameters and Partition Coefficients Included in CHEMBASE

Physicochemical Parameters (14 parameters)

1) Molecular Weight
2) Critical Pressure
3) Critical Volume
4) Critical Temperature
5) Boiling Point
6) Melting Point
7) Molar Volume
8) Aqueous Solubility
9) Vapor Pressure
10) Antoine constants
11) Henry's Law constant
12) Liquid Density
13) K_{ow} (Octanol/Water Partition Coefficient)
14) K_{oc} (organic carbon/water partition coefficient)

Bioconcentration Parameters (3 Parameters)

1) Aquatic Bioconcentration Factor (BCF)
2) Plant Bioconcentration Factor (PBCF)
3) Terrestrial Bioconcentration Factor (TBCF)

Reaction Parameters[a] (7 Parameters)

1) Reaction Rate constant for air
2) Reaction Rate constant for ground water
3) Reaction Rate constant for surface water
4) Reaction Rate constant for soil
5) Reaction Rate constant for sediment
6) Reaction Rate constant for biota
7) Reaction Rate constant for suspended solids

CHEMBASE Calculated Fields

1) Vapor pressure at a selected temperature using the Antoine Equation[b]
2) Dimensionless media partition coefficients[c]:
   - air/water
   - air/soil
   - water/sediment

[a] Temperature dependence of vapor pressure is calculated using the empirical Antoine vapor pressure equation.

[b] Reported as either a reaction half-life or first-order reaction rate constant

[c] Calculated to provide an illustration of chemical partitioning based on default values for organic carbon content, soil porosity, and moisture content.

4.3 Selection of CHEMBASE Parameter Values

CHEMBASE parameter values were selected based on a critical review of various literature sources and the compilation and selection of the pertinent physicochemical parameters. Given the discrepancies in the literature values for physicochemical parameters, a strict criteria was followed in selecting parameter values for inclusion in CHEMBASE.

In selecting parameter values, experimental values were given greater weight than calculated parameter values. When differences in reported parameter values spanned about 30% or less (for K_{ow}, K_{oc} and BCF the log values were compared) the experimental values were averaged. When differences among reported values were greater than 30% further analysis of the original references was conducted to ascertain the reason for the discrepancy. In numerous cases it was found that there were large uncertainties in the measured or estimated parameter values reported in the literature. Values that appeared to be most acceptable, as judged by the confirmation of reported values by multiple studies, were selected for input into CHEMBASE.

All CHEMBASE parameter values were first entered onto hard copy forms before being entered into CHEMBASE. CHEMBASE field values were checked against the parameter forms for each chemical and any entry errors were corrected. CHEMBASE values were also checked against values reported in a number of references of compiled physicochemical parameter including recent references by Mackay et al. (1992, 1993a,b, 1995), Montgomery et al. (1990); Howard et al., (1989,1990, 1991), Lyman et al. (1990), the SRC CHEMFATE Database (1994), and the Toxicological Profiles published by the ATSDR (1990). Beta versions of CHEMBASE were reviewed by the ARB, OEHHA and the UCLA research team and based on these reviews the CHEMBASE software was updated as deemed necessary.

4.4 Completeness of CHEMBASE Parameter Values

Compilation of parameter values for CHEMBASE has revealed that there are serious data gaps in the literature. The percent of parameter values, unavailable in the literature, for the twenty four physicochemical parameters of the CHEMBASE chemicals is plotted in Figure 4.1. The most significant data gap is for critical constants (i.e. critical temperature, volume and pressure), vapor pressure-temperature dependence, BCF's for plants and terrestrial animals and degradation rate constants (most significantly for the soil, sediment and biota compartments). The lack of critical properties curtails the use of corresponding-state type correlations for estimation of ITF values.

Also, noticeable is the limited availability of BCFs for plants and terrestrial organisms, 5% and 18%, respectively. A global view of the level of lacking data is provided in Figure 4.2 in which the various CHEMBASE parameters were grouped into the following categories: physicochemical parameters, BCFs and Reaction rate constants. The percent of unavailable parameter values is largest for the BCF's followed by the reaction rate constants and the basic physicochemical parameters. Finally, it is worth noting that with the exception of the atmospheric compartment, there are no reliable methods available to predict the environmental reaction rate constants for other media.

Figure 4.1 Profile of Unavailable Literature Data for CHEMBASE Chemicals

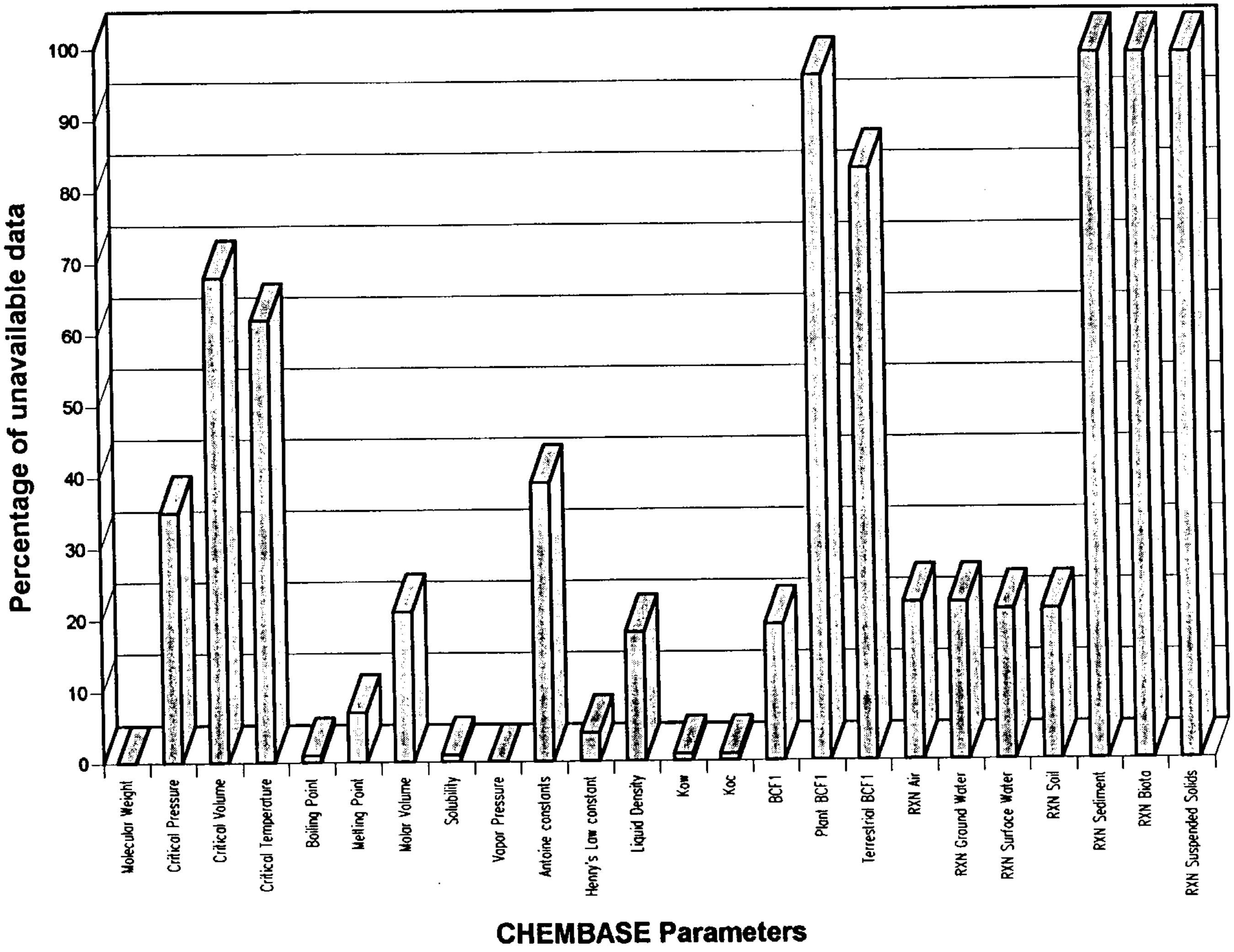
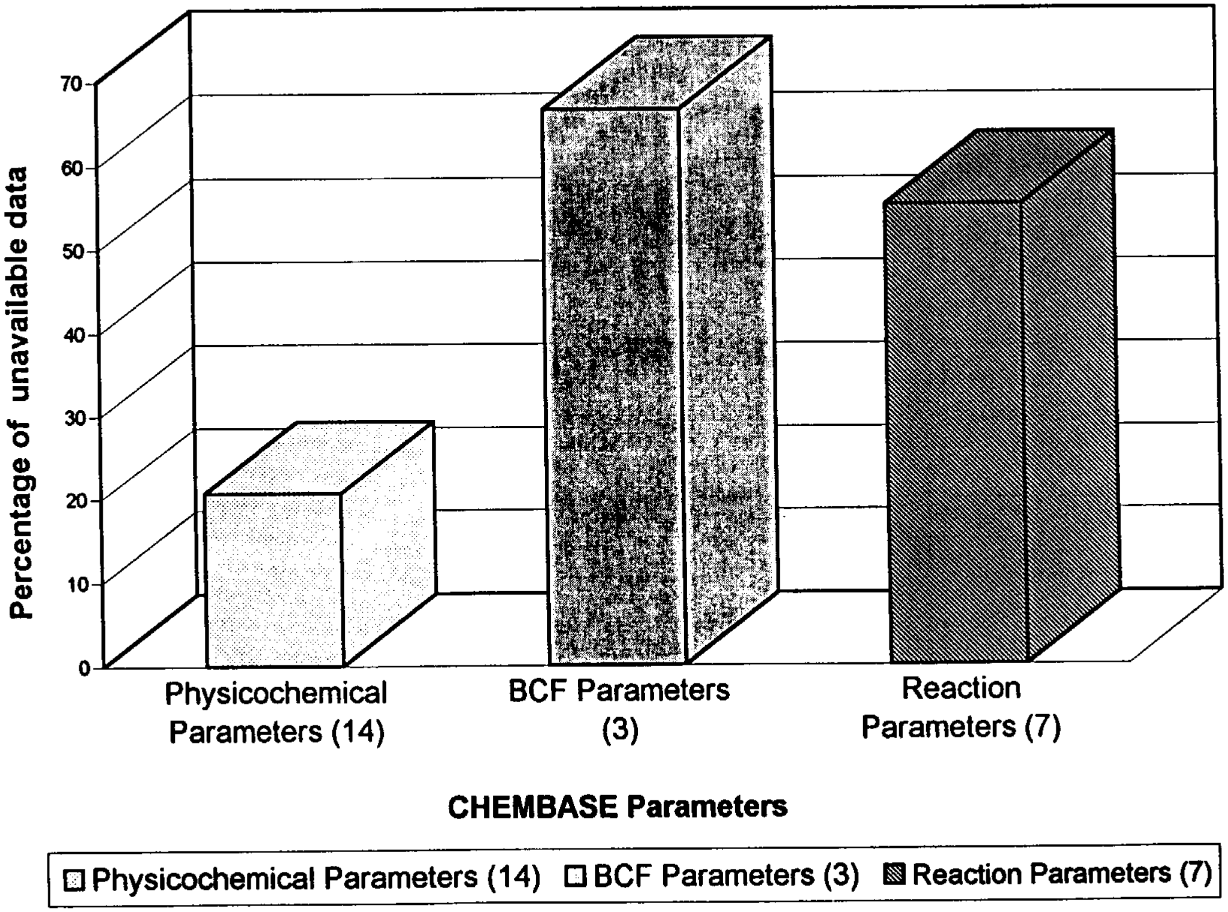


Figure 4.2 Global View of Unavailable Literature Data for CHEMBASE Chemicals



5. THE CHEMICAL PROPERTY PREDICTOR (CPP)

5.1 Overview

Methods for predicting various chemical-specific physicochemical properties and partition coefficients may be divided into two general categories: 1) theoretical estimation methods and 2) empirical correlations (Bruggemann et al. 1990). Empirical correlations are widely used in environmental analysis and can be developed for specific chemical classes. In the following section the development of quantitative structure-activity relationships (QSAR's) is briefly discussed followed by a description of the molecular descriptors and CPP correlations developed in this study. In the CPP, all the estimation methods are based on empirical correlations between ITFs and selected molecular descriptors.

5.2 QSAR as a Tool for Prediction of Intermedia Transfer Factors

Quantitative structure activity relationships (QSAR's) generally refer to any mathematically or statistically defined functional models that relate physicochemical, biological or toxicological properties to structural or structure-related parameters (Bruggemann et al. 1990). As recognized by Koch and Nagel (1983), the fundamental premise for all QSARs is that variations in a specific activity within a selected group of chemicals that share similar structural characteristics can be related to differences in the molecular or structural parameters of these chemicals.

Over the last two decades, various QSARs have been proposed to correlate the aqueous solubility, octanol-water partition coefficient, Henry's law constant, bioconcentration factor, and several other environmentally important parameters (e.g., ARB, 1994; Lyman et al. 1990; Mackay et al. 1992, 1993a,b; Dearden, 1990; Dunn, 1986; and references therein). QSARs have proved to be valuable for multipathway exposure analysis since they allow ITFs to be estimated in the absence of experimental data.

5.3 Development of Chemical Class-Specific CPP Algorithms

5.3.1 Overview of Approach and Methodology

ITF correlations that encompass several chemical classes have generally low correlation coefficients unless they involve multiple correlating parameters or structural parameters which are not readily available to the user. By contrast, ITF correlations which are chemical class-specific are typically more accurate and generally simpler since they require generally one or at most two correlating parameters. In order to maintain the simplicity and ease of use of the CPP, wherever possible, chemical-class specific correlations from the literature or newly developed correlations were utilized. It should be noted that for certain chemical classes (for example, anhydrides) it is not possible to establish simple class-specific correlations, either due to lack of experimental data, absence of fundamental structural regularity among members of a specific chemical class or lack of correlation with molecular descriptors or other ITFs. In the absence of chemical class-specific correlations, the CPP utilizes literature correlations that are most suitable for the classes or ITFs in question. However, one should note that general chemical class correlations provide less accurate estimates.

5.3.2 Molecular Descriptor Selection Criteria

Structural characteristics of chemicals can be described with various molecular descriptors and these can be used in correlating ITF values for different chemical classes. Various molecular descriptors have been reported in the literature in relation to the calculation of ITFs (Meylan, 1992; Lyman et al. 1990, Dearden 1990; Bruggemann et al., 1988, 1990; Hansch and Leo, 1979;; and references therein). Examples are molecular volume, the number of specific atoms (e.g., carbon or chlorine), surface area (defined in various ways) and molecular connectivity indices.

Two criteria were adopted for selecting specific molecular descriptors for use in the CPP QSAR correlations: (a) the descriptors should be calculable from straightforward algorithms or available from the literature and/or other accessible sources (e.g., chemical databases); and (b) preference should be given to molecular descriptors which can be correlated with the desired intermedia transfer factors using simple correlations. The simplest molecular parameters used in the CPP include molecular weight, molar volume and critical volume. Other descriptors include simple count of the number of functional groups or atoms of a specific type and molecular connectivity indices (Kier and Hall, 1976; Lyman et al., 1990; Dunnivant et al., 1992; Bruggemann et al., 1986, 1988, 1990; Reid et al, 1977, 1987). The molecular connectivity indices provide a set of structural parameters that can be used to correlate various physicochemical parameters, for various chemical classes, with a high degree of accuracy (e.g., Sabljić et al., 1993; Sabljić, 1989; Dearden, 1990; and references therein). Although a number of such correlations are included in the CPP, a module capable of calculating connectivity indices is not included in the present version of the ITFP.

5.4 Physicochemical Parameters and Partition Coefficients

5.4.1 Overview

The physicochemical parameters and partition coefficients included in the CPP are listed in Table 5.1. A brief discussion of the parameters listed in Table 5.1 is provided in the subsequent sections along with a brief account of some of the methods that may be useful for estimating these parameters.

Table 5.1 List of Major CPP Parameters

Symbol	Parameter Description
V_M	Molar Volume
S	Aqueous Solubility
K_{ow}	Octanol/Water Partition Coefficient
K_{oc}	Soil organic carbon/water partition coefficient
BCF	Bioconcentration Factor (Aquatic species)
BMF	Biomagnification Factor for Finned Fish (BMF)

5.4.2 Molar Volume

The molar volume (V_M) is the volume of one mole of a liquid compound at the normal boiling temperature expressed in the CPP in units of cm^3/mole. The molar volume of organic compounds is often used in solubility, K_{ow} and molecular mass diffusivity correlations. Common estimation methods include:

i. The Le Bas group contribution method (Reid et al. 1977);
ii. Critical volume correlation ($V_M = aV_C^b$; where a and b are constants and V_C is the critical volume; Reid et al. 1977);
iii. Approximation from the mass density (i.e., $V_M = MW/\rho$; where MW is the molecular weight and ρ is the chemical mass density).

The Le Bas method (Reid et al., 1977) is essentially a group contribution method, in which the molar volume of a chemical is the sum of the volume increments of all atoms, rings, and multiple bonds. The empirical correlation of V_M with the critical volume is recommended by Reid et al. (1977). The use of this correlation, however, is limited since the critical volume is unavailable for most of the air toxics of interest. When using molar volume correlations to estimate specific physicochemical properties, it is important to determine the molar volume using the same procedure utilized in the derivation of the corresponding property-molar volume correlation.

5.4.3 Vapor Pressure

The saturation vapor pressure, P_v, is a measure of the volatility of a chemical in its pure state and is an important determinant of the rate of vaporization and estimating various other ITFs (e.g., Henry's law constant). Vapor pressure can be estimated from various correlations (Burkhard et al., 1985; Hawker, 1989, 1990; Reid et al., 1977; Stephonson and Malanowski, 1987.) and group contribution methods (Reid et al., 1987). However, the current version of the ITFP only considers the estimation of vapor pressure as a function of temperature (in CHEMBASE) using the Antoine equation

$$\ln(P_v) = A + \frac{B}{T+C} \tag{5.1}$$

where A, B and C are the Antoine constants and T is the temperature. Thus, for chemicals for which the Antoine constants are available, the vapor pressure can be calculated for the temperature of interest.

5.4.4 Aqueous Solubility

Aqueous solubility, S (e.g., units of mass/vol) has been correlated with a variety of molecular descriptors. Some of the popular empirical correlation for estimating solubility include:

1. Solubility-molar volume correlations for individual chemical classes (e.g., Miller et al. 1984, 1985; Kamlet et al. 1988);
2. Solubility-molecular surface area for individual chemical classes (e.g., Hawker and Connell 1988; Dunnivant et al. 1992; Andren et al., 1987);
3. Solubility-K_{ow} correlations (e.g., Mackay et al. 1980; Chiou,1982a; Miller et al. 1985);
4. Solubility-molecular connectivity indices correlations (e.g., Lyman et al., 1990; Sabljic et al., 1993; Mailhot and Peters, 1988; Nirmalakhanda and Speece, 1989); and
5. Group contribution methods (e.g., Banerjee and Howard, 1988).

In the ITFP correlations of the type 1, 3 are utilized. Correlations of type 4 can be more accurate and could be included in future versions of the CPP with the addition of a module to calculate molecular connectivity indices and a database of connectivity indices values for CHEMBASE chemicals.

5.4.5 Octanol-Water Partition Coefficient

The octanol-water partition coefficient is an important parameter used in the assessment of environmental fate and transport for organic chemicals because octanol is a surrogate for lipid phase or natural organic carbon in the environment. The octanol-water partition coefficient (K_{ow}) is defined as the equilibrium ratio of the concentration of a chemical in the octanol phase to its concentration in the aqueous phase in a two-phase octanol/water system:

$$K_{ow} = C_o / C_w \qquad (5.2)$$

where C_o is the concentration in octanol phase and C_w the concentration in aqueous phase, both in units of mass/volume or mol/volume. Commonly applied empirical correlations for estimating K_{ow} include:

1. K_{ow}-molar volume correlations for individual chemical classes (e.g., Lyman et al., 1990; and references therein);
2. K_{ow}-molecular surface area correlations for specific chemical classes (e.g., Hawker and Connell 1988, Dunnivant et al. 1992);
3. K_{ow}-aqueous solubility correlations (e.g., Lyman et al. 1990 and references therein);
4. Group contribution methods using summation of organic fragment parameters (e.g., Leo et al. 1971, Hansch and Leo 1979); and
5. Correlation of K_{ow} with molecular connectivity indices (e.g., Mailhot and Peters, 1988; Sabljic et al., 1993; Patil, 1991; Gusten et al., 1991).

In the CPP correlations of type 1-3 and 5 are utilized. The majority of the correlations, however, are of type 1 and 3.

5.4.6 Henry's Law Constant

The Henry's law constant is an important parameter for the evaluation of chemical partitioning between air and water and is required as an input parameter in most multimedia models. The Henry's law constant for a given chemical (H) is defined as

$$H=\frac{P_{vp}}{C_w} \qquad (5.3)$$

where P_{vp} is the partial pressure of the chemical at the system temperature, and C_w is the concentration of the chemical in the aqueous phase in equilibrium with the air phase. The Henry's law constant can be correlated with molecular descriptors such as molecular connectivity indices and polarizability factors (e.g., Nirmalakhandan and Speece, 1988; Brunner et al., 1990; Sabljic and Gusten, 1989) and also estimated from group contribution approaches (e.g., Pividal and Sandler, 1990). Although various methods have been proposed to estimate the Henry's law constant (e.g., Dunnivant et al., 1992), these methods were found to be inconvenient or too complex for use in the current version of the ITFP software. Finally, it is noted that for sparingly water soluble organics, given the assumption of ideal solution, the Henry's law constant can be approximated from the vapor pressure/solubility ratio (Mackay, 1991; Lyman et al., 1990). Henry's law constants are reported in CHEMBASE when available and the corresponding dimensionless water/air partition coefficient can be estimated for the temperature of interest.

5.4.7 Bioconcentration Factor

The traditional measure of a chemical's potential to accumulate in an organism is the bioconcentration factor (BCF). The BCF which is defined as

$$\mathrm{BCF} = \frac{\text{Equilibrium concentration of chemical in the receptor}}{\text{Average concentration of chemical in the environmental medium}} \tag{5.4}$$

only accounts for uptake across external membranes from the media in which the receptor is directly exposed. The BCF does not account for uptake via the food chain and it is also important to note that BCF values are medium-specific and species-specific. BCFs are typically correlated with K_{ow}, S, and K_{oc} (Lyman et al. 1990, Isnard and Lambert 1988; Veith et al., 1979; Chiou, 1985).

5.4.8 Organic Carbon/Water Partition Coefficient

The natural organic carbon/water partition coefficient (K_{oc}) is a parameter used to predict the soil/water linear adsorption coefficient. K_{oc} is defined as

$$K_{oc} = \frac{\text{(mg chemical adsorbed/kg organic carbon)}}{\text{(mg chemical dissolved/L of solution)}} \tag{5.5}$$

K_{oc} is typically correlated with K_{ow} or aqueous solubility S. The empirical correlation between K_{oc} and K_{ow} is particularly useful because of the wide availability of K_{ow} values (Karickhoff et al.

1979; 1981). Also, given K_{oc} values, the soil adsorption capacity [e.g., mg/Kg soil] can be estimated from $q=K_{oc}\chi C_w$, where χ is the mass fraction of organic carbon in the soil and C_w is the chemical concentration in the aqueous phase [e.g., mg/L]. It is noted, however, that simple K_{ow}-K_{oc} and K_{oc}-solubility and Koc-BCF correlations are inadequate for nonpolar chemicals (Lyman et al., 1990; Southworth and Keller, 1986; Chiou et al., 1979, 1983; Kenaga, 1980a,b, Kenaga and Goring, 1980; Karickhoff, 1979; Mackay, 1982) and various other alternatives have been proposed. Such alternatives include correlations with molecular connectivity indices and the addition of structural correction factors to account for polar interactions (Meylan et al., 1992) and group contribution methods (e.g., Ames et al., 1995). The current version of the CPP does not include correlations for polar organics but such correlations can be added given the modular structure of the ITFP.

6. THE CHEMICAL PROPERTY PREDICTOR

6.1 Overview and Outline of Methodology

The chemical property predictor (CPP) contains a variety of algorithms to estimate the following parameters: molar volume, aqueous solubility, K_{ow}, K_{oc}, BCF and BMF. The first four parameters are integrated within the CPP. The biomagnification factor for finned fish (BMF) can be estimated using a stand-alone module. The BMF module allows the determination of the chemical concentration in the fish as a function of time, accounting for fish growth and biomagnification via a linear food chain model. The CPP modules require user-input of basic parameter values. The CPP software provides the user with default and/or recommended range of parameter values. The CPP software is described in section 8.3 and the relevant input screens are shown in Appendix E. The procedure used to identify the various physicochemical parameters listed in Table 5.1 is described briefly in section 6.2 along with the list of the correlations included in the CPP software.

6.2 CPP Algorithms for Aqueous Solubility, K_{ow}, K_{oc} and BCF

An extensive literature search of algorithms for the prediction of the physicochemical properties described in section 5 was conducted and relevant published QSAR estimation methods were evaluated and compiled. In addition, solubility and K_{ow} data were critically evaluated and compiled for individual chemical classes (Tables 6.2-6.5). Data compiled from different references were reviewed and the original sources were traced before the selection was made. When multiple values were reported for a given parameter, these were averaged when it was judged to be appropriate (see section 4.3). For each of the chemical classes a regression analysis was then performed to derive simple solubility-molar volume, K_{ow}-molar volume and K_{ow}-solubility correlations. These correlations are of the following general form:

$$\mathrm{Log}(S) = aV_m + b \tag{6.1}$$

$$\mathrm{Log}(S) = f(\mathrm{Log}K_{ow}) + g \tag{6.3}$$

$$\mathrm{Log}(K_{ow}) = cV_m + d \tag{6.2}$$

$$\mathrm{Log}(BCF) = I(\mathrm{Log}K_{ow}) + J \tag{6.4}$$

in which the parameters a,b,c,d,f,g,I,J are correlation constants. The above correlations for the various CPP chemical classes are provided in Table 6.1-6.3. In addition to the above correlations, various correlations for K_{oc}, K_{ow} and BCF were compiled from the literature and incorporated into the CPP. The various literature correlations utilized in the CPP are given in Tables 6.4-6.8.

As described in section 8.3, the CPP is constructed such that the user can select the correlation which is most appropriate for the chemical class under consideration. This initial compilation of QSARs in the user-friendly CPP software illustrates the utility of the ITFP. As new and improved methods are developed, they can be easily added to future versions of the ITFP given its modular structure.

TABLE 6.1

CPP Derived Aqueous Solubility Correlations

Chemical Class	Solubility-Molar Volume Correlations	Solubility-K_{ow} Correlations
Chloroalkanes	LogS = -0.0216V_m + 3.611 r^2=0.831; n =22	LogS = -0.929LogK_{ow} + 3.392 r^2=0.910; n=19
Chloroalkenes	LogS = -0.0280V_m + 3.788 r^2 = 0.975; n = 9	LogS = -1.151LogK_{ow} + 3.642 r^2=0.964; n= 9
Benzenes & Alkylbenzenes	LogS = -0.0255V_m + 3.812 r^2=0.923; n=23	LogS = -1.077LogKow + 3.592 r^2=0.935; n=22
Phenol & Chlorophenol	LogS= -0.0397Vm) + 7.201 r^2=0.983; n=13	LogS = -1.1043LogK_{ow} + 4.876 r^2=0.924; n=13
Chlorobenzenes	LogS=-0.0487Vm + 6.639 r^2=0.983; n=12	LogS = -1.905LogK_{ow} + 6.627 r^2=0.915; n=12
PAHs	LogS = -0.0352V_m + 4.815 r^2=0.804; n=48	LogS = -1.480LogK_{ow} + 4.645 r^2=0.821; n=48
PCBs	LogS = -0.0252V_m + 3.125 r^2=0.762; n=42	LogS = -1.020LogK_{ow} + 2.414 r^2=0.710; n=41
Alphatic & Aromatic Ethers	LogS = -0.0267V_m + 5.421 r^2=0.820; n=11	LogS = -1.121LogK_{ow} + 3.712 r^2=0.960; n=11
Chlorinated Dioxins	LogS = -0.0413V_m + 5.452 r^2=0.945; n=14	LogS = -0.981LogK_{ow} + 1.4 r^2=0.845; n=14
Chlorinated Dibenzofurans	LogS = -0.0474V_m + 7.083 r^2=0.970; n=7	LogS = -1.892LogK_{ow} + 6.51 r^2=0.984; n=7

V_m - LeBas molar volume (cm^3/mol);
S - aqueous solubility (mol/m^3)
r^2 - correlation coefficient
n - number of chemicals
Note: S-K_{ow} are also used in the CPP to estimate K_o

Table 6.2
CPP Derived K_{ow}-Molar Volume Correlations

Chemical Class Correlations	Correlation
Chloroalkanes	$\text{Log}K_{ow} = 0.0213V_m - 0.103$ $r^2 = 0.880$; n = 19
Chloroalkenes	$\text{Log}K_{ow} = 0.0237V_m - 0.031$ $r^2=0.988$; n=10
Benzenes & Alkylbenzenes	$\text{Log}K_{ow} = 0.0234V_m - 0.164$ $r^2=0.964$; N=22
Phenol & Chorophenol	$\text{Log}K_{ow} = 0.0343V_m - 1.856$ $r^2 =0.970$; n=13
Chlorobenzenes	$\text{Log}K_{ow} = 0.0253V_m + 0.041$ $r^2=0.992$; n=12
PAHs	$\text{Log}K_{ow} = 0.0234V_m - 0.0347$ $r^2 =0.950$;n=48
PCBs	$\text{Log}K_{ow} = 0.0194V_m + 0.695$ $r^2 =0.773$;n=42
Alphatic & Aromatic Ethers	$\text{Log}K_{ow} = 0.0278V_m - 2.216$ $r^2 =0.802$; n=13
Chlorinated Dioxins	$\text{Log}K_{ow} = 0.0378V_m - 2.992$ $r^2 =0.906$; n=14
Chlorinated Dibenzofurans	$\text{Log}K_{ow} = 0.0230V_m + 0.143$ $r^2 =0.915$; n=8

Note:
V_m - LeBas Molar Volume (cm^3/mol)
r^2 - correlation coefficient
n - number of chemicals

Table 6.3
CPP Derived BCF-K_{ow} Correlations^(a)

Chemical Class	BCF Correlation
Aromatics and Chlorinated aromatics.	$\text{LogBCF} = 0.982\text{Log}K_{ow} - 1.349$ $r^2=0.852$; n=13
Polyaromatic Hydrocarbons (PAHs)	LogBCF = 0.564LogKow + 0.477 $r^2=0.941$; n=13
Chlorinated Hydrocarbons	$\text{LogBCF}=0.791\text{Log}K_{ow} - 0.798$ $r^2=0.899$; n=10
Mixed class: PAHs, aromatics, chlorinated hydrocarbons, chlorinated aromatics, PCBs, DDT, DDE	$\text{LogBCF}=0.857\text{Log}K_{ow} - 0.798$ $r^2=0.896$; n=35

Note: r^2 - correlation coefficient ; n - number of chemicals

(a) Based on BCF data from Veith et al. (1979) and CHEMBASE data.

Table 6.4
Aqueous Solubility Correlations

Chemical Class	Solubility Correlation (S - Solubility)	Reference
Alkanes	$\mathrm{Log}(1/S) = 1.237\mathrm{Log}K_{OW} + 0.248$ S - mol/l; $r^2 = 0.908$; n = 16	Hansch et al. (1968)
Alkenes	$\mathrm{Log}\ 1/S = 1.294\mathrm{Log}K_{OW} - 0.248$ S - mol/l; $r^2 = 0.908$; n = 12	Hansch et al. (1968)
Alkynes	$\mathrm{Log}(1/S) = 1.294\mathrm{Log}K_{OW} - 1.043$ S - mol/l; $r^2 = 0.908$; n = 7	Hansch et al. (1968)
Halobenzenes:	$\mathrm{Log}S = -0.9874\mathrm{Log}K_{OW} - 0.0095T_m + 0.7178$ S - mol/l; T_m - melting temperature, °C, for $T_m < 25°C$, $T_m = 25°C$ is used $r^2 = 0.99$; n=35	Yalkowsky et al. (1979)
Chlorinated Benzenes	$\log S = -0.678(n_{cl}) - 4.13$ S - solubility in mol/l ;n_{cl} - number of chlorine atoms $r^2 = 0.975$; n=17	Miller et al. (1984)
Polyaromatic Hydrocarbons	$\mathrm{Log}S = -0.881\mathrm{Log}K_{OW} - 0.01T_m - 0.012$ S - mol/l; T_m - °C; for $T_m < 25°C$ use $T_m = 25°C$ $r^2 = 0.979$; n=32	Yalkowsky and Valvani (1979)
PAHs, Dioxins, Chlorinated hydrocarbons, aromatics	$\mathrm{Log}S = -1.37\mathrm{Log}K_{OW} + 7.26$ S - μmol/l $r^2 = 0.903$; n = 41	Banerjee et al. (1980)
PCBs	$\mathrm{Log}S = -0.785(n_{Cl}) - 1.72$ S - mol/l $r^2 = 0.956$; n=12	Miller et al. (1984)
Chlorinated Dibenzo-p-dioxins	$\mathrm{Log}S = 5.03 - V/29.9$ S - mol/m^3; V - molar volume, cm^3/mol	Shiu et al. (1988)
Note: r^2 - correlation coefficient ; n - number of chemicals		

Table 6.5
Octanol/Water Partition Coefficient Correlations

Chemical Class	K_{ow} Correlation	Reference
General	$LogK_{OW} = 0.04 - 0.6 LogS + 0.32\, ^1\chi$ S - mol/l; r^2=0.91 ; n=115	Mailhot and Peters (1988)
Alkanes	$LogK_{OW} = 0.79 + 0.020V_L$ V_L = molar volume cm^3/mol r^2 = 0.746; n =17	Mailhot and Peters (1988)
Alkenes	$LogK_{OW} = 0.27 + 0.970\, ^1\chi$ $^1\chi$ - first order connectivity index r^2 = 0.992, n = 9	Mailhot and Peters (1988)
Amines, Ethers, & Ketones:	$LogK_{OW} = -1.55 + 0.99\, ^1\chi$ $^1\chi$ - 1st order connectivity index r^2 = 0.957 ; n = 49,	Mailhot and Peters (1988)
Overall for halogenated hydrocarbons, alcohols, aromatics, amines, phenols, alkanes, ketones, alkenes, ethers, organophosphates	$LogK_{ow} = 0.94 - 0.69LogS$ S - mol/l;r^2 =0.91; n=258	Mailhot and Peters (1988)
Overall for halogenated hydrocarbons, alcohols, aromatics, amines, phenols, alkanes, ketones, alkenes, ethers, organophosphates	$LogK_{OW} = 5 - 0.67LogS$ S - µmo/l; r^2 =0.97; n=34	Chiou et al., (1977)
Overall for alkylbenzenes, halogenated benzenes, PCBs, PBBs, PCDFs and PCDDs	$LogK_{ow}=0.959 - 0.806LogS$ S - mol/l ; r^2 =0.96; n =55	Andren et al (1987)
Halogenated Hydrocarbons	$LogK_{OW} = 0.96 - 0.72LogS$ S - moles/l ; r^2 =0.944; n =65	Mailhot and Peters (1988)
Organophosphates	$LogK_{OW} = 0.39 - 0.77LogS$ S - moles/l; r^2 = 0.751; n = 13,	Mailhot and Peters (1988)
Chlorosubstituted Aromatics	$LogK_{ow} = (n + 1)^b LogK^\circ_{OW}$ n = number of chlorine atoms in ring portions; $logK^\circ_{ow}$ - $logK_{ow}$ of the parent compound ; a,b - empirical constants given in Table 6.6 below.	Kaiser (1983)
Chlorinated Dibenzo-p-dioxins	$LogK_{ow} = -1.63 + (V/32.1)$ V-molar volume, cm^3/mol	Shiu et al. (1988)

Table 6.6
Constants for the Kaiser (1983) Solubility-K_{ow} Correlation

Chemical Class	r^2	N	$\log K^{\circ}_{ow}$	b
biphenyls	0.96	10	3.964	0.2538
benzenes	0.991	13	2.147	0.4556
phenols	0.987	10	1.482	0.6634
anilines	0.995	8	0.978	0.991
pyridines	0.956	13	0.709	0.9926
nitrobenzenes	0.995	8	1.881	0.4508

Table 6.7
Organic Carbon/Water Partition Coefficient Correlations

Chemical Class	K_{oc} Correlation	Reference
nonionic organic compounds	$\mathrm{Log}K_{oc} = -0.729 \log S + .001$ S - moles/liter; $r^2 = .996$; n=12	Chiou et al (1983)
chlorinated hydrocarbons	$\mathrm{Log}K_{oc} = -0.557 \log S + 4.277$ S - µmoles/liter; $r^2=0.99$; n=15	Equation 4-7 Lyman et al. (1990)
General for aromatics, polynuclear aromatics, triazines and dinitroaniline herbicides	$\mathrm{Log}K_{oc} = 0.937 \log K_{OW} - 0.006$ S - moles/liter; $r^2 = 0.95$; n=19	Equation 4-9 Lyman et al. (1990)
Polynuclear aromatics	$\mathrm{Log}K_{oc} = \log K_{OW} - 0.21$ S - moles/liter; $r^2=1.00$; n=10	Equation 4-10 Lyman et al. (1990)
Variety of insecticides, herbicides and fungicides	$\mathrm{Log}K_{oc} = 1.029 \log K_{OW} - 0.18$ S - moles/liter; $r^2=0.91$; n=13	Equation 4-12 Lyman et al. (1990)
Non-polar organics	$\mathrm{Log}K_{oc} = 0.53\ {}^1\chi + 0.62$ ${}^1\chi$ - 1st order connectivity index $r^2=0.956$; n=64	Meylan et al. (1992)
General	$\mathrm{Log}K_{oc} = 0.544 \mathrm{Log}K_{OW} + 1.377$ $r^2 = 0.74$; n =45	Equation 4-8 Lyman et al. (1990)
General	$\mathrm{Log}K_{oc} = 0.63 \mathrm{Log}\ K_{OW}$ $r^2=0.74$; n=45	Karickhoff et al. (1979)

Table 6.8
Bioconcentration Factor for Aquatic Organisms

Chemical Class	BCF Correlation	Reference
General	$BCF = (K_{OW})f_l$ f_L - lipid fraction	Mackay (1982)
General	$LogBCF = 0.8LogK_{OW} - 0.52$ $r^2 = 0.904$; n=107	Isnard (1988)
General	$LogBCF = 0.76LogK_{OW} - 0.23$ $r^2=0.823$; n =84	Equation 5-2 Lyman et al. (1990)
General	$LogBCF = 1.119LogKoc - 1.579$ $r^2=0.757$; n=13	Equation 5-4 Lyman et al. (1990)
General	$LogBCF = LogK_{OW} - 1.32$ $r^2=0.95$; n=36	Mackay (1982)
General	$LogBCF = 2.791 - 0.564LogS$ S - ppm;	Kenaga (1980)
Hydrophobic organic chemicals (Log $K_{OW} > 6$)	$Log\ BCF = 0.0095 (Log\ K_{OW})^4 - 0.244 (Log\ K_{OW})^3 + 1.95 (Log\ K_{OW})^2 - 5.12\ Log\ K_{OW} + 5.37$ $r^2=0.87$; n=41	Hawker et al. (1990)

6.3 The Bioaccumulation Module

6.3.1 Overview

Several studies over the past 10 years (e.g., Chiou 1985; Thomann 1989; Clark et al., 1990; Barber et al., 1987, 1991, 1994; Gobas et a., 1987, 1993; and references therein) have indicated that the concentration of organic toxins in fish (e.g. PCB's) can be as much as 100,000 times greater than the corresponding ambient water concentrations. This phenomenon has been attributed to the uptake of the toxin via the water and food pathways.

