3751

VALANCE MOLECULAR CONNECTIVITY MODEL IN THE PREDICTION OF COMPARTMENTAL DISTRIBUTION OF SELECTED AROMATIC POLLUTANTS

by

G. Feryal Menemenli

B.Sc. in Chem., Boğaziçi University, 1977

M.Sc. in Chem., Boğaziçi University, 1980

Submitted to the Institute of Environmental
Sciences, in partial fulfillment of the
requirements for the degree of
doctor of philosophy
in
Environmental Sciences

Boğaziçi University

1987

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

VALANCE MOLECULAR CONNECTIVITY MODEL IN THE PREDICTION OF COMPARTMENTAL DISTRIBUTION OF SELECTED AROMATIC POLLUTANTS

APPROVED BY

Prof. Dr. Yüksel İnel .... Yüksel İnel
(Thesis Supervisor)

Doç. Dr. Rıdvan Tokay ....

Y. Doç. Dr. Orhan Yenigün .... Orhan Yenigün

DATE OF APPROVAL
February 1987

To

Prof. Dr. Yüksel İnel

ACKNOWLEDGEMENTS

It is my greatest pleasure to record here a dept which I can never repay to Prof. Dr. Yüksel İnel who with his encouraging helpfulness has been a source of enthusiasm all through my university years and all through this work and gave me the inspiration of a deeper perception of life. So in grateful acknowledgement I dedicate this work to him, hoping that he may find in these pages - insufficient though they are - something not quite unworthy of his generosity.

I take this opportunity to express my sincere gratitude to the members of the Thesis Committe Doç. Dr. Rıdvan Tokay and Y. Doç. Dr. Orhan Yenigün for their critical reading of the manuscripts.

I also take this opportunity to express my indebtedness to Eczacıbaşı Pharmaceuticals Company for their Support in the Completion of this work and also to Mr. Ayhan Suskun for his encouraging and understanding attitude throughout this work

My thanks are also due to Mr. Semih Kayalı for his invaluable contributions to and incessant efforts for the preparation of this work, and to my colleagues Miss Ürfet Orhon, Mrs. Pınar Orcan and to all other members of the Eczacıbaşı Research Laboratories for their assistance and cooperation throughout this work.

Finally, I wish to gratefully acknowledge Mrs. Nermin Demir for her impeccable typing of this manuscript and Miss Ayşe Turgut for her valuable help in typing out various tables.

TABLE OF CONTENTS

Page

ACKNOWLEDGEMENT iii

ABSTRACT ix

ÖZET xiii

LIST OF FIGURES xv

LIST OF TABLES xxiii

LIST OF SYMBOLS xxx

I. INTRODUCTION 1

II.GRAPH THEORY AND ITS APPLICATIONS 10
- II.1 Historical Background and its Development 10
- II.2 Theory
  - II.2.1 Graph Theory and Representation of Molecules 17
  - II.2.2 Assembling the Atom Connectivity Matrix 21
  - II.2.3 The Atom Connectivity Matrix Characteristic Polynomial and its Physico-Geometric (Topological) Significance 33
  - II.2.4 Development and Use of Topological Indices 40
  - II.2.5 The Addivity Function and the Topological İndices 49
- II.3 Valance Molecular Connectivity Index 56
  - II.3.1 Significance of Delta Values
  - II.3.2 Valance Molecular Connectivity and the treatment of Heteroatoms 64

Page

II.3.3 Valance Molecular Connectivity and the Development of Extended Connectivity Terms 71

III. ECOKINETICS IN RELATION TO VALANCE MOLECULAR CONNECTIVITY 77
III.1 Approaches to Environmental Exposure Analysis 77
III.1.1 Environmental Compartmentalization 81
III.1.2 Evaluation of Fugacity Capacities 87
III.1.2.1 Fugacity Capacity for the Atmosphere Z_a 89
III.1.2.2 Fugacity Capacity for Water, Z_w 91
III.1.2.3 Fugacity Capacity for Sorbed Phases (Soil, Sediment or Suspended Solids) Z_s, Z_{sd}, Z_{ss} 92
III.1.2.4 Fugacity Capacity for Biotic Phases (Z_b) 96
III.1.3 Description of the Model Used 98
III.2 Relationship of Valance Molecular Connectivity to Partition Coefficient, Solubility and Vapor Pressure 99

IV. DEVELOPMENT OF THE VALANCE CONNECTIVITY MODEL FOR THE PREDICTION OF ENVIRONMENTAL COMPARTMENTALIZATON OF VARIOUS BENZENE DERIVATIVES 107
IV.1 The Valance Connectivity Approach 107
IV.1.1 Evaluation of Valance Molecular Connectivity Indices 131
IV.1.2 Correlations 138
IV.1.3 Results of the Multivariable Regression Analysis 163
IV.2 Evaluation of Compartmental Distributions in Terms of Valance Molecular Connectivity Indices 189

Page

IV.2.1 Evaluation of ln K_{OW}, ln S and ln P in Terms of Valance Molecular Connectivity Indices 190
IV.2.2 Evaluation of Fugacity Capacity Constans in Terms of Valance Molecular Connectivity Indices 204
  IV.2.2.1 Derivation of the Expression for the Fugacity Capacity Constant for Air 204
  IV.2.2.2 Derivation of the Expression for the Fugacity Capacity Constant for Soil 205
  IV.2.2.3 Derivation of the Expression for the Fugacity Capacity Constant for Water 206
  IV.2.2.4 Derivation of the Expression for the Fugacity Capacity Constant for Biota 207
  IV.2.2.5 Derivation of the Expression for the Fugacity Capacity Constant for Suspended Solids 208
  IV.2.2.6 Derivation of the Expression for the Fugacity Capacity Constant for Sediment 210
IV.2.3 Specimen Calculations 211
  IV.2.3.1 Calculation of Fugacity Capacities According to Level I Fugacity Model 212
  IV.2.3.2 Calculation of Fugacity Capacities According to Valance Molecular Connectivity Model 215
IV.3 Evaluation of the Compartmental Distribution in Terms of Valance Molecular Connectivity Indices 220

V.DISCUSSION OF THE RESULTS 223
V.1 Tabulation of the Results 223
V.2 General Evaluation of the Results 312

Page

V.2.1 Valance Molecular Connectivity Indices and the Future Requirements 316

V.2.2 Predicted Environmental Distribution of Various Aromatic Hydrocarbons in Comparison to the Results Obtained from Level I Fugacity Calculations 318

V.3 Conclusions and the Future Research Needs Regarding VMCI Model 400

APPENDIX I

Evaluation of Vapor Pressures for Unsubstituted Polycylic Aromatic Hydrocarbons I-i

APPENDIX II

Computer Programs II-i

APPENDIX III

Outputs for Fugacity Capacity Constants Calculated by Level I Fugacity and VMCI Models III-i

BIBLIOGRAPHY

ABSTRACT

The main purpose of this work is to develop a mathematical model based on the Valance Molecular Connectivity theory which is initiated as an extension of graph theory having its roots especially in structure-activity studies concerning drug-design and toxicity prediction in pharmaceutical chemistry, to evaluate the compartmental distribution of various aromatic pollutants in the environment.

During the last decade concerns have been expressed as to the "best way" to assess the potential hazards posed by exposure to chemical substances. In response to these concerns, the chemical group of OECD initiated a hazard assessment project to examine the available methods for hazard assessment of chemicals. The main purpose being to determine how information on the ultimate fate and effects of a chemical can be derived from the set of premarket data, the group accepted four models for the estimation of exposure potentials of

chemicals within environmental compartments of major concern. All of the four models accepted by OECD chemical group was based on the concept of fugacity and essentially needed the following data

- molecular weight
- water solubility
- vapor pressure
- soil sorption constant
- octanol-water partition coefficient

However, the availability and precission of the set of data proposed, especially for chemicals which have rather large and complicated structures was a drawback of these models. Hence, a reasonable model to evaluate this distribution quantitatively without needing such hard-to-gather data would have been a remarkable advance in prediction of environmental hazards that are going to be caused by unknown chemicals irrespective of size and conformation.

In this work a new mathematical model (VMCI) based only on the topological characteristics of molecules is developed in order to evaluate the distribution of chemicals within various compartments of the environment such as air, soil, water, biota, suspended solids and sediment.

The Valance Molecular Connectivity Index, which is the basis of this new model is known to correlate significantly with a number of structure dependent physicochemical properties, and by this work it has now been shown to have a high degree of correlation also with water solubilities, vapor pressures and partition coefficients hence with the partitioning properties of molecules.

As a result, by comparing the two completely different methods of evaluation (VMCI and Level I Fugacity Models) this work proved that it is possible to predict the compartmental distribution of any aromatic compound quantitatively within a high accuracy just by considering the molecular geometry.

The superiority of this model compared to fugacity dependent models accepted by OECD lies in the fact that it does not require the physical data such as solubility, vapor pressure or partition coefficient. Relevantly another superiority comes out to be the ability to stay as accurate when even very complicated molecules are investigated while for fugacity dependent models accuracy diminishes due the difficulties in obtaining the experimental data.

ÖZET

Bu çalışmada Çizit Kuramının bir parçası olarak son yıllarda özellikle farmasötik kimya dalında yapı-etki ilişkilerinin incelenmesinde yaygın olarak kullanılan Valans Moleküler Konektivite İndeks'lerine bağlı matametiksel bir modelin geliştirilmesi amaçlanmıştır.

Bu model yardımı ile Polisiklik Aromatik Hidrokarbonlar (PAH), Alkilbenzenler, Poliklorine Siklik Aromatik Hidrokarbonlar (PCB) ve Halojen Substitüye Benzenlerin çevredeki denge dağılımlarının hesaplanması ve böylece bu kimyasalların çevrenin çeşitli kompartmanlarında (hava, toprak, su, biota, asılı madde ve sediment) hangi bağıl konsantrasyonlara ulaşacakları hesaplanmıştır.

Son yıllarda atık olarak çevreye giren ve sağlığı tehdit eden çeşitli maddelerin çevredeki dağlımının sudaki çözünürlükleri, buhar basınçları ve oktanol-su oranı katsayıları gibi fiziko-kimyasal bazı özelikleri kullanılarak hesaplanması OECD Çevre Analiz Grubu tarafından ele alınmış ve bu amaçla Mackay tarafından geliştirilen maddenin bir fazdan kaçınım yatkınlığı il-

kesine dayalı "fugasite Modeli" esas olarak belirlenmiştir.

Bu çalışma ile geliştirilen matamatiksel modelin bu konuya katkısı ise, sözkonusu dağılımı, yukarıda sözü edilen ve özellikle çevre bilimlerinin ilgi alanına giren büyük moleküller için literatürde bulunması zor olan birçok fiziko-kimyasal parametreye gereksinim olmadan hesaplayabilme kolaylığını sağlamasıdır.

Sözü edilen dört aromatik grup üzerinde yapılan detaylı bir istatistikî inceleme sonucu elde edilen veriler OECD tarafından benimsenen fugasite modeli ile elde edilen verilerle karşılaştırıldığında modelin yüksek bir korrelasyonla çalıştığı gözlenmiş ve bu tür hesapların yapılabilmesi için sadece moleküler geometri ve moleküler ağırlığın yeterli olacağı kanıtlanmıştır.

LIST OF FIGURES

		Page
FIGURE II.1	Chemical Graphs of Propane and Benzene Where Atoms are Represented by Vertices and Bonds by Edges	19
FIGURE II.2	The Adjancency Matrices for Three Types of Chemical Graphs Having Different Configurations	22
FIGURE II.3	Examples for the Hydrogen-Suppressed ACM's	28
FIGURE II.4	The Wiener İndex Calculated by Summing Up the Number of Bonds That Would Have to be Traversed in Travelling Along the Molecule From Every Atom to Very Other Atom.	44
FIGURE II.5	Evaluation of Randic Molecular Connectivity Index	46
FIGURE II.6	Smolenskii Addivity Function for i-butane Showing That A Path of Length k, Contains A Total of k Connected Edges of the Graph.	51
FIGURE II.7	Atoms and Hydrides Defined by δ and δ^v Values	62
FIGURE III.1	Unit World Designed by Mackay and Neely	83

Page

FIGURE III.2 Plot of the Logarithm of the Partition Coefficient Versus the Molecular Connectivity İndex for 24 Esters Nine Carboxylic Acids, 49 Alcohols, 28 Amines, 16 Ketones and 12 Ethers With the Corresponding Regression Line 103

FIGURE III.3 Plot of Natural Logarithm of Solubility Versus the Connectivity İndex for 51 Alcohols (+) and 18 Hydocarbons (x) With Corresponding Regression Lines. 104

FIGURE IV.1 Plot of the Logarithm of the Partition Coefficient Versus Zero Order Valance Molecular Connectivity İndex $({}^{o}X^{v})$ for Groups I,II, III and IV 154

FIGURE IV.2 Plot of the Logarithm of the Partition Coefficient Versus First Order Valance Molecular Connectivity İndex $({}^{1}X^{v})$ for Groups I, II, III and IV 155

FIGURE IV.3 Plot of the Logarithm of the Partition Coefficient Versus Second Order Valance Molecular Connectiviy İndex $({}^{2}X^{v})$ for Groups I, II, III and IV 156

FIGURE IV.4 Plot of the Logarithm of Vapor Pressure Versus Zero Order Valance Molecular Connectivity İndex $({}^{o}X^{v})$ for Groups I, II, III and IV 157

Page

FIGURE IV.5 Plot of the Logarithm of Vapor Pressure Versus First Order Valance Molecular Connectivity Index ($^1\chi^v$) for Groups I, II, III and IV 158

FIGURE IV.6 Plot of the Logarithm of Vapor Pressure Versus Second Order Valance Molecular Connectivity Index ($^2\chi^v$) for Groups I, II, III and IV 159

FIGURE IV.7 Plot of the Logarithm of Solubility Versus Zero Order Valance Molecular Connectivity Index ($^0\chi^v$) for Groups I, II, III and IV 160

FIGURE IV.8 Plot of the Logarithm of Solubility Versus First Order Valance Molecular Connectivity Index ($^1\chi^v$) for Groups I, II, III and IV 161

FIGURE IV.9 Plot of the Logarithm of Solubility Versus Second Order Valance Molecular Connectivity Index ($^2\chi^v$) for Groups I, II, III and IV 162

FIGURE V.2 Plot of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Polycyclic Aromatic Hydrocarbons (PAH) 323

Page

FIGURE V.2.1.1 Equilibrium Distribution (%) in Air For PAH's 324

FIGURE V.2.1.2 Equilibrium Distribution (%) in Soil for PAH'S 325

FIGURE V.2.1.3 Equilibrium Distribution (%) in Water for PAH's 326

FIGURE V.2.1.4 Equilibrium Distribution (%) in Biota for PAH's 327

FIGURE V.2.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment for PAH's 328

FIGURE V.2.2.1 Mass Distribution (%) in Air for PAH's 329

FIGURE V.2.2.2 Mass Distribution (%) in Soil for PAH's 330

FIGURE V.2.2.3 Mass Distribution (%) in Water for PAH's 331

FIGURE V.2.2.4 Mass Distribution (%) in Biota for PAH's 332

FIGURE V.2.2.5 Mass Distribution (%) in Suspended Solids for PAH's 333

FIGURE V.2.2.6 Mass Distribution (%) in Sediment for PAH's 334

FIGURE V.2.3.1 Concentration (ppm) in Air for PAH's 335

FIGURE V.2.3.2 Concentration (ppm) in Soil for PAH's 336

FIGURE V.2.3.3 Concentration (ppm) in Water for PAH's 337

FIGURE V.2.3.4 Concentration (ppm) in Biota for PAH's 338

FIGURE V.2.3.5 Concentration (ppm) in Suspended Solids and Sediment for PAH's 339

Page

FIGURE V.3 Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Alkylbenzenes 340

FIGURE V.3.1.1 Equilibrium Distribution (%) in Air for Alkylbenzenes 341

FIGURE V.3.1.2 Equilibrium Distribution (%) in Soil for Alkylbenzenes 342

FIGURE V.3.1.3 Equilibrium Distribution (%) in Water for Alkylbenzenes 343

FIGURE V.3.1.4 Equilibrium Distribution (%) in Biota for Alkylbenzenes 344

FIGURE V.3.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment for Alkylbenzenes 345

FIGURE V.3.2.1 Mass Distribution (%) in Air for Alkylbenzenes 346

FIGURE V.3.2.2 Mass Distribution (%) in Soil for Alkylbenzenes 347

FIGURE V.3.2.3 Mass Distribution (%) in Water for Alkylbenzenes 348

FIGURE V.3.2.4 Mass Distribution (%) in Biota for Alkylbenzenes 349

FIGURE V.3.2.5 Mass Distribution (%) in Suspended Solids for Alkylbenzenes 350

FIGURE V.3.2.6 Mass Distribution (%) in Sediment for Alkylbenzenes 351

Page

FIGURE V.3.3.1 Concentration (ppm) in Air for Alkylbenzenes 352

FIGURE V.3.3.2 Concentration (ppm) in Soil for Alkylbenzenes 353

FIGURE V.3.3.3 Concentration (ppm) in Water for Alkylbenzenes 354

FIGURE V.3.3.4 Concentration (ppm) in Biota for Alkylbenzenes 355

FIGURE V.3.3.5. Concentration (ppm) in Suspended Solids and Sediment for Alkylbenzenes 356

FIGURE V.4. Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Polychlorinated Biphenyls (PCB) 357

FIGURE V.4.1.1 Equilibrium Distribution (%) in Air for PCB's 358

FIGURE V.4.1.2 Equilibrium Distribution (%) in Soil for PCB's 359

FIGURE V.4.1.3 Equilibrium Distribution (%) in Water for PCB's 360

FIGURE V.4.1.4 Equilibrium Distribution (%) in Biota for PCB's 361

FIGURE V.4.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment for PCB's 362

FIGURE V.4.2.1 Mass Distribution (%) in Air for PCB's 363

Page

FIGURE V.4.2.2 Mass Distribution (%) in Soil for PCB's 364

FIGURE V.4.2.3 Mass Distribution (%) in Water for PCB's 365

FIGURE V.4.2.4. Mass Distribution (%) in Biota for PCB's 366

FIGURE V.4.2.5 Mass Distribution (%) in Suspended Solids for PCB's 367

FIGURE V.4.2.6 Mass Distribution (%) in Sediment for PCB's 368

FIGURE V.4.3.1 Concentration (ppm) in Air for PCB's 369

FIGURE V.4.3.2 Concentration (ppm) in Soil for PCB's 370

FIGURE V.4.3.3 Concentration (ppm) in Water for PCB's 371

FIGURE V.4.3.4 Concentration (ppm) in Biota for PCB's 372

FIGURE V.4.3.5 Concentration (ppm) in Suspended Solids and Sediment for 'PCB's 373

FIGURE V.5. Plots of Equilbrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Halogen Substituted Benzene Derivatives 374

FIGURE V.5.1.1 Equilibrium Distribution (%) in Air for Halobenzenes 375

FIGURE V.5.1.2 Equilibrium Distribution (%) in Soil for Halobenzenes 377

Page

FIGURE V.5.1.3 Equilibrium Distribution (%) in Water for Halobenzenes 378

FIGURE V.5.1.4 Equilibrium Distribution (%) in Biota for Halobenzenes 380

FIGURE V.5.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment for Halobenzenes 381

FIGURE V.5.2.1 Mass Distribution (%) in Air for Halobenzenes 382

FIGURE V.5.2.2 Mass Distribution (%) in Soil for Halobenzenes 383

FIGURE V.5.2.3 Mass Distribution (%) in Water for Halobenzenes 385

FIGURE V.5.2.4 Mass Distribution (%) in Biota for Halobenzenes 386

FIGURE V.5.2.5 Mass Distribution (%) in Suspended Solids for Halobenzenes 388

FIGURE V.5.2.6 Mass Distribution (%) in Sediment for Halobenzenes 390

FIGURE V.5.3.1 Concentration (ppm) in Air for Halobenzenes 392

FIGURE V.5.3.2 Concentration (ppm) in Soil for Halobenzenes 393

FIGURE V.5.3.3 Concentration (ppm) in Water for Halobenzenes 394

FIGURE V.5.3.4 Concentration (ppm) in Biota for Halobenzenes 396

FIGURE V.5.3.5 Concentration (ppm) in Suspended Solids and Sediment for Halobenzenes 398

LIST OF TABLES

		Page
TABLE I.1	Use of Valance Connectivity Indexes in Structure Activity Relationship Studies.	6
TABLE II.1	Equivalent Terms Used by Mathematicians and Chemists When Describing Graph Theoretical Concepts.	20
TABLE II.2	ACMCP's for Complete Molecules	35
TABLE II.3	p(G,k) Values and Hosoya Index for the Graphs Corresponding to all the Possible Isomers of the Lower Members of Saturated Hydrocarbons (N = 1-6)	48
TABLE II.4	Entropies, Heat Capacities and Heats of Formations for the Homologous Series of Hydrocarbons From Methane to Undecane Calculated by Using Smolenskii Index	53
TABLE II.5	Use of Valance Connectivity Indexes in Structure Activity Relationship Studies	57

		Page
TABLE II.6	Substituent Parameters for Molar Refraction (R_m)	67
TABLE II.7	Valance Delta (δ^V) Values for Heteroatoms	68
TABLE II.8	Boiling Points of Alkyl Halides.	70
TABLE III.1	Unit World Compartment Volumes, Densities	99
TABLE III.2	Summary of Regression Equations, Correlation Coefficients and Standart Deviations	102
TABLE IV.1	Compilation of Physical and Chemical Data for Various Groups of Benzene Derivatives	110
TABLE IV.2	Calculated Valance Molecular Connectivity Indices for PAH, PCB, Halogen and Alkyl Substituted Benzene Derivatives	135
TABLE IV.3	Input Data Used in Multiple Regression Analysis	142
TABLE IV.4	Results of the Regression Analysis (y=mx+n) Showing the Correlation of Valance Molecular Connectivity Indices With log K_{OW}, log S, log P	146
TABLE IV.5	Results of the Two Variable Regression Analysis for Y = log K_{OW}	151

Page

TABLE. VI.6 Results of the Two Variable Regression Analysis for $Y = \log S$ 152

TABLE IV.7 Results of the Two Variable Regression Analysis for $Y = \log P$ 153

TABLE IV.8 Multiple Regression Equations for Halogen Substituted Benzenes Derivatives Where $Y = \ln K_{ow}$ 166

TABLE IV.9 Multiple Regression Equations for Halogen Substituted Benzene Derivatives Where $Y = \ln S$ 167

TABLE IV.10 Multiple Regression Equations for Halogen Substituted Benzene Derivatives Where $Y = \ln P$ 168

TABLE IV.11 Multiple Regression Equations for Alkylbenzenes Where $Y = \ln K_{ow}$ 169

TABLE IV.12 Multiple Regression Equations for Alkylbenzenes Where $Y = \ln S$ 170

TABLE IV.13 Multiple Regression Equations for Alkylbenzenes Where $Y = \ln P$ 171

TABLE IV.14 Multiple Regression Equations for PCB Where $Y = \ln K_{ow}$ 172

Page

TABLE IV.15 Multiple Regression Equations for PCB Where Y = ln P 173

TABLE IV.16 Multiple Regression Equations for PCB Where Y = ln S 174

TABLE IV.17 Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons Where $Y = \ln K_{OW}$ 175

TABLE IV.18 Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons Where Y = ln P 176

TABLE IV.19 Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons Where Y = ln S 177

TABLE IV.20 Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for $Y = \ln K_{OW}$ 178

TABLE IV.21 Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for Y = ln S 179

TABLE IV.22 Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for Y = ln P 180

TABLE IV.23 Three Variable Regression Equations for Alkylbenzenes and PAH's (Groups I and III) Where $Y = \ln k_{OW}$ 181

Page

TABLE IV.24 Three Variable Regression Equations for Alkylbenzenes and PAH's (Groups I and III) Where Y = ln S 182

TABLE IV.25 Three Variable Regression Equations for Alkylbenzenes and PAH's (Groups I and III) Where Y = ln P 183

TABLE IV.26 Multiple Regression Equations for Groups I (Halobenzenes), II (Alkylbenzenes), III (PAH) and IV (PCB) together Where Y = ln K_{OW} 184

TABLE IV.27 Multiple Regression Equations for Groups I (Halobenzenes), II (Alkylbenzenes), III (PAH) and IV (PCB) together Where Y = ln P 187

TABLE IV.28 Multiple Regression Equations for Groups I (Halobenzenes), II (Alkylbenzenes), III (PAH) and IV (PCB) together Where Y = ln S 188

TABLE IV.29 Selected Regression Equations Defining ln K_{OW}, ln S and ln P for Groups I, II, III, IV and for all Groups Together Depending on the Correlation Coefficients. 193

TABLE IV.30 Calculated and Observed Values for ln K_{OW}, ln S and ln P for Alkylbenzenes. 197

Page

TABLE IV.31 Calculated and Observed Values for ln K_{OW}, ln S and ln P for Unsubstituted Polycyclic Aromatic Hydrocarbons 198

TABLE IV.32 Calculated and Observed Values for ln K_{OW}, ln S and ln P for Polychlorinated Biphenyls (PCB) 199

TABLE IV.33 Calculated and Observed Values for ln K_{OW}, ln S and ln P for Halogen Substituted Benzene Derivatives 200

TABLE IV.34 Fugacity Capacity Constants Evaluated by Valance Molecular Connectivity (A) and Level I Fugacity (B) Approaches for p-difluorobenzene 219

TABLE IV.35 Output for the Compartmental Distribution of Benzene Calculated by Level I Fugacity Model 222

TABLE IV.36 Output for the Compartmental Distribution of Benzene Calculated by VMCI Model 22

TABLE V. Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models 224

TABLE V.2 MPD Test Data for Hazard Assessment Accepted by OECD Exposure Analysis Group 315

Page

TABLE V.3. Comparison of Ortho-, Meta-, Para- substituted Benzene Derivatives in Terms of Correlation of Data 321

TABLE I. Boiling and Melting Point Data for Unsubstituted Polycyclic Aromatic Hydrocarbons I-ii

TABLE II. Evaluated Vapor Pressures of Unsubstituted Polycyclic Aromatic Hydrocarbons I-v

LIST OF SYMBOLS

G	a graph as a function
$\bar{\pi}$	Operator that generates lines in a graph
$A=\left[a_{ij}\right]$	Adjacency Matrix
$\vert ACM \vert$	Atom Connectivity Matrix Characteristic Polynomial
Z	Hosoya Index
f(G)	Smolenskii Index.
δ	Number of non-hydrogenic bonded neighbours, irrespective of multiplicity of bonding
δ^{v}	Number of valance electrons (Z_v) not involved in bonds to hydrogen.
X	Simple molecular connectivity index
$^{0}\chi^{v}$	Zeroth order valance molecular connectivity index
$^{1}\chi^{v}$	First order valance molecular connectivity index
$^{2}\chi^{v}$	Second order valance molecular connectivity index
a_i	Coefficients of the regression equations where $i=1,2,\ldots n$
C_a	Equilibrium concentration of chemical in the air phase
C_b	Equilibrium concentration of chemical in the biota phase
C_i	Equilibrium concentration of chemical in each phase