Uptake of a toxin via water only is termed bioconcentration. The bioconcentration factor (BCF) is defined by Eq. 5.4. One of the most important pathways of toxin accumulation in fish is by uptake through the gills. In this process, the organic toxin partitions to the lipid phase of the finned fish in a thermodynamically driven process. According to Thomann (1989) bioconcentration is the most significant uptake mechanism for chemicals with a log $K_{ow} < 5.0$. For toxins with log Kow > 5.0, uptake via food is also a significant mechanism (Thomann, 1989). The tendency for a chemical accumulate in the organism from both food and water is defined as **bioaccumulation.** The bioaccumulation factor (BAF) is defined as

$$BAF = \frac{\mu g \ chemical/g \ organism}{\mu g \ chemical/ml \ water} \tag{6.3.1}$$

The density of the organism is often taken to be equal to 1g/ml and thus the BAF is generally considered to be dimensionless. It is important to note that bioaccumulation is a physically driven process (uptake by feeding) whereas bioconcentration is a thermodynamically driven process. Bioaccumulation is hypothesized to arise because of bioaccumulation of the toxin rich feed (Gobas et al., 1993) in the gastro intestinal tract (GIT). Food digestion in the GIT alters the composition of the consumed food while attempting to metabolize it. In the case of hydrophobic, non-metabolizable food (prey saturated with high K_{ow} toxins). The resulting build up of chemical in the GIT results in an increase in the fugacity of the food to a level that exceeds the fugacity of chemical in the water phase.

In the ITFP a dynamic linear food chain model is used to estimate the bioaccumulation factor (BAF) for finned fish (Vohra, 1996). Detailed case studies were performed and the model accuracy was evaluated by comparing the ITFP BAF module results to available experimental data and the FGETS (Food and Gill Exchange of Toxic Substances) model of Barber et al. (1994).

6.3.2 Model Framework

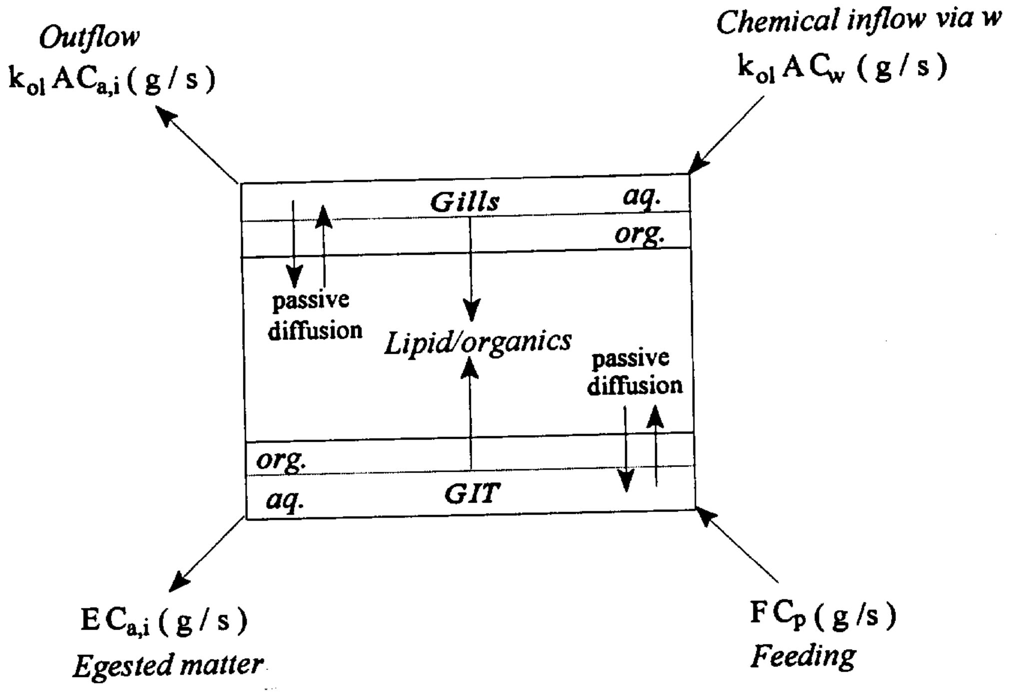
A chemical balance on a fish can be expressed mathematically as

$$\frac{d(C_{ai}W_i)}{dt} = k_i^{ol}A_i(C_{amb} - C_a*) + \sum_{p=1}^{N_{prey}} C_{a,p}F_{i,p} - E_i C_{ei} \tag{6.3.2}$$

where C_{ai} and C_{amb} are the average chemical concentrations in the organism (µg toxin/g-fish) and in the surrounding water (µg toxin/ml water), respectively, C_a* is the average chemical concentration in the aqueous fraction of the fish (µg toxin/g-fish) that would be in equilibrium with the water, and $C_{a,p}$ and C_{ei} are the chemical concentrations in the prey (µg toxin/g-prey) and in the egested matter (µg toxin/g-feces), respectively. The weight of the organism is denoted by W_i (g), A_i is the interfacial area for mass transfer (cm ^{2}), k^{ol}_i is the overall aqueous side mass transfer coefficient (cm/s), F_i is the feeding rate of the prey "p" to fish 'I' (g/s) and E_i is the rate of fecal matter egestion (g/s).

The first term in equation (6.3.2) represents the net accumulation of chemical 'a' in an organism 'I' of weight W, on a total body burden basis. The second term represents the net transfer rate of chemical 'a' into the organism via the gills. The third term represents the net uptake via food where it is possible to have multiple prey species for a given predator I. The last term represents the loss of chemical due to excretion. In general, the *total body burden* concentration in an organism, may be expressed as the weighted average of the concentrations in each compartment of that organism. The organism may be represented as a composite body made up of a lipid phase, non-lipid organic phase and an aqueous phase (see Figure 6.3.1), with these phases assumed to be in thermodynamic equilibrium.

Figure 6.3.1. Mass Transfer and Chemical Partitioning of in Finned Fish.



Following the development of Barber et al. (1994) the average concentration of a toxin in he entire fish body, C_{ai}, can be expressed as

$$C_{ai} = f_a C_a + f_L C_L + f_o C_o \qquad (6.3.3)$$

where the subscripts a, L and o denote the organism's aqueous phase, lipid matter and non-lipid organic matter, respectively. The mass fraction of compartment I in the finned fish is denoted by $_{Fi}$ and C_i is the concentration of toxin 'a' in compartment I. Subject to the assumption of internal equilibrium among the compartments of the fish, the fish/ambient water partition coefficient can be written as

$$K_f = = \frac{C_{ai}}{C_a} = f_a + K_L f_L + K_o f_o \qquad (6.3.4)$$

where K_L and K_o are lipid phase/water and non-lipid organic matter/water partition coefficients defined as

$$K_i = \frac{C_i}{C_a} \tag{6.3.5}$$

where the subscripts I denotes the lipid or non-lipid organic phase and the concentrations Ci and Ca are in identical units (e.g., µg chemical/g fish). At equilibrium $C_a \approx C_w$ (i.e. the aqueous phase in the fish behaves like water) and thus

$$BCF = K_f = \frac{C_{ai}}{C_w} = f_a + K_L f_L + K_o f_o \tag{6.3.6}$$

Subsequently, from the above expression for the BCF EQ. 6.3.2 can be rewritten as

$$\frac{d(C_{ai}W_i)}{dt} = k_i^{ol} A_i (C_w - \frac{C_{ai}}{K_f}) + \sum_{p=1}^{N_{prey}} C_{a,p} F_{i,p} - E_i C_{ei} \tag{6.3.7}$$

Equation 6.3.7 can be simplified by relating the excretion rate to the ingestion term:

$$E_i = (1-\alpha_f)F_i \tag{6.3.8}$$

where α_f is the dimensionless food assimilation efficiency. Also, the chemical concentration in the excreted matter is expressed by

$$C_{ei} = C_a f_a + C_o f_o \tag{6.3.9}$$

in which f_i is the volume fraction of compartment I. Equation 6.3.8 implies that food which is not digested is simply excreted and in writing Eq. 6.3.9 it is assumed that there is no lipid content in the fecal matter. If one assumes that the local concentration C_{ei} is in equilibrium with the fish total body concentration then C_{ei} can be expressed as

$$\frac{C_{ei}}{C_{ai}} = \left(\frac{K_e}{K_f}\right) \tag{6.3.10}$$

where K_e is the chemical excreted matter/water partition coefficient (i.e., $K_e=C_{ei}/C_w=f_a+f_LK_L$).

In general, the predator feeds on a number of different organisms ranging from other smaller fish to plankton. The most general approach to describe chemical accumulation through the food chain is by a "food web" model where a set of species depend on each other for food. Each species' overall diet consists of some fraction of other species in the food web. Consequently, for a biological system containing N species and age classes, one needs to solve, N^2 number of ordinary differential equations similar to (6.3.2). Although a food web is a more realistic description of a natural ecosystem, various studies (e.g., Thomann, 1989; Vohra, 1996; and references therein) indicate that the feeding of many piscivorous fish, may be approximated via a linear "food chain" as illustrated schematically in Figure 6.3.2.

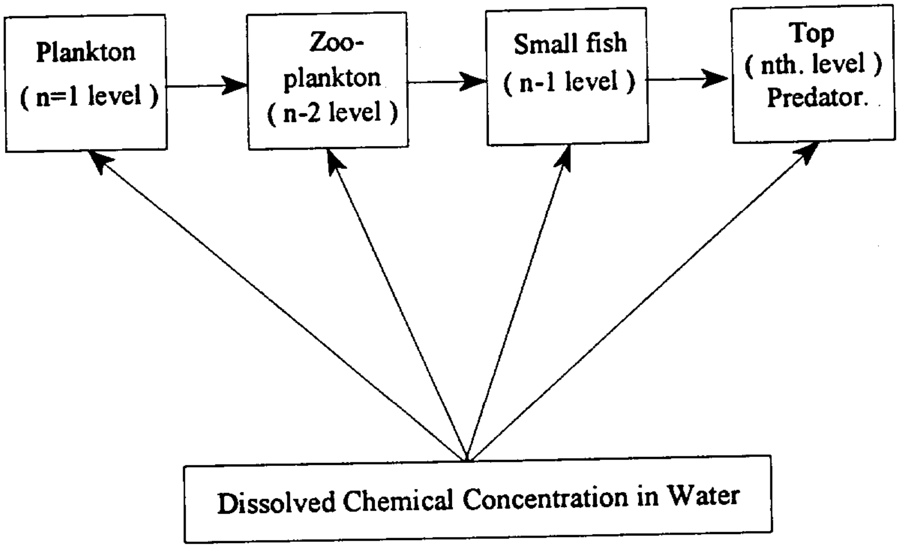


Figure 6.3.2. Example of a Linear Food Chain Model

The linear food chain model assumes that the diet of an N^{th} level predator, may be approximated as consisting entirely of the (N^{th} -1) level predator. As a result, an N^{th} level food chain has only N ODE's rater than N^2 ODE's. Evidence for a food chain rather than a food web, is also verified in field studies of Norstrom (1976) and Connolly (1985). Consequently, the use of a simple linear food chain model in the ITFP is believed to be appropriate for estimating BAFs for screening-level multimedia analysis.

In order to simplify the linear food chain model, the overall chemical concentration in the total feed, $C_{p,}$ can be written as

$$C_p = \sum_{p=1}^{N_{prey}} f_{i,p} C_{a,p} \qquad (6.3.11)$$

where the index p represents the different prey and plankon species in the food chain and $f_{i,p}$ represents the fraction of prey p that predator I consumes. Therefore, the diet of the predator needs to be specified. Substituting the prey concentration in Eq. 6.3.7 gives

$$\frac{d(C_{ai} W_i)}{dt} = k_i^{ol} A_i (C_w - \frac{C_{ai}}{K_f}) + \left[1 - (1 - \alpha_f) (\frac{K_e}{K_f}) (\frac{C_{ai}}{C_p})\right] C_p F_p \qquad (6.3.12)$$

where C_w os the chemical concentration in the surrounding water (μg toxin / ml water), α_f is the mass of food absorbed/mass ingested (food assimilation efficiency), F_p is the total feeding rate of the prey 'p' to fish 'I' (g/s) and K_e is the dimensionless partition coefficient for fecal matter. Mass balance equations similar to Eq. 6.3.12 also hold for the prey species and the resulting set of ordinary differential equations is solved numerically in the BAF module to obtain the BAF for the predator and the prey species. It is noted that when the only prey is plankton or benthic organisms, the BAF is equal to the BCF. Also, in the BAF module, the plankton and benthic organisms are assumed to be in local equilibrium with their aquatic environment.

In implementing the BAF model the allometric approach recommended by Thomann (1989) was followed since it was observed that many of the growth and feeding equations of the more detailed FGETS model (Barber et al., 1991, 1994) follow simple allometric behavior. Such an approach allows a reduction in the number of required model parameters. It is interesting to note, however, that Eq. 6.3.12 reduces to a number of models previously published in the literature. For example, if the food uptake terms were set to zero, then the mass balance is identical to the one developed by Mackay (1982). The so called "first order chemical uptake rate constant from water" is simply the overall mass transfer coefficient multiplied by the interfacial area and divided by the organisms weight. The concentration driving forces in both equations are therefore identical.

The BAF module employs several different K_{ow} and K_{oc} correlations, thus increasing the utility of the module. The BAF module has a built-in set of parameters for the following finned fish species: (1) Salmon; (2) Trout; (3) Striped Bass; (4) Yellow Perch; (5) Atlantic Croaker; (6) White Perch; and (7) Alewife. The estimation of BAF module parameters is discussed in Appendix D.

7. THE INTERMEDIA TRANSPORT PARAMETER PREDICTOR

7.1 Overview of the Intermedia Transport Parameter Predictor Algorithms

The intermedia transport parameter predictor (ITPP) adapts various models of intermedia transport phenomena in order to estimate the values of selected intermedia transfer factors. The intermedia transport parameters modules in the ITPP are listed in Table 7.1. The corresponding algorithms are described in the following sections and the software is described in section 8.4.

Table 7.1
Summary of ITPP Modules in the ITFP Software

Parameter	Reference
Dry Deposition Velocity (Air/Soil)	Sehmel and Hodgson (1980)
Dry Deposition Velocity (Air/Water)r	Williams (1982)
Dry Deposition Velocity (Air/Vegetation)	Slinn (1982)
Molecular Diffusion Coefficient in Air	Fuller (1966) Gustafson and Dickhut (1994a)
Molecular Diffusion Coefficient in Water	Wilke and Chang (1955) Hayduk and Laudie (1974) Hayduk et al. (1982) Gustafson and Dickhut (1994b)
Effective Diffusion Coefficient in the Soil Matrix	Ryan and Cohen (1990)
Effective Diffusion Coefficient in Sediment	Ryan and Cohen (1990)
Soil Volatilization Half-Life	Mayer et al. (1974)

Parameter	Reference
Rain Scavenging Coefficient for Particle-Bound Chemicals	Tsai et al. (1991)
Rain Scavenging Coefficient for Gaseous Chemicals	Tsai et al. (1991)
Air-Side Mass Transfer Coefficient	ARB (1994)
Water-Side Mass Transfer Coefficient	Brustaert (1975)
Air/Soil Gaseous Deposition Velocity	ARB (1994)
Air/Leaf Mass Transfer Coefficient	Van de Water (1995) Paterson et al. (1991) Bacci et al. (1990) (Section 7.4.5)
Environmental Partition Coefficients: - Air/Water - Air/Soil - Water/Sediment - Water/Suspended Solids	Section 7.2
Air/Leaf Partition Coefficient	Mackay et al. (1981) Paterson and Mackay (1994) Bacci et al. (1990)
Soil/Root Partition Coefficient	Mackay et al. (1981)
Gas/Particle Partitioning	Junge (1977) Bidleman and Foreman (1987) Pankow (1991)

7.2 Environmental Partition Coefficients

The dimensionless chemical partition coefficient between environmental compartment a and environmental compartment b is defined by the following expression:

$$H_{ab} \equiv \left(\frac{C_a}{C_b} \right)_{eq} \tag{7.2.1}$$

where H_{ab} is the dimensionless partition coefficient between compartment a and compartment b, C_a is the concentration of the contaminant in compartment a [e.g., mol/m^3] in equilibrium with the concentration of the contaminant in compartment b, C_b [e.g., mol/m^3].

The partition coefficient between any two compartments can be conveniently calculated using the fugacity approach (Mackay, 1981). Accordingly, the concentration in compartment I is written as (Mackay, 1981)

$$C_i = f_i Z_i \tag{7.2.2}$$

where C_i is the concentration of the contaminant in compartment I [e.g., mol/m^3], f_i is the fugacity of the contaminant in compartment I [e.g., Pascal], and Z_i is the fugacity capacity of compartment I [e.g., mol/m^3/Pascal]. At equilibrium, the fugacity of the chemical is the same in compartment a and compartment b (i.e., f_a=f_b). Thus, Eq. 7.2.1 can be written as

$$H_{ab} = \frac{Z_a}{Z_b} \tag{7.2.3}$$

The problem of obtaining partition coefficients is thus converted to the problem of obtaining expressions for the fugacity capacities for the various environmental media.

7.2.2 The Air and Water Compartments

The fugacity capacities for the air and water compartments can be written (in consistent units) as (Mackay, 1981)

$$Z_{air} = \frac{1}{RT_a} \tag{7.2.4}$$

$$Z_{water} = \frac{1}{H} \tag{7.2.5}$$

where Z_{air} is the fugacity capacity of the air [e.g., mol/m^3/Pascal], R is the ideal gas constant [e.g., J/mol/K], T_a is the absolute temperature of the air [K], Z_{water} is the fugacity capacity of water [e.g., mol/m^3/Pascal] and H is the Henry's Law constant for the chemical in the water phase [e.g., Pascal m^3/mol].

7.2.3 The Biota Compartment

The bioconcentration factor (BCF), which is often used to estimate contaminant concentrations in aquatic organisms (see section 5.57) when contaminant uptake is via the water phase only (Kenaga and Goring, 1980; Kenaga, 1980; Mackay, 1982), is defined as

$$\mathrm{BCF} = \frac{C_b}{C_w} \tag{7.2.6}$$

where C_b and C_w are the concentrations (in identical units) of the chemical in the biota and water phases, respectively. The bioconcentration factor can be expressed in terms of the fugacity capacities using Eqs. 7.2.3 and 7.2.6:

$$\mathrm{BCF} = \frac{Z_b}{Z_w} \tag{7.2.7}$$

where Z_b and Z_w are is the fugacity capacities [e.g., mol/m^3/Pascal] of the fish and water phases, respectively.

The fugacity capacity of the fish, Z_b, can be written in terms of the bioconcentration factor:

$$Z_b = \frac{\mathrm{BCF}}{H} \tag{7.2.8}$$

where H is the Henry's Law constant. Correlations of BCF with the octanol water partition coefficient, K_{ow}, are available in the literature (e.g., Mackay et al., 1982; Chiou, 1985; Barber et al., 1988; Lyman et al., 1990; and references therein). It is noted, however, that bioaccumulation of contaminants via the food chain can be important for chemicals with a high K_{ow}. A module that allows one to estimate chemical uptake via both the water phase and ingestion as a function of time, was developed for the ITPP as a stand-alone module (section 6.3 and Appendix C).

7.2.4 Suspended Solids

Particles suspended in water are assumed to contain an organic carbon phase that sorbs dissolved chemicals. The fugacity capacity of the suspended solids (Cohen et al., 1990) is given as

$$Z_{sus} = \frac{K_{oc}\,\chi_{oc}^{sus}\,\rho_{sus}}{H} \tag{7.2.9}$$

where Z_{sus} is the fugacity capacity of the sorbed phase [e.g., mol/m^3/Pascal], K_{oc} is the organic carbon/water partition coefficient [cm^3 of solution/g of organic carbon], χ_{oc}^{sus} is the mass fraction of the organic carbon in the suspended solids and ρ_{sus} is the density of the suspended solids [e.g, g/cm^3].

7.2.5 Multi-Component Media

The overall chemical concentration in a matrix consisting of n phases (e.g., soil and sediment) is defined as

$$C_m = \sum_{i=1}^{n} \theta_i C_i \tag{7.2.10}$$

where θ_i is the volume fraction of phase I and C_m and C_i are the chemical concentration (both in the same units) in the multiphase matrix and in phase I, respectively. The overall chemical concentration in the matrix (Eq. 7.2.10) can be written in terms of the fugacities and fugacity capacities (using Eq. 7.2.1) as

$$f_m Z_m = \sum_{i=1}^{n} \theta_i f_i Z_i \tag{7.2.11}$$

where Z_m and f_m are the fugacity and fugacity capacity of the matrix, respectively. The matrix fugacity capacity can be related to the individual phase fugacities by applying the local equilibrium assumption (i.e. $f_i = f_m$):

$$Z_m = \sum_{i=1}^{n} \theta_i Z_i \tag{7.2.12}$$

which can be used to calculate the fugacity capacity of the soil, sediment and plant compartments. For example, Eq. 7.2.12 can be applied to the soil compartment to yield an expression for the fugacity capacity of the soil matrix:

$$Z_{sm} = \frac{\theta_a^s}{RT_a} + \frac{\theta_s^s \chi_{oc}^s K_{oc}}{H} + \frac{\theta_w^s}{H} + \theta_r^s Z_{pr} \tag{7.2.13}$$

where θ_a^s , θ_s^s , θ_w^s θ_r^s are the volume fractions of the soil-air, soil-solids, soil-water and plant roots (in the soil), respectively, R is the ideal gas constant [e.g., J/mol/K], T_a^s is the temperature of the air in the soil [K], K_{oc} is the organic carbon partition coefficient [cm^3 of solution/g organic carbon], χ_{oc}^s is the mass fraction of the organic carbon in the soil solids, H is the Henry's Law Constant for water at the conditions of the soil [e.g., Pascal m^3/mol] and Z_r^s is the fugacity capacity of the roots in the soil [e.g., mol/m^3/Pascal].

Similarly, Eq. 7.2.12 can be used to write the fugacity capacity of the sediment matrix:

$$Z_{sed} = \frac{\theta_s^{sed} \chi_{oc}^{sed} K_{oc}}{H} + \frac{\theta_w^{sed}}{H} \qquad (7.2.14)$$

where θ_s^{sed} and θ_w^{sed} are the volume fractions of the sediment-solids and sediment-water, respectively, and χ_{oc}^{sed} is the mass fraction of the organic carbon in the sediment solids.

Finally, the fugacity capacity of the plant foliage and roots can be written as

$$Z_{pf} = \frac{\theta_a^{pf}}{RT_a} + \frac{\theta_w^{pf}}{H} + \frac{\theta_l^{pf} K_{ow}}{H} \qquad (7.2.15)$$

$$Z_{pr} = \frac{\theta_a^{pr}}{RT_a} + \frac{\theta_w^{pr}}{H} + \frac{\theta_l^{pr} K_{ow}}{H} \qquad (7.2.16)$$

where θ_a^{pf}, θ_l^{pf} ,θ_w^{pf} are the volume fractions of air, lipid and water phases in the plant foliage, respectively, and θ_a^{pf}, θ_l^{pr}, θ_w^{pr} are the volume fractions of air, lipid and water phases in the plant root compartment, respectively.

7.2.6 Gas/particle Partitioning

Air toxics can exist in the atmosphere in either a gaseous form and/or in an aerosol-bound form. Simple relationships to estimate the gas/aerosol particle partitioning of organic chemicals were proposed by various investigators (e.g., Junge, 1977; Yamasaki et al., 1982; Pankow, 1987, 1991). For example, the following expression for the equilibrium gas/particle partitioning coefficient can be derived based on the convention on the correlation of Junge (1977):

$$H_{gp} = \frac{P_{sat}}{b S^{(p)}} \qquad (7.2.17)$$

where H_{gp} is the dimensionless gas/particle partition coefficient, P_{sat} is the saturation pressure of the chemical at the ambient temperature [atm], $S^{(p)}$ is the total surface area of particles per unit volume of air [cm^2/cm^3] and b is a constant [$atm \cdot cm^3/cm^2$] that depends on the chemical molecular weight, the surface concentration associated with a monolayer coverage and the difference between the heats of desorption from the surface and the liquid phase. In the ITFP the default value for the Junge correlation constant b=0.1292 [mm Hg cm^3/cm^2] was selected as suggested by Pankow (1987).

The dependence of gas/particle partitioning on temperature was investigated in a later study by Yamasaki et al. (1982) who defined the following partition function:

$$K_Y \equiv \frac{G}{P/M^{(p)}} \qquad (7.2.18)$$

where K_Y is the Yamasaki sorption equilibrium constant [$\mu g/cm^3$], $M^{(p)}$ is the total mass of particulate matter per unit volume air [$\mu g/cm^3$], G is the chemical concentration in the vapor phase [mol/cm^3] and P is the chemical concentration in the particle phase [mol/cm^3]. Based on measurements in Osaka, Japan, over the course of a year, Yamasaki et al.(1982) defined the following partition function:

$$\log(K_Y) = \frac{m_y}{T} + b_y \qquad (7.2.19)$$

where T is the temperature [K] and b_y and m_y are the empirical parameters. Equation 7.2.19, as demonstrated by Pankow (1987), is the equivalent of a linear Langmuir adsorption isotherm.

In a subsequent study, Pankow (1991) correlated the inverse of the Yamasaki partition coefficient with temperature. Accordingly, the particle/gas partition coefficient was defined as

$$K_P \equiv \frac{P/M^{(p)}}{G} = K_Y^{-1} \qquad (7.2.20)$$

where K_p, the Pankow sorption equilibrium constant [$cm^3/\mu g$], was correlated with temperature by the following empirical equation:

$$\log K_P = m_p/T + b_p \qquad (7.2.21)$$

In the ITPP, values of m_p and b_p which are listed in Table 7.2 were obtained for the compounds studied by Pankow (1987, 1991), Bidleman and Foreman (1987) and Bidleman et al. (1986).

Table 7.2
Temperature Dependence of Gas/Particle Partitioning

Compound	m_p	b_p
Phenanthrene, Aanthracene	4117	-18.45
Me-phenanthrene, Me-anthracene	3365	-15.46
Fluoranthene	4421	-18.52
Pyrene	4183	-17.55
Benzo(a)fluorene, Benzo(b)fluorene	4554	-18.49
Chrysene, Benz(a)anthracene, Triphenylene	5826	-21.89
Benzo(b)fluoranthene, Benzo(k)fluoranthene	5693	-20.24
Benzo(a)pyrene, Benzo(e)pyrene	4864	-16.99
α-hexachlorocyclohexane	2755	-14.286
Hexachlorobenzene	3328	-16.117
Aroclor 1254	4686	-19.428
Chlordane	4995	-21.01
p,p'-DDE	5114	-21.048
p,p'-DDT	5870	-22.824

Adapted from Pankow (1987) and Bidleman and Foreman (1987).

Note that: $\zeta_p \equiv \frac{P/M^{(p}}{G}$ and $ogK_p = \frac{m_p}{T} + b$

where P is the concentration in the air bound to the particle phase [mol/cm^3], G is the concentration in the gas phase [mol/cm^3], $M^{(p)}$ is the mass concentration of particulate in air [µg/cm^3] and T is the temperature [K].

7.3 Environmental Diffusion Coefficients

The molecular diffusion mass flux due to concentration gradients is defined by Fick's Law as

$$J_A = -D_{AB}\, dC_A/dx \tag{7.3.1}$$

in which J_A is the diffusion flux of compound A [e.g., mg/m^2·s], C_A is the concentration of the chemical in the given medium (single phase or multiphase matrix), dC_A/dx is the concentration gradient along the x direction and D_{AB} is the molecular mass diffusion coefficient of component A in medium B [e.g., units of cm^2/s].

7.3.1 Molecular Mass Diffusion Coefficient in Air

The molecular mass diffusion coefficient in air can be estimated from the correlation of Fuller et al. (1966):

$$D_{BA} = \frac{10^{-3} T^{1.75} \sqrt{M_r}}{P\,(V_A^{1/3} + V_B^{1/3})^2}\ , \quad \mathrm{cm^2/s}\ , \quad \text{where } M_r = \frac{M_A + M_B}{M_A M_B} \tag{7.3.3}$$

in which the subscripts B and A denote the solute (e.g., air toxic) and air, respectively, T is temperature (K), M is molecular weight, P is the pressure [atm], and V_A and V_B are the molar volumes [cm^3/mol] for air and the solute in question (e.g., Air toxic), respectively.

For polyaromatic hydrocarbons, Gustafson and Dickhut (1994), proposed the following specific empirical correlation:

$$D_{BA} = 0.18 \times 10^{0.00283T} V_B^{-0.213} \quad ,\mathrm{cm^2/s} \tag{7.3.4}$$

where T is the temperature [°C] and V_B is the molar volume [cm^3/mol].

7.3.2 Molecular Diffusion Coefficient in Water

The molecular mass diffusion coefficient in water can be estimated using any of the following empirical methods.

Wilke and Chang (1955)

$$D_{BW} = \frac{7.4 \times 10^{-8}(\phi_W M_W)^{1/2} T}{\eta_W \; V_B^{0.6}} \quad , \quad cm^2/s \tag{7.3.5}$$

where M_W is molecular weight of water [g/mol], T is temperature [K], η_W is viscosity of water [cP], V_B is molar volume of solute B (e.g., air toxic) at its normal boiling temperature [cm^3/mol], and ϕ_W is the solvent association factor which equals 2.6 for water (Wilke and Chang, 1955).

Hayduk and Laudie (1974)

$$D_{BW} = \frac{13.26 \times 10^{-5}}{\eta_W^{1.14} \; V_B^{0.589}} \; , \quad cm^2/s \tag{7.3.6}$$

where η_W is viscosity of water [cP] (1 cP=1 poise=1g/cm.s) and V $_B$is the solute molar volume [cm^3/mol].

Hayduk et al. (1982)

$$D_{BW} = 1.25 \times 10^{-8}(V_B^{-0.19} - 0.292)T^{1.52}\eta_W^{\epsilon^*} \quad , \quad cm^2/s \tag{7.3.7}$$

where V_B is the solute molar volume [cm^3/mol], η_W is viscosity of water (cP), and $\epsilon^* = (9.58/V_B) - 1.12$.

For polyaromatic hydrocarbons (PAHs), the following empirical equation was proposed by Gustafson and Dickhut (1994):

$$D_{BW} = \frac{4.864 \times 10^{-3}}{\mu_w^{0.905} V_B^{1.32}} \quad ,cm^2/s \tag{7.3.8}$$

where μ_w is the water viscosity [cP] and V_B is the molar volume [cm^3/mol].