C_o	Equilibrium concentration of chemical in the octanol phase
C_s	Equilibrium concentration of chemical in the soil phase
C_{sd}	Equilibrium concentration of chemical in the sediment phase
C_{ss}	Equilibrium concentration of chemical in the suspended solid phase
C_w	Equilibrium concentration of chemical in the water phase
f	Fugacity
f_a	Fugacity in air
f_b	Fugacity in biota
f_s	Fugacity in soil
f_{sd}	Fugacity in sediment
f_{ss}	Fugacity in suspended solids
f_w	Fugacity in water
H	Henry's Law constant
K	Partition coefficient
K_{oc}	Soil organic carbon-water partition coefficient
K_{ow}	n-Octanol-water partition coefficient
K_p	Soil sorption coefficient
K_{p_s}	Soil-water partition coefficient
$K_{p_{sd}}$	Sediment-water partition coefficient
$K_{p_{ss}}$	Suspended solids-water partition coefficient

M_i	Amount of moles in each compartment
M_T	Total amount of moles
M_V	Molar volume
M_W ,M.Wt	Molecular weight
n	Number of compounds used for correlation
% OC	Percent of organic carbon
P	Vapor pressure
P_1	Vapor pressure at temperature T_1
P_2	Vapor pressure at temperature T_2
P_3	Vapor pressure at temperature T_3
P_i	Mass partitioning of chemical for each compartment
P_i'	Equilibrium partitioning of chemical for each compartment
R	Gas constant
r	Correlation coefficient
S	Aqueous solubility
T	Absolute temperature
T_B	Boiling point temperature in ^{o}K
T_M	Melting point temperature in ^{o}K
V	Volume
V_a	Volume of the air compartment
V_b	Volume of the biota compartment

V_i	Volume of each compartment
V_s	Volume of the soil compartment
V_{sd}	Volume of the sediment compartment
V_{ss}	Volume of the suspended solids compartment
V_w	Volume of the water compartment
Z	Fugacity capacity
Z_a	Fugacity capacity of chemical for the air compartment
Z_b	Fugacity capacity of chemical for the biota compartment
Z_i	Fugacity capacity of chemical for each phase
Z_s	Fugacity capacity of chemical for the soil compartment
Z_{sd}	Fugacity capacity of chemical for the sediment compartment
Z_{ss}	Fugacity capacity of chemical for the suspended solids compartment
π	Hydrophobic substituent constant
ρ	Density
ρ_a	Density of air
ρ_b	Density of biota
ρ_s	Density of soil
ρ_{ss}	Density of suspended solids
ρ_w	Density of water
ρ_{sd}	Density of sediment

I. INTRODUCTION

I- INTRODUCTION

During the past two decades, the study of Quantitative-Structure-Activity-Relationships (QSAR)is being used extensively in pharmacology, especially in drug design and toxicity prediction. The recent developments in this area made this approach a valuable tool also for the prediction of environmental hazards.

It is clear that, the number of organic chemicals currently used, are produced on commercial scale amounts to several tens of thousands per year and no doubt, many new ones will be introduced in increasing amounts in the future. Hence, for the past few years, the concern over the potential hazard of these compounds has led to a considerable amount of scientific research mainly on the partitioning behaviour of these compounds which plays a major role in the environment. Since each of these compounds can not be extensively

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

tested experimentally both in organisms and ecosystems, the prediction of environmental behaviour of these compounds to day, are largely based on various approaches in QSAR. Therefore, the efforts for the estimation of certain structure related physicochemical properties of these compounds through QSAR are gaining importance. Conceivably, the most explicit demonstration of the interactive role played by the molecular environment on biologic activity is observed in the action of drugs. It was Hansch[1] who first proposed that biologic activity very often depends parabolically on the lipid-aqueous phase partition coefficient of the compound in question and defined a hydrophobicity factor (π) which measures logarithmic changes in the partition coefficient. By applying the measured π constants, Hansch has been able to obtain startling correlations of molecular structure with the observed activity in most in vivo and in vitro biological tests. The basic Hansch equation, the starting point of many later correlations, was derived[1] by considering the general case of a drug applied to any biological system. In any biological test, only two quantities may be measured; the amount of compound given (the dose) and the biologic activity obtained (the response). And the response is determined by the structure, that is by the physicochemical properties of the compound. For example It has long been recognized that the absorption and ensuing transport of a drug or any compound from the applied phase to a sensitive site or another phase is governed largely by a lipophillic-hydrophillic balance that can be expressed in terms of the corresponding partition coefficient. It is later demonstrated by Collander[2,3] that the rate of transport of many organic compounds from one phase to another is proportional to the logarithim of their partition coefficients between an organic solvent and water. One primary function of Hansch analysis and other structure-activity methods is to predict optimal molecular or structural characteristics for the design of chemical agents to improve or optimize biological activity. On the other hand, the utility of these methods for studying the dynamics of molecules concerning, for example-the transport through different environmental phases, can not be disregarded.

This work, using an entirely different approach, based on the topological characteristics of molecules, will discuss the extent to which we can use our present understanding of intermolecular interactions to explain and ultimately predict the environmental behaviour in congeneric sets of environmentally hazardous chemical compounds. So, inorder to achieve this goal, a methematical model based on topological characteristics of the molecules is set up and a sound expression relating compartmantal behaviour of a group of molecules with their topology dependent molecular properties is derived.

For the purpose of predicting those properties, many workers used various approaches in QSAR investigations. The use of various molecular orbital concepts[4-6], quantum statistical approximations and many other new types of substituent constants[7] which joined the ranks of σ , π and E_s in Hansch type QSAR studies are among them.

Despite the limited and quantitative nature of the majority of structure-activity relations observed in the first half of XX. century, the justification of the hypothesis that the activity or the behaviour of a substance is a function of its structural features, must be regarded as a general outcome of such relations.

In the simplest case, we know that the structural formula of a molecule conveys a lot of information about the molecule it represents. And it tells us not only which atoms are present but also gives an indication of the way they are linked together. The structural formula thus, gives information about the topology of a molecule, i.e. the way the constituent atoms are connected in space. The structural formula, however, is not the only way of presenting this information. Recent developments in the representation of chemical species have made possible a wide variety of methods to be developed. Among them, there are certain mathematical formulas known as topological indices, which provide a convenient means of encoding, into one comperatively simple mathematical formula, the topological structure of any chemical species. In view of the importance of many of the conceivable uses of topological indices such as in cancer research or in drug design, it is not surprising that they have evoked a great deal of interest recently in the field of environmental sciences. One of the most informative topological indices proposed to date was put forward in 1976 by Kierr and Hall[8] which are known as valance molecular connectivity indices. This concept was used widely in structure activity analysis of drug molecules.

Table I.1 shows several investigations in structure- activity relationship analysis of drugs by using valance molecular connnectivity. This work evaluates the concept of valance molecular connectivity as a means for predicting the possible compartmental distribution of environmentally hazardous chemical substances. The mathematical model set up is based on a large group of substituted benzene derivatives which includes PAH, PCB and halogen substituted benzenes. The hazardous aspects of benzene and its derivatives has long been recognized and have been extensively studied. The biological effects of benzene and its simple derivatives may range from odor sensation

Table I.1. Use Of Valance Connectivity Indexes İn Structure Activity Relationship Studies

Study	Molecules	Reference
Toxicity of anesthetics	Ethers	9
Anesthetic potency	Ethers, ketones	10
Barbiturate potency	Barbiturates	11
Partition coefficient	Hydroxyureas	12
Carminative activity	Alcohols, esters	13
Chromatographic retention	Alcohols	14
Hückel pi electron enrgy	Aromatic hydrocarbons	15
Taste threshold	Alcohols carbonyls, acids, esters	16
Bitter taste	Amino acids, peptides	17
Boiling point	Alcohols, amines,halides	18
Solubuluties		18
Molar refraction		18
General anesthetics	Mixed	19
Cytochrome conversion	Phenols	20
Sweet taste	Nitroanilines	20
Enzyme inhibition	Benzyl alcohols	20
Toxicity	Phenyl phosphates	20
Odor	Benzaldehydes, nitrobenzenes	21
Hallucinogenic activity	Phenylisopropyl amines	22
Mutagenicity	Nitrosamines	23
Serotonin antagonists	Phenalkylamines	24
Serotonin antagonists	Lysergic acid amides	25
Muscarinic antagonists	Amines	26
Antimicrobial activity	Phenyl propyl ethers	27
Chromatgraphic retention	Mixed	28
General anesthetics	Halocarbons	29
Hallucinogenic agents	Phenethylamines	30
Monoamine oxidase inhibitors	Hydrazines	31
Hormone class	Steroids	32
Reductase inhibitors	Benzohydroxamic acids	33

to production of lesions in blood, liver kidney and nervous tissue. In addition to being toxic to mammals, many of these derivatives show marked biological activity on a wide variety of other organisms including bacteria, plants, insects and fungi. The type and intensity of this effect varies with the nature and the position of the substituent on the benzene ring.

In study of the relationship of structure and physical properties to activity one generally examines not only the positional isomerism, or steric and inductrometric effects of these substituents but also the effects of these substituents on the physical properties of molecules such as vapor pressure, solubility and partition coefficients so that a bridge between these structure dependent properties and the activity can be set up . From the point of wiew of an environmentalist, on the other hand, this approach concering mathematical manuplation of several of these structure dependent molecular parameters may as well lead to a compact representation of possible distribution of these compounds in the environment.We know that, every physicochemical property which is additive in the broadest sense of the word, is a function of the number and sort of valancy bonds or energy units of the molecules exhibiting the particular property.

It is also obvious that in a congeneric series, when it is inconvenient or impossible to obtain parameters for a series of molecules, a model that is independent of these parameters can be used, assuming that the various substituent groups contribute additively and linearly to the specific property.

In this work, such a model, based on the graph theoretical evacation of zero to second order valance melocular connectivity indices is developed to predict the compartmental behaviour of a series of substituted benzene derivatives including PAH, PCB and halogen substituted benzene derivatives. Those indices when evaluated according to Mackay's level I fugacity model, have led to an expression of type

$$Z = C \exp A$$

where Z is the fugacity capacity for a certain compartment and C and A are semiempirical constants determined through the appropriate use of valance molecular connectivity indices.

Hence, by simple physicogeometric evaluation of zero to second order valance molecular connectivity indices, one can easily predict amounts, concentrations mass and equilibrium partitioning values for a specific member of the congeneric series.

As a result, it clearly appears that by the application of graph theory real advonces should be expected also in the field of environmental sciences provided that the deserved attention is payed to different modifications of the capacity for molecular binding, which is readily susceptible to calculation whatever the complexity of the given structure is.

"The atoms were dancing before my eyes.......my mental eye..... could now distinguish larger structures of manifold conformation; long rows...... all twining and twisting in snake-like motion. But look! What was that? One of the snakes had seized hold of his own tail, and the form whirled mockingly before my eyes."

Kekulé 1858

II. GRAPH THEORY
AND
ITS APLICATIONS

II. GRAPH THEORY AND ITS APPLICATIONS

II.1. HISTORICAL BACKGROUND AND ITS DEVELOPMENT

Graphs were first invented in the mid 1730's by Euler, who used idealized networks to solve a celebrated problem of his time known as the Königsberg bridge problem. Since then, graphs have been employed in a variety of different contexts, such as Kirchoff's electrical circuits and recently the theory has developed into an important branch of mathematics with many applications to a large number of other disciplines. Thus, today graph theory is making a significant impact in many fields such as economics, psychology, nuclear and theoretical physics, linguistics, sociology and mathematical biology.

The use of graphs to depict molecules was the first application of graph theory to chemistry. This represented a major advance and has been claimed to be the most fruitful scientific discovery ever made. The importance of this discovery can hardly be over-emphasized since it has provided the necessary conceptual framework in which modern organic and later inorganic chemistry could develop and thus, has been directly responsible for the foundation and phenomenal growth of chemistry over the last century.

The originator of this idea, namely the graphical representation of molecules is quite difficult to pinpoint. Although a number of workers had similar thoughts on the subject at about the same time, the first use of the term 'structural formula' in its modern sense is due to the Russian chemist Butlerov (1861)[70] and recently it is recognized that all covalent structures may be represented by either a two or a three-dimensional graph.

A graph is an abstract mathematical concept, probably most easily visualized as a collection of points and lines, drawn so that pairs of points are connected together. A graph thus provides not only the chemical constitution but also the complete topology of the molecule it represents. In this mode of representation the vertices stand for the time average position of the atomic nuclei while the edges symbolize the valance bonds connecting the nuclei.

Graph theory, which Is sufficiently broad in scope to serve as a foundation for the representation and categorization of large numbers of chemical systems, has been successfully employed in a number of problems which arrise from studies of chemical structure. So, the advantage of the use of its techniques in chemistry lies in its exceptional versatility in both the depiction and categorization of molecular structure.

In recent years, a large number of nomenclature systems based on graph theory have been devised both for the representation and for the computer searching of structures. Depending on the nature of the problem to be tackled, these systems have represented molecular structures by codes, matrices or polynomials[71]. This representation has provided the basis for an efficient technique for searching files of chemical compounds stored in coded form.

Fugmann et. al.[72], a few years later took this concept one step further and attempted to represent the chemical concepts and their interrelations in graph theoretical language. On the other hand, methods based on the representation of structures by matrices and polynomials have also proved their value in computerizing chemical information. This new mode of representation, due to Spialter[73] was based on the so-called atom connectivity matrix (ACM) for a molecule and was essentially a method of representing the graph of the molecule in matrix form as will be illustrated in the foregoing sections.

Another system was developed by Lederberg and his co-workers[74] which is known as the Dendritic Algorithm (DENDRAL) method which uses a line representation for molecules consisting of letters, dots and other typographical symbols. The importance of this method lies in its successful application to the interpretation of mass spectra by matching the structures[75] and to the enumeration of structural isomers.

The use of graphs to represent complex chemical systems is comparatively recent. During the last decade graphs have been increasingly employed to represent a great deal of information about systems which are often very complicated, in quite a convenient and concise way. From these studies, useful information on the differences in the stereoisomerizations for alternative mechanisms and the relative energy relationships involved has emerged:

At the beginning of 70's intentions were made to investigate the applicability of the mathematical apparatus of Graph Theory (GT) to the Hückel's molecular orbital theory (HMOT)[76,77]. As an interesting outcome of this treatment, it has been shown that the problem of Hückel orbital energies can be completely reduced to the adjacency matrix eigenvalue problem in GT. In other words, the spectrum of eigenvalues obtained from the graphical approach were found to be so closely related to the energy levels obtained from the Hückel matrix that, the terms eigenvalue and energy level are used interchangeably in this context since then. On the other hand, it is clear that, quantities derived from the Hückel theory, including a number of indices such as charge density, bond order etc. are determined by the topology of the species considered. So, it has been observed that most aspects of MO theory put forward by Hückel, have a very close connection with the graphical (topological) representation of molecular species.

Today, we know that those indices may also be derived from the characteristic polynomials in graph theory.

Hence, because of its unique way of encoding the topological structure of a molecule, graph theoretical approach, as well as Hückel theory has found one of its prime applications in the derivation of physical properties of chemical species by the use of those indices.

Graph theory also proved of benefit in kinetic studies on the reactivity of chemical species because incipient or partial bonds which are formed during a chemical reaction can be represented by means of fractional connectivity entries in this method.

So, this mode of representation enabled graph theory to represent a whole series of chemical states of a molecule by the appropriate sequence of matrices the aggragate sum of which represents the total molecule.

The next major advance parallel to this idea, led to the application of Additivity Principle to graph theory. This, the concept that the chemical components of molecules could display fixed characteristics in series of molecules, have led to a number of new and useful indices which are topological in nature for predicting the additive physicochemical properties of molecules. Hence, graph theoretical approach constituted a reasonable and useful mathematical model for the prediction of quantitative structure activity relationships (QSAR). However, up to late 70's graph theory, within its limitations, was mostly applied to and had been succesful with small, straight chain molecules. When those limits went beyond the need for a simple filing and coding system for chemical species and larger molecules, aromatic compounds and especially heteroatoms were considered, some modifications on the model, involving the electrical nature of bonds, was required to be done as to take care of size effects, conformational differences and presence of heteroatoms. In other words, the model to be set up should go beyond the structural fact of adjacency, which is the basis of graph theory and should consider the count of valance electrons participating in σ , π and lone pair orbitals on each atom.

Among the few approaches to accomplish the encoding of such structural differences, the approach of Kierr and Hall[78], proposing the idea of using "valance molecular connectivity" instead of "simple atom connectivity" have found its prime application in the derivation of physical properties of molecules and consequently in QSAR studies. Their approach quantized the molecular structure encoding information about size, branching, cyclization, unsaturation and heteroatom content.

This approach constitutes the basic theory on which this work has been set up. Hence, in addition to the possible applications of graph theory which have been summarized above, This work underlines another specific area in which graph theory is likely to have an important impact in the coming decade; that is the determination of the types of functions relating quantitatively the structural characteristics of a substance to its behaviour in the environment. In other words, the environmental techology....

II.2. THEORY

II.2.1. GRAPH THEORY AND REPRESENTATION OF MOLECULES

As we all know, chemical pictographs or molecular diagrams are the natural language in which chemists describe molecules and reactions thereof. In this mode of representation, the essential components are the constituent atoms and the bonds between them.

Consider molecules as being "connected collections of readily recognizable local assemblies of atoms", such as chains, n-membered rings, functional groups etc., and to such local assemblies, assign characterisctic symbols with suitable additional symbolism to describe their interconnections.

This method of describing molecular pictographs is based on some sort of topological mapping of the individual atoms and the bonds between them.

It appears likely that such a representation based only on atoms and interconnecting bonds is the simplest mathematical transformation of a chemical pictograph.

This class of representation is initially based on a special matrix construction which is then converted by standart algebraic techniques to a derivative form which has interesting and useful properties.

A graph; in more general terms, is a mathematical structure which may be used to depict the topology of any given system. A chemical graph on the other hand, is defined as a set of points, known as vertices, and set of lines, known as edges, which connect pairs of vertices. So, in a chemical graph the vertices represent atoms and edges represent the bonds between them. Figure II.1 shows chemical graphs representing the molecules of propane and benzene.

Since the chemical graph provides a pictorial representation of the topology of a chemical species it is regarded as the first stage in the construction of the topological index for the species.

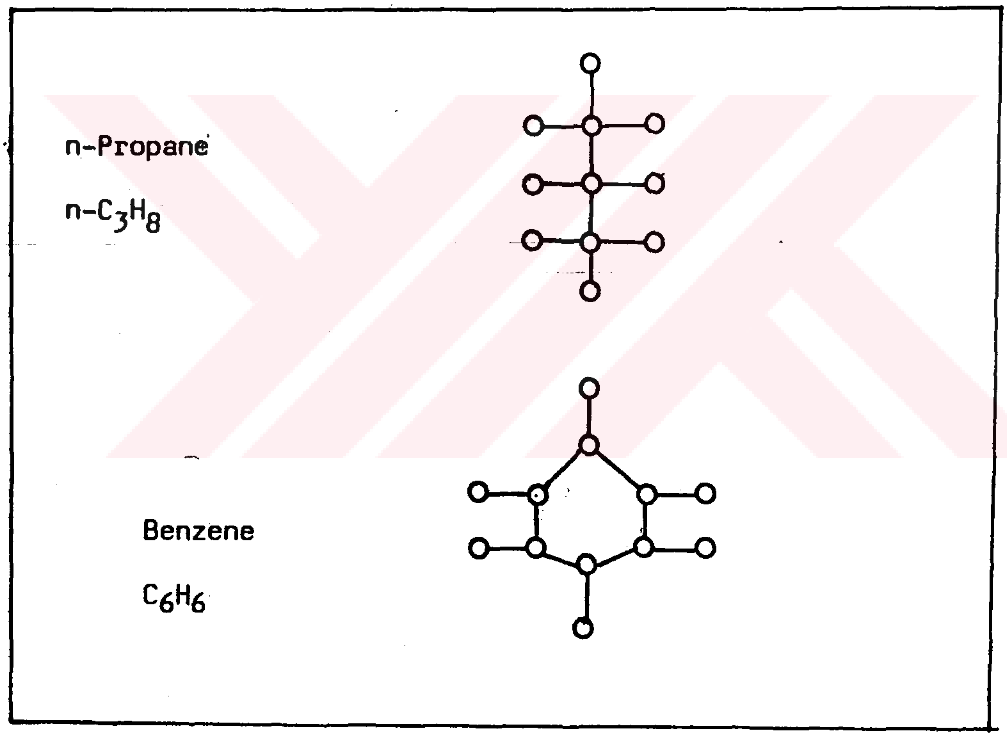


Fig. II.1.: Chemical graphs of propane and benzene where atoms are represented by vertices and bonds by edges.

In this context, a graph can be defined as "an abstract mathematical concept which can be visualized as, a collection of points and lines drawn so that pairs of points are connected together." So before going further to the details,.to make the terminology clear in the following discussion on the derivation of some basic graph theoretical concepts, we should have a look at some of the equivalent terms used by mathematicians and chemists when describing chemical graphs listed in table II.1.

Table II.1. : Equivalent terms used by mathematicians and chemists when describing graph theoretical concepts.

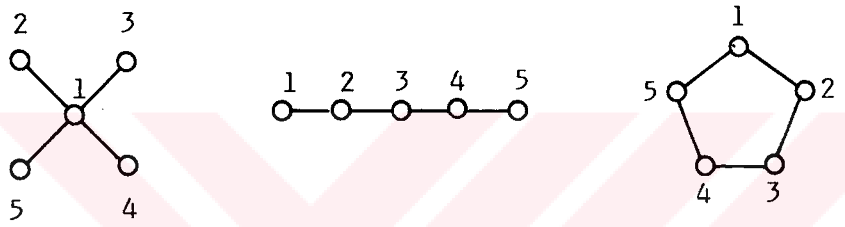
MATHEMATICAL TERM	CHEMICAL TERM
Chemical graph	Structural formula
Vertex	Atom
Edge	Chemical bond
Degree of a vertex	Valancy of an atom
Adjacency matrix	Topological matrix
Bipartite graph	Alternant molecule
Cycle with n vertices	n- Annulene
Chain with n vertices	n- Polyene
Eigenvalue	Energy level

II.2.2: ASSEMBLING THE ATOM CONNECTIVITY MATRIX

A graph G, may be defined as " a set X, of points, together with an operator (Γ) which generates the lines in the graph, by mapping points of X into neighbouring points[92] ". A graph, which now may be represented symbolically as $G = (X, \Gamma)$, thus gives all the neighbourhood relations for the set X. Here, the function of Γ , is to create from X, a new set Y, consisting of unordered pairs of X, the members of which are the vertices of the graph, while the members of set Y represents the edges.

The following approach based on the topology of the molecule assimilates a covalently bonded molecule with a graph whose vertices (points) are the atoms and whose edges (lines) are the covelent bonds. The structure or the topology of the molecule is then uniquely encoded in the adjacency matrix of its graph. By definition, the adjacency matrix $A = \left[a_{ij}\right]$ of a graph G with P points $V_1, V_2 \ldots V_p$ is the binary matrix in which $a_{ij} = 1$ when V_i and V_j are adjacent (bonded in chemical terminology) and $a_{ij} = 0$ otherwise, including the main diagonal elements. This implies that, all adjacency matrices must be symmetrical about the principle diagonal, which itself will always consist only of zero entries.

Figure II.2. illustrates the structure of adjacency matrices for three different types of chemical graphs having the configurations of a star, a chain and a ring



$$\begin{array}{c|ccccc|}
 & 1 & 2 & 3 & 4 & 5 \\
1 & 0 & 1 & 1 & 1 & 1 \\
2 & 1 & 0 & 0 & 0 & 0 \\
3 & 1 & 0 & 0 & 0 & 0 \\
4 & 1 & 0 & 0 & 0 & 0 \\
5 & 1 & 0 & 0 & 0 & 0
\end{array}
\qquad
\begin{array}{c|ccccc|}
 & 1 & 2 & 3 & 4 & 5 \\
1 & 0 & 1 & 0 & 0 & 0 \\
2 & 1 & 0 & 1 & 0 & 0 \\
3 & 0 & 1 & 0 & 1 & 0 \\
4 & 0 & 0 & 1 & 0 & 1 \\
5 & 0 & 0 & 0 & 1 & 0
\end{array}
\qquad
\begin{array}{c|ccccc|}
 & 1 & 2 & 3 & 4 & 5 \\
1 & 0 & 1 & 0 & 0 & 1 \\
2 & 1 & 0 & 1 & 0 & 0 \\
3 & 0 & 1 & 0 & 1 & 0 \\
4 & 0 & 0 & 1 & 0 & 1 \\
5 & 1 & 0 & 0 & 1 & 0
\end{array}$$

Fig. II.2. : The adjancency matrices for three types of chemical graphs having different configurations.

A different but related matrix which also encodes uniquely the structure of the molecule put forward by Spialter[73,79], is the Atom Connectivity Matrix. This matrix differs from the adjacency matrix in two respects:

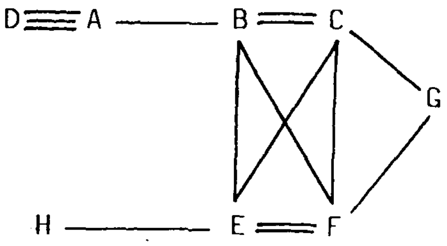
- On the main diagonal the chemical elements are displayed instead of zeros which contain no information.
- Off the main diagonal, bond parameters describing the bonds, such as bond orders 1,2,3 (or fractional ones) are displayed.

Hence, the Atom Connectivity Matrix, simply known as ACM becomes some sort of topological mapping of the individual atoms and the bonds between them. So, it is a universal symbolism which, with only two simple rules, allows ready transformation of the usual two dimensional pictorial molecular representation into a unique mathematical expression.

RULE I: Sketch the molecule with all the atoms (or radicals, nuclei etc.) and interatomic connectivities (bonds, bond orders, force constants, ionic character, dipole moments, vectorial components etc.) to be incorparated into the ACM.

RULE II: Construct the matrix array composed of mathematical elements a_{ij} , where i and j are integers defining the row and the column respectively. In the diagonal elements where i = j, are placed symbols for the atoms, radicals, electron charges or other groups making up the molecular formula in any order. In the respective off-diagonal positions where $i \neq j$, are placed the connectivity parameter between the groups in question.

To describe the assembling of the ACM array let us take the hypothetical "molecule" which had been previously used by L. Spialter[11],



where connectivities pictured are conventional bond orders.

The procedure, step by step is as follows;

1- The eight atoms in question are placed into the diagonal elements of an 8x8 matrix in any order.