7.3.3 The Effective Chemical Diffusion Coefficient in the Soil Matrix

The diffusion flux of chemicals in the soil matrix can often be described in terms of the total chemical concentration in the soil matrix (i.e., where C_m is used in Eq. 7.2.10). When the soil phases are assumed to be in local equilibrium, and given the reasonable assumption of negligible diffusion along the soil solids, the effective chemical diffusivity in the soil matrix is given by (Jury et al., 1983; Ryan and Cohen, 1990)

$$D_m^s = \frac{\dfrac{\theta_a^s D_a}{\tau_a} + \dfrac{\theta_w^s D_w}{\tau_w H_{aw}^*}}{\theta_a^s + \dfrac{\theta_w^s}{H_{aw}^*} + \theta_s^s H_{sa}^*} \qquad (7.3.9)$$

where θ_a^s and θ_w^s are the volume fractions of the soil-air and soil-water, respectively, D_a and D_w are the chemical molecular mass diffusivities [e.g. cm^2/s] in the soil-air and soil-water, respectively, τ_a and τ_w are the tortuosities of the soil-air and soil-water phases, respectively, H_{aw}^* and H_{sa}^* are the dimensionless air/water and soil-solids/air partition coefficient in the soil matrix, respectively. Finally, the tortuosity parameters in Eq. 7.3.9 can be estimated using the following empirical correlations (Ryan and Cohen, 1990):

$$\tau_a = \frac{\left(\theta_a^s + \theta_w^s\right)^2}{\left(\theta_a^s\right)^{2.3}} \qquad (7.3.10)$$

$$\tau_w = \frac{\left(\theta_a^s + \theta_w^s\right)^2}{\left(\theta_w^s\right)^{2.3}} \qquad (7.3.11)$$

7.3.4 The Effective Diffusion Coefficient in the Sediment Matrix

The effective chemical diffusion coefficient for the sediment matrix, D_m^{sed}, is given by Eq. 7.3.9 and the tortuosity for the water phase is given by Eq. 7.3.11 where volume fraction of air is set to zero in both equation. Thus, the following expression is obtained for the effective chemical diffusion coefficient in the sediment:

$$D_m^{sed} = \frac{\left(\theta_w^{sed}\right)^{1.3} D_w}{\theta_w^{sed} + \theta_s^{sed} H_{sw}} \tag{7.3.12}$$

where H_{sw} is the dimensionless solids/water partition coefficient.

7.4 Interfacial Mass Transfer of Volatile Air Toxics

7.4.1 The Air/Water Mass Transfer Coefficients

The traditional approach to calculating the interfacial mass flux of a compound between air and water phases is to use the two-film theory in which it is assumed that the concentrations immediately on either side of the interface are in equilibrium as can be expressed by the dimensionless Henry's law constant (Lewis and Whitman, 1924). The mass flux, N [e.g., g/cm^2.s], can be expressed as

$$N = K_G (C_g - H_{aw}C_l) = K_L (C_l - C_g/H_{aw}) \tag{7.4.1}$$

where K_G and K_L are the overall mass transfer coefficients [cm/s] for the gas and liquid phase, respectively, H_{aw} is a dimensionless Henry's law constant, and C_g and C_l are the chemical concentrations in gas and liquid phases, respectively. The overall mass transfer coefficients for the gas and liquid phase can be defined as

$$1/K_G = 1/k_g + H_{aw}/k_l \tag{7.4.2}$$

$$1/K_L = 1/k_l + 1/H_{aw}k_g \tag{7.4.3}$$

where k_g and k_l are the gas-side and liquid-side mass transfer coefficients [cm/s], respectively. Predictive equations that can be used to estimate k_g and k_l are discussed in the sections 7.4.2 and 7.4.3.

7.4.2 Air/Water - Air Side - Mass Transfer Coefficient (k_g)

Numerous theories and empirical equations have been proposed to estimate k_g. The theoretical expressions for k_g as proposed by Brutsaert (1975) are particularly useful for estimating k_g. For a rough surface, k_g is given by

$$\frac{k_g}{U_{10}} = C_D^{1/2}\left[\epsilon_D^{+}\left(C_D^{-1/2} - 5\right) + 7.3\ Re_o^{0.25}\ Sc_a^{1/2}\right]^{-1},\quad Re_o > 2 \tag{7.4.4}$$

and for a smooth surface, k_g is given by

$$\frac{k_g}{U_{10}} = C_D^{1/2}\left[\epsilon_D^{+}\left(C_D^{-1/2} - 13.5\right) + 13.6\ Sc_a^{2/3}\right]^{-1},\quad Re_o < 0.13 \tag{7.4.5}$$

in which the Schmidt number, Sc_a, is given by the ratio ν_a/D_a, where D_a is molecular diffusivity in air (Section 7.2), U_{10} is the wind speed at a reference height (usually 10 meters), C_D is the wind drag (or stress) coefficient, ϵ_D^{+} is the ratio of the eddy momentum diffusivity (ϵ_m) to the eddy mass diffusivity (ϵ_D), often approximated to be near unity, and Re_o is the roughness Reynolds number. Although Eqs.7.4.4 and 7.4.5 are strictly applicable to a neutral atmospheric condition they are probably still satisfactory even under very unstable, but apparently not under stable conditions (Brutsaert, 1975). In the ITFP Eqs. 7.4.4 and 7.4.5 are used and thus the estimation of k_g should be considered suitable for a neutral condition and for screening-level analysis for non-neutral conditions. A more complex approach for non-neutral conditions is possible (Brutsaert, 1975) but is not considered in the current version of the ITFP. It should be noted that, within the context of screening-level analysis, as is the case for example in the CAPCOA (CAPCOA, 1992) and CalTox (DTSC, 1993) models, the application of Eqs. 7.4.4 and 7.4.5 is sufficient, especially for sparingly soluble hydrophobic organic compounds.

The use of Eqs. 7.4.4 and 7.4.5 requires the wind-drag coefficient, C_D, defined as (Wu, 1980)

$$C_D = \left(\frac{U_W^{*}}{U_{10}}\right)^2 \left(\frac{\rho_w}{\rho_a}\right) = \left(\frac{U_a^{*}}{U_{10}}\right)^2 \tag{7.4.6}$$

in which ρ_a and ρ_w are the air and water densities, respectively, U_W^{*} is the surface shear velocity given by

$$U_W^{*} = \sqrt{\frac{\tau_s}{\rho_w}} \tag{7.4.7}$$

where τ_a is the shear stress imparted by the wind on the water surface, and $U_{10}$is the wind speed measured at a reference height (usually 10m) above the water surface. It is noted that the water-side and air-side friction velocities U_w^* and U_a^* , respectively, are related through the simple relation $\rho_a(U_a^*)^2 = \rho_w(U_w^*)^2$ which arises from the condition of stress continuity at the air/water interface.

The roughness Reynolds number, Re_o, is defined by

$$Re_o = U_a^* z_o/\nu_a \tag{7.4.8}$$

where z_o is the effective surface roughness height and ν_a is the kinematic viscosity of air. The effective surface roughness height can be estimated using the following correlation(Wu, 1980):

$$z_o = 1.468\text{x}10^{-5}(U^*_a)^2/g \qquad , \text{cm} \tag{7.4.11}$$

where g=981, cm/s^2. The following alternate correlations were proposed by Brutsaert (1975)

for a smooth surface:

$$z_o \approx 0.135(\nu_a/U^*_a) \quad , \quad \text{cm} \tag{7.4.9}$$

and for a rough surface,

$$z_o = a(U^*_a)^b \quad , \quad \text{cm} \tag{7.4.10}$$

in which U^*_a is the air-side friction velocity [cm/s] and ν_a is the kinematic viscosity [cm/s$^{2]}$. The parameters a and b are given by $a = 1.69\times10^{-2}$ and $b = -1$ for $U^*_a \leq 6.89$ cm/s, and $a = 1.65\times10^{-4}$, b=1.4 for $U^*_a > 6.89$ cm/s (Jirka and Brutsaert, 1984).

For a large water fetch, the wind-stress coefficient near neutral conditions can be estimated from (Wu, 1980)

$$C_D = 8.5\times10^{-4} \quad , \qquad U_{10} < 5 \text{ m/s} \tag{7.4.12}$$

$$C_D = [0.85 + 0.11\ (U_{10} - 5)]\times10^{-3} \quad , \quad 5 \text{ m/s} \leq U_{10} \leq 20 \text{ m/s} \tag{7.4.13}$$

$$C_D = 2.5\times10^{-3} \quad , \qquad U_{10} > 20 \text{ m/s} \tag{7.4.14}$$

Another convenient correlation for k_g, determined based on laboratory measurements in a small wind-wave tank (fetch < 3m) under near neutral conditions, was proposed by Mackay and Yeun (1983):

$$\frac{k_g}{U_a^*} = 46.2 \times 10^{-3}\ Sc_a^{-0.67} \qquad (7.4.15)$$

Eq. 7.4.15 which was developed based on short fetch data yields k_g values which are about 20%-40% higher than predicted by Eqs. 7.4.4 and 7.4.5, possible due to differences in surface roughness in the short fetch wind-wave tank relative to long-fetch conditions.

7.4.3 Air/Water - Liquid Side - Mass Transfer Coefficient (k_l)

The water-side mass transfer coefficient, k_l, for large water bodies (i.e., reservoirs, lakes, oceans) can be estimated using the theoretical correlation of Cohen and Ryan (1985), which was found to be in excellent agreement with available data for a water-side friction velocity in the range of 0.5-6 cm/s,

$$k_l/U_w^* = a\ Sc_w^{-n} \qquad (7.4.16)$$

in which Sc_w is the Schmidt number given by the ratio ν_w/D_w where ν_w is the water kinematic viscosity and D_w is the chemical molecular mass diffusivity in water. The constants a and n are weak functions of the dimensionless water surface velocity U_s^+ ($U_s^+ = U_s/U_w^*$, in which U_s is the wind-induced surface water velocity), given by

$$a = a_0 - a_1 \ln U_s^+ \qquad (7.4.17)$$

$$n = n_0 - n_1 \ln U_s+ \qquad (7.4.18)$$

where

$$a_0 = 0.0969;\ a_1 = 0.0105 \qquad (7.4.19)$$

$$n_0 = 0.5778;\ n_1 = 0.0177 \qquad (7.4.20)$$

For a long fetch (say ≥ 30m), the surface velocity is equal to about 3.5% of the wind speed (i.e., $U_s = 0.035\ U_{10}$), while for short fetch (say less than about 10m), $U_s \approx 0.020\ U_{10}$ (Wu, 1975;

Plate and Friedrich, 1984). Eq. 7.4.19 was found to be in excellent agreement with laboratory data from wind-wave facilities with an average error of about 16 percent.

The prediction of k_l in flowing water bodies (e.g., rivers) requires consideration of the river current and the river depth (Cohen, 1986b). There are numerous studies on the reaeration coefficient in flowing streams (O'Connor, 1983; Lyman et al., 1990), and the water-side mass transfer coefficient k_l can be estimated from the reaeration coefficient, k_v [e.g., hr^{-1}], by using the following relationship:

$$k_l = \left(\frac{D}{D_o}\right)^{1/2} h\, k_v \qquad (7.4.21)$$

in which h is the depth of the water body [e.g., m], D is the mass diffusivity of the compound of interest (e.g., air toxic), D_o is the molecular mass diffusivity of oxygen at the temperature at which k_v is known and h is the river depth (Cohen, 1986b). Although various correlations have been proposed in the literature to estimate k_v, most require knowledge of the bed slope (Lyman et al., 1990). Thus, in the ITFP the following more convenient empirical correlation, which was recommended by Shen et al. (1993), is utilized

$$k_v = 0.2205\ (1.024)^{T-20}\ U_s^{0.67}\ h^{-1.85} \quad , \quad hr^{-1} \quad . \qquad (7.4.22)$$

in which T is the temperature [°C], U_s is the water current [m/s], and h is the water depth [m].

7.4.4 Dry Deposition of Gaseous Chemicals to Soil Surface

Air toxics that are present in the vapor phase in the atmosphere can transported to the soil surface by dry deposition. Following the approach adapted by Cohen et al. (1990; see also, ARB, 1994), the dry deposition velocity for gases is proportional to $D_a^{2/3}$ (where D_a is the chemical molecular diffusivity in air). Thus, if the dry deposition velocity for a given reference chemical is known, the deposition velocity for the chemical of interest can be estimated using the equation

$$V_{d_B} = V_{d_A} \left(\frac{D_B}{D_A}\right)^{2/3} \qquad (7.4.23)$$

where V_{d_B} is the dry deposition velocity of the chemical, V_{d_A} is the dry deposition velocity of a reference chemical for which a measured value of the deposition velocity is available, at the desired meteorological and surface conditions, D_B is a diffusion coefficient of the chemical of interest, and D_A is a diffusion coefficient of the reference chemical.

7.4.5 The Air/Leaf mass Transfer Coefficient

The uptake of gaseous air toxics by plants through the leaf can be estimated by the following compartmental chemical mass balance

$$V_L \frac{dC_L}{dt} = K_{LA} A_L (C_L - C_A H_{LA}) \tag{7.4.24}$$

$$V_L \frac{dC_L}{dt} = K_{AL} A_L (C_A - C_L H_{AL}) \tag{7.4.25}$$

where V_L is the volume of the leaf compartment [m^3], C_L is the concentration in the leaf compartment [mol/m^3], C_A is the chemical vapor phase concentration [mol/m^3], K_{LA} and K_{AL} are the overall leaf-side and overall air-side mass transfer coefficients [m/hr] for mass transfer across the air/leaf interface, and H_{LA} and H_{AL} are the dimensionless leaf/air and air/leaf partition coefficients (note: $H_{LA}=H_{AL}^{-1}$).

The mass transfer coefficients can be estimated based on the reported mass transfer data of Bacci et al. (1990) for the uptake of organics by azalea leaves. Paterson et al. (1991) analyzed the results of Bacci et al. (1990) using the following kinetic expression:

$$\frac{dC_L}{dt} = k_1 C_A - k_2 C_L \tag{7.4.26}$$

where k_1 is the uptake constant [hr^{-1}] and k_2 is the clearance rate constant [hr^{-1}]. By comparing Eqs. 7.4.24-7.4.26 it can be shown that the clearance constant k_2, which was experimentally measured by Bacci et al. (1990), is related to the overall mass transfer coefficients given as

$$K_{LA} = \frac{V_L}{A_L} k_2 \qquad (7.4.27)$$

$$K_{AL} = \frac{V_L}{A_L} H_{LA} k_2 \qquad (7.4.28)$$

where H_{LA} is the dimensionless leaf/air partition coefficient. In order to estimate the mass transfer coefficients from Equations 7.4.27 and 7.4.28, a value for the clearance rate, k_2, is required. Paterson et al. (1991) correlated k_2 with the octanol/air partition coefficient using an expression of the form:

$$k_2 = \frac{1}{\tau_L + \tau_A H_{OA}} \qquad (7.4.29)$$

where τ_L and τ_A are correlation constants related to the mass transfer coefficients and H_{OA} is the dimensionless octanol/air partition coefficient. The octanol/air partition coefficient can be evaluated from

$$H_{OA} = \frac{K_{OW}}{H_{AW}} \qquad (7.4.30)$$

where K_{OW} is the octanol/water partition coefficient and H_{AW} is the dimensionless air/water partition coefficient. In order to estimate the mass transfer coefficients , the ITFP utilizes the default values of 126 hr for τ_L and 5×10^{-6} hr for τ_A recommended by Paterson et al. (1991) and the volume to area ratio (V_L/A_L) is required as an input by the user.

7.4.6 Soil Volatilization Half-Life

The soil volatilization half-life is defined as the time for the mass of a chemical originally present in the soil to decrease to half of its initial value due to volatilization. The volatilization half-life depends on a number of different factors including the initial and boundary conditions on the soil column and the soil properties. In order to provide a ranking of the relative volatilization time scale for different chemicals, the ITFP utilizes a simple diffusion model in which volatilization is the only process of chemical removal from the soil matrix. In this model the soil column is assumed to be initially contaminated with a uniform concentration C_0 [e.g., mol/m^3] with an impermeable bottom boundary. At the soil/atmosphere interface, mass transfer resistance on the air-side is assumed to be negligible. According to the above scenario, the initial mass of the chemical placed in the soil and the total amount volatilized at time t are given by

$$M_0 = LAC_0 \tag{7.4.36}$$

$$M_v = \int_{t_0}^{t} N(t)Adt \tag{7.4.37}$$

where A is the surface area of the soil [e.g., m^2] and N(t) is the volatilization flux at the soil/air interface [e.g., mol/m^2/hr]. The mass of the chemical remaining in the soil (at any time t) is given by

$$M_t = M_o - M_v \tag{7.4.35}$$

where M_0 and M_t are the total initial and final amounts [e.g., mol], respectively, of the chemical in the soil at time t, and M_v is the mass [e.g., mol] of the chemical that has volatilized.

The volatilization half-life is defined as the time when $M_t/M_0 = ½$ which can be obtained from the following implicit equation

$$\frac{M_t}{M_0} = \frac{1}{2} = 1 - \frac{1}{LAC_0}\int_{t_0}^{t} N(t)Adt \tag{7.4.38}$$

where the volatilization flux N(t) is given by the following expression (Mayer et al., 1974):

$$N(t) = \frac{\overline{D}C_0}{\sqrt{\pi \overline{D}t}}\left[1 + 2\sum_{n=1}^{n=\infty}(-1)^n \exp\left(-(n)^2\frac{L^2}{\overline{D}t}\right)\right] \tag{7.4.39}$$

where $\overline{D}$ is the effective diffusivity in the soil matrix [e.g., m^2/hr] as defined in Eq. 7.3.9. The volatilization half-life is obtained by combining Eqs. 7.4.38 and 7.4.39 resulting in the following implicit equation for $t_{1/2}$,

$$\frac{1}{2} = \frac{\sqrt{\overline{D}}}{L\sqrt{\pi}} \int_{t_0}^{t_{1/2}} t^{-1/2}\left[1 + 2\sum_{n=1}^{n=\infty} (-1)^n \exp\left(-(n)^2 \frac{L^2}{\overline{D}t}\right)\right] dt \qquad (7.4.40)$$

Since the parameters n, $\overline{D}$, t and L are always positive, the series in Eq. 7.4.41 converges rapidly. Equation 7.4.41 is solved numerically in the ITFP yielding the volatilization half-life given user-input of selected chemical and soil properties.

7.5 Dry Deposition Velocity of Particle-Bound Chemicals

7.5.1 Overview

The flux of particle-bound pollutants from the atmosphere can be represented by the following equation:

$$N_d = V_d C_p^{(a)} \qquad (7.5.1)$$

where $C_a^{(p)}$ is the mass of the pollutant in the particle phase per unit volume of air [e.g. $\mu g/m^3$], and V_d is the overall particle deposition velocity [e.g., m/s]. The overall deposition velocity for the particle-bound chemical is defined by the following equation:

$$V_d = \int_0^{\infty} V_d(a)F(a)da \qquad (7.5.2)$$

where $V_d(a)$ is the deposition velocity for a particle of diameter a and F(a) is the normalized chemical distribution defined such that

$$\int_0^{\infty} F(a)da = 1 \qquad (7.5.3)$$

where F(a)da is the mass fraction of the chemical present in particle phase in the size range a to a+da. For semi-volatile organics it is usually assumed that the organics are adsorbed onto the surface of the atmospheric particles. For this case, the mass of the chemical-bound to atmospheric particles is linearly proportional to the surface area of the particles (Junge, 1977; Pankow, 1987) and thus F(a)da is given by

$$F(a)da = \frac{S^{(p)}(a)}{S_T^{(p)}} \tag{7.5.4}$$

where $S^{(p)}(a)$ is the surface area of particles of diameter a per unit volume of air [e.g., cm^2/cm^3] and $S_T^{(p)}$ is the total surface area of the particle phase per unit volume [e.g., cm^2/cm^3]. Alternatively, F(a)da may be taken to be proportional to the mass of atmospheric particles (Pankow, 1987). For this case the expression for F(a)da is given by

$$F(a)da = \frac{M^{(p)}(a)}{M_T^{(p)}} \tag{7.5.5}$$

where $M^{(p)}(a)$ is the mass of particles with diameter a per unit volume of air [e.g., g/cm^3] and $M_T^{(p)}$ is the total mass of the particle phase per unit volume [e.g., g/cm^3]. The particle size distribution function can be used to estimate $S^{(p)}(a)$, $S_T^{(p)}$, $M^{(p)}(a)$ and $M_T^{(p)}$ (Appendix D).

In the ITPP, three models are available for calculating the dry deposition velocity to various surfaces. Dry deposition velocity from the atmosphere to a vegetative canopy is estimated using the model of Slinn (1982). The dry deposition velocity to a water surface is estimated using the model of Williams (1982). Dry deposition to a surface which can be characterized by a known roughness height is estimated by the model of Sehmel and Hodgson (1980). A brief description of the algorithms is given in the following sections.

7.5.2 Dry Deposition to Vegetative Canopies: The Slinn Model

The model of Slinn (1982) can be used to calculate the dry deposition velocity of particles to a vegetative canopy in the ITFP. In the Slinn model, the vegetative canopy is modeled as a collection of cylinders with a specified collection efficiency. The overall mass transfer resistance can then be written as the sum of the canopy resistance and the resistance of the canopy:

$$r_o = r_a + r_c \tag{7.5.6}$$

where r_o is the overall mass transfer resistance [e.g., hr/m], r_a is the mass transfer resistance above the canopy [e.g., hr/m] and r_c is the mass transfer resistance within the canopy [e.g., hr/m]. The dry deposition velocity can then be written in terms of the mass transfer resistance:

$$V_d^V(a) = \frac{1}{r_o} + V_g(a) \tag{7.5.7}$$

where $V_d(a)$ is the dry deposition velocity of particles of diameter a [e.g., m/hr] and $V_g(a)$ is the gravitational settling velocity of particles with diameter a [m/hr].

The gravitational settling velocity can be estimated using Stokes Law:

$$V_g(a) = \frac{g a^2 \rho_p}{18 \mu_a} \tag{7.5.8}$$

where g is the gravitational constant [m/sec^2], a is the diameter [m], ρ_p is the particle density [kg/m^3] and μ_a is the air viscosity [kg/m/sec].

The mass transfer resistance above the canopy, r_a, is given as

$$r_a = \frac{u_r - u_h}{u_v^{*2}} \tag{7.5.9}$$

where u_r is the mean wind speed at the reference height of 10 meters [m/hr], u_h is the mean wind speed at the height of the canopy [m/hr] and u_v^* is the friction velocity in the vegetative canopy [m/hr].

The mass transfer resistance of the canopy is given by

$$r_c = \frac{u_h}{u_v^{*2}} \frac{1}{\sqrt{\xi_c}} \left[\frac{1 + \sqrt{\xi_c} \tanh\left(\gamma_v \sqrt{\xi_c}\right)}{\sqrt{\xi_c} + \tanh\left(\gamma_v \sqrt{\xi_c}\right)} \right] \tag{7.5.10}$$

in which ξ_c is the dimensionless collection efficiency of the vegetative canopy and the parameter γ_v is defined by:

$$\gamma_v = h_c \left[\frac{c_d \alpha u_0}{K_0} \right]^{1/2} \tag{7.5.11}$$

where C_d is the dimensionless drag coefficient in the canopy, α is the collection area per unit volume of the canopy [1/m], u_o is the characteristic wind speed in the canopy [m/hr], h_c is the height of the canopy [m] and K_o is the average turbulent diffusivity in the canopy [m^2/hr].

The collection efficiency of the canopy can be estimated by

$$\begin{aligned} \xi_c &= \bar{E} R_R \\ \bar{E} &= \bar{E}_{IN} + \bar{E}_{IM} + \bar{E}_B \end{aligned} \tag{7.5.12}$$

where R_R is the fractional reduction in collection caused by rebound, $\bar{E}_{IM}$ is the efficiency of the impaction process, $\bar{E}_{IN}$ is the efficiency of the interception process and $\bar{E}_B$ is the efficiency of the Brownian diffusion collection process. Specific details regarding the calculation of the mass transfer resistances, the collection efficiencies, the turbulent diffusivity and the overall deposition velocity can be found elsewhere (Slinn, 1982; Clay, 1992; Van de Water, 1995).

7.5.3 Dry Deposition to Water Surfaces: The Williams Model

The dry deposition velocities of particles to water surfaces is estimated in the ITPP using the model proposed by Williams (1982). In the Williams model, particle deposition is considered for two types of water surfaces, broken and smooth. For each type of surface, the atmosphere is divided into two layers, a turbulent layer and a deposition layer. The resulting equation for the overall deposition velocity for particles of diameter a is (Williams, 1982):

$$\begin{gathered} v_d^w(a) = (1 - \Phi)k_{as}^w(a)\left(1 - \frac{\delta(a)}{\gamma(a)}\right) + \\ \Phi k_{ab}^w(a)\left(1 - \frac{\beta(a)}{\alpha(a)}\right) + v_{gd}(a) \end{gathered} \tag{7.5.13}$$

where Φ is the fraction of the water surface that is broken, k_{as}^w is the mass transfer coefficient in the turbulent layer for smooth surfaces [m/hr], k_{ab}^w is the mass transfer coefficient in the turbulent layer for broken surfaces [m/hr] and V_{gd} is the gravitational settling velocity for dry particles [m/hr].

The parameters δ, γ, β and α are given by:

$$\begin{gathered} \alpha(a) = \Phi k_{bs}^w(a) + \Phi k_{ab}^w(a) + \Phi v_{gw}(a) + \\ (1 - \Phi)\left(k_{as}^w(a) + k_{ss}^w(a) + v_{gw}(a)\right) + \frac{\Phi(1 - \Phi)}{k_m^w(a)} \cdot \\ \left(k_{as}^w(a) + k_{ss}^w(a) + v_{gw}(a)\right)\left(v_{gw}(a) + k_{bs}^w(a) + k_{ab}^w(a)\right) \end{gathered} \tag{7.5.14}$$

$$\begin{gathered} \beta(a) = \Phi k_{ab}^w(a) + v_{gd}(a) + \\ (1 - \Phi)\left(k_{as}^w(a) - v_{gd}(a)\right) + \\ \frac{\Phi(1 - \Phi)}{k_m^w(a)}\left(k_{as}^w(a) + k_{ss}^w(a) + v_{gw}(a)\right)\left(k_{ab}^w(a) + v_{gd}(a)\right) \end{gathered} \tag{7.5.15}$$

$$\gamma(a) = (1 - \Phi)\left(k_{ss}^w(a) + v_{gw}(a) + k_{as}^w(a)\right) \tag{7.5.16}$$

$$\begin{gathered} \delta(a) = (1 - \Phi)k_{as}^w(a) + \\ \Phi\left(k_{ab}^w(a) - \frac{\beta}{\alpha}\left(k_{ab}^w(a) + k_{bs}^w(a) + v_{gw}(a)\right)\right) + v_{gd}(a) \end{gathered} \tag{7.5.17}$$

where Φ is the fraction of the water surface that is broken, k_{as}^{w}, k_{ab}^{w}, k_{ss}^{w}, and k_{m}^{w} are the mass transfer coefficients [m/hr] in the turbulent layer for smooth surfaces, in the turbulent layer for broken surfaces, in the deposition layer for smooth surfaces and in the deposition layer for broken surfaces, respectively, and [m/hr], k_{bs}^{w} is the mass transfer coefficient [m/hr] in the lateral mass transfer coefficient in the turbulent layer and V_{gd} and V_{gw} are the deposition velocities [m/hr] for dry and wet particles, respectively. The above parameters can be estimated as described below.

The fraction of the water surface that is broken, Φ, is given by (Wu, 1979)

$$\Phi = 1.7\times10^{-6}\,U_{10}^{3.75} \tag{7.5.18}$$

where U_{10} is the wind velocity measured at 10m [m/s].

The gravitational settling velocities, V_{gd} and V_{gw}, are given by Stokes law:

$$v_{gi} = \frac{g\cdot a_i^2 \rho_{p,i}}{18\,\mu_a} \tag{7.5.19}$$

where the subscript I represents either the dry particle (I=d) or the wet particle (I=w), g is the gravitational constant [m/s^2], a_i is the particle diameter [m], μ_a is the viscosity of the air [kg/m/s] and $\rho_{p,i}$ is the density of the particles [kg/m^3]. The particle diameter of particles in the deposition layer can increase due to condensation of water as estimated below (Fitzgerald,1975):

$$\begin{aligned} a_w &= a && \text{for relative humidity} = 0\% \\ a_w &= 4.5\,a^{1.04} && \text{for relative humidity} = 99\% \\ a_w &= 23\,a^{1.5} && \text{for relative humidity} = 100\% \end{aligned} \tag{7.5.20}$$

where a and a_w are the diameters [m] of the the dry and wet particles, respectively.

The expression for k_{ss}^{w} is given by (Slinn and Slinn 1980)

$$k_{ss}^{w} = \left(\frac{u_{af}^{2}}{\kappa U_{10}}\right)\left[10^{-(3/St_p)} + Sc_p^{-1/2}\right] \tag{7.5.21}$$

where κ is the von Karman constant (κ=0.4), u_{af} is the air-side friction velocity [m/hr], St_p is the Stokes number defined by

$$St_p = \frac{u_{af}^2 V_{gw}}{g \upsilon_a} \qquad (7.5.22a)$$

where V_{gw} is the gravitational settling velocity of wet particles, g is the gravitational constant [m/s^2] and υ_a is the kinematic viscosity of air [m^2/s] and Sc_p is the particle Schmidt number given by:

$$Sc_p = \frac{\upsilon_a}{D^p(a)} \qquad (7.5.22b)$$

where $D^p(a)$ is the diffusivity of the particle [m^2/s]. Little information is available concerning k_{bs}^w, the mass transfer coefficient to a broken surface in the deposition layer. Thus, following Williams (1982), k_{bs}^w and k_{as}^w are assumed to be equal.

The mass transfer coefficients in the turbulent layer, k_{as}^w, k_{ab}^w and k_m^w [m/hr], are given by (Hess and Hicks, 1975)

$$k_{as}^w = k_{ab}^w = k_m^w = \frac{\kappa u_{af}}{\ln\left(\frac{z_0^w}{z_u}\right)} - \Psi_h\left(\frac{z}{L}\right) \qquad (7.5.23)$$

in which u_{af} is the air-side friction velocity [m/hr], z_0^w is the roughness length of the water surface [m], κ is the von Karman constant, $\Psi_H(z/L)$ is the stability dependent correction parameter for particles [dimensionless] and z_u is defined as

$$z_u = \frac{D_c'}{\kappa u_a^*} \qquad (7.5.24)$$

where $D_c^{\prime}$ is the effective diffusivity of the particles [m^2/hr]. Finally, the evaluation of the stability parameter, the friction velocity, the effective diffusivity and the roughness length of the water surface is discussed elsewhere (Williams, 1982).

7.5.4 Dry Deposition to Soil Surfaces: The Sehmel and Hodgson Model

In the ITFP the model of Sehmel and Hodgson (1980) is used to calculate the dry deposition velocity of particles to soil surfaces where the user has information on the surface roughness. In this model the deposition velocity is expressed as

$$V_d(a) = \frac{V_{gd}}{1 - 1/\alpha} \tag{7.5.25}$$

where V_{gd} is the gravitational settling velocity [m/sec] given by Stoke's equation:

$$V_{gd} = \frac{g \cdot a^2 \rho_p}{18\, \mu_a} \tag{7.5.26}$$

where g is the gravitational constant [m/s^2], a is the particle diameter [m], μ_a is the air phase viscosity [kg/m/s] and ρ_p is the density of the particles [kg/m^3].

The dimensionless mass transfer resistance, α, is given by

$$\alpha = \exp\left(-v_{gd} \frac{\beta}{u_*} \right) \tag{7.5.27}$$

where u^* is the friction velocity [m/sec] and β is the mass transfer resistance given by

$$\beta = \int_{z_r^+}^{z_s^+} \frac{dz^+}{\frac{1}{\nu}\left(\epsilon + \overline{D}\right)} + \gamma \tag{7.5.28}$$

where z^+ is the dimensionless height defined as

$$z^+ = z\frac{u^*}{\nu} \tag{7.5.29}$$

z_r^+ is the reference height at which the concentration is known (C_{ref}) and z_s^+ is the height of the deposition surface. The air kinematic viscosity [m^2/sec] is denoted by ν, γ is the integrated resistance of the deposition surface, $\overline{D}$ is the Brownian diffusivity [m^2/sec] and ϵ is the particle eddy diffusivity [m^2/sec] assumed to be equal to the eddy difusivity of momentum and thus given by

$$\epsilon = \kappa u^*\left(z + z_0\right) \tag{7.5.30}$$

where it is assumed that is assumed to be equal to the eddy diffusivity of momentum which is where κ is the von Karman constant (κ=0.4). The Brownian diffusivity is given by

$$\overline{D} = \frac{K_bT}{6\pi\mu a}\left(1 + \frac{10^{-4}}{pa}(6.32 + 2.01\exp(-2190pa))\right) \tag{7.5.31}$$

where K_b is the Boltzmann constant, p is the pressure [cm of Hg] and a is the particle radius.

For a variety of different surfaces Sehmel and Hodgson proposed the following correlation for the surface resistance integral, γ,

$$\begin{gathered}\gamma = -\exp(-378.051 + 16.498\ln(Sc) + \\ \ln\tau^+\left[-11.8178 - .28628\ln\tau^+ + .32262\ln\left(\frac{d}{z_0}\right) - \right. \\ \left. .33850\ln\left(\frac{\overline{D}}{z_0u^*}\right)\right)\right] - 12.8044\ln d\end{gathered} \tag{7.5.32}$$

where d is the particle diameter [cm], u^* is the friction velocity [cm/sec], Sc is the Schmidt number ($\nu/\overline{D}$), z_0 is the aerodynamic surface roughness [cm] and τ^+ is the dimensionless relaxation time defined as

$$\tau^{+} = \frac{\rho_p d^2}{18\mu}\frac{(u^{*})^2}{\nu}\times 10^{-8} \tag{7.5.33}$$

Finally, the expression for the lower limit of the surface resistance integral, γ,

$$\gamma = \frac{\nu}{\overline{D}}\left(\frac{d}{2}\frac{u^{*}}{\nu}-\frac{u^{*}}{\nu}\right) \tag{7.5.34}$$

is used if the value of γ, as calculated by Eq. 7.5.32, is below the value given by Eq. 7.5.34.

7.6 Rain Scavenging

7.6.1 Overview

The depletion of air toxics from the atmosphere during rainfall, due to rain scavenging (in the absence of all other intermedia processes), is often represented by a simple mass balance as given below (Tsai et al., 1991),

$$(1-\theta_r)V_a\frac{dC_a}{dt} = C_a^{(g)}H_{wa}\hat{R}A_{sf}\Lambda_g + C_a^{(p)}\hat{R}A_{sf}\Lambda_p \tag{7.6.1}$$

where the left hand side represents the rate of change of the chemical mass from the atmosphere due to rain scavenging [mol/hr], θ_r is the volume fraction of the rain water in the atmosphere, V_a is the volume of the atmospheric compartment [m^3], C_a is the overall chemical concentration in the atmospheric compartment [mol/m^3], $C_a^{(g)}$ is the chemical concentration in the gas-phase [mol/m^3], $C_a^{(p)}$ is the concentration the chemical associated with the particle phase [mol/m^3], H_{wa} is the dimensionless chemical water/air partition coefficient, $\hat{R}$ is the rate of rainfall [m/hr], A_{sf} is the terrestrial surface area of the modeled region [m^2], Λ_g is the dimensionless rain scavenging coefficient for the chemical in the gas phase and Λ_g is the dimensionless rain scavenging coefficient for particle-bound contaminant. The particle size distribution can change significantly; thus, the rain scavenging coefficient for particle-bound chemicals, Λ_p will vary during a given rain event (Tsai et al., 1991). Therefore, in the current version of the ITFP the initial upper limit value of Λ_p is estimated. The temporal variation in Λ_p can be obtained using the detailed model of Tsai et al. (1991); however, such a detailed approach is beyond the needs of a screening-level analysis. The scavenging coefficients are estimated in the ITFP using the algorithms described in sections 7.6.2 and 7.6.3.