A							
	B						
		C					
			D				
				E			
					F		
						G	
							H

2- The appropriate connectivities are placed at the intersections of rows and columns for the respective atoms. For example,

a- The triple bond between A and D appears on the matrix as;

A			3				
	B						
		C					
3			D				
				E			
					F		
						G	
							H

(3 appears at the cross points for row and column 1 and 4 governed by A and D)

b- The complex interplay between the atoms B, C, E and F where both double and single bonds appear can be entered into the ACM as follows;

A							
	B	2		1	1		
	2	C		1	1		
			D				
	1	1		E	2		
	1	1		2	F		
						G	
							H

c- The three membered ring involving C, F and G would appear as;

A							
	B						
		C			1	1	
			D				
				E			
		1			F	1	
		1			1	G	
							H

The total ACM assambled for the hypothetical molecule in accordance with the principles examplified above can then be written as follows after filling out the zeros for the cases where there is no bonding.

A	1	0	3	0	0	0	0
1	B	2	0	1	1	0	0
0	2	C	0	1	1	1	0
3	0	0	D	0	0	0	0
0	1	1	0	E	2	0	1
0	1	1	0	2	F	1	0
0	0	1	0	0	1	G	0
0	0	0	0	1	0	0	H

The resulting matrix is symmetric about the diagonal line of the atoms and each half of the matrix represents the total connectivity of the whole molecular system. Thus, the resulting ACM, independent of atom-ordering priorities, numbering conventions, language etc., is a complete, compact representation of the molecular pictograph. A few illustrative examples of ACM's are given in figure II.3.

It is to be noted that the ACM for large molecules may appear as a formidable array. However itis possible to make a significant saving in the size of the ACM by noting that its greatest application will probably be to organic molecules. Since hydrogen atoms except in rare cases (such as perhalocarbons) constitute a large proportion of the atoms in most organic structures and since they have a bond order connectivity of unity, it has been found possible and convenient to omit them from the ACM with no significant loss in general, for a majority of applications.

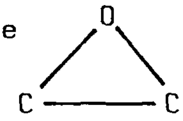
MOLECULE		
NAME	STRUCTURE (H-suppressed)	ACM
N-Butane	C-C-C-C	$\begin{vmatrix} C & 1 & 0 & 0 \\ 1 & C & 1 & 0 \\ 0 & 1 & C & 1 \\ 0 & 0 & 1 & C \end{vmatrix}$
Acetaldehyde	C-C=O	$\begin{vmatrix} C & 1 & 0 \\ 1 & C & 2 \\ 0 & 2 & 0 \end{vmatrix}$
Ethylene oxide		$\begin{vmatrix} C & 1 & 1 \\ 1 & C & 1 \\ 1 & 1 & 0 \end{vmatrix}$

Figure II.3.: Examples for the hydrogen-suppressed ACM'S.

In essence, how the chemist draws the original molecule, its atoms and their connectivities determines also the ACM and its relative order of approximation to the molecular structure. These concepts can probably best be explained by selecting specific applications to other molecular types such as free radicals, ions, ionic salts, sandwich compounds etc. Following examples will be devoted to simple structure inexing of such structures. Since the rules are self-evident, discussion will be kept to a minimum.

1- Free Radicals

$$R^{\bullet} = \begin{vmatrix} R & 1 \\ 1 & \varepsilon \end{vmatrix}$$

2- Ions

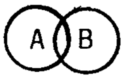
$$A^{+3} = \begin{vmatrix} A & 1 \\ 1 & ch^{+3} \end{vmatrix}$$

3- Ionic Salts

$$(A^{+})\ (B^{-}) = \begin{vmatrix} A & 0 & 1 & 0 \\ 0 & B & 0 & 1 \\ 1 & 0 & ch^{+1} & 0 \\ 0 & 1 & 0 & ch^{-1} \end{vmatrix}$$

This convention shows a zero order bond between A^+ and B^-.

4- Clathrates

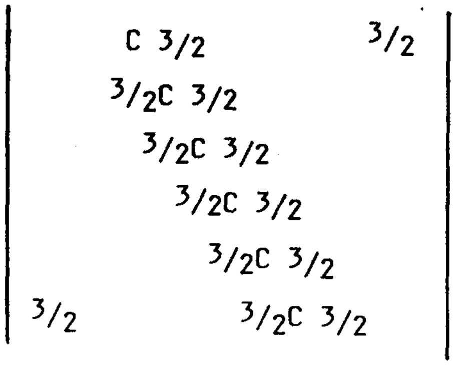


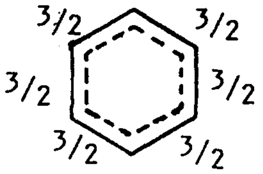
$$= \begin{vmatrix} ACM_A & 0 \\ 0 & ACM_B \end{vmatrix}$$

Where ACM_A and ACM_B are the ACM's for components A and B. Inclusion compounds and linked ring chains wherein no specific bonds can be drawn between two seperate molecular entities mechanically joined may be combined into one ACM with zero off-diagonal elements between them.

5- Resonance hybrids and delocalized species

These species, where connectivities are of fractional orders can be transformed into their ACM's by using fractional entries. The extension of this technique to benzene in its delocalized form is;

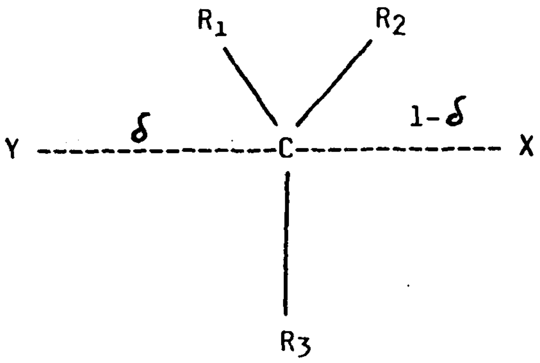

C 3/2
3/2
3/2C 3/2
3/2C 3/2
3/2C 3/2
3/2C 3/2
3/2
3/2C 3/2


3/2
3/2
3/2
3/2
3/2
3/2

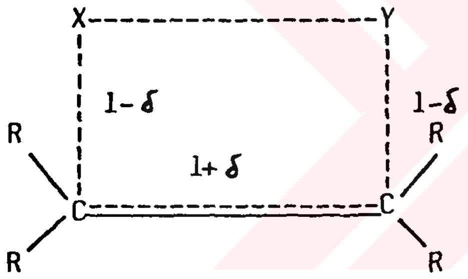
Here, since a bonding electron corresponds to one-half of a bond order unit, the C-C bonds in the ring have a bond order of $^3/_2$

6- Transition states

Transition states, which are non-stable molecular species are expressed by a continuously changing parameter , which varies from 0 to 1 during the course of a reaction. Two typical examples, one for an SN_2 reaction and another for a four centered (E_1) elimination is given below.



$$\begin{vmatrix} C & 1 & 1 & 1 & 1-\delta & \delta \\ 1 & R_1 & 0 & 0 & 0 & 0 \\ 1 & 0 & R_2 & 0 & 0 & 0 \\ 1 & 0 & 0 & R_3 & 0 & 0 \\ 1-\delta & 0 & 0 & 0 & X & 0 \\ \delta & 0 & 0 & 0 & 0 & Y \end{vmatrix}$$



$$\begin{vmatrix} R & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & C & (1+\delta) & 0 & (1-\delta) & 0 & 1 & 0 \\ 0 & (1+\delta) & C & 1 & 0 & (1-\delta) & 0 & 1 \\ 0 & 0 & 1 & R & 0 & 0 & 0 & 0 \\ 0 & (1-\delta) & 0 & 0 & X & \delta & 0 & 0 \\ 0 & 0 & (1-\delta) & 0 & \delta & Y & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & R & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & R \end{vmatrix}$$

7- Macromolecules

Polymers of n-mer type yield ACM's by taking the n th. power of the ACM for the basic building block or monomeric unit, assuming zero order or non-localized bonding between the monomeric units.

II.2.3. THE ATOM CONNECTIVITY MATRIX CHARACTERISTIC POLYNOMIAL AND ITS PHYSICO-GEOMETRIC (TOPOLOGICAL) SIGNIFICANCE

It is clear from the above discussion that, matrix notation for a molecule has certain excellent storageability characteristics. However, it is also evident that the stroge simplicity of the matrix formulation carries with it certain serious limitations such as,

a) A group of matrices cannot be universally ordered, that is, there is no method for organizing a collection of matrices in some numerical sequence defined by the matrices themselves.

b) The identity of the molecule represented by the pictograph is independent of how one cares to number or name the atoms in the molecule. This is not the case with a matrix representation.

c) Matrices require very complex computer operations for searching and comparison.

d) ACM implies only what the chemist draws, and it is assumed that the chemist means what he draws and draws what he means.

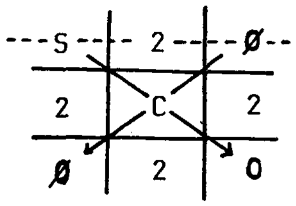
So, a scheme to overcome these disadvantages was what we needed for better storageability characterisitics. One of the concepts proposed, appeared to meet these requirements except for the last cited difficulty above. This quantity derivable from the ACM is the Atom Connectivity Matrix Characteristic Polynomial (ACMCP). This polynomial is obtained by evaluating the matrix as a determinant through the usual mathematical techniques,such as decomposition into minors and the summation of factor-cofactor products or by matrix operations not requiring direct expansion[80]. This procedure, known as the "determinantal polynomial" or the "value of the determinant"in matrix calculus, is expressed as;

$$|ACM| = ACMCP = \sum_{P(i)} (-1)^{v} \quad a_{1i_1} \cdot a_{2i_2} \cdots\cdots a_{ni_n}$$

where; $|ACM|$ is the value of the determinant of ACM, a_{ni_n} is the element in row n, column i_n , i_n is the column subscript, v is the number of inversions and the indicated algebraic sum is taken over all possible permutations of the subscripts. This range of summation is denoted by P (i).

The following example equates the molecular pictorgraph for carbonyl sulfide, to the analogous ACMCP determined in accordance with the above definition.

S = C = O



ACM = S (CO - 2.2) - 2.(2.O -2.0) + 0 (2.2 - C.0)

ACMCP = SCO - 4S - 4O

Other examples of ACMCP's for complete simple molecules are shown in table II.2.[80]

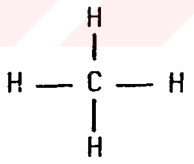
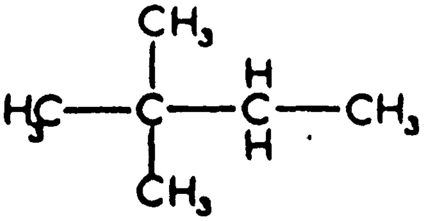
MOLECULE	PICTOGRAPH	ACMCP
Methane	 $H-\underset{H}{\overset{H}{C}}-H$	$CH^4 - 4H^3$
Acetylene	$H-C=C-H$	$C^2 H^2 - 2CH - 9H^2 + 1$
Formaldehyde	$H_2C = O$	$CH^2O - 2HO - 4H^2$
Cyanogen	$N \equiv C - C \equiv N$	$C^2N^2 - 18CN - N^2 + 81$
Ketene	$HC = C = O$	$C^2H^2O - 4CH^2 - 4H^2O -$ $2CHO + 8H$

Table II.2. : ACMCP's for complete molecules

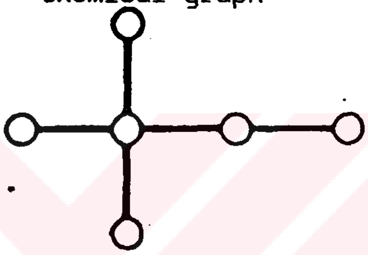
The numerical coefficients obtained in ACMCP have certain physical significance in being combinatorial products of connectivities in bonds and around ring configurations in the molecule under consideration.

As a general outcome of the evaluation of characteristic polynomials for chemical species, it has been understood that this kind of representation contains a great deal of useful information about the species it represents. For example, when this polynomial is set equal to zero and solved as a polynomial equation, a number of characteristic roots or eigenvalues are obtained which can be used in the same sense as energy levels derived from the Hückel matrix. The following scheme illustrates the sequence of steps required to derive the eigenvalues for 2,2-dimethylbutane. Due to this close relationship between molecular orbital theory as put forward by Hückel and graph theory, a fair amount of research on this topic has been carried out to derive the topology determined quantities derivable from Hückel theory by the graph theoretical approach. Those efforts have revealed that those two matrices are equivalent and that they

Structural formula



Chemical graph



Topological matrix

$$\begin{array}{c|cccccc} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 1 & 1 & 0 \\ 3 & 0 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 1 & 0 & 0 & 0 & 0 \\ 5 & 0 & 1 & 0 & 0 & 0 & 1 \\ 6 & 0 & 0 & 0 & 0 & 1 & 0 \end{array}$$

Characteristic polynomial

$$x^6 - 5x^4 + 3x^2$$

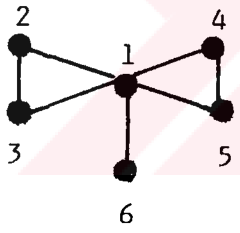
Spectrum of eigenvalues

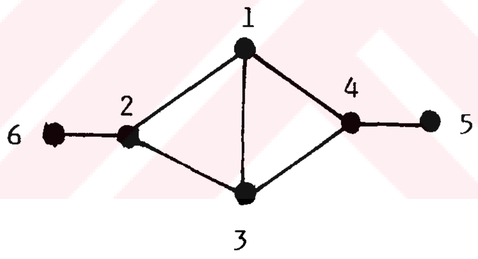
$-2{\cdot}075$, $-0{\cdot}835$, $0{\cdot}0$

$0{\cdot}0$, $+\,0{\cdot}835$, $+\,2{\cdot}075$

will therefore always possess corresponding eigenvalues or energy levels. This result in turn implied that all topological indices derived from the Hückel matrix can also be derived by means of the topological indices (eigenvalues) obtained from the topological matrix.

However, it was later realized that this polynomial does not always give a unique characterization of the chemical species in all possible cases. The fact that two non-isomorphic chemical graphs such as;





may have the same set of eigenvalues, pointed out to an important drawback in the use of the characteristic polynomials to characterize chemical species. Hence, in order to overcome this drawback, the conventional methods for distinguishing the carbon skeletons of the structural isomers of hydrocarbons have gained attention and as a useful outcome of these studies a new topological index Z is defined and proposed as another candidate for classifying saturated hydrocarbons with respect to their topological nature[81]. Index, Z, is proposed for a connected graph G, representing the carbon skeleton of the set of the numbers p (G,k), which is the number of ways in which such k bonds are so chosen from G that no two of them are connected. This approach has been the start of a new era in the development of graph theory, after which it has become an important tool in characterization of molecular properties.

II.2.4. DEVELOPMENT AND USE OF TOPOLOGICAL INDICES

One of the most important tools in the topological method of making chemical predictions are known as indices. Indices are derived from algorithims or procedures for converting the topological structure of a molecule into a single characteristic number.

This approach is based on the determination of the properties of basic fragments found in many molecules and the combination of these fragmental properties in ways that depend on the make up of the molecule in question. These properties are usually determined by analyzing a set of molecules that are similar to the specific group of molecules that is being studied. Here, the object is to relate a rather ill-defined concept of overall structure to rigorously defined molecular behavior. This technique is based on the assumption that molecular structure can be characterized mathematically and precisely and that the mathematically determined parameters of molecules can be correlated with the molecules' experimentally measured properties. The only thing to do is to choose a mathematical way of assigning numbers to molecules and than correlate those numbers with the vast data base of known chemical properties. In this way the properties of well known molecules serve as a tool for predicting the properties of molecules that do not yet exist. The key to the method lies in finding the index that correlates best with the chemical property being studied.

Due to the promising correlations obtained between the topological indices and the topology dependent molecular properties, the search for new and useful topological indices has in recent years gained importance and it is now being increasingly realized that those indices have all sorts of practical applications. For example, other than being a sorting device in the coding of chemical formulae, further work on its usefulness in this domain may prove graph theory to play an important part in the search for new drugs that should possess specific structural features or in the prediction of certain patterns of behaviour due to certain structural similarities and in this context it might also be useful in predicting the degree to which various pollutants might spread in the environment and the harm they might do once they have spread.

The topological analysis of a molecule begins with a drawing in which the atoms are depicted as points and the bonds linking them are depicted as straight lines. Once the chemical graph has been drawn, derivation of topological index is a matter of obtaining a number that characterizes the graph. This number must have the same value for a given molecule no matter how the molecule's graph is drawn or labelled. A number of this type is reffered to by mathematicians as a graph invariant. One of the earliest graph invariants or topological indices is known as vertex or carbon number which chemists have been relying on for certain correlations for more than a century without realizing that they were using what is infact a simple topological index. Later, in the mid forties, the need for other indices that are able to distinguish effectively between branched and unbranched molecules and among branched molecules having different branching structures together with the concept that a whole series of chemical states of a molecule may be represented by an appropriate sequence of matrices and that the "state" of a molecule could be represented by a summation of the "states" of the component parts of the molecule have led *to a number of new and useful indices of topological nature* for characterizing the physicochemical properties of molecules.

The first topological index capable of characterizing the "branchedness" of molecules was put forward by Harry Wiener (1947). The Wiener index is based on the graph theoretical notion of distance. Wiener showed that the distance between any two vertices is equal to the number of edges one would traverse in taking the shortest route possible through the molecule's graph from one of the vertices to the other. Hence, Wiener index of *a molecule is equal to the sum of the graph theoretical dis*tances between all pairs of atoms in the molecule (fig. II.4(a)). This index correlated surprisingly well with such properties as boiling point, (fig. II.4(b)) viscosity, surface tension and refractive index. In later years it has been shown to correlate very well **also** with the energies of the bonding electrons in certain types of complex molecules. This seemed to

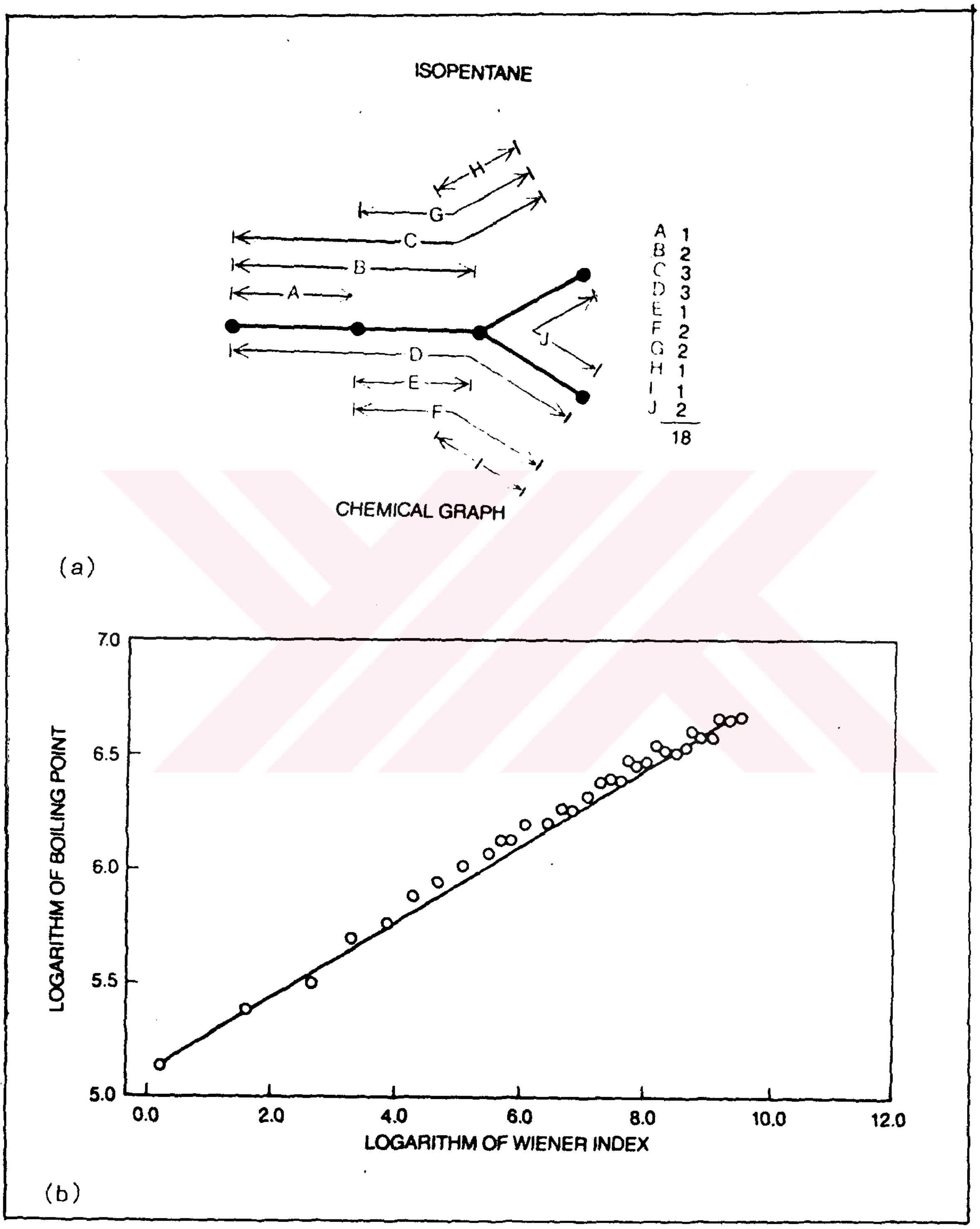


Figure II.4. : *The Wiener index is calculated by summing up the number* of bonds that would have to be traversed in travelling along the molecule from every atom to very other atom.

be a very important result, because the energy levels of molecule's bonding electrons are directly responsible for a great deal of the molecule's chemical behaviour.

Just as the Wiener index depends on the topological concept of distance, in the beginning of seventies another index that is dependent on the concept of degree which is more sensitive to shape was introduced by M. Randic (1975) known as the molecular-connectivity index. According to Randic, the degree of any vertex is equal to the number of other vertices to which it is attached. More spesifically the value of an edge is equal to the reciprocal of the square root of the product of the degrees of the two vertices. So, the Randic index is equal to the sum of the values of all molecules edges (fig. II.5.).

After Randic proposed his molecular connectivity index, other investigators noted that in some cases better correlations could be obtained by focusing on the component parts of molecule. In this way, other connectivity indices that are applicable to particular molecular substructures that may be of importance in determining specific behavioral charac-

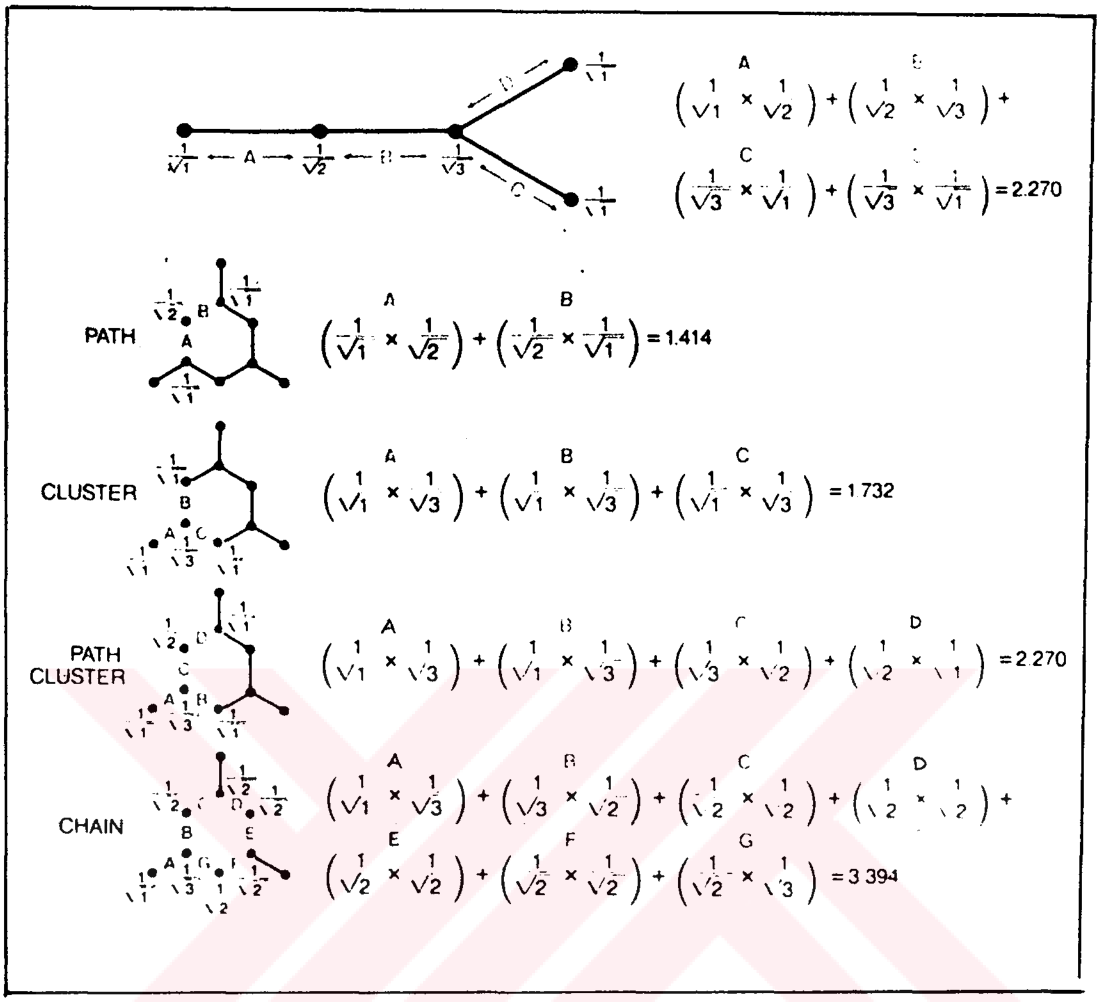

A
B
C
D
=2.270
PATH
=1.414
CLUSTER
=1.732
PATH CLUSTER
=2.270
CHAIN
E
F
G
=3.394

Figure II.5. : Evaluation of Randic Molecular Connectivity Index

teristics have been developed. For example the Hosaya index put forward by H. Hosoya (1971) is one of the most important topological indices proposed. The Hosoya index which is used for the characterization of many molecular properties is formally defined by the equation

$$Z = \sum_{k=0}^{m} p(G,k)$$

where Z represents the index, p(G,k) is the number of ways in which k edges of the chemical graph can be chosen so that no two of them are direcly connected and the summation extends over all the m edges of the graph.

One of the most important aspects of the Hosoya index has been its correlation with the boiling points of the species represented and the evaluation of the index for a large number of molecules has shown that the boiling points of organic substances are proportional to the value of the index for the species in question. Since it provides a measure of the topological nature of the chemical graph especially in regard to its branching and cyclization features, the Hosoya index has found a significant role also in other areas such as determining the Kekulé structures or evaluating Hückel energy levels in given species due to its close interrelation to the characteristic polynomial. The evaluated indices and their relation to the boiling points for the lower members of normal and isomeric parrafins are given in table II.3. in increasing order of the Hosoya index Z.