7.6.2 Rain Scavenging Coefficient for Particle-Bound Phase

The removal of particle-bound pollutants by rain scavenging can be determined from a chemical mass balance on raindrops as they travel to the ground. The change in the chemical concentration in a single raindrop as it travels from the cloud base is determined from the following chemical mass balance (Tsai et al., 1991)

$$\frac{d\left(C_w^{(p)}\ \pi D_d^3/6\right)}{d\tau} = \int_0^\infty E(a, D_d) \left(\frac{\pi D_d^2 L_c}{4L_c/V_t}\right) C_a^{(p)} F(a)da \qquad (7.6.2)$$

where $C^{(p)}_w$ and $C^{(p)}_a$ are the chemical concentration in the particle-bound form in rain water [e.g., ng/m^3 of water] and in the air phase [ng/m^3 of air], respectively, $E(a,D_d)$ is the collection efficiency of a particle of diameter a by a raindrop of diameter D_d, $F(a)$ is the mass fraction distribution of the chemical in the particle phase defined such that $F(a)da$ is the mass fraction of the chemical within the size fraction a to a+da, τ is the travel time of a raindrop from the cloud base [e.g., s], L_c is the height of the cloud base above ground level [e.g., m] and V_t is the raindrop terminal velocity (m/s) estimated from Easter and Hales (1984)

$$V_t(D_d) = 40.55D_d \qquad ;D_D \leq 0.001m \qquad (7.6.3)$$

$$V_t(D_d) = 130D_d^{1/2} \qquad ;D_d > 0.001m \qquad (7.6.4)$$

where D_d is the diameter of a raindrop [m].

The collection efficiency can be approximated by the empirical correlation of Ryan and Cohen (1986) which was validated using field rain scavenging data for PAHs (Tsai et al., 1991). The collection efficiency is given by the following equation:

$$E(a) = \left[\frac{S - \frac{1}{12}}{S + \frac{7}{12}} \right]^{1.5} \quad , \quad a > 1.35\ \mu m \tag{7.6.5}$$

$$E(a) = 0.0005 \quad , \quad 0.09\ \mu m \le a \le 1.35\ \mu m \tag{7.6.6}$$

$$E(a) = 0.125/(0.5 + a)^2 \quad , \quad a < 0.9\ \mu m \tag{7.6.7}$$

where $S = 0.1038a^2$ and a is the particle diameter [cm].

Given experimental data for F(a), the average chemical concentration in the particle-bound form can be obtained by integrating Eq. 7.6.2 over the spectra of raindrop sizes and particle sizes, between $\tau = 0$ (i.e., cloud base) and $\tau = L_c/V_t$ (i.e., the time to reach ground level). Accordingly, the following expression for the chemical concentration in rainwater, at ground level, $\overline{Cw_f}$, is obtained

$$\overline{Cw_f} = \overline{Cw_o} + \frac{C_a}{V_r} \int_0^{\infty} \frac{3}{2} \frac{L_c}{D_d} \left[\int_0^{\infty} E(a)F(a)d(a) \right] \frac{\pi D_d^3}{6} N_{D_d} dD_d \tag{7.6.8}$$

in which C_a is the atmospheric mass concentration of the chemical in the particle-bound phase [e.g., ng/m^3], $\overline{Cw_o}$ is the average initial concentration at the cloud base, V_r is the volume of rain per volume of air given by

$$V_r = \int_0^{\infty} \frac{\pi D_d^3}{6} N_{D_d} dD_d \tag{7.6.9}$$

where N_D is the raindrop size distribution expressed such that $N_D dD$ is the number of raindrops per unit volume of air, between diameters D_d and $D_d + dD_d$. The raindrop size distribution, N_{D_d}, can be approximated by the Marshall-Palmer (1948) distribution.

$$N_{D_d} = N_o\, e^{-cD_d} \tag{7.6.10}$$

in which $N_o = 0.08$ cm^{-4} and $C = 41R_{Rain}^{-0.21}$ where the rate of rainfall, R_{Rain}, is expressed in units of cm/hr.

In the absence of field data for F(a), an appropriate correlation for F(a), as described in section 7.2.6, along with the particle size distribution can be utilized using the rain scavenging model of Tsai et al. (1991). In this approach it is assumed that the chemical distribution in the particle phase (due to adsorption) is weighted with respect to the particle surface area. Accordingly, the rain scavenging coefficient:

$$\Lambda_p = \frac{\overline{C_w^{(p)}}}{C_a^{(p)}} \tag{7.6.11}$$

can be obtained by considering the washout ratio at the beginning of the rain event. In the ITFP the user can specify the chemical distribution within the particle phase using discrete particle size fractions. However, for chemicals that partition to the particle phase by adsorption (e.g., semi-volatile organics) an a priori predictive approach can be used since the mass of the chemical in the different particle size fractions is proportional to the particle surface area. For this latter case, the analysis of Tsai et al. (1991) leads to the following expression for Λ_p,

$$\Lambda_p = \frac{\int_0^\infty \left\{ C_{wo}^{(p)} + \frac{3}{2}\,\frac{C_s^{(p)} L_c}{2D_d} \int_0^\infty E(a,D_d)\,\frac{\pi D_d^2}{4}\,n(a)da \right\} \frac{\pi D_d^3}{6}\,N_{D_d} dD_d}{C_a^{(p)}\,V_r} \tag{7.6.12}$$

where Eq. 7.6.12 provides an estimate of the initial upper limit value of Λ_p. The particle size distribution is denoted by n(a) and $C_s^{(p)}$ is the concentration of the surface-bound chemical expressed on a surface-area basis (e.g., ng chemical /m^2 of particle; i.e., $C_s^{(p)} = C_a^{(p)}/S_t$ where S_t is the surface area of particles per unit volume of air).

7.6.3 Rain Scavenging Coefficient for Gas Phase Contaminant

Air toxics which are in the gas phase can be removed from the atmosphere by rain scavenging. The concentration of the scavenged chemical in rain water at ground level, relative to the maximum attainable concentration, due to simple physical partitioning, is denoted by the gaseous rain scavenging coefficient defined as (Tsai et al., 1991):

$$\Lambda_g = \frac{C_{ws}^{(g)}}{H_{wa} C_a^{(g)}} \tag{7.6.13}$$

where $C_{ws}^{(g)}$ and $C_a^{(g)}$ are the chemical concentrations [e.g., mol/m^3] in the rain drop (at ground level) and in the gas phase, respectively, and H_{wa} is the dimensionless water/air partition factor.

The chemical concentration in rain at the ground surface can be obtained from a chemical mass balance on a single raindrop (Tsai et al.,1991):

$$\frac{\pi D_d^3}{6} \frac{dC_w^{(g)}}{dt} = \pi D_d^2 K_{owa} \left(C_a^{(g)} H_{wa} - C_w^{(g)} \right) + \frac{k_{wd} \pi D_d^3 C_w^{(g)} \zeta}{6} \tag{7.6.14}$$

where the left hand side represents the accumulation of contaminant in a raindrop with diameter D_d [e.g., m], $C_w^{(g)}$ is the chemical concentration of the contaminant in the raindrop [e.g., mol/m^3], H_{wa} is the dimensionless water/air partition coefficient, K_{owa} is the overall mass transfer coefficient [m/hr] from the atmosphere to the raindrop, k_{wd} is the first order reaction rate of the chemical in the raindrop [e.g., 1/hr] and ζ the stoichiometric coefficient which equals +1 for a production reaction and -1 for a degradation reaction.

The chemical concentration in the drop at ground level is obtained by integrating Eq. 7.6.14 from tine t=0 to t=τ_h (i.e., the time it takes a raindrop to travel from the height of the cloud to the ground surface) resulting in the following expression (Clay, 1992; Tsai et al., 1991):

$$C_{ws}^{(g)} = \frac{K_{owa} H_{wa} C_a^{(g)}}{K_{owa} + \zeta k_{wd} D_d/6} - \left(\frac{K_{owa} H_{wa} C_a^{(g)}}{K_{owa} + \zeta k_{wd} D_d/6} - C_{w0}^{(g)} \right) \cdot \exp\left(\frac{\tau_h \cdot \left(6K_{owa} + \zeta k_{wd} D_d \right)}{D_d} \right) = \Gamma(D_d) \tag{7.6.15}$$

where $C_{w0}^{(g)}$ is the initial chemical concentration in the raindrop [e.g., mol/m^3] and τ_h is the time of travel to ground level determined from $\tau_h = h_A/V_t$ where h_A is the height of the cloud base [e.g., m] and V_t is the terminal velocity of the raindrop [e.g., m/hr] (Clay, 1992). Equation 7.6.15 must be integrated over the spectrum of raindrop sizes to obtain the overall chemical concentration in rain at the ground surface. Accordingly, the following expression is obtained for the rain scavenging coefficient:

$$\Lambda_g = \frac{1}{C_a^{(g)} H_{wa}} \left[\frac{\int_0^\infty \Gamma(D_d)(\pi D_d^3/6) N_{D_d} dD_d}{V_r} \right] \tag{7.6.16}$$

in which $\Gamma(D_d)$ designates the RHS of Eq. 7.6.15, N_{D_d} is the raindrop size distribution function defined such that $N_{D_d} dD_d$ is the number of raindrops with diameter in the size range D_d to $D_d + dD_d$ and V_r is the rain volume defined by Eq. 7.6.9.

8. ITFP SOFTWARE: STRUCTURE AND USER GUIDE

8.1 Overview

The intermedia transfer factor predictor (ITFP) was programmed in Microsoft Visual Basic Version 3.0 using custom controls for convenience and flexibility. For example, the CSTEXT custom control from Crescent Software was used for all the "input fields". The ELASTIC and INDEXTAB controls from VideoSoft were used for "panels" and "tabs" respectively. The SSHDATA control from Sheridan Software Systems was used to control access to the CHEMBASE database. Finally, PC-Install™ from 20/20 Software was used to create the installation routine.

The most basic element in the ITFP is the "label". Labels are used to display database values, describe input fields and designate units. Labels cannot accept input, though clicking on labels containing reference numbers in CHEMBASE will bring up the "References" window. Labels are typically white or transparent and their color cannot be changed.

Another common element in the ITFP is the "input field". Input fields allow the user to enter numbers required by the program to perform its calculations. Input fields are associated with labels that describe the input field and designate the appropriate units. Most of the input fields in the ITFP will not allow non-numeric input, though the characters "E", "e", "+" and "-" can be entered for input fields that allow scientific notation. Various input fields have minimum and maximum limits selected to represent reasonable physical constraints. If the entered number is not in the appropriate range, a message will appear displaying the appropriate range and returning the user to the appropriate field. The color of input fields can be changed by selecting the "Input Fields" option from the "Color" menu.

"Command buttons" allow the user to go from window to window, from panel to panel and to execute various commands. These buttons are grey with blue text and a three dimensional appearance. Command buttons do not accept input, though labels containing previously estimated values are associated with many command buttons in the ITPP main window. Various windows in the ITFP have descriptive labels at the bottom of the screen that will change depending on which command button the cursor happens to be over.

Input fields, labels and command buttons are placed on "tabs" and "panels". Tabs allow the user to select from a variety of options by clicking on the tab labels located at the top of each tab. Panels allow sequential access to input fields and command buttons and have more active space then tabs. The currently displayed panel can only be changed by clicking on the appropriate command button. The color of grey panels cannot be changed, though the color of other panels and tabs can be changed by selecting "Primary" or "Secondary" option from the "Color" menu.

Tabs and panels are combined to form the windows of the ITFP. These windows are arranged in the hierarchical structure shown in Figure 8.1. The introductory window (Figure 8.2) allows the user to access any of the three main windows: the CHEMBASE window, the selection window for the Chemical Property Predictor (CPP) or the main window for the Intermedia Transfer Parameter Predictor (ITPP). A brief description of the windows of the ITFP is given below.

8.2 CHEMBASE Software: Overall Structure and User Guide

The main window of CHEMBASE is shown in Figure 8.3 The parameters in the database are divided into the following categories:

1. Physical/Critical
2. Solubility/Vapor Pressure
3. Density
4. Partition Coefficients
5. Media
6. Aquatic BCFs
7. Plant BCFs
8. Terrestrial BCFs
9. Reactions Rate Constants
10. Comments

Information available for the selected compound appears in labels next to the appropriate units. By clicking on the "Browse" arrows at the bottom right hand corner of the screen, it is possible to scroll through the database one chemical at a time or proceed immediately to the first or last chemical in the list. Alternatively, the "Find" button on the left hand side of the screen allows the user to search through the database by chemical name or CAS registration number. Chemicals in the database are listed in alphabetical order with numbers listed before letters. (e.g., 1,1,1 trichloroethane is listed before benzene)

In addition to accessing the database, the main CHEMBASE window also has a number of useful features. If values for the Antoine Equation are available, for example, the user can automatically calculate the vapor pressure for any input temperature for which the Antoine equation

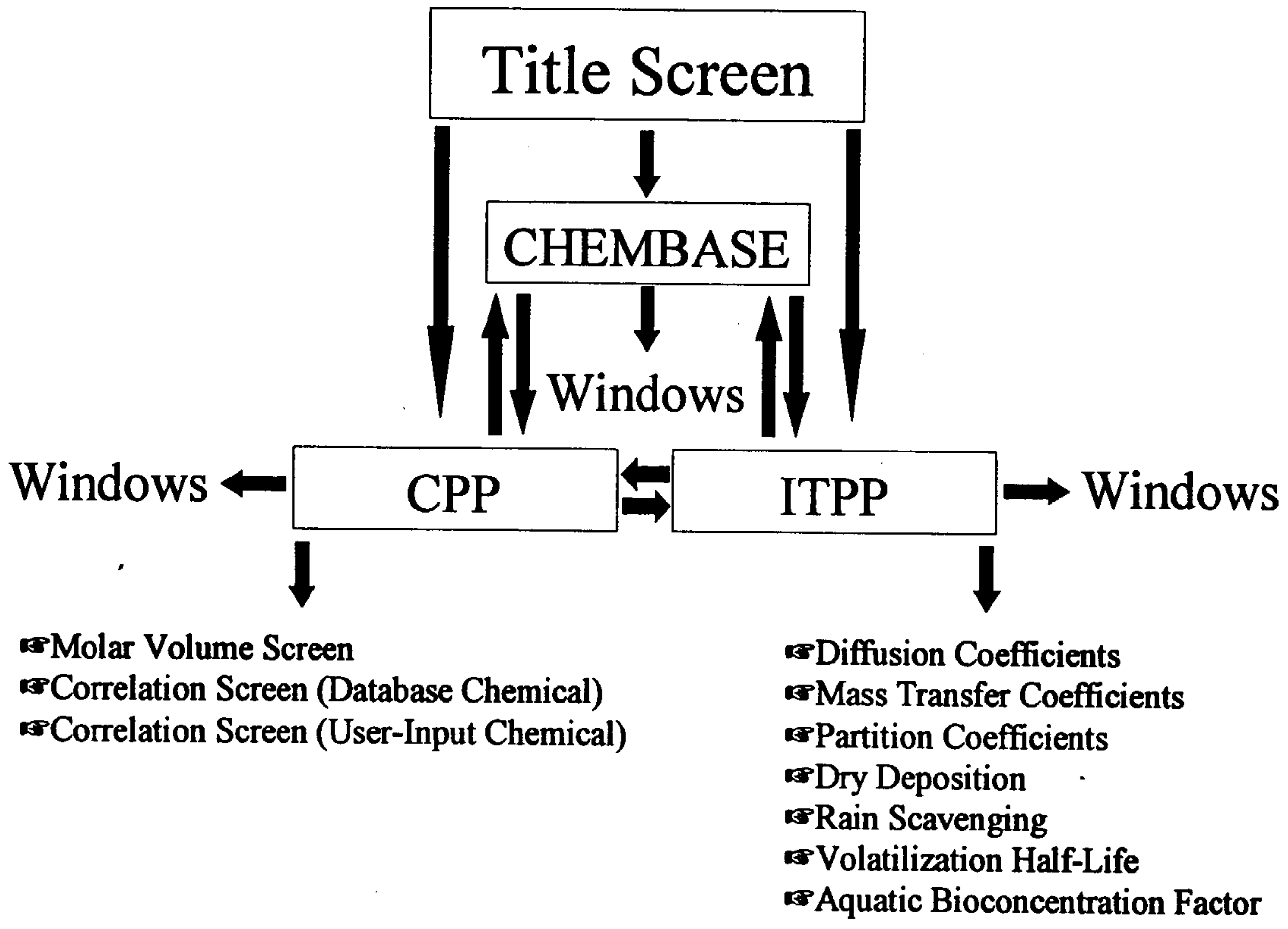
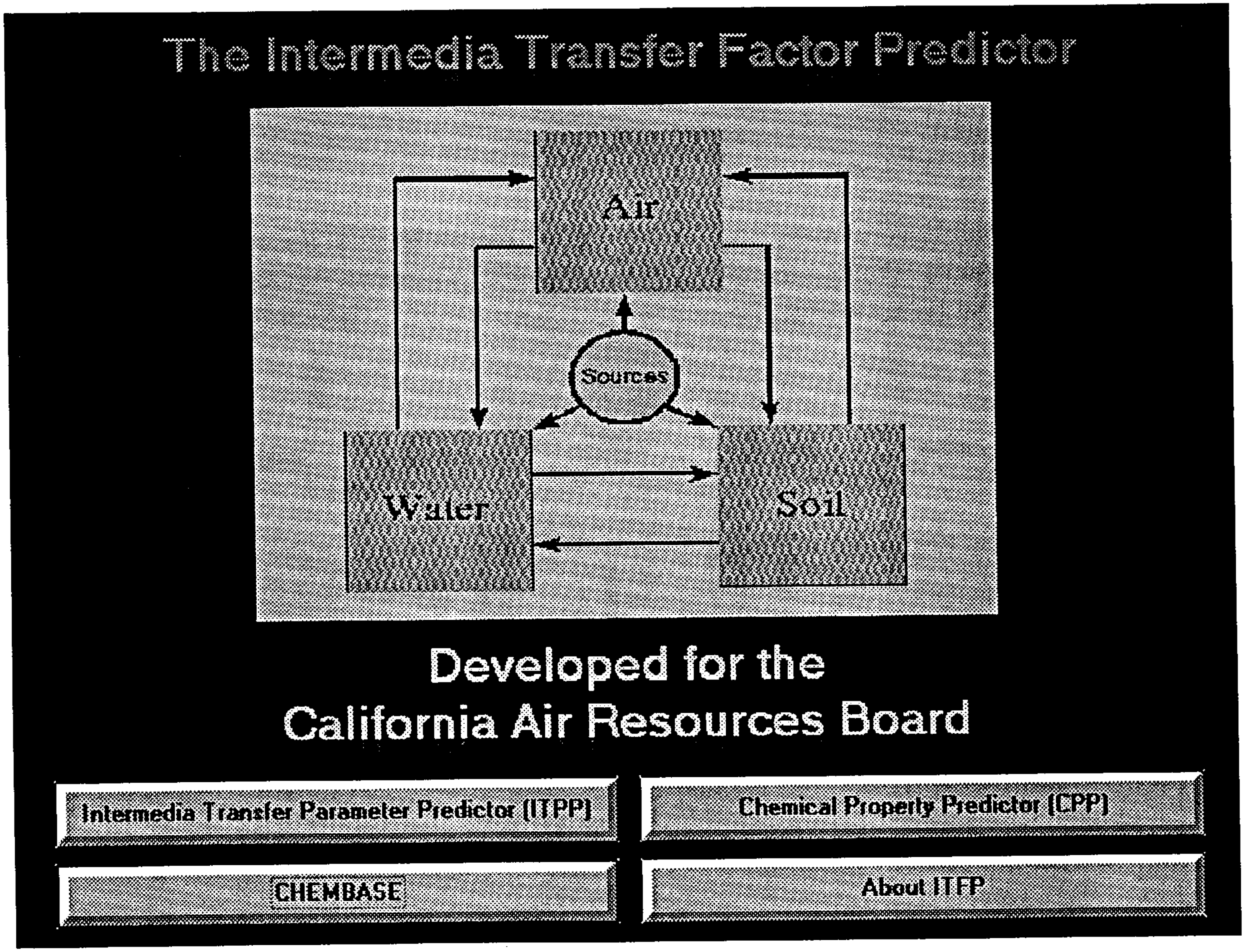


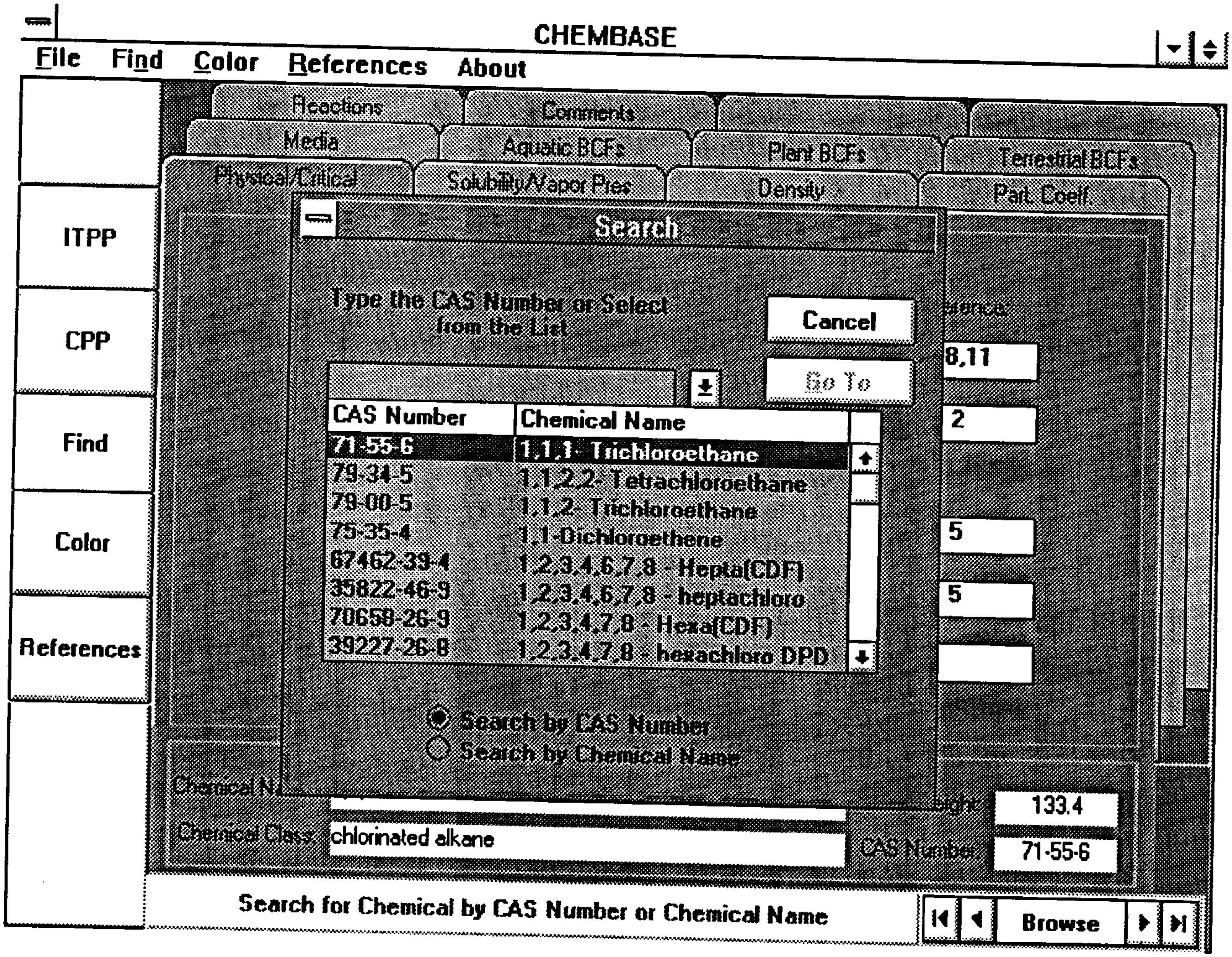
Figure 8.1 Structure of the ITFP



The Intermedia Transfer Factor Predictor

Developed for the
California Air Resources Board

Figure 8.2 ITFP Main Window



Type the CAS Number or Select from the List

CAS Number	Chemical Name
71-55-6	1,1,1- Trichloroethane
79-34-5	1,1,2,2- Tetrachloroethane
79-00-5	1,1,2- Trichloroethane
75-35-4	1,1-Dichloroethene
67462-39-4	1,2,3,4,6,7,8 - Hepta(CDF)
35822-46-9	1,2,3,4,6,7,8 - heptachloro
70658-26-9	1,2,3,4,7,8 - Hexa(CDF)
39227-26-8	1,2,3,4,7,8 - hexachloro DPD

● Search by CAS Number
○ Search by Chemical Name

8,11

2

5

5

Chemical Class: chlorinated alkane

133.4

CAS Number: 71-55-6

Search for Chemical by CAS Number or Chemical Name

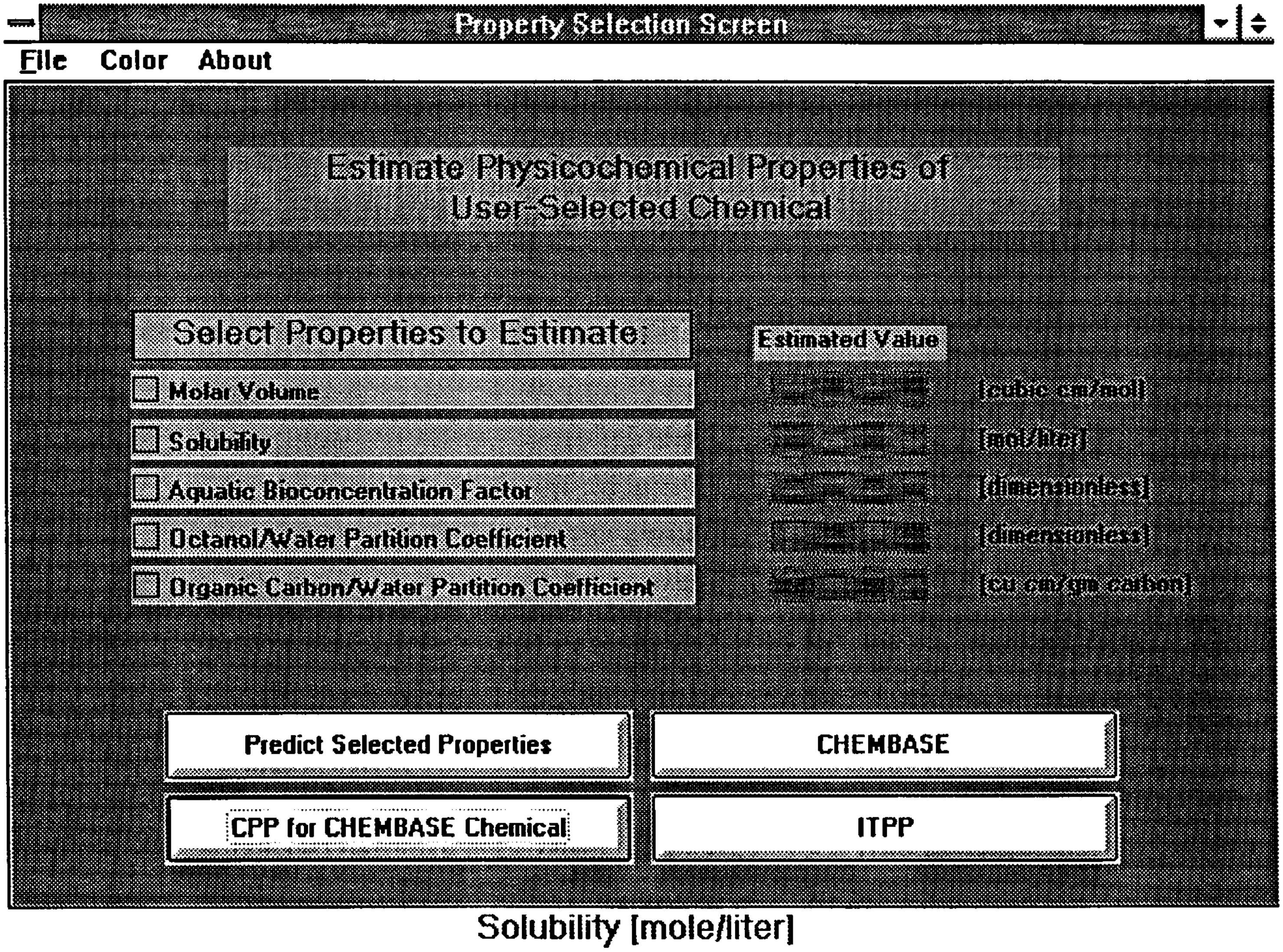
Figure 8.3 CHEMBASE Main Window

is valid. Also, the dimensionless environmental partition coefficients for the selected chemical can be quickly estimated for user-selected temperatures. Finally, the first order reaction rate constants can be calculated from or converted to reaction half-lives by clicking on "Chemical Reaction Half-Lives" or "Pseudo-First Order Environmental Degradation Rate Constants", respectively.

8.3 Overall Structure and Use of the Chemical Property Predictor (CPP)

The Property Selection Window of the CPP with the User-Selected chemical panel and the CHEMBASE chemical panel are shown in Figures 8.4 and 8.5, respectively. The principal distinction between using the CPP for a user-selected chemical as opposed to a CHEMBASE chemical is that the values predicted for user-selected chemicals are retained as the user "Browses" the database. Another difference is that CHEMBASE values for the correlation variables are automatically displayed in the appropriate input fields. Finally, the "molar volume" option is not allowed for CHEMBASE chemicals because calculated values for the molar volume are already in CHEMBASE.

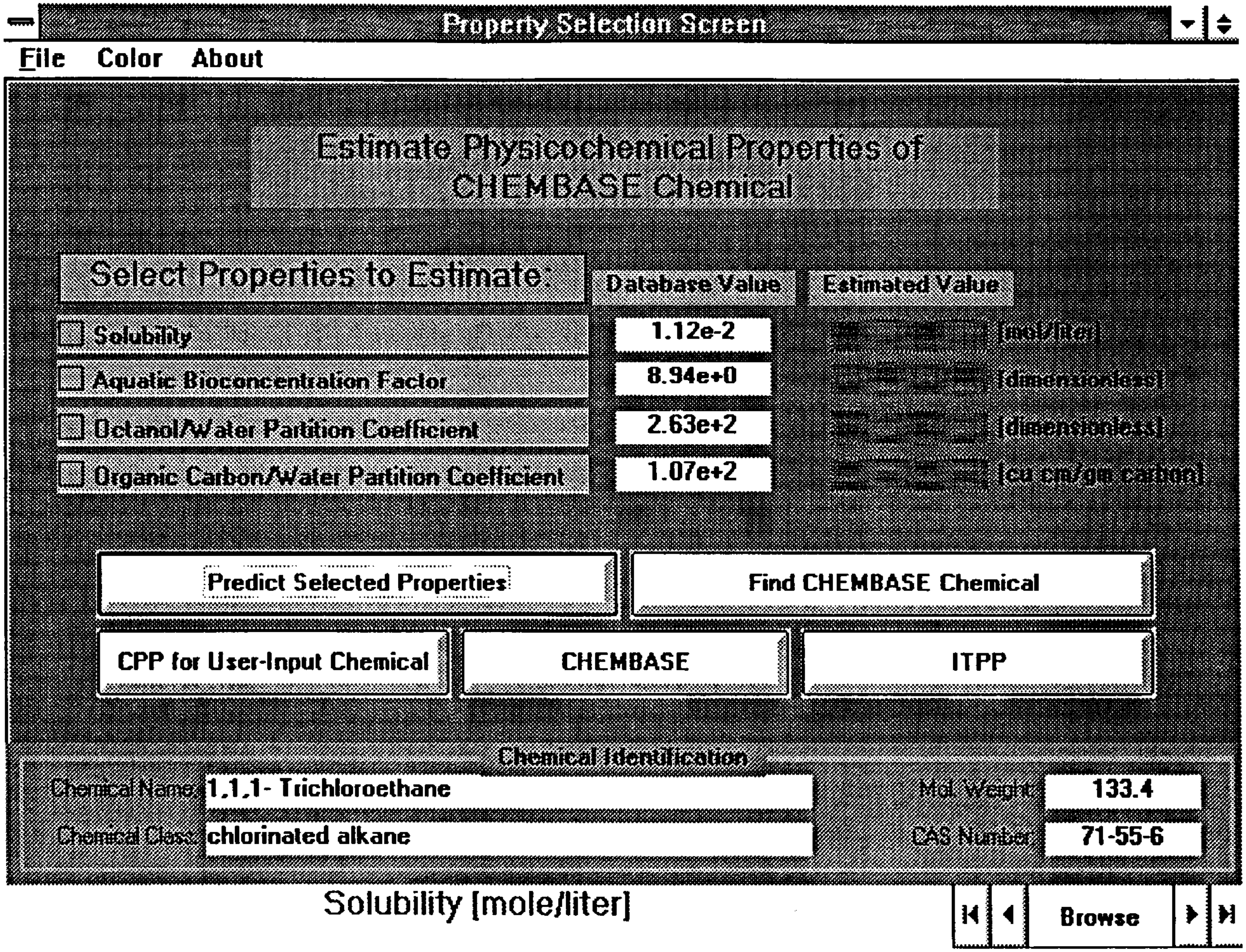
As shown in Figures 8.4 and 8.5, the "Property Selection" window allows the user to estimate the molar volume, solubility, Bioconcentration factor, octanol/water partition coefficient or organic carbon/water partition coefficient by checking the desired properties and clicking the "Predict Selected Properties" button. If no properties are selected, a message will direct the user to select one or more of the listed CPP parameters. Additional features of the "Property Selection" window allow the user to "Browse" the database, go to CHEMBASE or the ITPP and toggle between using the CPP for a CHEMBASE chemical or a user-selected chemical. It is noted, however, that the database cannot be directly accessed from any of the other CPP windows. The CPP also has three windows used to contain the various correlations. The first correlation window is the "Molar Volume" estimation window shown in Figure 8.6. Here the user can estimate the molar volume of a compound if its chemical structure or critical volume is known. The CPP uses the Le Bas method for estimating the molar volume from chemical structure (Reid et al., 1977) and the method of Tyn and Calus (Reid et al., 1977) for estimating the molar volume using the critical volume. Both of these methods are discussed by Reid et al. (1977). To facilitate the use of the Le Bas method, the CPP keeps track of the molecular weight as additional atoms are added to the molecule. Comparison of the final molecular weight with the molecular weight of the compound can be used to verify that the information has been entered correctly. The number of atoms and ring structures will be remembered by the CPP the next time the user enters the "Molar Volume" estimation window.



☐ Molar Volume [cubic cm/mol]
☐ Solubility [mol/liter]
☐ Aquatic Bioconcentration Factor [dimensionless]
☐ Octanol/Water Partition Coefficient [dimensionless]
☐ Organic Carbon/Water Partition Coefficient [cu cm/gm carbon]

Solubility [mole/liter]

Figure 8.4 CPP with User-Selected Panel



Estimate Physicochemical Properties of CHEMBASE Chemical

Select Properties to Estimate:	Database Value	Estimated Value
☐ Solubility	1.12e-2	[mol/liter]
☐ Aquatic Bioconcentration Factor	8.94e+0	[dimensionless]
☐ Octanol/Water Partition Coefficient	2.63e+2	[dimensionless]
☐ Organic Carbon/Water Partition Coefficient	1.07e+2	[cu cm/gm carbon]

Chemical Identification

Chemical Name: 1,1,1- Trichloroethane
Chemical Class: chlorinated alkane
Mol. Weight: 133.4
CAS Number: 71-55-6

Solubility [mole/liter]

Figure 8.5 CPP with CHEMBASE-Selected Chemical Panel

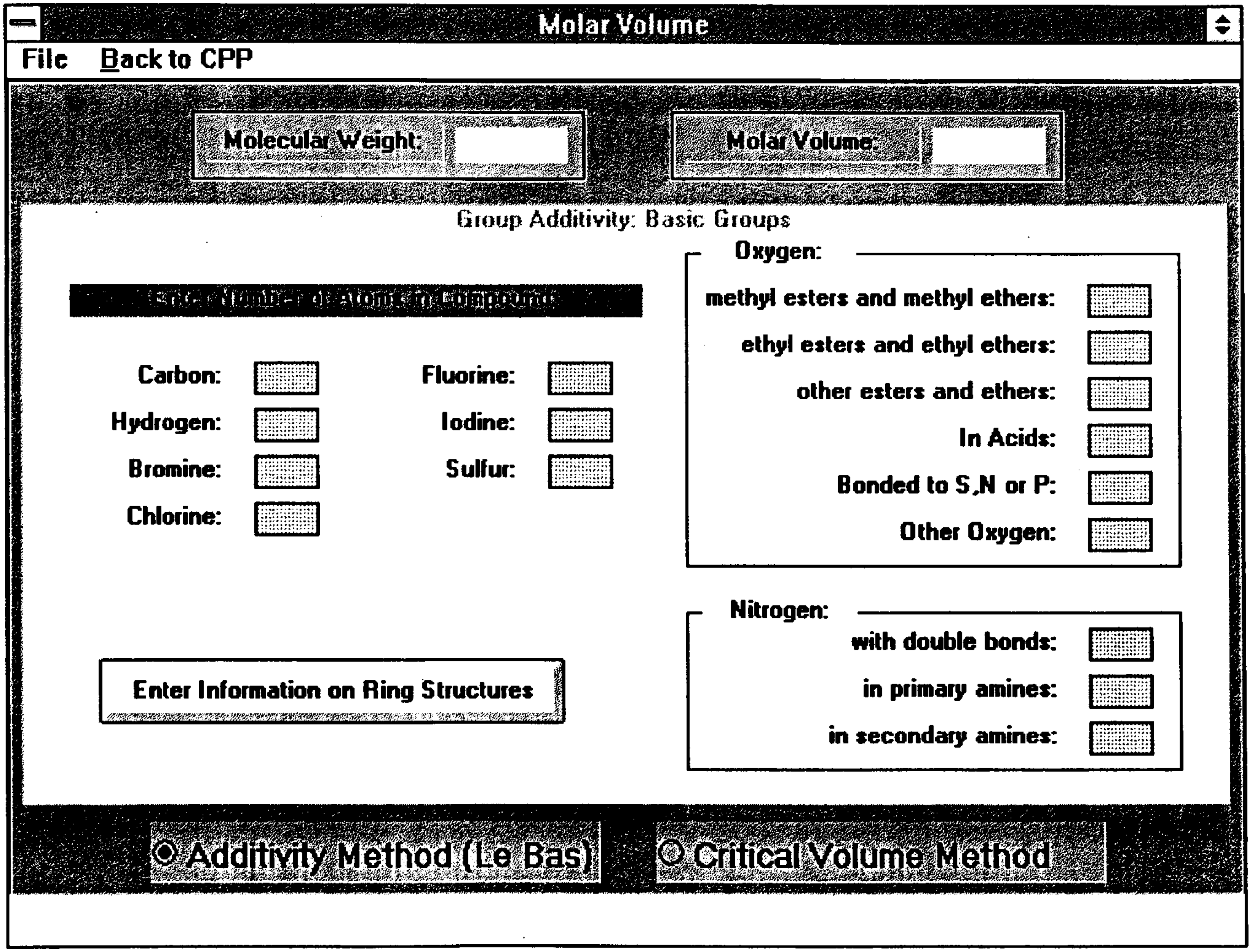


Figure 8.6 Primary Molar Volume Estimation Window

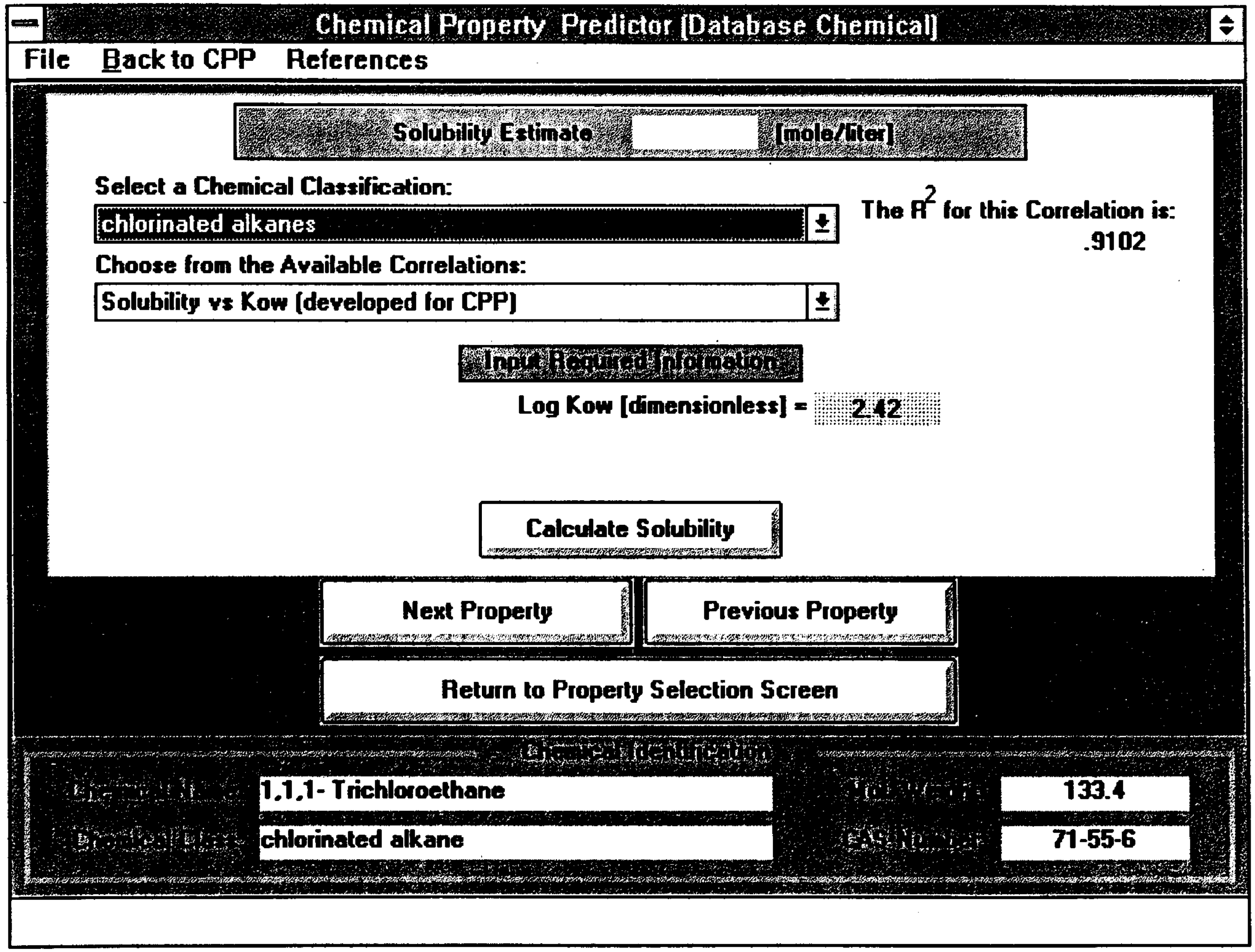
The CPP correlation windows consist of four main windows (Figures 8.7-8.10):

1. Solubility
2. Aquatic Bioconcentration Factor (BCF)
3. Octanol/Water Partition Coefficient (K_{ow})
4. Organic Carbon/Water Partition Coefficient (K_{oc}).

Each one of the CPP property windows includes a list of chemical classifications, a list of available correlations for the selected chemical classification, a value for the r^2 of the correlation (if it is available) and an input field (or fields) for the correlation variables. If a value for the correlation variable is available in CHEMBASE or has been entered previously, it will automatically appear in the input field. The correlations available in the "Property Predictor" windows are a mixture of correlations found in the literature and correlations developed for the CPP. Detailed information about the CPP correlations is provided in section 6.2.

When the "Property Predictor (CHEMBASE chemical)" window first appears on the screen, the CPP selects the appropriate correlations for the chemical class of the selected CHEMBASE chemical. For example, if a compound has a CHEMBASE classification "chlorinated alkane" and there are correlations available for "chlorinated hydrocarbon", the CPP will automatically display the correlation for this chemical class.

If a CHEMBASE chemical is selected then the chemical identification (Chemical name, CAS number, chemical class and molecular weight) is provided at the bottom of the chemical property estimation window. Once a correlation is selected (base on the chemical class) the user is prompted for the required input parameters. For a selected CHEMBASE chemical the required input information is supplied by the CPP if it is available in CHEMBASE. Once the required input information is entered by the user (or the CPP), the estimated physicochemical property is displayed at the top of the window.



Solubility Estimate [mole/liter]

Select a Chemical Classification: chlorinated alkanes

Choose from the Available Correlations: Solubility vs Kow (developed for CPP)

The R^2 for this Correlation is: .9102

Log Kow [dimensionless] = 2.42

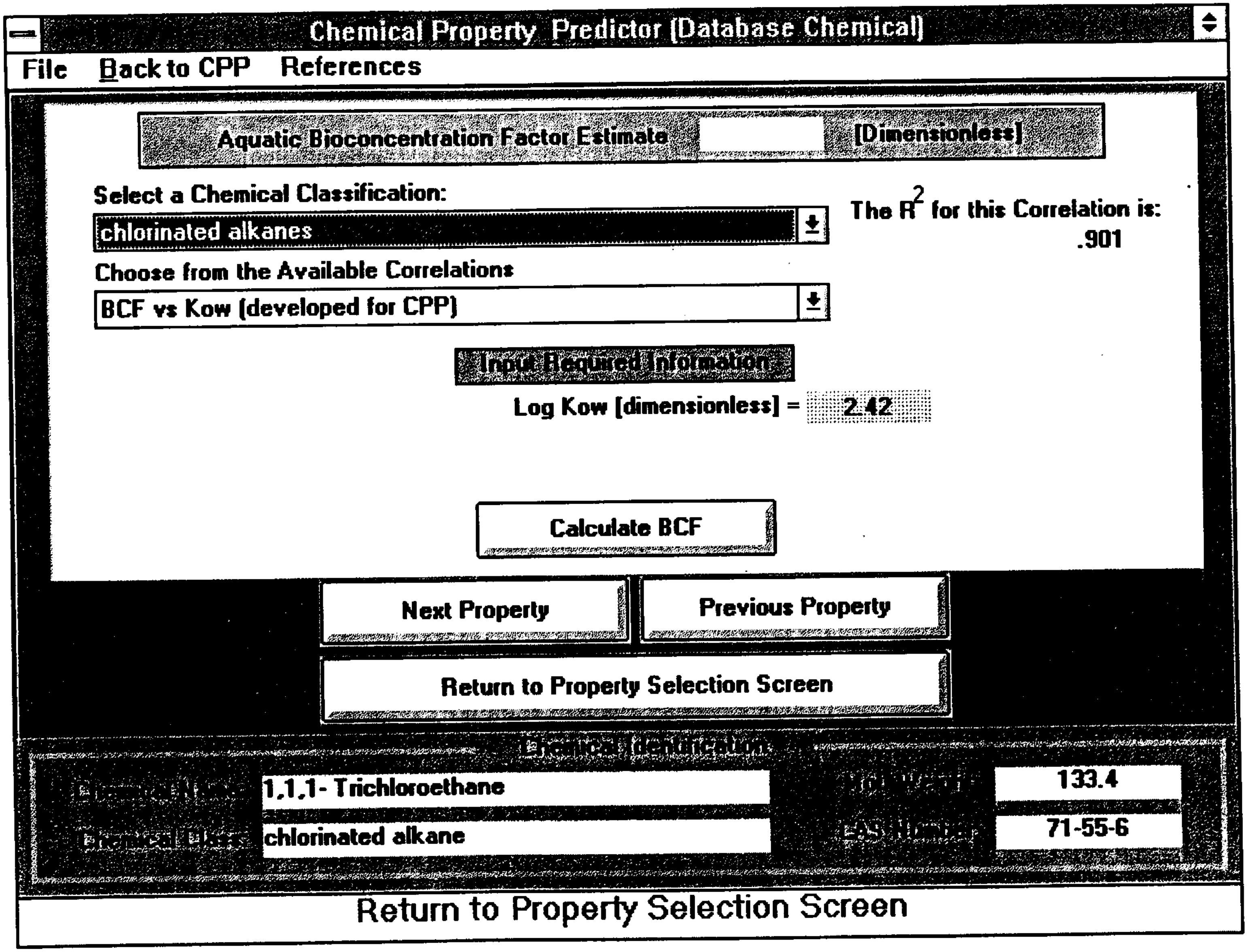
Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Weight: 133.4

CAS Number: 71-55-6

Figure 8.7 Solubility Estimation Window



Aquatic Bioconcentration Factor Estimate [Dimensionless]

Select a Chemical Classification: chlorinated alkanes

Choose from the Available Correlations: BCF vs Kow (developed for CPP)

The R^2 for this Correlation is: .901

Log Kow [dimensionless] = 2.42

Chemical Identification

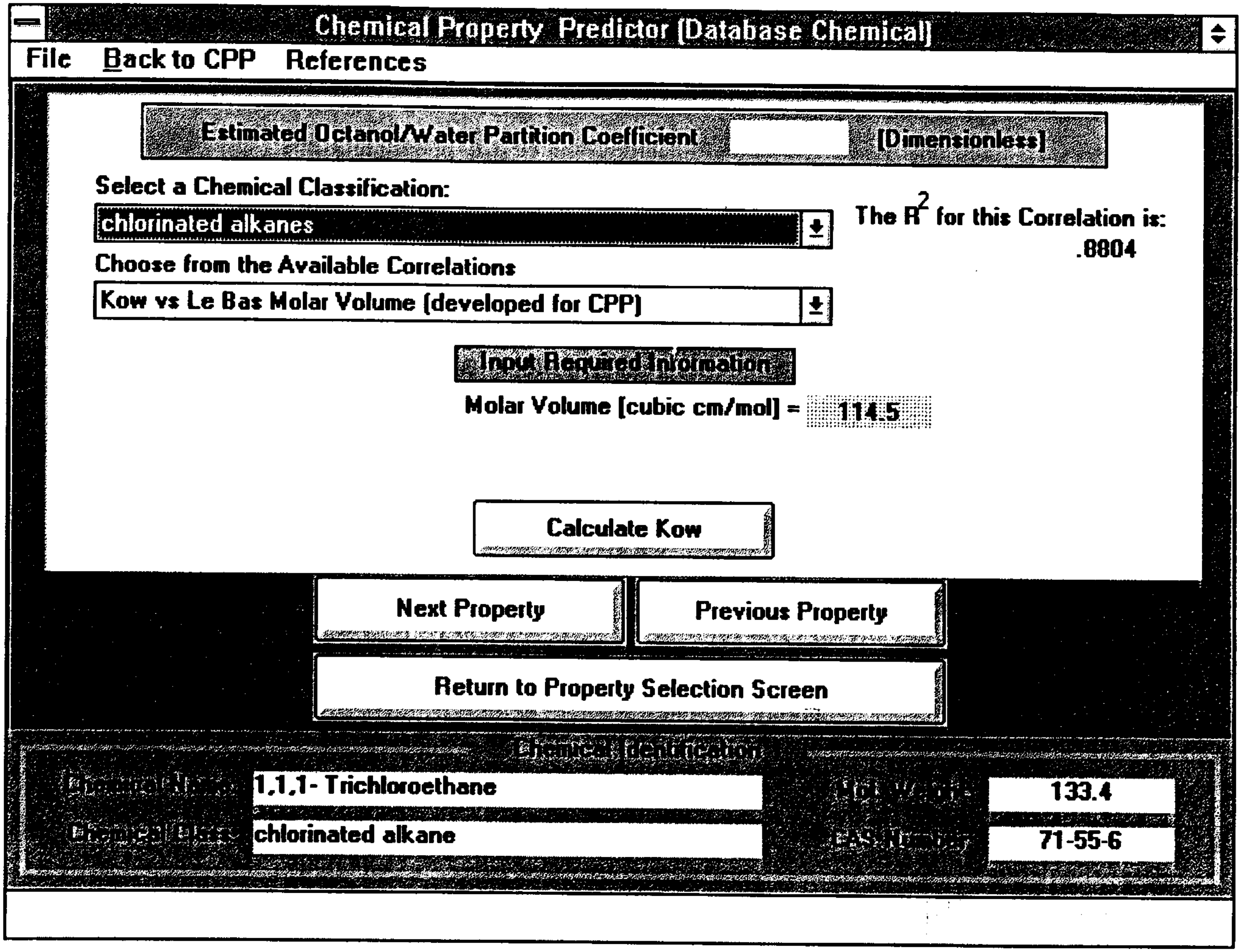
Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Weight: 133.4

CAS Number: 71-55-6

Figure 8.8 Aquatic Bioconcentration Factor Estimation Window



Estimated Octanol/Water Partition Coefficient [Dimensionless]

Select a Chemical Classification: chlorinated alkanes

The R^2 for this Correlation is: .8804

Choose from the Available Correlations: Kow vs Le Bas Molar Volume (developed for CPP)

Molar Volume [cubic cm/mol] = 114.5

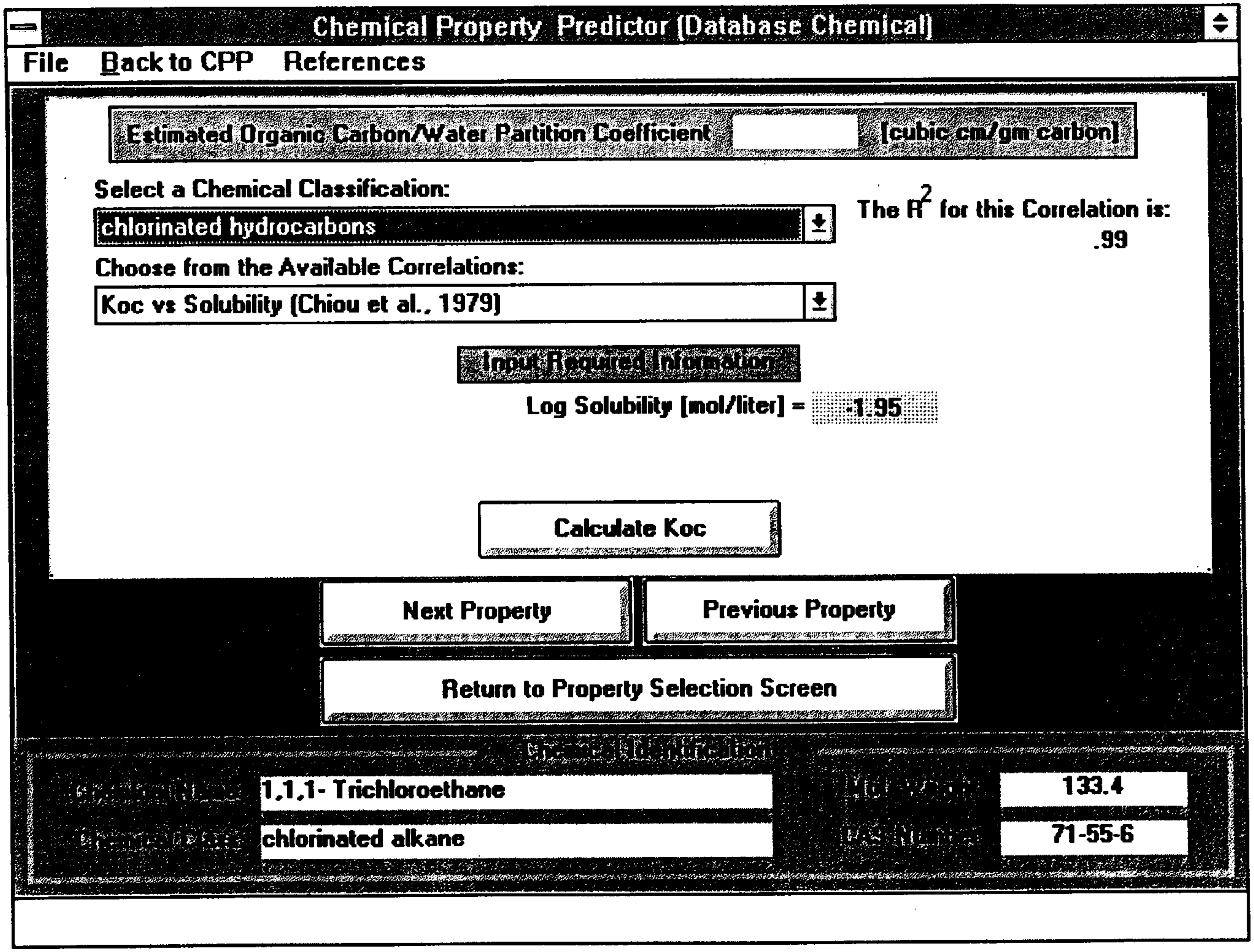
Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Weight: 133.4

CAS Number: 71-55-6

Figure 8.9 Octanol/Water Partition Coefficient Estimation Window



Estimated Organic Carbon/Water Partition Coefficient [cubic cm/gm carbon]

Select a Chemical Classification: chlorinated hydrocarbons

Choose from the Available Correlations: Koc vs Solubility (Chiou et al., 1979)

The R^2 for this Correlation is: .99

Log Solubility [mol/liter] = -1.95

Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Wgt.: 133.4

CAS Number: 71-55-6

Figure 8.10 Organic Carbon/Water Partition Coefficient Window

8.4 Intermedia Transfer Parameter Predictor (ITPP): Overall Structure and User Guide

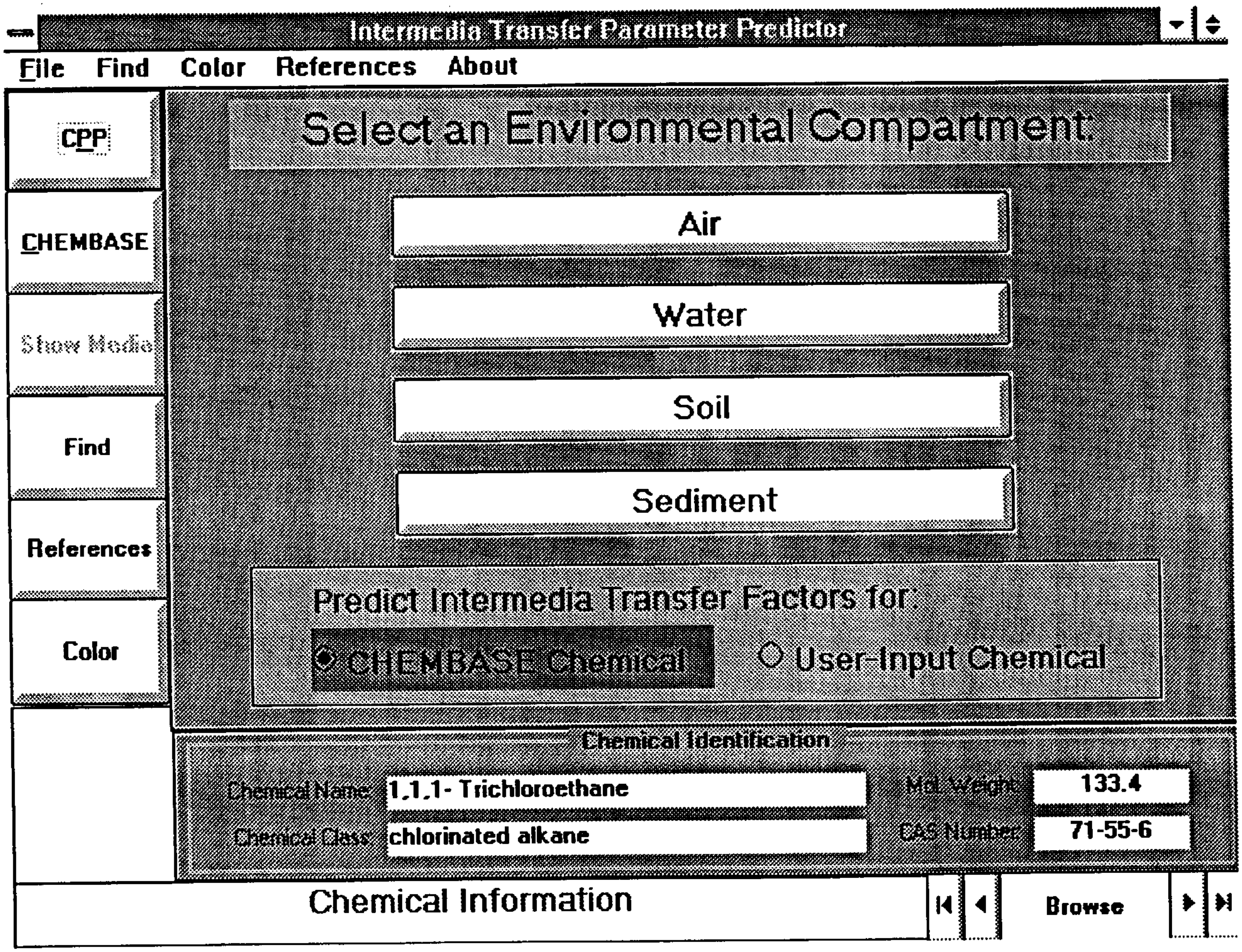
The main window of the Intermedia Transfer Parameter Predictor (ITPP) is shown in Figure 8.11. In this main window the intermedia transfer parameters are categorized by environmental media: "Air", "Water", "Soil" and "Sediment". For the sake of convenience, "Diffusion Coefficients" are found under all four headings while other intermedia transfer parameters are found only under the most appropriate headings. (e.g., the air/soil partition coefficient is found both under "Air" and "Soil") Also, clicking the "Show Media" button on the left hand side of the screen or the "Return to Media Selection" tab displays the media selection menu.

Once an environmental media has been selected, buttons containing the available intermedia transfer parameters appear on the screen as shown for example in Figure 8.12 for the Air/Soil window. Pressing one of these buttons directs the user to the window for calculating that intermedia transfer parameter. The intermedia transfer parameter modules currently available in the ITPP include see section 7):

1. Dry Deposition to Soil, Water and Vegetation
2. Diffusion Coefficients in Air, Water, Soil and Sediment
3. Volatilization Half-Life in Soil
4. Rain Scavenging of Gaseous and Particle-Bound Pollutants
5. Air/Water, Air/Soil and Air/Vegetation Mass Transfer Coefficients
6. Air/Water, Air/Soil, Air/Vegetation, Water/Suspended Solids, Water/Sediment, Soil/Root and Gas/Particle Partition Coefficients
7. Bioconcentration Factors for Fish

In addition, there is a stand-alone module for estimating chemical bioaccumulation in finned fish (as described in Appendix C). The windows used to predict these intermedia transfer parameters are discussed briefly below.

The water, soil and vegetation **Dry Deposition** modules of the ITPP follow the models proposed by Williams, (1982) Sehmel and Hodgson (1980) and Slinn, (1982), respectively. These windows use models of dry deposition published in the literature to estimate the dry deposition velocity. The above dry deposition models require parameters such as the wind speed, air temperature and roughness height for the deposition surface. Input fields for the model parameters are placed onto separate panels by type and can be accessed through the command buttons at the



● CHEMBASE Chemical ○ User-Input Chemical

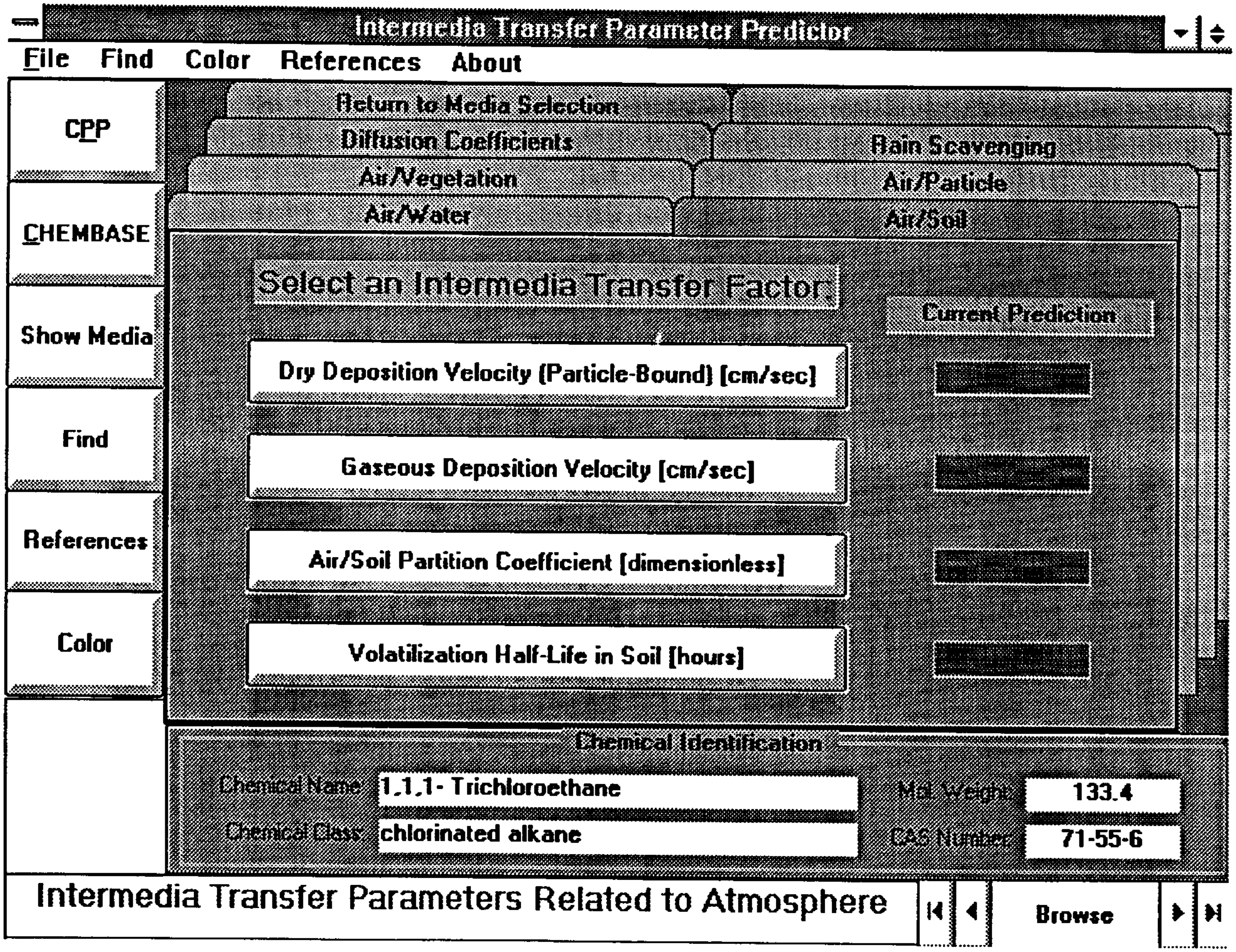
Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Weight: 133.4

CAS Number: 71-55-6

Figure 8.11 ITPP Main Window



Chemical Name: 1,1,1- Trichloroethane

Chemical Class: chlorinated alkane

Mol. Weight: 133.4

CAS Number: 71-55-6

Figure 8.12 ITPP Media Selection Tabs and Air/Soil ITF Window bottom of the screen. Recommended values for some of the required parameters were taken from the respective papers and appear in the input fields. Tri-modal particle size distribution functions are required to estimate the dry deposition velocity and these can be input by the user or selected from a list of distributions published by Whitby (1978).

The Diffusion Coefficient estimation module can estimate the molecular diffusion coefficients for the selected chemical in air and water. The effective diffusion coefficients in the soil and sediment matrices can also be estimated. The method of Fuller (1966) is used to estimate the molecular diffusion coefficient in air. The Wilke-Chang (Wilke and Chang, 1955), Hayduk and Laudie (Hayduk and Laudie, 1974) and Hayduk (Hayduk et al., 1982) methods are available for estimating the molecular diffusion coefficients in water. The soil and sediment matrix diffusion coefficients are calculated using the method outlined by Jury (1983) and Cohen and Ryan (1990). The input fields for the parameters required by these correlations are classified by media (air, water, soil and sediment) and placed on separate panels accordingly. Reasonable values for parameters such as the organic carbon fraction of soil appear in the input fields automatically, though these values can be changed by the user.

The Volatilization Half-Life estimation module estimates the time it takes for half the mass of a chemical that is initially uniformly distributed down to a certain depth to be removed by diffusion in the absence of chemical reaction. The module uses analytical solutions to the diffusion equation published by Mayer, Letey and Farmer (1974) to keep track of the total mass remaining in the soil as a function of time. When the chemical mass in the soil reaches half of the initial value, the half-life is displayed in the appropriate label. Note that the initial concentration of the chemical in the soil is not required as input for this module.

The Rain Scavenging window uses the rain scavenging model of Tsai and Cohen (1991) to estimate the initial rain scavenging coefficient for particle-bound chemicals and the rain scavenging coefficient of gaseous chemicals. In this model, the raindrop size distribution is approximated using the method of Marshall and Palmer (1948). Other parameters required by the model such as the rate of rainfall have input fields and allowable ranges. Note that the rain scavenging coefficient for particle-bound chemicals requires the same tri-modal particle size distribution as the dry deposition modules. Rain Scavenging is a dynamic process and in the ITPP the calculated rain scavenging coefficient for particle-bound chemicals is the initial value at the beginning of the rain event.

The deposition velocity of gaseous chemicals and the **air/water, air/leaf mass transfer coefficients** can be estimated from the "Mass Transfer Coefficient" estimation window. The gaseous dry deposition velocity is calculated using the deposition velocity of a reference chemical and the ratio of the Schmidt number to the 2/3 power (ARB, 1994). The overall air/water mass transfer coefficient can be calculated using two film resistance theory (Lewis and Whitman, 1924) if the single phase mass transfer coefficients for the air and water phases can be calculated. The air-side mass transfer coefficient can be estimated using the methodology of Brutsaert (1975) or Mackay and Yeun (1983). The water-side mass transfer coefficient can be estimated using the methodology of Cohen and Ryan (1985) for large lakes or reservoirs or Shen et al. (1993) for flowing streams. The above algorithms are discussed in greater detail elsewhere (Cohen et al., 1994). The overall air/leaf mass transfer coefficient is estimated from mass transfer resistances based on the study of Paterson et al. (1991) as discussed in section 7.4.

The environmental partition coefficients can be estimated from the "Partition Coefficient" estimation window. The partition coefficients are estimated using the fugacity capacity method of Mackay and coworkers (1991). Using this methodology, all of the environmental partition can be estimated using, the K_{oc}, the K_{ow}, the Henry's law constant, the temperature and the volume fractions of various environmental components (air, water, organic carbon or lipid/octanol). In addition, empirical correlations for plant partition coefficients are also available (Bacci, 1990; Paterson and Mackay, 1994; Paterson et al., 1991).

The "Gas/Particle Partitioning" estimation window is separate from the "Partition Coefficient" window for the sake of convenience. From this window, the user can select either the Junge method (1975) or the method described by Pankow (1991). The Junge method allows the user to estimate gas/particle partitioning using only the vapor pressure of the chemical, the surface area concentration of atmospheric particles and the Junge correlation coefficient. The surface area concentration of the atmospheric particles can be estimated from the tri-modal particle size distribution function used in the dry deposition and rain scavenging modules if the particles are assumed spherical or if the specific surface area of the aerosol is known. The value for the Junge correlation constant varies with the class of chemical but a reasonable average value taken from the literature (Pankow, 1987) automatically appears in the appropriate input field. The saturation pressure must be supplied by the user unless it is available in CHEMBASE. The Pankow correlation can only be used for the chemical classes for which the gas/particle partitioning has been measured. A list of chemicals for which the correlation parameters are known is given in a scrollable ITPP list (Pankow, 1991; Bidleman and Foreman, 1987).

Finally, the "Aquatic Bioconcentration Factor" estimation window is identical to the "Property Predictor" windows used in the CPP for the estimation of Aquatic Bioconcentration Factors.