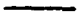
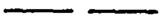
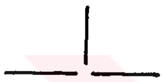
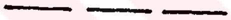
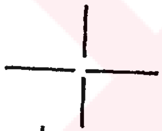
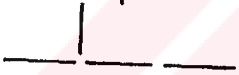
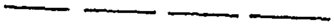
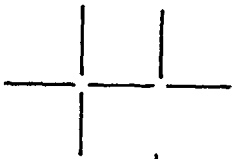
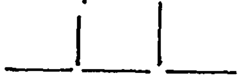
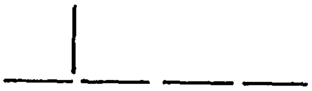
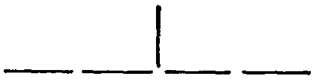
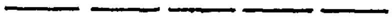
N	Graph (G)	k= 0	1	2	3	Z_G	bp ^{o}C
1		1	0	0	0	1	-161.7
2		1	1	0	0	2	-88.6
3		1	2	0	0	3	-42.2
4		1	3	0	0	4	-11.7
		1	3	1	0	5	- 0.5
5		1	4	0	0	5	9.5
		1	4	2	0	7	27.9
		1	4	3	0	8	36.1
6		1	5	3	0	9	49.7
		1	5	4	0	10	57.9
		1	5	5	0	11	60.2
		1	5	5	1	12	63.5
		1	5	6	1	13	68.7

Table II.3. p(G,k) values and Hosoya İndex for the graphs corresponding to all the possible isomers of the lower members of saturated hydrocarbons (N=1-6).

II.2.5. THE ADDIVITY FUNCTION AND THE TOPOLOGICAL INDICES

The idea that the chemical components of molecules could display more or less fixed characteristics in series of molecules arose in the late nineteenth century. Up to sixties extensive investigations were undertaken to correlate the thermodynamic parameters of molecules with topological structure. This work was initiated by Parks and Huffman who attempted to calculate the thermodynamic proporeties of molecules from those of their component parts. Each of the various groupings of a molecule were thought to contribute a fixed amount to the thermodynamic constants of the molecule. During the later years this method was greatly elaborated by many subsequent workers in this field. The first topological formulation of the additivity principle put forward by Smolenskii[82] in 1964 has the advantage of being not only elegant but possibly also one of the most useful indices ever proposed. Smolenskii's formulation is based on the idea that the individual pyhsico-chemical properties of hydrocarbons can be determined by the structure of individual small sections of the molecule .

According to this formulation, any additive property may be divided into seperate components which constitute the contributions made by each individual C-C and C-H bond as well as by each interaction between them, assuming the contributions made by the individual bonds are constant.

The Smolenskii index is defined by the general expression

$$f(G) = a_0 + \sum_{k=1}^{m} a_k \, |X_k|$$

for calculating the additive properties of the hydrocarbons where f(G) is the property to be calculated for each graph G of a set of graphs representing a series of molecules, m is the number of edges in G, a_0 and a_k are the experimentally determined constants for the physicochemical property under investigation and X_k is any section of the graph G which consists of k edges. The index f(G) is this determined by a summation of the possible edge sequences, each multiplied by an appropriate constant, in the chemical graph G Figure II.6. illustrates this index for i-butane

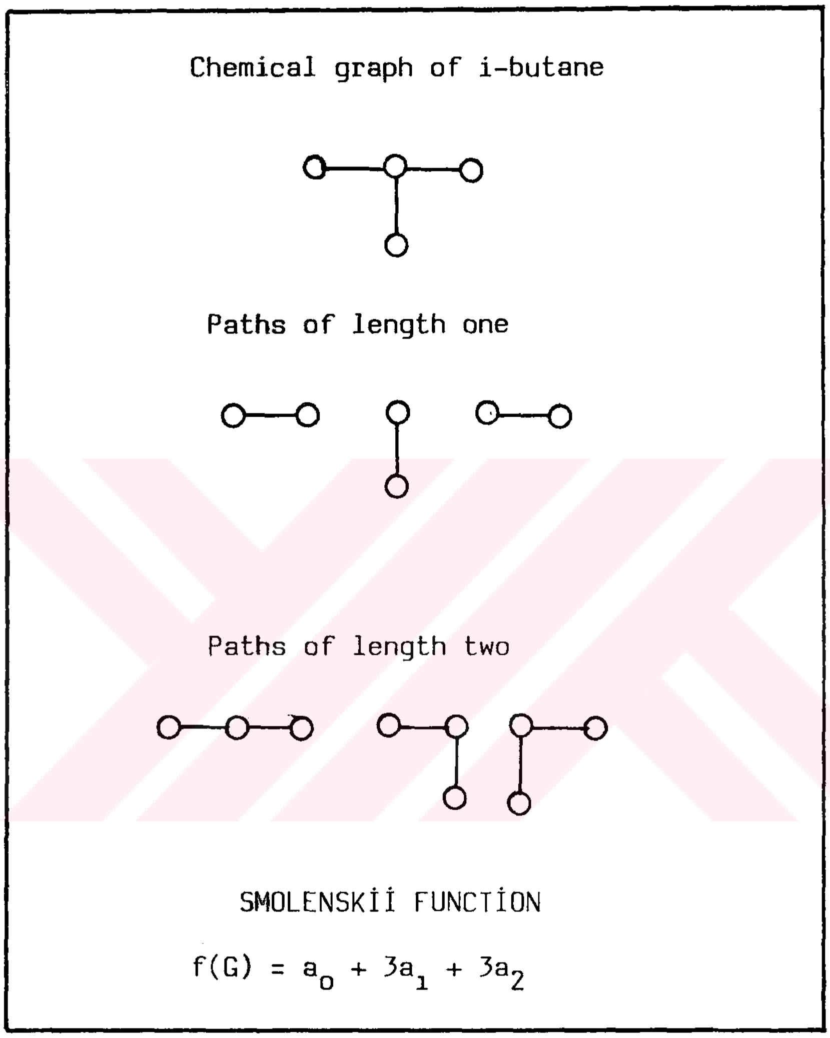

Chemical graph of i-butane
Paths of length one
Paths of length two
SMOLENSKİİ FUNCTİON
$f(G) = a_0 + 3a_1 + 3a_2$

Figure II.6. : Smolenskii addivity function for i-butane. Note that a path of length k, contains a total of k connected edges of the graph.

The Smolenskii index has proved its value in practice in several studies concerning the calculation of additive properties in hydrocarbons and its great usefulness lies in the fact that, once the constants a_0 to a_m have been determined from a small number of sample molecules, the index can be used to predict the additive properties of all the remaining molecules of the same general type. As an example of the kinds of results obtained using this index, table II.4.,lists the heats of formation , heat capacities and entropies for a set of hydrocarbons calculated by using Smolenskii index.[83] For the purpose of comparison, the tables also give the known experimental values. The results show that the index provides a reliable means of estimating those additive thermodynamic properties within a homologous series of saturated hydrocarbons.

As can be seen, topological indices can model an incredibly wide range of physical, chemical and biological phenomena. Although it has not yet been possible to tell in advance with complete certainty which index will be most suited

Table II.4. : Entropies, heat capacities and heats of formation for the homologous series of hydrocarbon from methane to undecane calculated by using Smolenskii index.[14]

COMPOUND	X_1	X_2	X_3	S		C_p		H_f	
				Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
1. Methane	0	0	0	43.98	44.5	7.44	8.5	16.3	17.89
2. Ethane	1	0	0	55.69	54.7	12.66	12.5	20.37	20.24
3. Propane	2	1	0	64.6	64.51	17.95	17.66	25.64	24.83
4. n-Butane	3	2	1	74.07	74.1	23.28	23.3	30.5	30
5. 2-Methylpropane	3	3	0	70.74	70.42	23.29	23.11	32.1	32.1
6. n-Pentane	4	3	2	83.53	83.5	28.61	28.6	35.37	34.9
7. 2-Methylbutane	4	4	2	80.75	82.1	28.68	28.4	36.56	36.5
8. 2,2-Dimethylpropane	4	6	0	74.08	73.1	28.71	28.8	39.75	40.2
9. n-Hexane	5	4	3	93	92.9	33.95	34	40.23	39.96
10. 2-Methylpentane	5	5	3	90.21	91	34.01	33.95	41.42	41.5
11. 3-Methylpentane	5	5	4	90.76	91.5	34.06	33.4	41.02	40.9
12. 2,2-Dimethylbutane	5	7	3	84.64	85.6	34.14	33.8	43.81	43.9
13. 2,3-Dimethylbutane	5	6	4	87.97	87.4	34.12	33.3	42.22	42.1
14. n-Heptane	6	5	4	102.46	102.2	39.28	39.4	45.09	44.89
15. 2,3-Dimethylpentane	6	7	6	97.98	99	39.51	38.43	46.68	46.3
16. 2,4-Dimethylpentane	6	7	4	96.89	94.8	39.41	40.8	47.48	48.1
17. 3,3-Dimethylpentane	6	8	6	95.2	95.1	39.57	39.6	47.87	47.6
18. 2,2,3-Trimethylbutane	6	9	6	92.41	91.6	39.63	39	49.06	48.6
19. 2-Methylhexane	6	6	4	99.60	100.4	39.35	39.3	46.29	46.4
20. 3-Methylhexane	6	6	5	100.22	101.8	39.39	39.1	45.88	45.9

Table II.4. : Cont.

COMPOUND	X_1	X_2	X_3	S		C_p		H_f	
				Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
21. 3-Ethylpentane	6	6	6	100.77	98.3	39.44	39.6	45.48	45.2
22. 2,2-Dimethylpentane	6	8	4	94.1	93.8	39.47	39.8	48.68	49
23. n-Octane	7	6	5	111.93	111.6	44.62	44.8	49.95	49.82
24. 2-Methylheptane	7	7	5	109.14	109.8	44.68	44.7	51.15	51.4
25. 3-Methylheptane	7	7	6	109.69	111.2	44.73	44.4	50.75	50.8
26. 4-Methylheptane	7	7	6	109.69	109.3	44.73	44.7	50.75	50.8
27. 2,2-Dimethylhexane	7	9	5	103.57	103.4	44.81	45	53.54	53.9
28. 3,3-Dimethylhexane	7	9	7	104.66	104.7	44.9	45.6	52.73	52.7
29. Isooctane	7	10	5	100.78	101	44.87	45	54.73	53.7
30. n-Nonane	8	7	6	121.39	121	49.95	50.2	54.82	54.7
31. 2-Methyloctane	8	8	6	118.61	119.2	50.01	50.1	56.01	56.3
32. 3-Methyloctane	8	8	7	119.15	120.6	50.06	49.8	55.61	55.7
33. 4-Methyloctane	8	8	7	119.15	120.1	50.06	50	55.61	55.8
34. 3-Ethylheptane	8	8	8	119.7	118.8	50.11	50.6	55.21	55.2
35. 4-Ethylheptane	8	8	8	119.7	118.3	50.11	50.9	55.21	55.2
36. n-Decane	9	8	7	130.86	130.4	55.29	55.7	59.68	59.67
37. 2-Methylnonane	9	9	7	128.07	128.5	55.35	55.5	60.87	61.2
38. 3-Methylnonane	9	9	8	128.62	129.9	55.4	55.2	60.47	60.7
39. 4-Methylnonane	9	9	8	128.62	129.5	55.4	55.4	60.47	60.7
40. 5-Methylnonane	9	9	8	128.62	128.2	55.4	55.3	60.47	60.7
41. Undecane	10	9	8	140.32	138.37	60.62	60	64.54	64.6

to any particular application, various indicies are already becoming known for their applicability in modelling size, shape, branching reactivity and a large number of other characteristics. Two areas in particular where topological indices appear to have a bright future are in designing new drugs and in tracking the fate of various pollutants in the environment and modelling their likely effects on living organisms.

We know now that indices work; it remains only to put them to work. And when the task becomes a matter of choosing the suitable index which correlate well with the ability of chemical pollutants to spread within air, water or soil or to pass from one of these environmental compartments to another the nature of the molecules in question requires an index which can take care of size effects, conformational differences and presence of heteroatoms. And this problem specifically involves the electrical nature of such bonds. In other words, the index which is going to be used must go beyond the structural fact of adjacency, which is the basis of graph theory and should consider the count of valance electrons participating in sigma, pi and lone pair orbitals on each atom. In the following sections of this work it is going to be proved that one of the most suitable approaches to accomplish the encoding of such structural differences is the use of valance molecular connectivity index which quantizes the molecular structure encoding information about size, branching cyclization, unsaturation and heteroatom content.

II.3. VALANCE MOLECULAR CONNECTIVITY INDEX

The growing use of molecular connectivity has resulted in an interest in the significance of elements of the method and the meaning of the calculated indices. Molecular connectivity is a method of quantitation of molecular structure which is developed in several stages, beginning with the index proposed by Randic[84], a treatment of unsaturation[85], a development of extended bond quantitation[86] and finally, the most useful addition for the medicinal and environmental chemist, a rational way of quantifying heteroatom concent[18]. The treatment of heteroatoms, introduced by Kierr and Hall[8] and called valance molecular connectivity brought molecular connnectivity into the role of a structure quantitation method useful in

QSAR analysis of drugs and environmentally hazardous chemicals.

Table II.5 shows the employment of valance molecular connectivity in several structure-activity relationship analysis of different molecules.