8.5 Notes Concerning ITFP Input Parameters

Calculations performed by the ITFP software require input parameters such as temperature, wind speed or organic carbon fraction as well as chemical properties such as the solubility or octanol/water partition coefficient. There are three different types of input parameters in the ITFP: chemical properties for a user-selected chemical, chemical properties for a database chemical and all other parameters. All of these parameters retain their values as one moves from window to window but differ in how they are affected by other changes. Parameters associated with a user-selected chemical, for example, do not change as the user browses the database. However, all changes to chemical properties made for a database chemical are refreshed as one browses the chemical database. The values of other parameters are always the most recently input value for these parameters. In the current version of the software, values of user-entered variables are not saved when the user exits the program.

Parameters related to the particle size distribution function of atmospheric aerosol particles have special features that require discussion. For intermedia transfer parameters that require this information (rain scavenging of particulate matter, dry deposition to water, soil and vegetation and gas/particle partitioning), average tri-modal particle size distributions published by Whitby (1978) are available in a scrollable list in the "Particle Parameters" panel. If one of these size distributions is selected, the appropriate values describing the tri-modal distribution are placed in the parameter fields. In order to change the values of these parameters, it is necessary to select the "User-Selected" particle size distribution from the scrollable list.

8.6 Colors

The colors in the ITFP software package can be customized to allow for personal preference. Once the colors have been changed, they will be remembered for subsequent use of the program.

8.7 Online ITFP and CHEMBASE References

Pertinent references that contain information on compounds and parameter correlations are given in CHEMBASE and the CPP. Reference information can be copied by using the mouse to highlight the desired reference and the Ctrl-C key to copy the information to the Windows clipboard.

8.8 Installation

The installation of the ITFP software is similar to the installation of most Windows compatible software. Place "ITFP disk 1" in the "a:" drive and run "a:\install.exe" from Windows and follow the prompts. The ITFP can be removed from the hard drive onto which it is installed by clicking the "Uninstall" icon that appears next to the ITFP icon. Uninstall will automatically remove all of the ITFP files from the hard disk. The minimum installation requirements for the ITFP software is 3.2 Mb of disk space, a VGA monitor, Windows 3.1 or higher operating system running on a 386 or higher CPU with at least 640Kb of RAM.

The ITFP BAF module is supplied as a stand-alone module on a single 1.44 Mb floppy disk. The software can be executed directly from the floppy disk or loaded onto a hard disk using the DOS copy command or the Windows file manager. Additional information on using and installing the software is available in the readme files.

9. REFERENCES

9.1 General ITFP References

Agency for Toxic Substances and Disease Registry (ATSDR), Toxicological Profile for ______, U.S. Department of Health & Human Services, Public Health Service,, Division of Toxicology/Toxicology Information Branch, Atlanta, Georgia, 1989-1995.

Air Resources Board, Development of Intermedia Transfer Factors for Toxic Air Pollutants, Volumes I - VIII, prepared by Cohen, Y. And A. M. Winer, March, 1994.

Air Resources Board/Office of Environmental Health Hazard Assessment, Health Risk Assessment Program, Version 1.1: Operating Instructions, March 1992. Prepared by Grant Chin and Narcisco Gonzalez.

Allen, D., Kaplan, I., and Yoram Cohen (Editors), Intermedia Pollutant Transport: Modeling and Field Measurements, Plenum Press, New York, 1989.

Ames, T. And E. Grulke, Group Contribution Method for Predicting Equlibria of Nonionic Organic Compounds between Soil Organic Matter and Water, Environmental Science and Technology, 29, 2273-2279, 1995.

Andren, A.W., W.J. Doucette and R.M. Dickhut, American Chemical Society, 2-33, 1987.

A&WMA, Total Exposure Assessment Methodology, Proceedings of the EPA/A&WMA Specialty Conference, November, 1989, Las Vegas, Nevada, Air &Waste Management Association, Pittsburgh, PA.

Bacci, B., Cerejeira, M.J., Gaggi, C., Chemello, G., Calamari, D., and Vighi, M., Bioconcentration of Organic Chemical Vapors in Plant Leaves: The Azalea Model, Chemosphere, 21, 525-535, 1990.

Banerjee, S. and Baughman, G., Bioconcentration Factors and Lipid Solubility, Environmental Science and Technology, 25, 536-539, 1991.

Banerjee, S. And P. H. Howard, Improved Estimation of Solubility and Partitioning through Correction of UNIFAC-Derived Activity Coefficients, Environmental Science and Technology, 22, 839-841, 1988.

Banerjee, S., Yalkowsky, S. H., Valvani, S.C., Water Solubility and Octanol/Water Partition Coefficient of Organics. Limitations of the Solubility-Partition Coefficient Correlation, Environmental Science and Technology, 14, 1227-1229, .

Barber M.C., Suarez L.A., Lassiter L.L., FGETS User's Manual and database, Environmental Research Laboratory Office of Research and Development, US E.P.A., 1987.

Barber M.C., Suarez L.A., Lassiter L.L., FGETS Version 3.0-12 User's Manual and Database, Environmental Research Laboratory Office of Research and Development, US E.P.A., 1994.

Barber M.C., Suarez L.A., Lassiter L.L., Modelling Bioaccumulation of Organic Pollutants in Fish with an Application to PCB's in Great Lake salmonids., Canadian Journal of Fisheries and Aquatic Sciences, 48, 318-337, 1991.

Bidleman, T.F. and Foreman, W.T., Vapor-Particle Partitioning of Semivolatile Organic Compounds, In: Sources and Fates of Aquatic Pollutants, Hites, R.A. and Eisenreich, S.J. (Eds.) American Chemical Society, Washington, D.C., 1987.

Bidleman T.F., Billings W., Foreman W., Vapor-Particle Partitioning of Semivolatile Organic Compounds: Estimates from Field Collections, Environmental Science and Technology, 20, 1038-1043, 1986.

Bruggemann R. and Munzer B., In Jochum et al. (eds): Physical Property Prediction in Organic Chemistry, Springer-Verlag, Berlin, 304-334, 1988.

Bruggemann R., Altschuh J., and Matthies M., Qsar for Estimating Physicochemical Data, in W. Karcher and J. Devillers (eds.): Practical Applications of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology, Kluwer Academic Publishers, Dordrecht, 197-211, 1990.

Brunner, S., E. Hornung, H. Santl, E. Wolff, O. G. Piringer, J. Altshuh and R. Bruggemann, Henry's Law Cosntants for Polychlorinated Biphenyls: Experimental Determination and Structure-property Relationships, Environmental Science and Technology, 24, 1751-1754, 1990.

Brutsaert, W., A Theory for Local Evaporation (or Heat Transfer) from Rough and Smooth Surfaces at Ground Level, Water Resources Research, 11(4), 543-550, 1975.

Buck, J.W., Whelan, G., Droppo, J.G., Strenge, D.L., Castleton, K.J., McDonald, J.P., Sato, C., Streile, G.P., Multimedia Environmental Pollutant Assessment System (MEPAS) Application Guidance: Guidelines for Evaluating MEPAS Input Parameters for Version 3.1. PNL-10395, Pacific Northwest, Richland, WA, 1995.

Burkhard L.P., Andren A.W., Armstrong D.E., Estimation of Vapor Pressures for Polychlorinated Biphenyls: a Comparison of Eleven Predictive Methods, Environmental Science and Technology 19, 500-507, 1985.

CAPCOA Air Toxics 'Hot Spots' Program, Risk Assessment Guidelines' Prepared for the AB 2588 Risk Assessment Committee of the California Air Pollution Officers Association (CAPCOA), July 1990.

CAPCOA, "Air Toxics "Hot Spots" Program Risk Assessment Guidelines", Prepared by the AB 2588 Risk Assessment Committee of the California Air Pollution Control Officers Association (CAPCOA), 1992.

Cheng, J.J., Droppo, J.G., Faillace, E.R., Granapragasm, E., Johns, R.A., Laniak, G., Lew, S., Mills, W.B., Strenge, D.L., Sutherland, J.F., Whelan, G., Yu, C., Benchmarking Analysis of Three Multimedia Models: RESRAD, MMSOILS, and MEPAS, Prepared by: USEPA, Athens, GA; Pacific Northwest Laboratory, Richland, WA; Argonne National Laboratory, Argonne, IL; University of Tennessee, Knoxville, TN; Tetra Teach, Inc., Lafayette, CA. Prepared for the U.S. Department of Energy, Office of Management, 1995.

Chiou, C.T., Freed, V.H., Schmedding, D.H., and Kohnert, R.L., Partition Coefficients and Bioaccumulation of Selected Organic Chemicals, <u>Environmental Science and Technology</u>, 11, 475-478, 1977.

Chiou, C.T., Peters, L.J., and Freed, V.H., A Physical Concept of Soil-Water Equilibria for Nonionic Organic Compounds, <u>Science</u>, 206, 831-832, 1979.

Chiou C.t., Partition Coefficients of Organic Compounds in Lipid-Water Systems and Correlations with Fish Bioconcentration Factors., <u>Environmental Science and Technology</u>, 19, 75-62, 1985.

Chiou, C.T., Porter, P.E., Schmedding, D.W., Partition Equilibria of Nonionic Organic Compounds between Soil Organic Matter and Water, <u>Environmental Science and Technology</u>, 17, 227-231, 1983.

Chiou, C., V. Freed, D. Schmedding, Kohnert, R., Partition Coefficient and Bioaccumulation of Selected Organic Chemicals, <u>Environmental Science and Technology</u>, 11, 475-478 1977.

Chiou C.T., Partitioning of Organic Chemicals in Octanol-Water System, <u>Environmental Science and Technology</u>, 16, 4-10, 1982a.

Chiou C.T., Schmedding D.W., Manes M., Partitioning Coefficients of Organic Compounds in Lipid-Water Systems and Correllations with Fish Bioconcentration Factors, <u>Environmental Science and Technology</u>, 16, 4-10, 1982b.

Chow, W. and K. K. Conor (Eds.), Managing Hazardous Air Pollutants: State-of-the-Art,, Lewis Publisher, Chelsea, MI, 1993.

Clark K.E, Gobas F.A.P.C., Mackay D., Model of Organic Chemical Uptake and Clearnace by Fish from Food and Water, Environmental Science and Technology, 24, 1203-1213, 1990.

Clay, R.E., Multimedia Environmental Distribution of Gaseous, Dissolved, and ParticleBound Pollutants, M.S. Thesis, Department of Chemical Engineering, UCLA, 1992.

Cohen, Y. and Ryan, P.A., Multimedia Modeling of Environmental Transport: Trichloroethylene Test Case, Environmental Science and Technology, 19, 412-417, 1985.

Cohen Y., Organic pollutant transport, Environmental Science and Technology, 20, 538-563, 1986a.

Cohen, Y., Intermedia Transport Modeling in Multimedia Systems, in Pollutants in a Multimedia Environment, Plenum Press, NY, 1986b.

Cohen, Yoram, Modeling of Pollutant Transport and Accumulation in a Multimedia Environment, in Geochemical and Hydrologic Processes and Their Protection: The Agenda for Long Term Research and Development, Draggan, S., J. J. Cohrssen, and R. E. Morrison (Eds), Praeger Publishing Company, New York, 1987.

Cohen, Y., Tsai, W., Chetty, S.L., and Meyer, G.J., Dynamic Partitioning of Organic Chemicals in Regional Environment: A Multimedia Screening-Level Modeling Approach, Environmental Science and Technology, 24(10), 1549-1558, 1990.

Cohen, Y., Allen, D.T., Clay, R.E., Rosselot, K., Tsai, W., Klee, H., and Blewitt, D., Multimedia Assessment of Emissions (MAB) from the AMOCO Corporation Yorktown Refinery (AMOCO/EPA Pollution Prevention Project), A&WMA 84th Annual Meeting and Exhibition, Paper #91-84.6, 1991.

Cohen, Y., Clay, R.E., Multimedia Partitioning of Particle-Bound Organics, The Journal of Hazardous Materials, 37, 507-526, 1994.

Cohen, Y., Van de Water, R., Environmental Distribution of Organics, Computer Techniques in Environmental Studies V, Vol. I: Pollution Modeling, Zanetti (Ed.), Computational Mechanics Publications, Southampton, UK, 1994.

Connolly J.P., Tonelli R., Modelling Kepone in the Striped Bass food Chain of the James River Estuary, Estuaries Coastal and Shelf Science, 20, 349-366, 1985..

Davis J.C., Randall D.J., Gill irrigation and pressure relationships in Rainbow Trout (Salmo gairdnrei). The Journal of the Fisheries Research Board of Canada, 30, 99-104, 1983.

Dearden, J.D., Practical Applications of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology, Karcher, W., Devillers, J., (Eds.), Kluwer Academic Publishers, Dordrecht, Holland, 1990.

Department of Toxic Substances Control, California Environmental Protection Agency, CalTox: A Multimedia Total Exposure Model for Hazardous Waste Sites - Technical Report, 1993.

Draggan, S., J. J. Cohrssen, and R. E. Morrison (Eds), Geochemical and Hydrologic Processes and Their Protection: The Agenda for Long Term Research and Development, Praeger Publishing Company, New York, 1987.

Dunn III W.J., Block J.H., and Pearlman R.S., Partition Coefficient: Determination and Estimation, Pergamon Press, New York, 1986.

Dunnivant F.M., Elzerman A.W., Jurs P.C., Hansen M.N., Quantitative Structure-property Relationships for Aqueous Solubilities and Henry's Law Constants of Polychlorinated Biphenyls, Environmental Science and Technology, 26, 1567-1573, 1992.

Easter, R.C. and Hales, J.M., in PLUVIUS: A Generalized One-Dimensional Model of Reactive Pollutant Behavior Including Dry Deposition, Precipitation Formation, and Wet Removal, Report PNL-4046 BD2, Battelle Pacific Northwest Lab, Richland, WA, 1984.

Fiedler, H. And K.-W. Schramm, QSAR Generated Octanol-Water Partition Coefficients of Selected Mixed Halogenated Dibenzodioxins and Dibenzofurans, Chemosphere, 20, 1597-1602, 1990.

Fitzgerald, J. W., Journal Applied Meteorology, 14, 1044, 1975.

Fuller, B.N., Schettler, P.D., and Giddings, J.C., A New Method for Prediction of Binary Gas-Phase Diffusion Coefficients, Industrial and Engineering Chemistry, 58, 19-57, 1966.

Gobas F.AP.C. and Mackay D., Dynamics of Hydrophobic Organic Chemical Bioconcentration in Fish, Environmental Science and Technology, 6: 495-504, 1987.

Gobas F.A.P.C., Xin Zhang and Ralph Wells., Gastrointestinal Magnification: The Mechanism of Bioaccumulation and Food Chain Accumulation of Organic Chemicals, Environmental Science and Technology, 27: 2885-2863, 1993.

Gustafson, K. E. And R. M. Dickhut, Molecular Diffusivity of Polycyclic Aromatic Hydrocarbons in Air, Journal of Chemical and Engineering Data, 39, 286-289, 1994a.

Gustafson, K. E. And R. M. Dickhut, Molecular Diffusivity of Polycyclic Aromatic Hydrocarbons in Aqueous Solution,Journal of Chemical and Engineering Data, 39, 281-285, 1994b.

Gusten H., Horvatic D., and Sabljic A., Modeling N-Octanol/Water Partition Coefficients by Molecular Topology: Polycyclic Aromatic Hydrocarbons and Their Alkyl Derivatives, Chemoshere, 23, 199-213, 1991.

Hansch C. and Leo A.J., Substituent Constants for Correlation Analysis in Chemistry and Biochemistry, John Wiley, New York, 1979.

Hansch, C., Quinlan, J.E., Lawrence, G.L., The Linear Free-Energy Relationships between Partition Coefficients and the Aqueous Solubility of Organic Liquids, Journal of Organic Chemistry, 33, 347-350, 1968.

Hawker, D., Description of Fish Bioconcentration Factors in Terms of Solvatochromic Parameters, Chemosphere, 20, 467-477, 1990.

Hawker D.W., Vapor pressure and Henry's Law Constants of Polychlorinated Biphenyls, Environmental Science and Technology, 23, 1250-1253, 1990.

Hawker D.W., the Relationship Between Octanol/Water Partition Coefficient and Aqueous Solubility in Terms of Solvatochromic Parameters, Chemosphere, 19, 1585-1593, 1989.

Hawker D.W. and Connell D.w., Octanol-water Partition Coefficients of Polychlorinated Bipheny Congeners, Environmental Science and Technology, 22, 382-387 1988.

Hayduk, W. and Laudie, H., Prediction of Diffusion Coefficients for Non-electrolytes in Dilute Aqueous Solutions, AIChE Journal, 20, 611, 1974.

Hayduk, W., Minhas, B.S., and Lan, J., Correlations for Prediction of Molecular Diffusivities in Liquid, The Canadian Journal of Chemical Engineering, 60, 295, 1982.

Hinds, William, C., Aerosol Technology Properties, Behavior and Measurement of Airborne Particles, John Wiley & Sons, New York 1982.

Holsen, T. M., Noll, K. E., Dry Deposition of Atmospheric Particles: Application of Current Models to Ambient Data, Environmental Science and Technology, 26, 1807-1815 1992.

Howard P.H., Jarvis W.F., Sage G.W., Basu D.K., Gary D.A., Meylan W., and Crosbie E.K., Fate and Exposure Handbook, Volumes I-III, Lewis Publishers, Inc., 1989-1990.

Isnard P. and Lambert S., Estimating Bioconcentration Factors from Octanol-water Partition Coefficient and Aqueous Solubility. Chemosphere, 17, 21-34, 1988.

Jirka, G.H. and Brutsaert, W., Measurements of Wind Effects on Water-Side Controlled Gas Exchange in Riverine Systems, in Gas Transfer at Water Surfaces, W. Brutsaert and G.H. Jirka (Eds.), D. Reidel Publishing Co., Dordecht, Holland, 1984.

Junge, C.B., in Fate of Pollutants in the Air and Water Environments, Part I, Suffet, I.H. (ed.), Wiley, N.Y., 7-26, 1977.

Jury, W.A., Spencer, W.F., Farmer, W.J., Journal of Environmental Quality, 12, 558, 1983.

Kaiser, K. L. E., Non-linear Function for the Approximation of Octanol/water Partition Coefficients of Aromatic Compounds with Multiple Chlorine Substitution, Chemosphere, 12, 1159-1167, 1983.

Kamlet, M. J., R. M. Doherty, P. W. Carr, D. Mackay, M. H. Abraham and R. W. Taft, Linear Solvation Energy Relationships. 44. Parameter Estimation Rules that Allow Accurate Prediction of Octanol/Water Partition Coefficients and Other Solubility and Toxicity Properties of Polychlorinated Biphenyls and Polycyclic Aromatic Hydrocarbons, Environmental Science and Technology, 22, 503-509, 1988.

Karickhoff S. W., Semi-Empirical Estimation of Sorption of Hydrophobic Pollutants on Natural Sediments and Soil., Chemosphere, 10, 833-846, 1981.

Karickhoff, S.W., Brown, D.S., and Scott, T.A., Sorption of Hydrophobic Pollutants on Natural Sediments, Water Research, 13, 241-248, 1979.

Kenaga, G.E. and Goring, C.A.I., Relationship Between Water Solubility, Soil Sorption, Octanol-Water Partitioning, and Concentration of Chemicals in Biota, Aquatic Toxicology, 13, 78-109, 1980.

Kenaga, G. E., Predicted Bioconcentration Factors and Soil Sorption Coefficients of Pesticides and Other Chemicals, Ecotox.Environ.Safety., 4, 26-38, 1980a.

Kenaga, G. E., Correlation of Bioconcentration Factors of Chemicals in Aquatic and Terrestrial Organisms with their Physical and Chemical Properties, Environmental Science and Technology, 14, 553, 1980b.

Kier L.B. and Hall L.H., Molecular Connectivity in Chemistry and Drug Research, Academic Press, N.Y., 1976.

Koch R. and Nagel M., Toxicol. Environ. Quantitative Approach to Drug Design (ed. J. Dearden), Elservier, Amsterdam, 1983.

Leo A., Hansch C., Elkins D., Partition coefficients and their uses, Chem. Rev., **71**, 525-616, 1971.

Lewis, W.K. and Whitman, W.G., Principles of Gas Absorption, Industrial and Engineering Chemistry, 16(12), 1215-1220, 1924.

Lyman, W.J., Reehl, W.F., and Rosenblatt, D.H., Handbook of Chemical Property Estimation Methods, American Chemical Society, Washington, D.C., 1982, 1990.

Mackay D., Shiu W-Y., and Ma K-C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Volume I, Lewis Publishers, Inc., Chelsea, MI, 1992.

Mackay D., Shiu W-Y., and Ma K-C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Volume II, Lewis Publishers, Inc., Chelsea, MI, 1993a.

Mackay D., Shiu W-Y., and Ma K-C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Volume III, Lewis Publishers, Inc., Chelsea, MI, 1993b.

Mackay, D., Bobra, A., Shiu, W.Y., and Yalkowsky, S.H., Relationships Between Aqueous Solubility and Octanol-Water Partition Coefficients, Chemosphere, 9, 701-711, 1980.

Mackay, D., Paterson, S., Environmental Science and Technology, 15, 1006-1014, 1981.

Mackay, D. and Yeun, A.T.K., Mass Transfer Coefficient Correlations of Volatilization of Organic Solutes from Water, Environmental Science and Technology, 17, 1983.

Mackay D. and S. Paterson, Environmental Science and Technology, 16, 645a 1982.

Mackay D., Correlation of Bioconcentration Factors, Environmental Science and Technology, 6, 274, 1982.

Mackay D., Multimedia Environmental Models. The Fugacity Approach., Chelsea. Michigan: Lewis Publishers Inc. 1991.

Mailhot, H. And R. H. Peters, Empirical relationships Between the 1-octanol/water Partition Coefficient and Nine Physicochemical Properties, Environmental Science and Technology, 22, 1479-1488, 1988.

Marshall, J. and Palmer, W., The Distribution of Raindrops with Size, Journal of Meteorology, 5, 165-166, 1948.

Mayer, R., Letey, J., Farmer, W.J., Models for Predicting Volatilization of Soil-Incorporated Pesticides, Soil Science Society of America Proceedings, 38, 563-568, 1974.

Meylan W., Howard H., and Boethling R.S., Molecular Topology/Fragment Contribution Method for Predicting Soil Sorption Coefficients, Environmental Science and Technology,26, 1560-1567, 1992.

Miller, M.M., Ghodbane, S., Wasik, S.P., Tewari, Y.B., Martire, D.E., Aqueous Solubilities, Octanol/Water Partition Coefficients, and Entropies of Melting of Chlorinated Benzenes and Biphenyls, Journal of Chemical and Engineering Data, 29, 184-190, 1984.

Miller, M.M., Wasik, S.P., Huang, G.L., Shiu, W.Y., and MacKay, D. Relationships between Octanol-Water Partition Coefficient and Aqueous Solubility, Environmental Science and Technology, 19, 522-529, 1985.

Montgomery, J.H. and Welkom, L.M., Groundwater Chemicals Desk Reference, Lewis Publishers, Inc., 60-64, 1990.

National Research Council (NRC), Human Exposure Assessment for Airborne Pollutants -- Advances and Opportunities, National Academy Press, Washington D.C., 1991.

Nirmalakhandan, N. N. and R. E. Speece., Prediction of Aqueous Solubility of Organic Chemicals Based on Molecular Structure. 2. Application to PNAs, PCBs, PCDDs, etc., Environmental Science and Technology, 23, 708-713, 1989.

Nirmalakhandan, N. N. and R. E. Speece.,Environmental Science and Technology, 222, 328, 1988.

Nirmalakhandran, N. N. And R. E. Speece, QSAR Model for Predicting Henry's Constant, Environmental Science and Technology, 22, 1349-1357, 1988.

Norstrom R.J., A.E. McKinnon, and A.S.W. DeFreitas., A Bioenergetics Based Model for Pollutant Accumulation by Fish. Simulation of PCB and Methylmercury Residue Levels in Ottawa River Yello Perch (Perca Flavescens)., The Journal of the Fisheries Research Board of Cananda, 33, 248-267, 1976.

O'Connor, D., Wind Effects of Gas-Liquid Transfer Coefficients, Journal of Environmental Engineering, 109(3), 731-752, 1983.

Onishi Y., Shulyer L., Cohen Y., Multimedia Modeling of Toxic Chemicals, Proceedings of the International Symposium on Water Quality Modeling of Agricultural and Non-Point Sources, Part II, Donn G. Decoursey (Editor), USDA ARS-81, pp 475-479, 1990.

Pankow, J.F., Review and Comparative Analysis of the Theories on Partitioning Between the Gas and Aerosol Phases in the Atmosphere, Atmospheric Environment, 21, 2275-2284, 1987.

Pankow, J., F., Common y-Intercept and Single Compound Regressions of Gas-Particle Partitioning Data vs 1/T, Atmospheric Environment, 25A, 2229-2239, 1991.

Paterson, S., Mackay, D., A model of Organic chemical Uptake by Plants from Soil and the Atmosphere, Environmental Science and Technology, 28, 2259-2266, 1994.

Paterson, S. and Mackay, D., Bacci, E., Calamari, D., Correlation of the Equilibrium and Kinetics of Leaf-AirExchange of Hydrophobic Organic Chemicals, Environmental Science and Technology, 25, 866-871, 1991.

Patil G.S., Correlation of Water Solubility and Octanol-water Partition Coefficient Based on Molecular Structure, Chemosphere, 22, 723-738, 1991.

Pividal, K. A. And S. I. Sandler, Neighbor Effects in the Group Contribution Method: Infinite Dilution Activity Coefficients of Binary Systems Containing Primary Alcohols, Journal of Chemical and Engineering Data, 35, 53-60, 1990.

Plate, E.J. and Friedrich, R., Reaeration of Open Channel Flow, Gas Transfer at Water Surfaces, W. Brutsaert and G.H. Jirka (Eds.), Dordecht, Holland, 1984.

Rao, P.S.C., Davidson, J.M., Estimation of Pesticide Retention and Transformation Parameters Required in Nonpoint Source Pollution Models, Environmental Impact of Nonpoint Source Pollution, 1980.

Reid, R.C., Prausnitz, J.M., and Poling, B.E., The Properties of Gases and Liquids, 4th Edition, McGraw-Hill Book Company, New York, 1987.

Reid, R.C., Prausnitz, J.M., and Sherwood, T.K., The Properties of Gases and Liquids, 3rd Edition, McGraw-Hill Book Company, New York, 1977.

Ryan, P.A. and Cohen, Y., Multimedia Transport of Particle-Bound Organics: Benzo(a)pyrene Test Case, Chemosphere, 15(1), 21-47, 1986.

Ryan, P. and Cohen, Y., Diffusion of Sorbed Solutes in Gas and Liquid Phases of Low-Moisture Soils, Soil Science Society of America Journal, 54, 2, 1990.

Sabljic, A. And H. Gusten, Predicting Henry's Law Constants for Polychlorinated Biphenyls, Chemosphere, 19, 1503-1511, 1989.

Sabljic A., Quantitative Modeling of Soil Sorption for Xenobiotic Chemicals, Environ. Health. Perspect., 83, 179-190, 1989.

Sabljic, A., H. Gusten, J. Hermens and A. Opperhulzen, Modeling Octanol/Water Partition Coefficients by Molecular Topology: Chlorinated Benzenes and Biphenyls, Environmental Science and Technology, 27, 1394-1402, 1993.

Sehmel, G.A., Particle and Gas Deposition: A Review, Atmospheric Environment, 14, 9831011, 1980.

Sheffield, A. E., Pankow, J. F., Specific Surface Area of Urban Atmospheric Particulate Matter in Portland, Oregon,Environmental Science and Technology, 28, 9, 1759-1766, 1994.

Shen, T., Schmidt, C.E., and Card, T., Assessment and Control of VOC Emissions from Waste Treatment and Disposal Facilities, Van Nostrand Reinhold Publishing, New York, New York, 1993.

Shiu W-Y., Ma K-C., Varhanickova D., and Mackay D., Chlorophenols and Alkyphenols: Aa Review and Correlation of Environmentally Relevant Properties and Fate in an Evaluative Environment, Chemosphere, 29, 1155-1224, 1994.

Shiu W.-Y., Doucette W., Gobas F.A.P.C., Mackay D., Andren A.W., 1988. Physical-Chemical Properties of Chlorinated Dibenzo-p-dioxins, Environmental Science and Technology, 22, 651-658, 1988.

Shiu W-Y, Mackay, D., A Critical Review of Henry's Law Constants for Chemicals of Environmental Interest, The Journal of Physical Chemistry Data, 10 , 1175-1199, 1982.

Slinn, W.G.N., Prediction for Particle Deposition to Vegetative Canopies, Atmospheric Environment, 16, 1785-1792, 1982.

Slinn, S. A., Slinn, W. G. N., Predictions for Particle Deposition on Natural Waters, Atmospheric Environment, 1013-1016, 1980.

South Coast Air Quality Management District (SCAQMD), Multipathway Health Risk Assessment Input Parameters Guidance Document, 1988.

Southworth, G. R. And J. L. Keller, Hydrophobic Sorption of Polar Organics by Low Organic Carbon Soils, Water.Soil.and.Air.Poll., 28, 239-248, 1986.

Swackhamer, D.L., Armstrong, D.E., Journal of Great Lakes Research, 1979.

Syracuse Research Corporation, Environmental Fate Data Base, Syracuse, NY, 1994.

Thomann R.V., Bioaccumulation Model of Organic Chemical Distribution in Aquatic Food Chains., Environmental Science and Technology , 23, 699-707, 1989.

Tsai, W., Cohen, Y., Sakugawa, H., and Kaplan, I., Dynamic Partitioning of Semi-Volatile Organics in Gas/Particle/Rain Phases During Rain Scavenging, Environmental Science and Technology, 25(12), 2012-2022, 1991.

U.S. EPA Office of Pesticides and Toxic Substances Exposure Evaluation Division PCGEM'S User's Guide Release 1.0, Sept., 1989.

Van de Water, R., Modeling the Transport and Fate of Volatile and Semi-Volatile Organics in a Multimedia Environment, M.S. Thesis, Department of Chemical Engineering, UCLA, 1995.

Cohen, Y. and R. van de Water, "Environmental Distribution of Organics," 267-278, in Computer Techniques in Environmental Studies V. Vol. I: Pollution Modeling, Zannetti (Ed.), Computational Mechanics Publications, Southampton, UK (1994).

Veith, G. D., D. L. Defoe and B. V. Bergstedt, Measuring and Estimating the Bioconcentration Factors of Chemicals in Fish,The Journal of the Fisheries Resources Board of Canada, 36, 1040-1048, 1979.

Vohra, Rajeev, Dynamic Partitioning and Intermedia Transport of Hydrophobic Chemicals in Aquatic Systems, M.S. Thesis, Department of Chemical Engineering, University of California, Los Angeles, 1996.

Whitby, K.T., The Physical Characteristics of Sulfur Aerosols, Atmospheric Environment, 12, 135-159, 1978.

Wilke, C.R. and Chang P., Correlation of Diffusion Coefficients in Dilute Solutions, AIChE Journal, 1, 264-70, 1955.

Williams, R.M., A Model of the Dry Deposition of Particles to Water Surfaces, Atmospheric Environment, 16, 1933-1938, 1982.

Wu, J., Wind-Induced Drift Current, Journal of Fluid Mechanics, 68, 49-70, 1975.

Wu, J., Oceanic Whitecaps and Sea State, Journal of Physical Oceanography, 9, 1064-1068, 1979.

Wu, J., The Wind-Stress Coefficient over Sea Surface Near Neutral Conditions - A Revisit, Journal of Physical Oceanography, 10, 727-740, 1980.

Yalkowsky, S.H., Orr, R.J., Valvani, S.C., Solubility and Partitioning: 3. The Solubility of Halobenzenes in Water, Industrial Engineering Chemistry Fundamentals, 18, 351-353, 1979.

Yalkowsky, S.H., Valvani, S.C., Solubilities and Partitioning: 2. Relationships between Aqueous Solubilities, Partition Coefficients, and Molecular Surface Areas of Rigid Aromatic Hydrocarbons, Journal of Chemical and Engineering Data, 24, 127-129, 1979.

Yamasaki, H., Kuwata, K., Miyamoto, H., Effects of Ambient Temperature on Aspects of Airborne Polycyclic Aromatic Hydrocarbons, Environmental Science and Technology, 16, 189-194, 1982.

APPENDIX A: ADDITIONAL CHEMBASE PARAMETER REFERENCES

Agency for Toxic Substances and Disease Registry (ATSDR), *Toxicological Profile for ______*, U.S. Department of Health & Human Services, Public Health Service,, Division of Toxicology/Toxicology Information Branch, Atlanta, Georgia, 1989-1995.

Air Pollution Control Association, Journal of the Air Pollution Control Association, Pittsburgh, 32, 1982.

Bondi, A., Van der Waals Volumes and Radii, Journal of Physical Chemistry, 68, 441, 1964.

Cohen, Y., Winer, A. M., Creelman, L., Stein, E., Kwan, A., and Chu, J., Development Of Intermedia Transfer Factors for Toxic Air Pollutants, Contract No. A032-170, California Air Resources Board, Vol. I-VII, 1994.

Dean, J. D., Lange's Handbook of Chemistry, 12nd Edition, McGraw-Hill Book Company, New York, 1985.

Environmental Fate Database by Syracuse Research Corporation, 1994.

Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M., Handbook of Environmental Degradation Rates, Lewis Publishers, Chelsea, Michigan, 1991.

Howard, P. H., Jarvus, W. F., Sage, G. W., Basu, D. K., Gray, D. A., Meylan, W., Crosbie, E. K., Handbook of Environmental Fate and Exposure Data For Organic Chemicals, Vol. I, Lewis Publishers, Chelsea, Michigan, 1989.

Howard, P. H., Sage, G. W., Jarvus, W. F., Gray, D. A., Handbook of Environmental Fate and Exposure Data For Organic Chemicals, Vol. II, Lewis Publishers, Chelsea, Michigan, 1990.

Howard, P. H., Michalenko, E. M., Jarvis, W. F., Basu, D. K., Sage, G. W., Meylan, W. M., Beauman, J. A., Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Vol. III, Lewis Publishers, Chelsea, Michigan, 1991.

Kurtz, D. A., Long Range Transport of Pesticides, Lewis Publishers, Chelsea, Michigan, 1990.

Lide, D. R., Handbook of Chemistry and Physics, 72nd Edition, CRC Press, Cleveland, Ohio, 1991-92.

Lyman, W. J., Reehl, W. F., Rosenblatt, D. H., Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, American Chemical Society Publishers, Washington DC, 1990.

Mackay, D., Shiu, W. Y., Ma, K. C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Oxygen, Nitrogen, and Sulfur Containing Compounds, Vol. IV, Lewis Publishers, Chelsea, Michigan, 1995.

Mackay, D., Shiu, W. Y., Ma, K. C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Volatile Organic Chemicals, Vol. III, Lewis Publishers, Chelsea, Michigan, 1993.

Mackay, D., Shiu, W. Y., Ma, K. C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs, Vol. I, Lewis Publishers, Chelsea, Michigan, 1992.

Mackay, D., Shiu, W. Y., Ma, K. C., Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans, Vol. II, Lewis Publishers, Chelsea, Michigan, 1992.

McKone, T. E., Daniels, J. I., Chiao, F. F., and Hsieh, D. P. H., Intermedia Transfer Factors for Fifteen Toxic Pollutant Released to Air Basins in California, Report No. UCRL-CR-115620, The California Air Resources Board and The Office of Environmental Health Hazard Assessment (CalEPA), 1993.

Montgomery, J. H., Welkom, L. M., Groundwater Chemicals Desk Reference, Lewis Publishers, Chelseas, Michigan, 1990.

Reid, R. C., Prausnitz, J. M., Sherwood, T. K., The Properties of Gases and Liquids, Third Edition, McGraw-Hill Book Company, New York, 1987.

Reid, R. C., Prausnitz, J. M., Sherwood, T. K., The Properties of Gases and Liquids, Fourth Edition, McGraw-Hill Book Company, New York, 1977.

Stephonson, R. M., Malanowski, A., Handbook of the Thermodynamics of Organic Compound, Elsevier, New York 1987.

U.S. E.P.A., Superfund Public Health Evaluation Manual, Office of Emergency and Remedial Response; Office of Solid Waste Emergency Response, Oswer Directive 9285.4-1, Washington, D.C., 1987.

Verschueren, K., Handbook of Environmental Data on Organic Chemicals, Second Edition, Van Nostrand Reinhold, New York, 1983.

Zwolinski, B. J., Wilhoit, R. C., Estok, G. K., Mahoney, G. B., Dregne, S. M., Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds, College Station: Thermodynamics Research Center, Department of Chemistry, Texas A & M University, 1971.

APPENDIX B: CPP Correlations developed for ITFP

B1. Overview

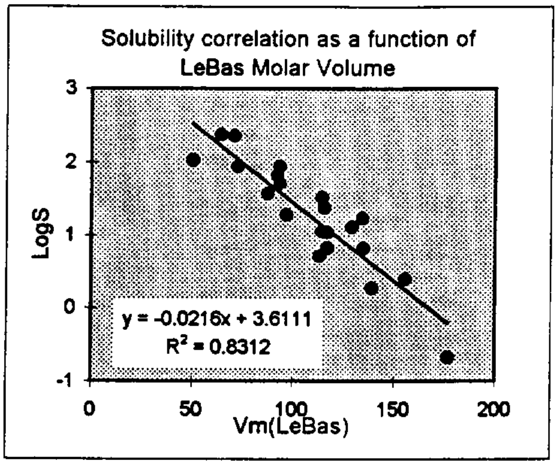
Chemical class-specific correlations for K_{ow}, solubility and BCF were developed for the CPP based on CHEMBASE data and additional data obtained from Mackay et al. (1992a,b, 1993, 1995) and BCF data presented Veith et al. (1979). Data for K_{ow}, solubility, BCF from the above compilations was selected as described in sections 4.3 and 6.2. The correlations presented in the Appendix complement the literature correlations used in the CPP as described in section 6.

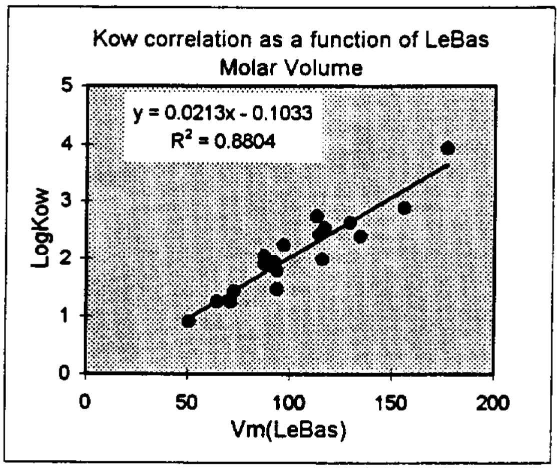
Table 1. Chloroalkanes

Compound	$V_{m(LeBas)}$ (cm³/mol)	S (mol/m³)	logS (mol/m³)	$\log K_{ow}$ (unitless)
1-Chlorobutane	117.1	6.64	0.822	2.54
1-Chloropentane	139.3	1.86	0.270	
1-Chloropropane	87.5	36.92	1.567	2.04
1,1-Dichloroethane	93.6	50.53	1.704	1.79
1,1,1,2-Tetrachloroethane	135.0	6.55	0.816	
1,2,3-Trichloropropane	129.3	12.88	1.110	2.63
2-Chlorobutane	117.1	10.80	1.033	
2-Chloropropane	87.5	37.88	1.578	1.90
Dichloromethane	71.0	228.40	2.358	1.25
Pentachloroethane	156.0	2.47	0.393	2.89
Hexachloroethane	177.0	0.21	-0.675	3.93
1,1,1-Trichloroethane*	114.5	11.21	1.050	2.42
1,1,2,2-Tetrachloroethane*	134.5	17.10	1.233	2.39
1,1,2-Trichloroethane*	114.5	32.98	1.518	2.42
1,2-Dichloroethane*	93.6	87.81	1.944	1.46
1,2-Dichloropropane*	115.8	23.90	1.378	1.99
Chloroethane*	72.7	88.03	1.945	1.43
Chloroform*	92.3	66.34	1.822	1.94
Chloromethane*	50.5	105.47	2.023	0.91
Carbon tetrachloride*	113.2	5.17	0.713	2.75
Chlorodibromomethane*	97.1	19.20	1.283	2.24
Methyl Chloride*	64.5	235.50	2.372	1.25

Note that * refers to chembase chemical.

Figure 1a-c. ITF Correlations for Chloroalkanes.





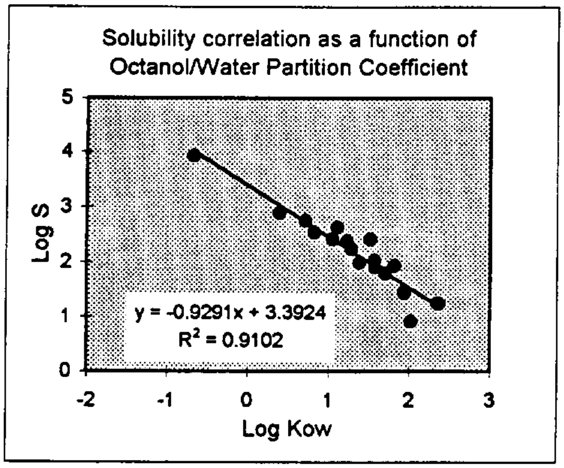


Table 2. Chloroalkenes

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
1,1-Dichloroethene*	86.2	25.787	1.411	2.13
1,3-Dichloroethylene	86.2			2.28
cis-1,2-Dichloroethene*	86.2	36.105	1.558	1.86
trans-1,2-Dichloroethene*	86.2	64.576	1.810	2.09
Tetrachloroethylene*	128.0	0.900	-0.046	3.00
Trichloroethylene*	107.1	8.370	0.923	2.42
Hexachloro-1,3-butadiene	206.8	0.013	-1.886	4.78
Hexachlorocyclopentadiene	210.1	0.007	-2.180	5.04
Vinyl chloride*	65.3	44.208	1.646	1.37

Note that * refers to chembase chemical.

Figure 2a-c. ITF Correlations for Chloroalkenes.

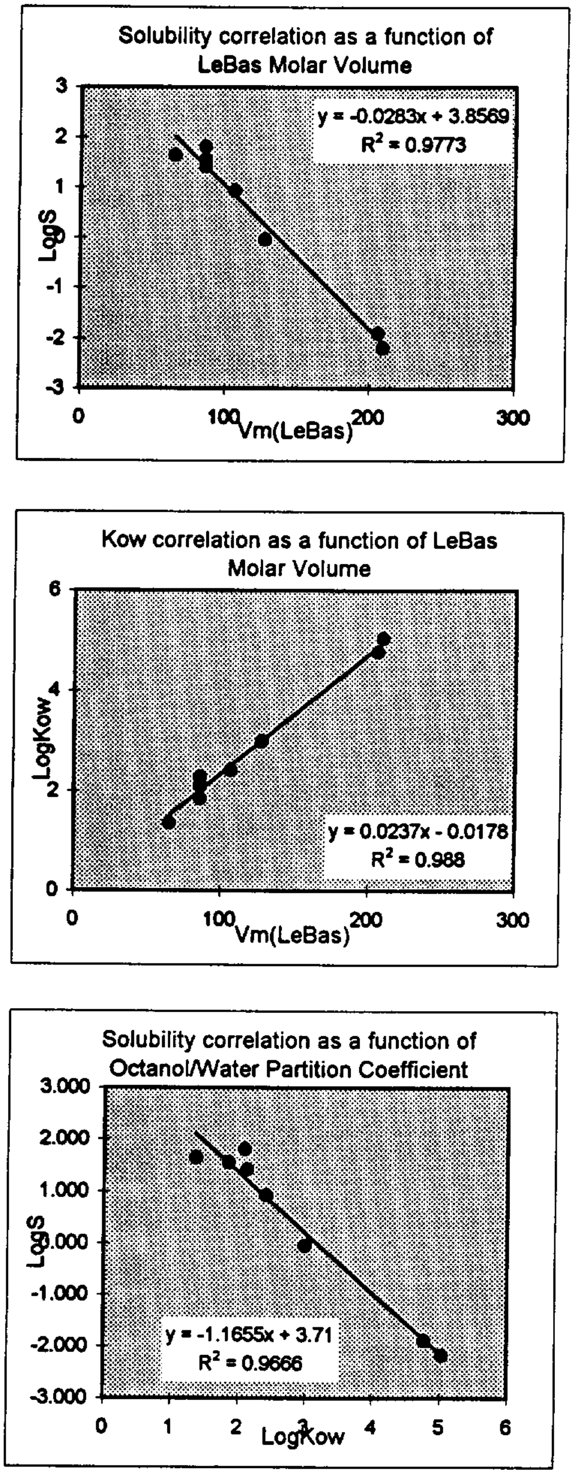


Table 3. Benzenes and Alkylbenzenes

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
Benzene*	96.0	22.788	1.358	2.13
Ethylbenzene*	140.4	1.413	0.156	3.13
Toluene*	118.2	5.590	0.747	2.69
Xylene (mixed)*	140.4	1.220	0.086	3.33
m-xylene*	140.4	1.525	0.183	3.20
o-xylene*	140.4	1.778	0.250	3.16
p-xylene*	140.4	1.781	0.251	3.18
1,2,3-Trimethylbenzene	162.6	0.585	-0.233	3.55
1,2,4-Trimethylbenzene	162.6	0.467	-0.331	3.63
1,3,5-Trimethylbenzene	162.6	0.427	-0.370	3.42
n-Propylbenzene	170.0	0.428	-0.369	3.69
iso-Propylbenzene	170.0	0.449	-0.348	3.56
1-Ethyl-2-methylbenzene	162.6	0.621	-0.207	3.53
1-Ethyl-4-methylbenzene	162.6	0.789	-0.103	3.63
iso-propyl-4-methylbenzene	184.8	0.174	-0.759	4.10
n-Butylbenzene	184.8	0.106	-0.975	4.38
iso-Butylbenzene	184.8	0.075	-1.125	4.01
sec-Butylbenzene	184.8	0.131	-0.883	
tert-Butylbenzene	184.8	0.237	-0.625	4.11
1,2,4,5-Tetramethylbenzene	184.8	0.026	-1.585	4.24
n-Pentylbenzene	207.0	0.024	-1.614	4.90
Pentamethylbenzene	207.0	0.105	-0.979	4.57
n-Hxylbenzene	229.2	0.006	-2.222	5.40

Note that * refers to chembase chemical.

Figure 3a-c. ITF Correlations for Benzenes and Alkylbenzenes.

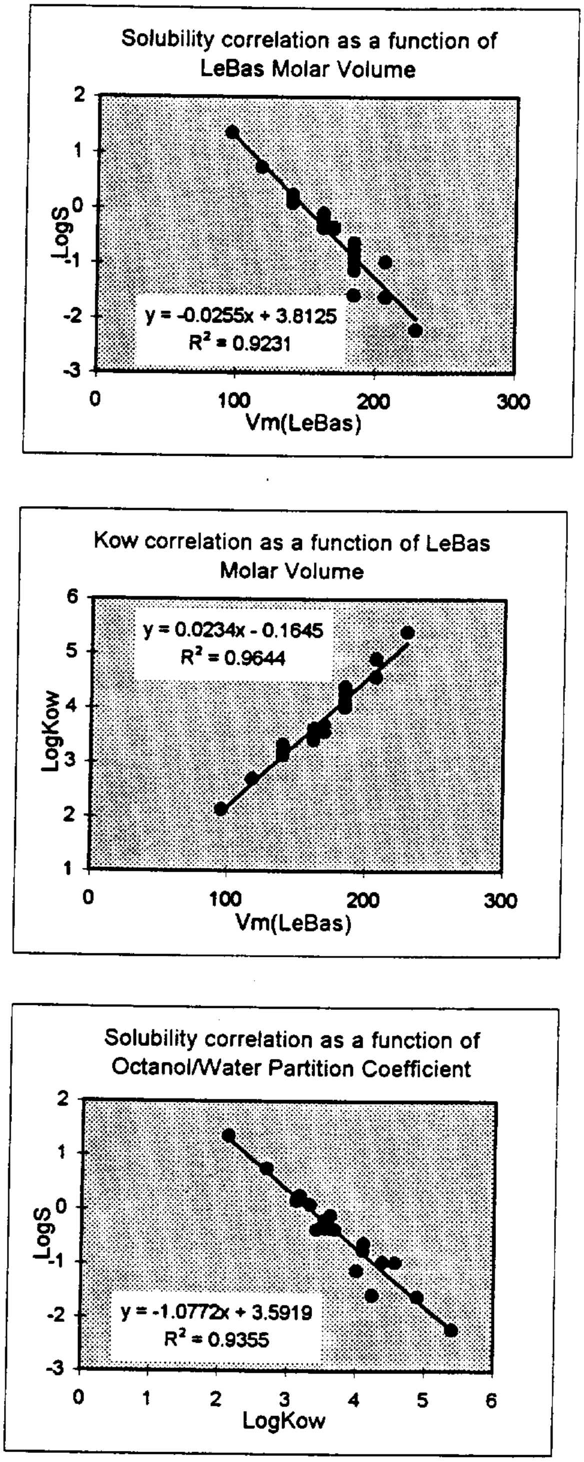


Table 4. Phenol and Chlorophenol

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
Phenol*	103.4	871.68	2.940	1.46
2-chlorophenol	124.3	185.78	2.269	2.21
3-chlorophenol	124.3	202.24	2.306	2.54
4-chlorophenol	124.3	203.24	2.308	2.47
2,4-chlorophenol	145.2	34.24	1.535	3.22
2,6-chlorophenol	145.2	16.10	1.207	3.01
3,4-chlorophenol	145.2	56.79	1.754	3.52
2,3,4-chlorophenol	166.1	2.53	0.403	3.81
2,4,5-chlorophenol	166.1	4.80	0.681	4.03
2,4,6-chlorophenol*	166.1	4.56	0.659	3.69
2,3,4,5-chlorophenol	187.0	0.72	-0.143	4.65
2,3,4,6-chlorophenol	187.0	0.79	-0.102	4.46
Pentachlorophenol*	207.9	0.06	-1.222	5.12

Note that * refers to chembase chemical.

Figure 4a-c. ITF Correlations for Phenol and Chlorophenol.

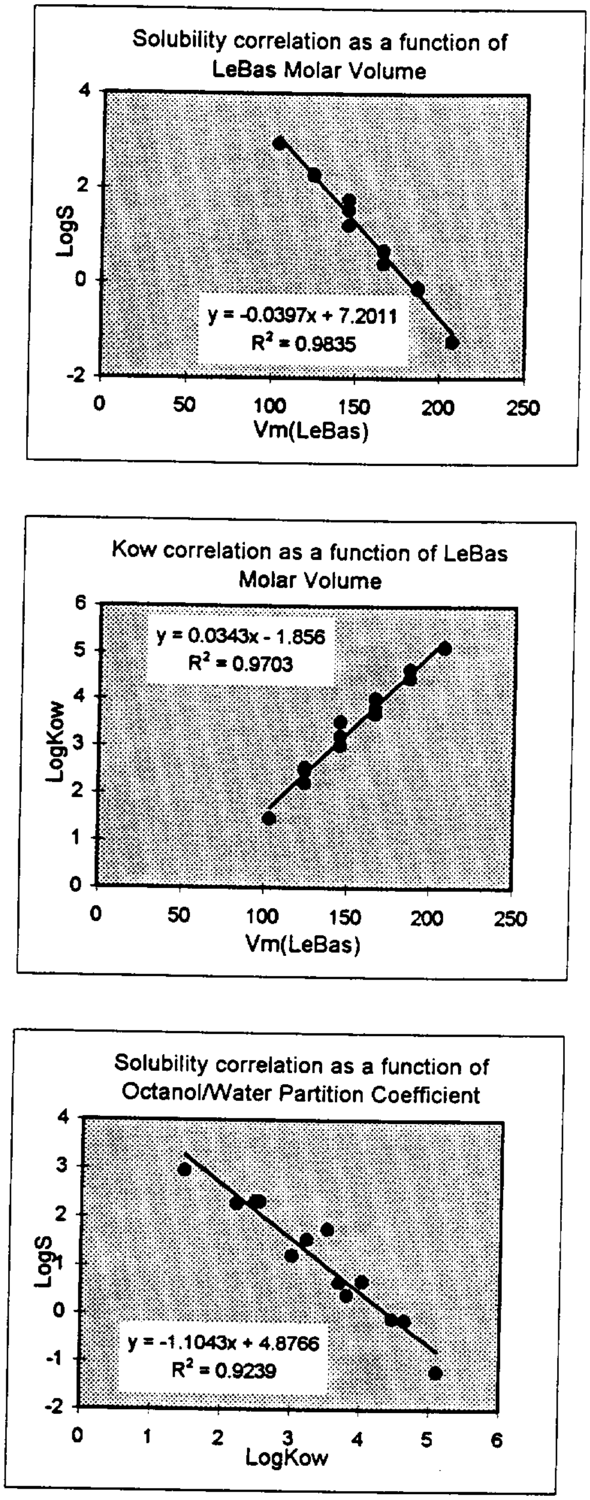


Table 5. Chlorobenzenes

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK$_{ow}$ (unitless)
Chlorobenzene	117	4.3E+0	0.632	2.93
1,2-Dichlorobenzene	138	1.0E+0	0.008	3.52
1,3-Dichlorobenzene	138	8.8E-1	-0.058	3.50
1,4-Dichlorobenzene*	138	5.6E-1	-0.256	3.54
1,2,3-Trichlorobenzene	159	9.8E-2	-1.008	4.09
1,2,4-Trichlorobenzene	159	2.0E-1	-0.705	3.99
1,3,5-Trichlorobenzene	159	3.7E-2	-1.437	4.20
1,2,3,4-Tetrachlorobenzene	180	3.5E-2	-1.453	4.58
1,2,3,5-Tetrachlorobenzene	180	1.6E-2	-1.804	4.66
1,2,4,5-Tetrachlorobenzene	180	2.1E-3	-2.681	4.61
Pentachlorobenzene	200	1.8E-3	-2.756	5.15
Hexachlorobenzene	221.4	1.8E-5	-4.750	5.53

Note that * refers to chembase chemical.

Figure 5a-c. ITF Correlations for Chlorobenzenes.

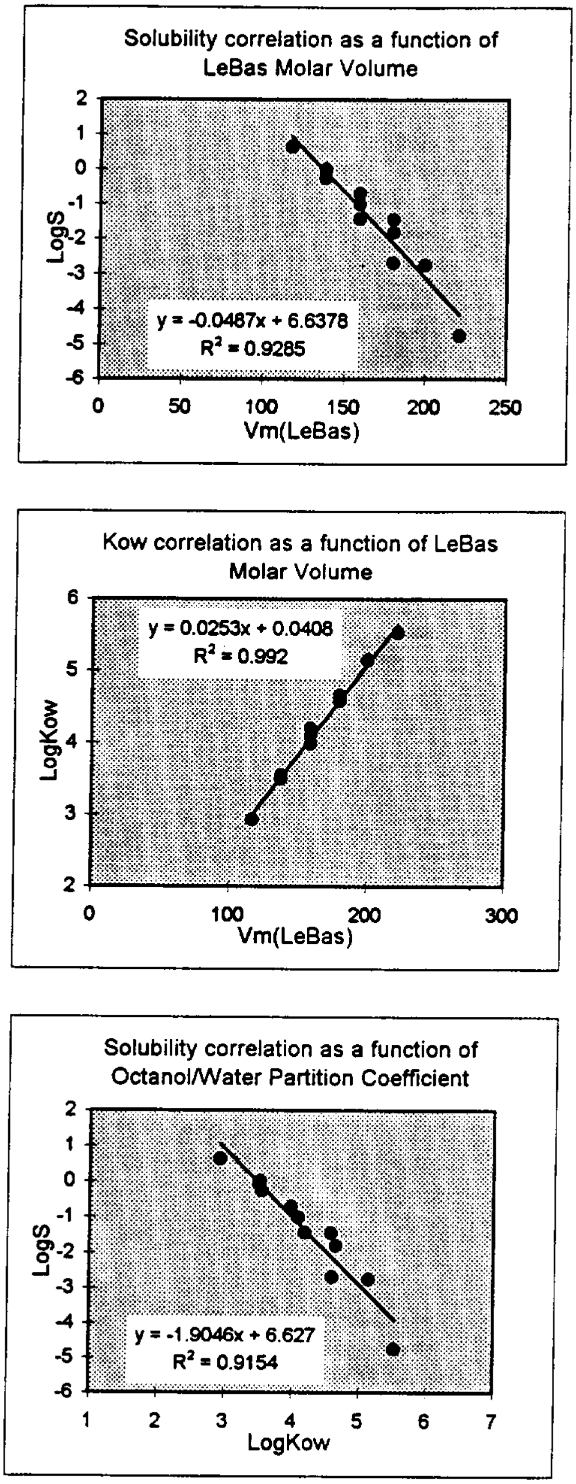


Table 6. PAHs

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
Indan	143.7	9.3E-1	-0.031	3.33
Naphthalene*	147.6	2.4E-1	-0.614	3.34
1-Methylnaphthalene	169.8	2.0E-1	-0.689	3.87
2-Methylnaphthalene	169.8	1.8E-1	-0.755	4.00
1,3-Dimethylnaphthalene	192.0	5.1E-2	-1.291	4.42
1,4-Dimethylnaphthalene	192.0	7.3E-2	-1.137	4.37
1,5-Dimethylnaphthelene	192.0	2.0E-2	-1.708	4.38
2,3-Dimethylnaphthalene	192.0	1.9E-2	-1.717	4.40
2,6-Dimethylnaphthalene	192.0	1.1E-2	-1.963	4.31
1-Ethylnaphthalene	192.0	6.8E-2	-1.164	4.39
2-Ethylnaphthalene	192.0	5.1E-2	-1.292	4.38
1,4,5-Trimethylnaphthalene	214.2	1.2E-2	-1.909	4.90
Bibenzyl	206.8	2.4E-2	-1.620	4.76
trans-Stilbene	221.6	1.6E-3	-2.793	4.81
Acenaphthene*	173.0	2.7E-2	-1.576	4.10
Acenaphthylene*	165.7	2.6E-2	-1.588	4.03
Fluorene*	188.0	1.1E-2	-1.963	4.18
1-Methyfluorene	210.0	6.1E-3	-2.218	4.97
Phenanthrene*	199.0	7.5E-3	-2.124	4.46
1-Methylphenanthrene	218.7	1.4E-3	-2.853	5.14
Anthracene*	199.2	3.1E-4	-3.511	4.49
9-Methylanthracene	219.0	1.4E-3	-2.867	5.42
2-Methylanthracene	219.0	1.7E-4	-3.762	5.15
9,10-Dimethylanthracene	241.0	2.7E-4	-3.566	5.65
Pyrene*	214.0	7.0E-4	-3.155	5.18
Fluoranthene*	217.0	1.2E-3	-2.923	5.20
Benzo[a]fluorene	240.0	2.1E-4	-3.682	5.75
Benzo[b]fluorene	240.0	9.2E-6	-5.034	5.75
Chrysene*	251.0	8.6E-6	-5.065	6.06
Triphenylene	251.0	1.9E-4	-3.725	5.45
p-Terphenyl	258.2	7.8E-5	-4.107	6.03
Naphthacene	251.0	2.5E-6	-5.603	5.91
Benz[a]anthracene*	248.0	4.8E-5	-4.317	5.90
Benzo[a]pyrene*	263.0	1.6E-5	-4.803	6.30
Benzo[e]pyrene	263.0	2.2E-5	-4.649	6.44
Perylene	263.0	1.6E-6	-5.800	6.50
Benzo[b]fluoranthene*	268.9	5.9E-6	-5.226	6.18
Benzo[j]fluoranthene	268.9	9.9E-6	-5.004	6.44
Benzo[k]fluoranthene*	268.9	3.2E-6	-5.499	6.59
7,12-DMBA	282.7	1.6E-4	-3.793	5.90
9,10-DMBA	282.7	1.7E-4	-3.770	6.93
3-Methylcholanthracene	296.0	1.1E-5	-4.966	6.42
Benzo[ghi]perylene*	277.0	9.4E-7	-6.026	6.72
D[a,c]A	300.0	5.7E-6	-5.240	7.19
D[a,h]A*	302.4	2.0E-6	-5.704	6.50
D[a,j]A	300.0	4.3E-5	-4.365	7.19
Indeno(1,2,3-cd)pyrene*	283.5	2.2E-4	-3.650	6.51
Coronene	292.0	4.7E-7	-6.332	6.50

Note that * refers to chembase chemical.

Figure 6a-c. ITF Correlations for PAHs.

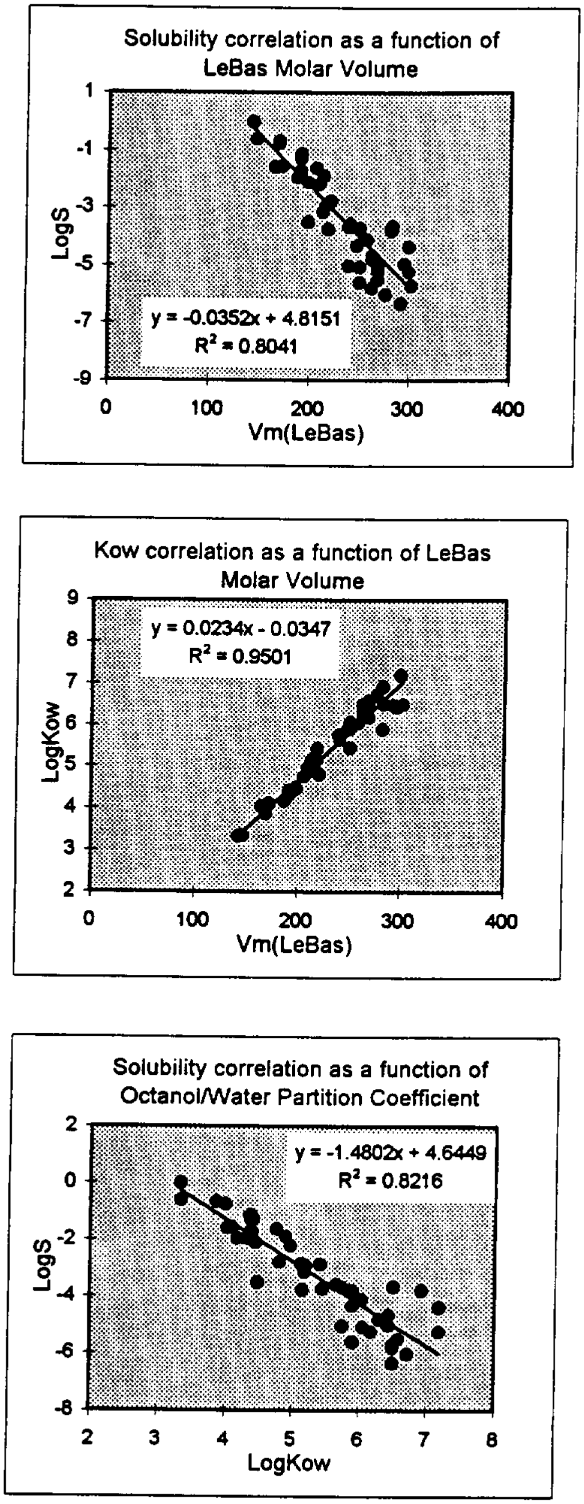


Table 7. PCBs

Compound IUPAC	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
0	184.6	4.8E-2	-1.317	3.88
1	205.4	2.5E-2	-1.602	4.48
2	205.4	1.3E-2	-1.889	4.50
3	205.4	6.9E-3	-2.164	4.50
4	226.4	6.0E-3	-2.222	4.98
7	226.4	5.4E-3	-2.269	4.97
8	226.4	4.8E-3	-2.316	4.91
9	226.4	9.0E-3	-2.047	5.10
10	226.4	6.3E-3	-2.202	5.00
11	226.4	3.5E-4	-3.456	5.30
18	247.3	1.8E-3	-2.743	5.62
26	247.3	9.8E-4	-3.008	5.18
28	247.3	4.8E-4	-3.315	5.58
29	247.3	4.9E-4	-3.311	5.80
30	247.3	8.6E-4	-3.065	5.52
33	247.3	3.0E-4	-3.519	5.80
40	268.2	1.2E-4	-3.934	5.80
44	268.2	4.3E-4	-3.368	6.00
47	268.2	1.9E-4	-3.731	5.90
52	268.2	1.7E-4	-3.768	6.10
53	268.2	2.2E-4	-3.652	5.55
54	268.2	4.1E-5	-4.390	5.86
60	268.2	2.0E-4	-3.702	6.24
61	268.2	5.8E-5	-4.235	6.18
66	268.2	2.0E-4	-3.702	6.13
75	268.2	3.1E-4	-3.506	6.03
86	289.1	1.3E-5	-4.870	6.38
87	289.1	3.2E-5	-4.500	6.50
88	289.1	3.7E-5	-4.435	6.50
101	289.1	3.4E-5	-4.474	7.10
104	289.1	4.8E-5	-4.321	5.37
110	289.1	5.4E-5	-4.267	6.26
116	289.1	3.1E-5	-4.509	6.65
3,3-Dichlorobenzidine*	255.8	N/A	N/A	N/A
DDD*	312.6	5.0E-4	-3.301	6.20
DDE*	305.2	3.8E-4	-3.424	7.00
DDT*	335.5	9.6E-6	-5.018	6.19
Aroclor 1016 (PCB)*	N/A	1.6E-3	-2.788	5.52
Aroclor 1221 (PCB)*	N/A	1.9E-2	-1.714	4.09
Aroclor 1232 (PCB)*	N/A	6.2E-3	-2.205	4.55
Aroclor 1248 (PCB)*	N/A	2.8E-4	-3.553	6.02
Aroclor 1254 (PCB)*	N/A	1.9E-4	-3.721	6.38
Aroclor 1260 (PCB)*	N/A	1.4E-5	-4.854	6.87

Note that * refers to chembase chemical.

Figure 7a-c. ITF Correlations for PCBs.

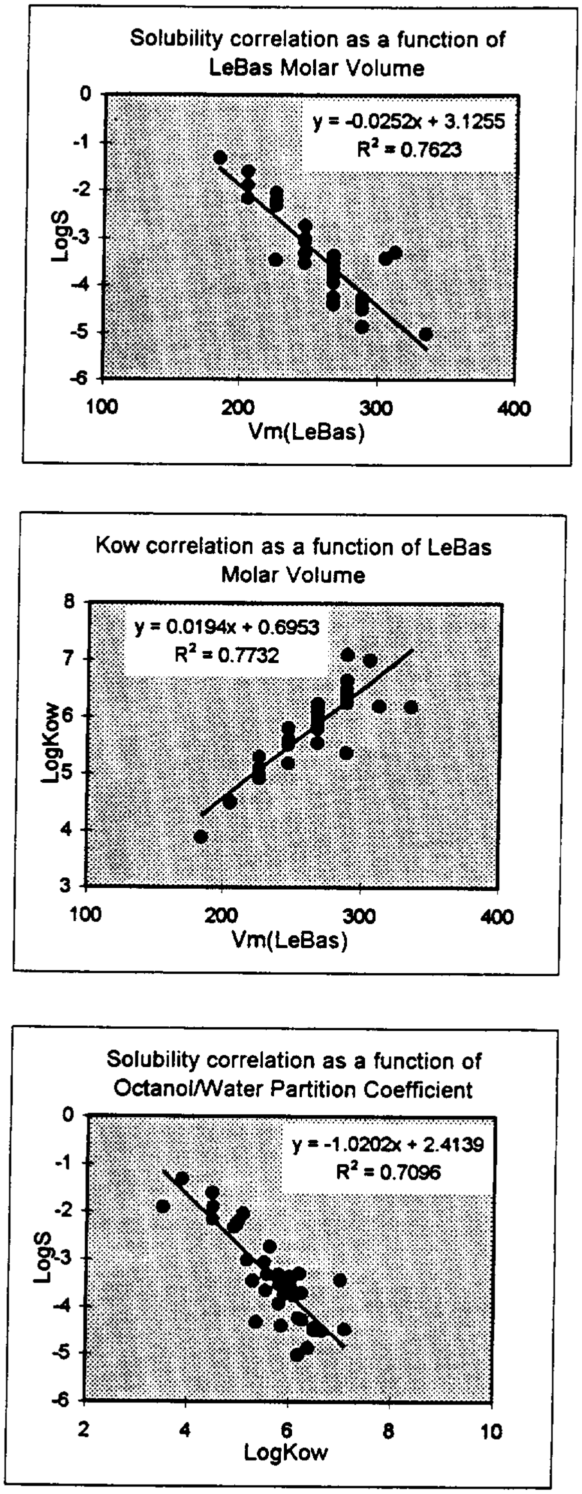


Table 8. Aliphatic and Aromatic Ethers

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK_{ow} (unitless)
Methyl ether	60.9	3.7E+3	3.567	0.10
Methyl t-butyl ether	127.5	4.1E+2	2.617	0.94
Di-n-propyl ether	151.6	4.1E+1	1.610	2.03
Di-isopropyl ether	151.6	6.3E+1	1.797	1.52
Di-n-butyl ether	196.0	1.8E+0	0.248	3.21
Butylethyl ether	150.5	6.4E+1	1.804	2.03
Propylene oxide	69.7	8.2E+3	3.914	0.03
1,4-Dioxane*	91.8			-0.42
Benzyl ethyl ether	173.6			2.64
Anisole (methoxybenzene)	137.3	1.6E+1	1.195	2.10
Phenetole (ethoxybenzene)	143.5	4.6E+0	0.661	2.68
Styrene oxide	138.0	2.3E+1	1.367	1.71
Cellosolve*	105.3	N/A	N/A	-0.33

Note that * refers to chembase chemical.

Figure 8a-c. ITF Correlations for Aliphatic and Aromatic Ethers.

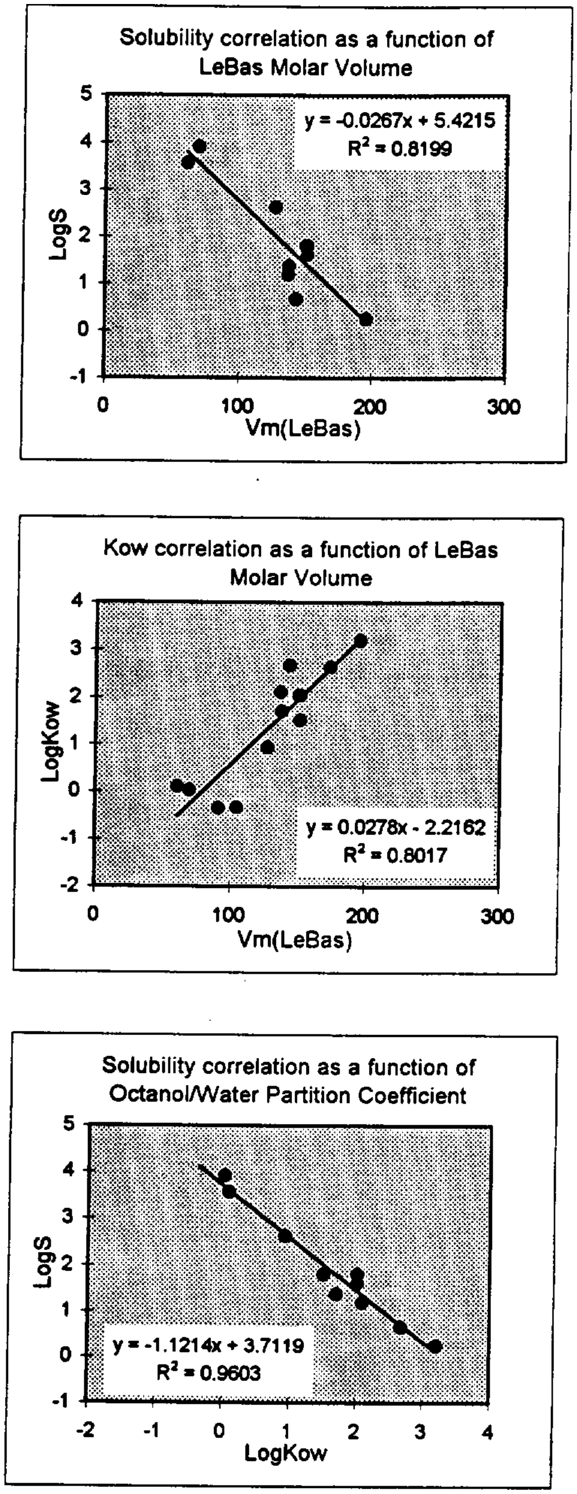
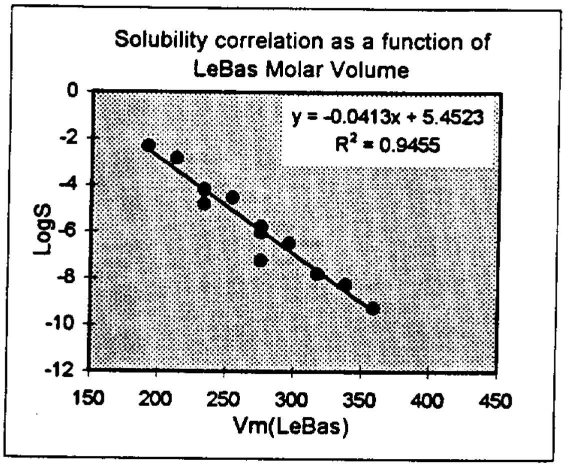


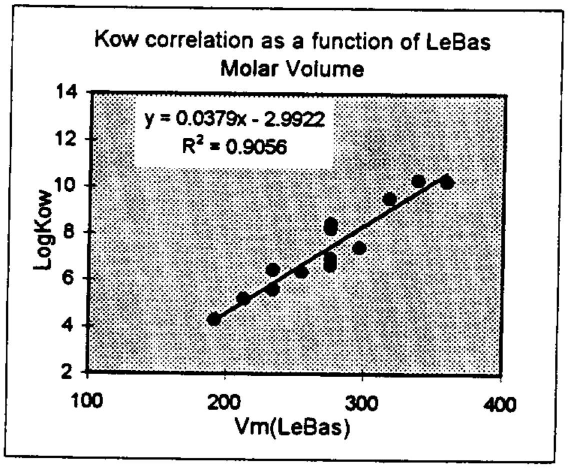
Table 9. Chlorinated Dioxins

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	$\log K_{ow}$ (unitless)
Dibenzo-p-dioxin (DD)	192.0	4.7E-3	-2.330	4.30
2-CDD	212.9	1.4E-3	-2.855	5.20
2,3-DCDD	233.8	5.9E-5	-4.230	5.60
2,7-DCDD	233.8	1.5E-5	-4.829	6.43
2,8-DCDD	233.8	6.6E-5	-4.180	5.60
1,2,4-T3CDD	254.7	2.9E-5	-4.534	6.35
1,2,3,4-TCDD	275.6	1.7E-6	-5.767	8.22
1,2,3,7-TCDD	275.6	1.6E-6	-5.788	6.90
1,3,6,8-TCDD	275.6	9.5E-7	-6.021	8.41
2,3,7,8-TCDD*	275.6	6.0E-8	-7.222	6.64
1,2,3,4,7-PCDD	296.5	3.3E-7	-6.482	7.40
1,2,3,4,7,8-H6CDD*	317.4	1.6E-8	-7.805	9.53
1,2,3,4,6,7,8-H7CDD*	338.3	5.7E-9	-8.245	10.32
OCDD*	359.2	5.5E-10	-9.261	10.26

Note that * refers to chembase chemical.

Figure 9a-c. ITF Correlations for Chlorinated Dioxins.





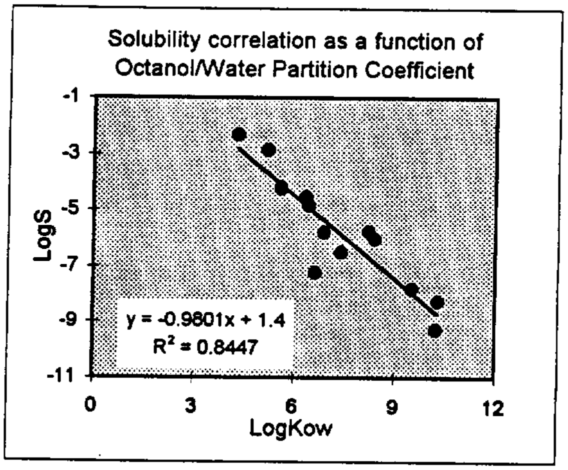


Table 10. Chlorinated Dibenzofurans

Compound	$V_{m(LeBas)}$ (cm^3/mol)	S (mol/m^3)	logS (mol/m^3)	logK$_{ow}$ (unitless)
Dibenzofuran (DF)	184.6	3.8E-2	-1.424	4.21
2,8-DichloroDF	226.4	6.1E-5	-4.214	5.62
2,3,7,8-TetrachloroDF*	268.2	1.4E-6	-5.860	6.31
2,3,4,7,8-PentachloroDF*	298.1	7.1E-7	-6.150	6.92
1,2,3,4,7,8-HexachloroDF*	310.0	2.7E-8	-7.570	7.70
1,2,3,4,6,7,8-HeptachloroDF*	330.9	3.2E-9	-8.500	7.92
1,2,3,4,7,8,9-HeptachloroDF	330.9	N/A	N/A	6.90
OctachloroDF*	351.8	9.0E-11	-10.050	8.54

Note that * refers to chembase chemical.

Figure 10a-c. ITF Correlations for Chlorinated Dibenzofurans.

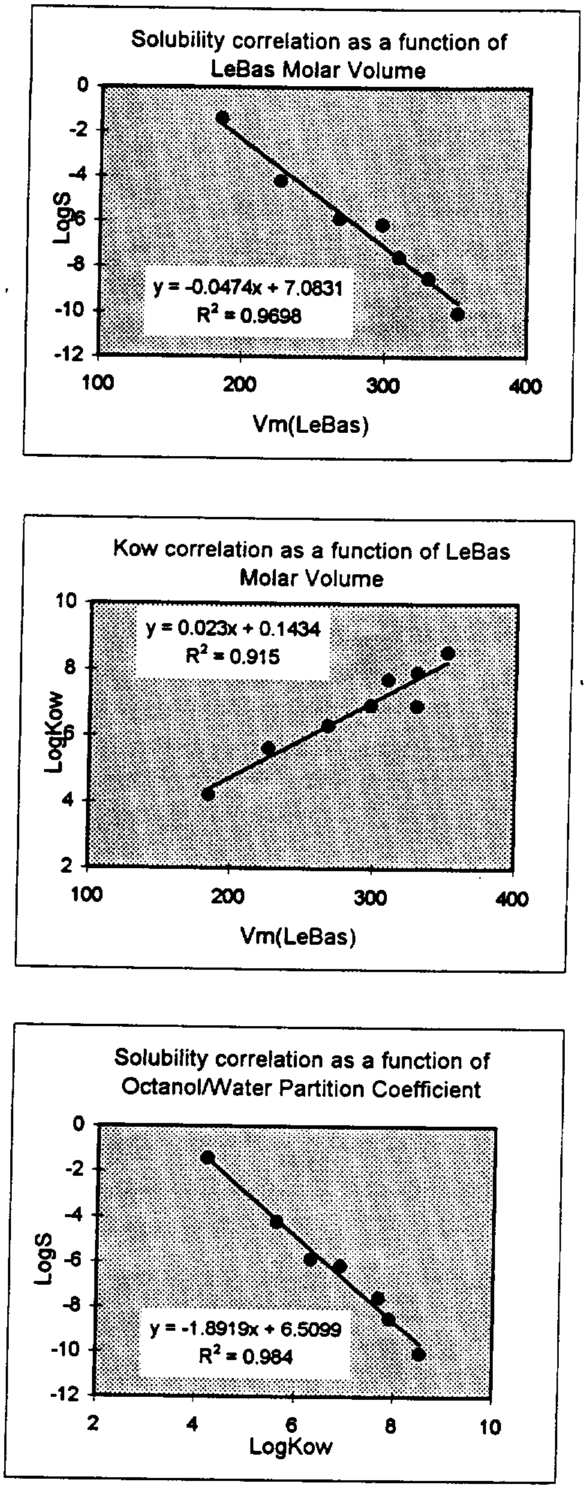


Table 11. BCF Correlation for Chlorinated Hydrocarbons.

Compounds	BCF	logKow	logBCF
Carbon tetrachloride*	3.00E+01	2.75	1.48
Carbon tetrachloride*	1.70E+01	2.75	1.24
Chloroform*	6.00E+00	1.94	0.78
1,2-Dichloroethane*	2.00E+00	1.46	0.30
Hexachloroethane	1.39E+02	3.93	2.14
Pentachloroethane	6.70E+01	2.89	1.83
Pentachloroethane	8.00E+00	2.39	0.90
1,1,1-Trichloroethane*	9.00E+00	2.42	0.95
1,1,2-Trichloroethylene*	1.70E+01	2.42	1.23
Tetrachloroethylene*	4.90E+01	3.00	1.69

Note that * refers to chembase chemical.

Figure 11. BCF correlation for Chlorinated Hydrocarbons.

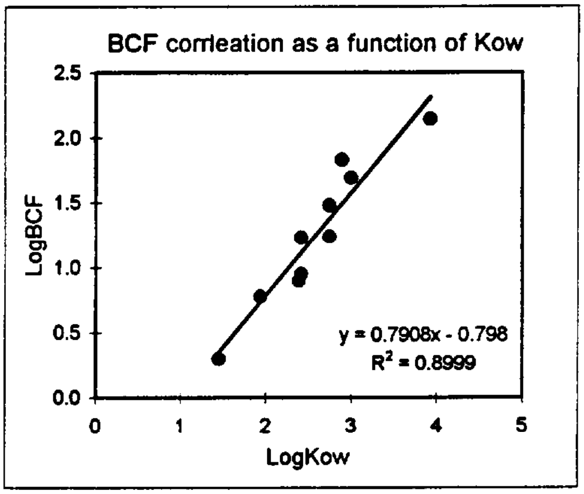


Table 12. BCF correlation for Mixed Aromatics.

Compound	BCF	logKow	logBCF
Benzene*	9.00E+00	2.13	0.95
1,2-Dichlorobezene	8.90E+01	3.52	1.95
1,3-Dichlorobenzene	6.60E+01	3.50	1.82
1,4-Dichlorobenzene*	2.49E+02	3.54	2.40
Hexachlorobenzene*	1.60E+04	5.53	4.20
Nitrobenzene*	6.02E+00	1.86	0.78
Pentachlorobenzene	3.40E+03	5.15	3.53
1,2,3,5-Tetrachlorobenzene	1.80E+03	4.66	3.26
1,2,4-Trichlorobenzene	2.80E+03	3.99	3.45
Ethylbenzene*	1.45E+02	3.13	2.16
m-xylene*	1.51E+01	3.20	1.18
o-xylene*	2.19E+01	3.16	1.34
p-xylene*	1.43E+01	3.18	1.16

Note that * refers to chembase chemical.

Figure 12. BCF correlation for Mixed Aromatics.

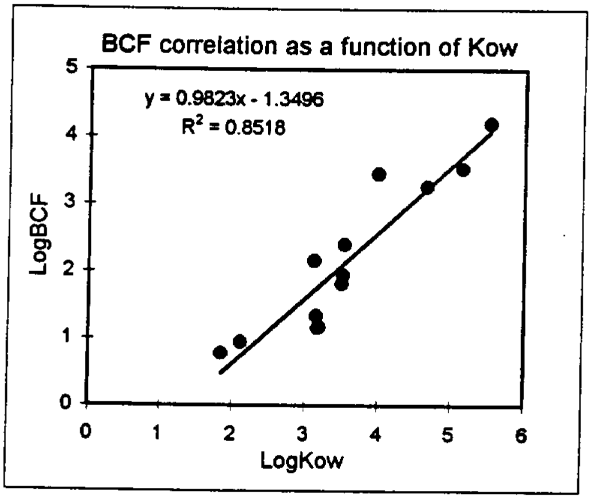


Table 13. BCF correlation for PAHs.

Compounds	BCF	logKow	logBCF
Acenaphthene*	3.89E+02	4.10	2.59
Naphthalene*	3.21E+02	3.34	2.51
Phenanthrene*	1.78E+03	4.46	3.25
Fluorene*	5.01E+02	4.18	2.70
Anthracene*	9.12E+02	4.49	2.96
Pyrene*	2.69E+03	5.18	3.43
Fluoranthene*	1.74E+03	5.20	3.24
Chrysene*	6.10E+03	6.06	3.78
Benz[a]anthracene*	1.02E+04	5.90	4.01
Benzo[b]fluoranthene*	1.00E+04	6.18	4.00
Benzo[k]fluoranthene*	1.32E+04	6.59	4.12
Benzo[ghi]perylene*	2.82E+04	6.72	4.45
Dibenz[a,h]Anthracene*	1.00E+04	6.50	4.00

Note that * refers to chembase chemical.

Figure 13. BCF correlation for PAHs.

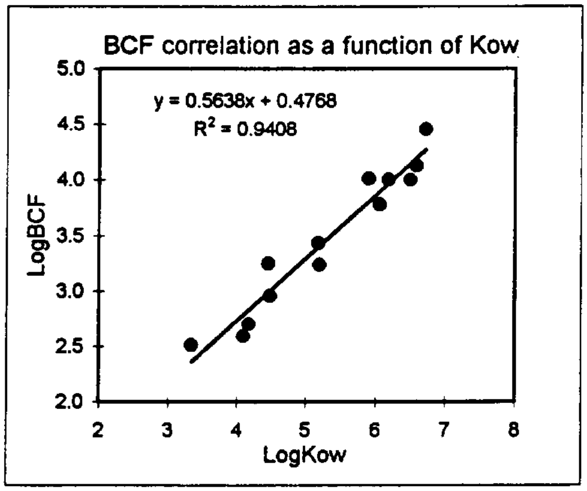
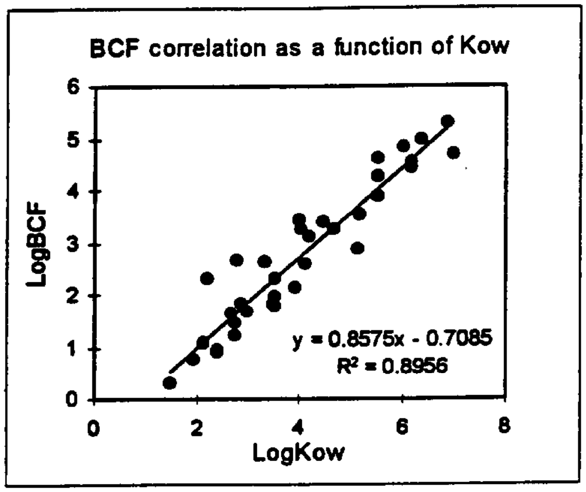


Table 14. BCF correlation for Mixed Chemicals.

Compounds	BCF	logKow	logBCF
Acenaphthene*	3.87E+02	4.10	2.59
Aroclor 1016*	4.25E+04	5.52	4.63
Aroclor 1248*	7.05E+04	6.02	4.85
Aroclor 1254*	1.00E+05	6.38	5.00
Aroclor 1260*	1.94E+05	6.87	5.29
Benzene*	1.26E+01	2.13	1.10
Carbon tetrachloride*	3.00E+01	2.75	1.48
Carbon tetrachloride*	1.74E+01	2.75	1.24
2-Chlorobenzene	4.50E+02	2.80	2.65
Chloroform*	6.00E+00	1.94	0.78
2-Chlorophenol	2.14E+02	2.21	2.33
p,p'-DDT	2.94E+04	6.19	4.47
o,p'-DDT	3.70E+04	6.19	4.57
p,p'-DDE	5.10E+04	7.00	4.71
1,2-Dichlorobezene	8.90E+01	3.52	1.95
1,3-Dichlorobenzene	6.60E+01	3.50	1.82
1,4-Dichlorobenzene*	6.00E+01	3.54	1.78
1,4-Dichlorobenzene*	2.15E+02	3.54	2.33
1,2-Dichloroethane*	2.00E+00	1.46	0.30
Fluorene*	1.30E+03	4.18	3.11
Hexachlorobenzene	7.76E+03	5.53	3.89
Hexachlorobenzene	1.85E+04	5.53	4.27
Hexachloroethane	1.39E+02	3.93	2.14
Naphthalene*	4.30E+02	3.34	2.63
Pentachlorobenzene	3.40E+03	5.15	3.53
Pentachloroethane	6.70E+01	2.89	1.83
Pentachlorophenol*	7.70E+02	5.12	2.89
Phenanthrene*	2.63E+03	4.46	3.42
1,2,3,5-Tetrachlorobenzene	1.80E+03	4.66	3.26
1,1,2,2-Tetrachloroethane*	8.00E+00	2.39	0.90
Tetrachloroethylene*	4.90E+01	3.00	1.69
Toluene*	4.30E+01	2.69	1.63
1,2,4-Trichlorobenzene	2.80E+03	3.99	3.45
1,1,1-Trichloroethane*	9.00E+00	2.42	0.95
2,4,5-Trichlorophenol	1.90E+03	4.03	3.28

Note that * refers to chembase chemical.

Figure 14. BCF correlation for Mixed Chemicals.



List of Abbreviated Chemical Names Used in Appendix B

7,12 DMBA - 7,12 Dimethylbenz[a]anthracene
9,10 DMBA - 9,10 Dimethylbenz[a]anthracene
CDD - Chloro-dibenzo-p-dioxin
DCDD - Dichloro-dibenzo-p-dioxin
DDD - 1,1 - dichloro - 2,2-bis(p-chlorophenyl)ethane)
DDE - 1,1 - dichloro - 2,2-bis(p-chlorophenyl)ethylene)
DDT - 1,1,1 - trichloro - 2,2 - bis (p-chlorophenyl)ethane)
D[a,j]A - Dibenz[a,j]anthracene
D[a,h]A - Dibenz[a,h]anthracene
D[a,c]A - Dibenz[a,c]anthracene
H6CDD - Hexachloro-dibenzo-p-dioxin
H7CDD - Heptachloro-dibenzo-p-dioxin
OCDD - Octachloro-dibenzo-p-dioxin
PCB - Polychlorinated Biphenyl
PCDD - Pentachloro-dibenzo-p-dioxin
T3CDD - Trichloro-dibenzo-p-dioxin
TCDD - Tetrachloro-dibenzo-p-dioxin

APPENDIX C: Parameter Estimation For the Bioaccumulation Factor Model

C1. Overview

In order to solve the overall governing biotic mass balance (6.3.12) is necessary to estimate several critical physical, gill and morphometric parameters. A number of investigators have proposed various empirical correlations to estimate various parameters needed to estimate the bioaccumulation of toxics in finned fish (e.g., Barber et al., 1991, 1994; Thomann 1989; and references therein). The main parameters required for the biotic mass balance are: $W(t)$, k_i^{ol}, A_i , $C_w(t)$, α_f , K_e, K_f (BCF), $C_{a,p}$, $F_{i,p}$. These parameters have been previously described in section 6.3 and in this Appendix algorithms for estimating these critical parameters are presented. The BAF module contains necessary model parameters for the following finned fish species: (1) Salmon; (2) Trout; (3) Striped Bass; (4) Yellow Perch; (5) Atlantic Croaker; (6) White Perch; and (7) Alewife. This set of species is believed to be adequate for assessing the potential for bioaccumulation in finned fish. For other species user-input of the appropriate parameters is required.

C2. Interfacial Biotic Surface Area for Mass Transfer A_i

In general A_i (the effective surface area for mass transfer through the gills) is only 60-80 % of the total lamellar surface area (Barber et. al 1991). Barber et al. (1991). approximate A_i [cm^2] as

$$A_i = 0.5\, S_g \qquad \text{(C-1)}$$

where S_g is the total lamellar surface area [cm^2] given by (Barber et al., 1991)

$$S_g = s_1 W^{s_2} \qquad \text{(C-2)}$$

Equation C-2 is an approximate expression for a wide set of fish species between the weights of 10g to 1000g. Barber et al. (1991) also report that studies over a wide range of fish species indicate that s_1 ranges from 0.8-11 [cm^2/g^{S2}] and s_2 ranges from 0.4-1.2.

C3. The Overall Liquid Side Mass Transfer Coefficient, k_l^{ol}

The overall liquid mass transfer coefficient for chemical transport from water to fish, via the gills, can be estimated using the following expression (Barber et al., 1991)

$$k_i^{ol} = \frac{D}{h}\left[\frac{1-0.99\exp(-0.66N_{gz})}{0.5N_{gz}}\right] \qquad \text{(C-3)}$$

where k_i^{ol} is the overall liquid -side mass transfer coefficient, D is the aqueous diffusivity of the chemical in water [cm^2/s], h is the hydraulic width of the gill lamellae [cm] which is the equivalent 'membrane half-thickness' for the lamellar gill channels, and N_{gz} is the lamellar Graetz number for the gill lamellae. The half thickness of the gill channels h [cm] can be approximated by (Barber et al., 1991)

$$h = 0.5(0.118\rho_1 W^{\rho_2})^{-1.19} \qquad \text{(C-4)}$$

where W is the fish mass [g] and the empirical parameters ρ_1 and ρ_2 have been reported to vary from 15 to 52.2 [cm/g$^{\rho 2}$] and -0.08 to -0.3 respectively (Barber et al., 1989). The lamellar Graetz number is obtained from (Barber, 1991)

$$N_{gz} = \frac{lD}{h^2V} \qquad \text{(C-5)}$$

Where l is the mean lamellar length [cm], D is the aqueous diffusivity [cm^2/s], h is the mean lamellar width [cm] and V is the velocity of the water flowing through the gills [cm/s]. The lamellar length is given by the allometric expression recommended by Barber et al. (1991)

$$l = 0.0188W^{0.294} \qquad \text{(C-6)}$$

Equation C-6 is reported to be applicable for a for a wide range of fish species. Finally, the velocity of water through the gills can be approximated as

$$V = \frac{\Delta P h^2}{3\eta_w l} \qquad \text{(C-7)}$$

where ΔP the pressure drop across the lamellae [N/cm^2] which is approximately 2.5x10 $^{-3}$ N/cm^2 (based on the rainbow trout studies of Davis and Randall (1983) and η_w is the viscosity of water

[m^2/s]. Clearly ΔP could vary for different species and thus the use of the above constants should only be regarded as an approximation.

C4. The Bioconcentration Factor BCF

The bioconcentration factor (BCF) was defined in section 6.3 as

$$\frac{C_{ai}}{C_a} = BCF = K_f = f_a + K_L f_L + K_o f_o \qquad \text{(C-8)}$$

and the aqueous and non-lipid fractions in finned fish can be estimated from (Barber et al., 1991)

$$f_a = \text{aqueous mass fraction} = 0.82 - 1.25\, f_L \qquad \text{(C-9)}$$

$$f_o = \text{non-lipid organic mass fraction} = 0.18 + 0.25 f_L \qquad \text{(C-10)}$$

It is important to note here that the BCF as defined in Eq. C-8 and in all subsequent correlations in the BAF module is based on a total body mass. It is also interesting to note that, as was observed by Thomann (1989), the lipid fraction appears to be only a weak function of the fish mass or growth rate. Therefore, as a simplification, the BAF module assumes that the lipid fraction of the fish is constant throughout the life of the fish.

Other relations to estimate the BCF are available in the literature and these are usually in the form of BCF-K_{ow} or BCF-K_{oc} correlations (see section 6.3). For example, MacKay (1982) proposed to following simple BCF correlation:

$$BCF = K_{ow} f_L \qquad \text{(C-11)}$$

According to the study of Isnard et al. (1988), the above relation is a good approximation for the BCF for log $K_{ow} < 6.0$. For more hydrophobic (log $K_{ow} > 6.0$) chemicals, Isnard et al. (1988) proposed the following alternative correlation that is based on a wider range of K_{ow} values and for a wide set of species:

$$\text{Log} BCF = 0.8 \text{Log } K_{ow} - 0.52 \qquad \text{(C-12)}$$

Correlation C-12 was derived for 107 hydrophobic organic toxins (K_{ow} range of 10^2 - 10^7) with a regression correlation coefficient of $r^2 = 0.904$. More recent studies (Hawker et al., 1990; Banerjee et al., 1991; Park et al., 1993) have suggested significant non linear behavior between the log BCF and the log K_{ow} for chemicals with a log $K_{ow} > 6.0$. Several explanations for the non linearity were provided, the most significant one being that for highly hydrophobic chemicals there is considerable transport resistance in the aqueous fractions of the fish (see for example, Hawker et al. (1990). A BCF-K_{ow} correlation that covers a wide range of K_{ow} values was proposed by Hawker et al. (1990)

$$\begin{aligned} \mathrm{LogBCF} &= 9.5 \times 10^{-3} (\mathrm{Log}K_{ow})^4 - 2.44\mathrm{x}10^{-1}(\mathrm{Log}K_{ow})^3 + 1.95(\mathrm{Log}K_{ow})^2 \\ &\quad - 5.12\mathrm{Log}K_{ow} + 5.37. \end{aligned} \tag{C-13}$$

The above correlation was based on 41 organic chemicals with K_{ow} values ranging from 10^2-$10^{8.2}$ with a correlation coefficient $r^2 = 0.87$.

Banerjee et al. (1991) report that the correlation of Hawker et al. (1990) is best suited for low melting point organics. For organic toxins that are solids at room temperature, Banerjee et al. (1991) proposed the following correlation,

$$\mathrm{Log\,BCF} = -1.13 + 1.02\mathrm{Log}(K_{ow}) + 0.84\mathrm{Log}S_{octanol} + 0.004(T_{mp}-25) \tag{C-14}$$

where, $S_{octanol}$ is the molar solubility of the toxin in octanol [mol toxin / liter solution] and T_{mp} is the toxin melting point [°C]. Both $S_{octanol}$ and T_{mp} need to be supplied by the user. The above expression was derived for a wide array of hydrophobic toxins with K_{ow} range from 10^2 - $10^{8.7}$ and a correlation coefficient $r^2 = 0.95$.

The BCF can also be estimated by employing the earlier expression presented by Chiou (1985):

$$\mathrm{LogBCF}_l = 0.957\mathrm{Log}K_{tw} + 0.245 \tag{C-15}$$

where K_{tw} is the triolein/water partition coefficient which was correlated with K_{ow}

$$K_{tw} = 1.27\, K_{ow} \qquad ; \mathrm{Kow} < 10^5 \tag{C-16a}$$

$$K_{tw} = 2.13 \times 10^2\, K_{ow}^{\,0.571} \qquad ; K_{ow} \geq 10^5 \tag{C-16b}$$

C5. K_e and K_{oc}

The overall species/water partition coefficient can be expressed as (Karickhoff et al., 1981)

$$K_e = f_a + f_o K_{oc} \tag{C-17}$$

where K_{oc}, the organic carbon/water partition coefficient, can be estimated from various correlations listed in section 6.3.

C6. Food Assimilation Efficiency

The food assimilation efficiency, α_f, is a species specific property. For most freshwater species it ranges from 0.2-0.9 (Barber et al., 1991).

C7. Estimating the biota growth W(t)

In general, the growth rate per gram organism can be expressed allometrically as (Thomann 1989),

$$G = \frac{1}{W}\frac{dW}{dt} = aW^{-b} \tag{C-18}$$

Where, G is the net organism growth rate coefficient [day $^{-1}$] and the parameters a and b are dimensionless allometric coefficients. Across a general food chain, Thomann (1989) suggests that a ~ 0.002 and b varies from 0.2 - 1.0. The above equation can be integrated to yield the following expressions for W(t):

for $b \geq 0$,

$$W(t) = (W_0^{\,b} + abt)^{\frac{1}{b}} \tag{C-19}$$

and for b=0

$$W(t) = \exp(at + \ln(W_0)) \tag{C-20}$$

where, W_o is the initial weight of the organism [g].

C8. Prey Consumption F_p (g (prey) / day)

The prey consumption per unit mass of predator can be expressed using the empirical expression proposed by Thomann (1989) and Norstrom et al. (1976)

$$F*_{i,i-1} = \frac{F_p}{W} = \frac{(G+r)}{\alpha_f} \qquad \text{(C-21)}$$

where, r is the organism's respiration rate constant [1/day] estimated as $r = \phi W^{-\gamma}$ where ϕ and γ are empirical constants that vary from 0.014 to 0.05 and 0.02 to 0.3, respectively, and α_f is the dimensionless food assimilation efficiency. If an allometric form for the respiration is also assumed (e.g. Thomann, 1989; Norstrom et al, 1976)), then Eq. C-22 can be expressed as (Vohra, 1996),

$$F*_{i,i-1} = \frac{F_p}{W} = \frac{(aW^{-b} + cW^{-d})}{\alpha_f} \qquad \text{(C-22)}$$

in which the parameters c and d, across a general food chain, are in the range of 0.014-0.05 and 0.2-0.3, respectively (Thomann, 1989).

APPENDIX D: THE PARTICLE SIZE DISTRIBUTION FUNCTION, SURFACE AREA AND VOLUME

D1. Particle Size Distribution Function

The dry deposition and wet deposition modules of the ITFP make use of information on the particle size distribution function. The particle size distribution function, n(a) [#/m^3], is defined by

$$\frac{n(a)}{a}\,da \equiv dN_t \qquad \text{(D-1)}$$

where a is the particle diameter [m] and N_t is the total number of particles per unit volume [#/m^3]. In order to obtain the number of particles in a size range d to $d+\Delta d$ Eq. D-1 must be integrated between the appropriate limits

$$N_{d,d+\Delta d} = \int_{d}^{d+\Delta d} dN_t = \int_{d}^{d+\Delta d} \frac{n(a)}{a}\,da \qquad \text{(D-2)}$$

The ITFP uses a tri-modal lognormal size distribution defined by (Whitby, 1978):

$$\begin{aligned} n(a) = {} & \frac{N_n}{(2\cdot\pi)^{.5}\log(\sigma_n)} \times \exp\left[-\frac{1}{2}\left(\frac{\log\left[\frac{a}{\alpha_n}\right]}{\log(\sigma_n)}\right)^2\right] + \\ & \frac{N_a}{(2\cdot\pi)^{.5}\log(\sigma_a)} \times \exp\left[-\frac{1}{2}\left(\frac{\log\left[\frac{a}{\alpha_a}\right]}{\log(\sigma_a)}\right)^2\right] + \\ & \frac{N_c}{(2\cdot\pi)^{.5}\log(\sigma_c)} \times \exp\left[-\frac{1}{2}\left(\frac{\log\left[\frac{a}{\alpha_c}\right]}{\log(\sigma_c)}\right)^2\right] \end{aligned} \qquad \text{(D-3)}$$

where a is the diameter, σ_i is the standard deviation of particle mode I, α_i is the geometric mean size of particle mode I, N_i is the total number of particles per volume of particle mode I and the subscripts n, a and c refer to the particles in nucleation, accumulation and coarse particle modes, respectively.

Equation D-3 allows for the input of various practical size distribution functions. If site-specific information concerning the particle size distribution function is not available, then the particle size distributions measured by Whitby (1978) can be used as reasonable approximations.

D2. Surface Area of Atmospheric Particles

As discussed in Section 7, the gas/particle partitioning of a contaminant in the atmosphere depends on the total surface area of atmospheric particulate and the temperature. The total surface area of particles in the atmosphere is determined by the particle size distribution function and the morphology of the individual particles. Accordingly, if the number of particles with a diameter in the range d to $d + \Delta d$ is $N_{d,d+\Delta d}$ [#/m^3], then the surface area of particles in that same size range per unit volume of air, $S^{(p)}(d)$ [cm^2/m^3], is given by

$$S^{(p)}(d) = A_{ap}(d) \cdot N_{d,d+\Delta d} \tag{D-4}$$

where $A_{ap}(d)$ is the average area of a particle in the size range d to $d + \Delta d$ [cm^2].

If the atmospheric particles are assumed to be spherical, then Eq. D-4 becomes

$$S^{(p)}(d) = \pi \left(d + \frac{\Delta d}{2} \right)^2 \cdot N_{d,d+\Delta d} \tag{D-5}$$

where $d + \Delta d/2$ represents the average particle diameter in the range d to $d + \Delta d$ [cm].

The total surface area of particles per volume of air in the atmosphere can then be obtained from

$$S_t^{(p)} = \sum_{m=1}^{m=k} \pi \left(d_m + \frac{\Delta d_m}{2} \right)^2 \cdot N_m \tag{D-6}$$

where $d_m + \Delta d_m/2$ represents the average diameter of size range m [cm], N_m is the number of particles in size range m [#/m^3] and k is the total number of size ranges.

D3. Volume Distribution of Particles

As an alternative to calculating the surface area using Equation D-6, it is possible to calculate the total surface area of particles, $S^{(p)}$, using the expression:

$$S_t^{(p)} = V_t^{(p)}\overline{\rho}^{(p)}\hat{A}_{ap} = M_t^{(p)}\hat{A}_{ap} \tag{D-7}$$

where $V_t^{(p)}$ is the total volume of particles per volume of air [$\mu m^3/m^3$], $\overline{\rho}^{(p)}$ is the average density of the particles [$\mu g/\mu m^3$], $\hat{A}_{ap}$ is the specific surface area of the particles [$cm^2/\mu g$] and $M_t^{(p)}$ is the total mass of particles per unit volume [$\mu g/m^3$].

The volume of particles in the atmosphere, $V_t^{(p)}$, can be estimated using the volume analog of Eq. D-6

$$V_t^{(p)} = \sum_{m=1}^{m=k} \frac{\pi}{6}\left(d_m + \frac{\Delta d_m}{2}\right)^3 \cdot N_m \tag{D-8}$$

Equation D-8 can be easily modified to calculate the total mass of particles per unit volume

$$M_t^{(p)} = \overline{\rho}_p \sum_{m=1}^{m=k} \frac{\pi}{6}\left(d_m + \frac{\Delta d_m}{2}\right)^3 \cdot N_m \tag{D-9}$$

where it is assumed that the density does not vary with particle size.

Typical densities of atmospheric particulate matter vary from 1 to 11 [g/cm^3] (Hinds, 1982). For example, the density of the coarse and fine modes of a typical urban aerosol have been reported to be 1.7 and 2.0 g/cm^3, respectively (Holsen and Knoll, 1992), while a default value of 1.5 g/cm^3 is usually assumed for the average particle density (Sehmel and Hodgson, 1980).

The specific area has been reported to be approximately constant for urban aerosols in the range 0.019 to 0.05 $cm^2/\mu g$] (Pankow, 1987; Sheffield and Pankow, 1994). In the ITFP the default surface area is set as $\hat{A}_{ap} = 0.05\ cm^2/\mu g$ based on a review of a number of field studies (Van de Water, 1995).