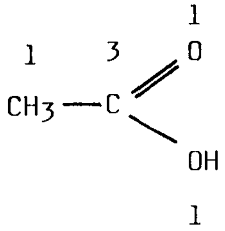
Table II.5. : -Use Of Valence Connectivity Indexes in Structure Activity Relationship Studies

Study	Molecules
Toxicity of anesthetics	Ethers
Anesthetic potency	Ethers, ketones
Barbiturate potency	Barbiturates
Partition coefficient	Hydroxyureas
Carminative activity	Alcohos, esters
Chromatographic retention	Alcohols
Hückel pi electron energy	Aromatic hydrocarbons
Taste thereshold	Alcohols, carbonyls,acids,esters
Bitter taste	Amino acids, peptides
Boiling point	Acohols,amines, halides
Solubilities	
Molar refraction	
General anesthetics	Mixed
Cytochrome conversion	Phenols
Sweet taste	Nitroanilines
Enyzme inhibition	Benzyl alcohols
Toxicity	Phenyl phosphates
Odor	Benzaldehydes, nitrobenzenes
Hallucinogenic activiy	Phenylisopropyl amines
Mutagenicity	Nitrosamines
Serotonin antagonists	Phenalkylamines
Serotonin antagonists	Lysergic acid amides
Muscarinic antagonists	Amines
Antimicrobial activity	Phenyl propyl ethers
Chromatographic retention	Mixed
General anesthetics	Halocarbons
Hallucinogenic agents	Phenethylamines
Monoamine oxidase inhibitors	Hydrazines
Hormone class	Steroids
Reductase inhibitors	Benzohydroxamic acids

The simple molecular connectivity index arrises from the assigment of numerical adjacency values to each atom other than hydrogen (the molecular skeleton) in a molecule. These values called δ values, are cardinal numbers ennumerating the presence of nonhydrogenic-bonded neighbors, irrespective of what the element is or what multiplicity of bonding is present. If we take acetic acid as an example and dissect the bonds describing each by two δ values, a term form each bond (C_{ij}) can be calculated according to $C_k = (\delta_i \cdot \delta_j)_k^{-1/2}$. When these terms are summed over the entire molecule it gives the simple molecular connectivity index of the first order.

$$^{1}\chi = \sum C_k = \sum (\delta_i \ \delta_j)_k^{-1/2}$$

Acetic Acid

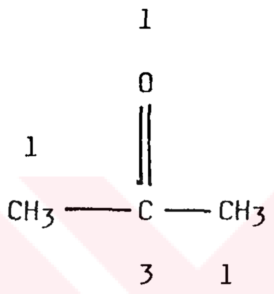


$$^{1}\chi = (1.3)^{-1/2} + (3.1)^{-1/2} + (3.1)^{-1/2}$$

$$= 1.732$$

If we evaluate this index also for the acetone molecule we can see that the set of values is the same as for acetic acid.

Acetone



$$\overset{1}{CH_3} - \underset{3}{\overset{\overset{1}{O}}{\overset{\|}{C}}} - \underset{1}{CH_3}$$

$$^1X = (1.3)^{-1/2} + (3.1)^{-1/2} + (3.1)^{-1/2}$$
$$= 1.732$$

So, it is clear that the ^1X value of 1.732 for both of these molecules is not sufficiently descriptive and the obvious difference in the structures is not encoded in this index.

Hence, instead of assigning simple numerical adjacency values, Kierr and Hall considered the count of the valance electrons participating in the sigma, pi and lone-pair orbitals on each atom, exlusive of bonds to hyrogen. In this case the index

($^1X^v$) is calculated by using valance delta (δ^v) values which is based on the number of valance electrons (Z^v) not involved in bonds to hydrogen. Thus;

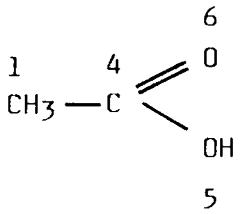
$$\delta_i^v = Z_i^v - h_i$$

Where h_i is the number of bonded hydrogens on atom i and the calculation of first order valance molecular connectivity index proceeds exactly as described for the simple molecular connectivity index such that;

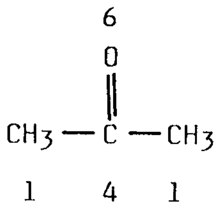
$$^1X^v = \sum (\delta_i^v \cdot \delta_j^v)_k^{-1/2}$$

When we assign δ^v values for acetic acid and acetone, we can see that the calculated $^1X^v$ values are clearly different for each structure. Hence, the necessary structural information is encoded in these values.

Acetic Acid



Acetone



$$^1X^v = (1.4)^{-1/2} + (4.6)^{-1/2} + (4.5)^{-1/2}$$

$$= 0.928$$

$$^1X^v = (1.4)^{-1/2} + (4.6)^{-1/2} + (4.1)^{-1/2}$$

$$= 1.204$$

II.3.1. SIGNIFICANCE OF DELTA VALUES

Studies have employed ${}^1X$ and ${}^1X^v$ indices singly and in concert as structural descriptors in QSAR analysis. Since molecular information encoded in these X values is derived from the δ values of the atoms, insight into the significance of molecular connectivity begins with analysis of the δ values.Within the context of molecular connectivity an atom in its valance state can be described by two cardinal numbers; δ the number of bonded neighbors (excluding hydrogen) and δ^v , the number of valance electrons (exluding those bonding the hydrogens)[78] .

This dual description of atoms is revealed in the matrix shown in fig. II.7 for second quantum level atoms in their valance states. Superimposed on the same matrix are the hydrides of these atoms. It is apparent that δ_i is a count of the nonhydrogen sigma bond electrons contributed by atom i and δ^v_i is a count of all valance electrons, including those sigma electrons (σ_i) ennumerated by δ_i. Thus the relationship is;

$$\delta^v_i = \delta_i + P_i + n_i = \sigma_i + P_i + n_i - h_i$$

where pi is the number of pi orbital electrons and n_i is the number of lone-pair electrons on atom i.

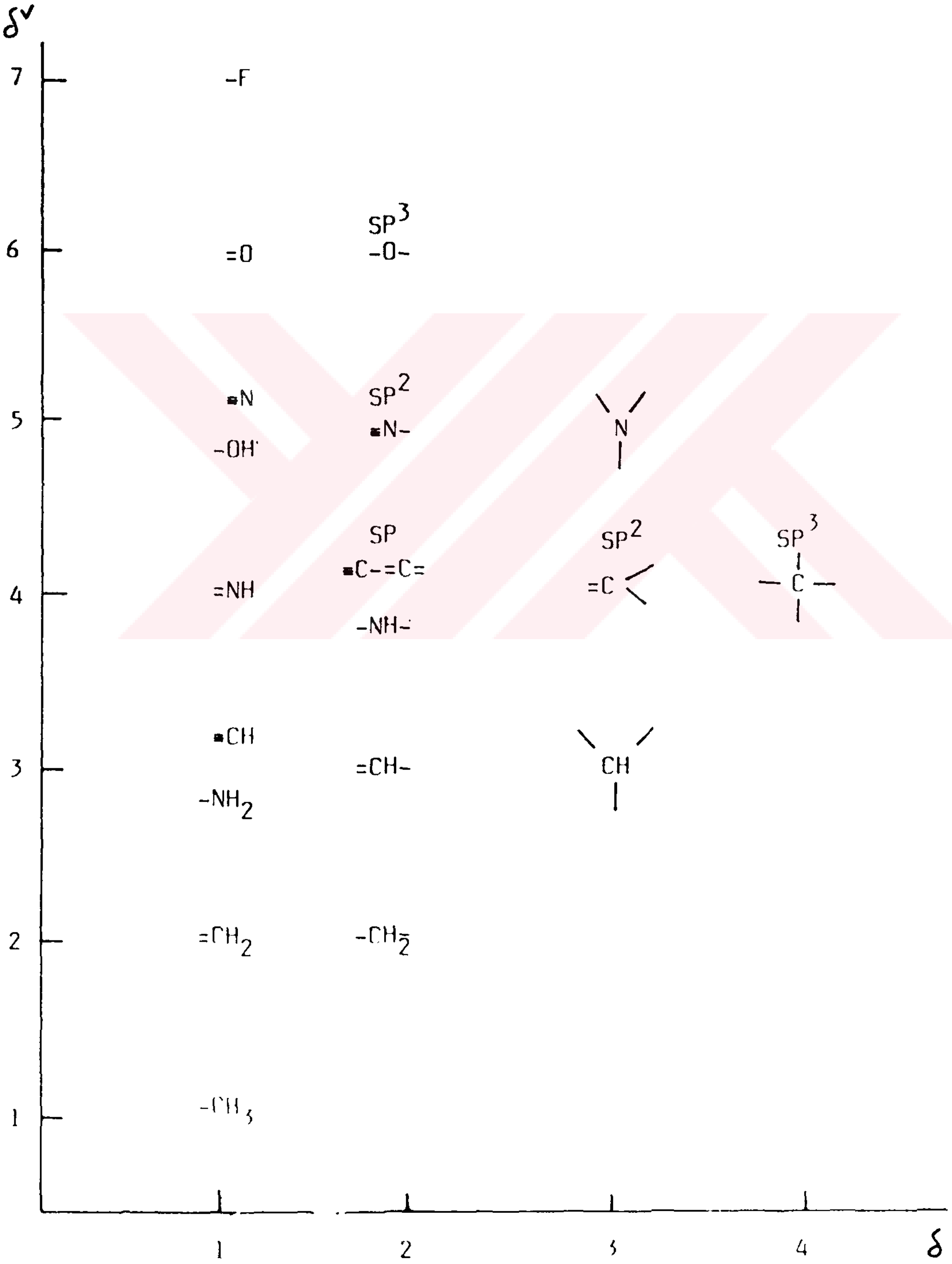


Figure II.7. : Atoms and hydrides defined by δ and δ^v values.

Hence the values of δ^v and δ depend on the element represented, its valance (hybrid) state and the number of bonded hydrogen atoms. Thus from fig. II.7, $\delta=2$; $\delta^v= 4,5$ and 6 describes an SP carbon an SP^2 nitrogen and SP^3 nitrogen respectively. On the other hand, $\delta^v=4; \delta=2,3$ and 4 describes an SP carbon, an SP^2 carbon, an SP^3 carbon respectively.

Hence, these two cardinal numbers δ and δ^v specify the hybrid states or valance states of any atom within a quantum level.

The δ^v value, when formulated into the $^1\chi^v$ value for a molecule, carries with it information relating to both volume and electronic character. Thus, an SP^3 nitrogen atom has a $\delta^v=5$. The cardinal number, 5, counts orbitals contributing to a spatial property, volume. The number 5 concurrently counts the number of valance electronic characteristics such as ionicity , bond dipole, partial atomic charge and bond strength. This duality in the information encoded in δ^v leads to a duality of structural information encoded in the derived $^1\chi^v$ values.

Hence, with the structural and physical significance of δ and δ^v revealed, it is possible to derive the bond index encoding information about structure and properties. The volume information encoded in $^1X^v$ values has been demonstrated on numerous occasions in the form of close correlations with volume related physical properties. Other studies showed that properties largely governed by electronic composition also correlate with $^1X^v$ indices (tableII.5).

II.3.2. VALANCE MOLECULAR CONNECTIVITY AND THE TREATMENT OF HETEROATOMS

In earlier studies using the molecular connectivity index to describe structural features, the heteroatoms such as oxygen or nitrogen were considered to contribute equally. This approach inevitably led to redundant values for isomers. An initial approach to the resolution of these redundancies was used in an alcohol solubility study by introducing a second regression variable simply as the contribution to total molecular connectivity index from the C— OH bond. This and similar approaches are now considered to be an interim or first-order solution to a more basic problem of calculating the molecular connectivity contribution of any atom other than carbon.

Recently, the extension of molecular connectivity to the treatment of heteroatom molecules was described. This approach mainly concerns the assignment of an atom connectivity term δ^v (by considering the valance electrons) for heteroatoms and testing the ability of δ^v to describe the atomic connectivity in heteroatoms so that the molecular connectivity indices bear some relationship to structure influencing physical or biological properties.

Assuming that intermolecular effects are minimal in influencing a physical property, it may be possible to relate the connectivity of various molecules, containing different heteroatoms with that property. This approach appears to be possible with molar refraction[28]. A comparison of X and X^v values with molar refraction provides a severe test of X^v values because they must recreate connectivity properties of carbon, nitrogen and oxygen in a self-consistent manner.

For twentyfive phenyl substituents including alkyls, ethers, amines, esthers, amides, ketones, an aldehyde, alcohol and a nitro group (table II.6) this relationship is evaluated to be

$$R_m = 2.656\ (\pm 0.593)\ X + 7.140(\pm 0.688)X^v - 0.958(\pm 0.518)$$

r= 0.990
s: 1.03
n: 25

This successful relationship illustrates the consistency of the oxygen and nitrogen connectivity parameters with the parameters established for the carbon atom.

On the other hand, since halogen atoms have an identical number of valance electrons, this prescription yields identical values of δ^v. So, it is necessary to derive empirical values of δ^v for

Table II.6 : Substituent Parameters for Molar Refraction (R_m)

Substituent	Molar Refraction		Connectivity Index	
	Obs.	Calc.	χ	χ^v
Methyl	4.7	4.14	0.577	0.500
Ethyl	9.4	9.58	1.115	1.06
Propyl	14.0	14.48	1.615	1.561
1-Methylethyl	14.0	13.30	1.488	1.443
Butyl	18.7	19.37	2.115	2.061
1,1-Dimethylethyl	18.5	16.29	1.789	1.750
Phenyl	24.3	22.84	3.150	2.161
Hydroxyl	1.5	2.17	0.577	0.224
Methoxyl	6.5	6.37	1.115	0.612
Ethoxyl	11.3	11.90	1.615	1.200
Propoxyl	15.9	16.80	2.115	1.700
1-Methylethoxyl	16.0	15.66	1.971	1.595
Butoxyl	20.7	21.69	2.615	2.200
Pentoxyl	25.3	26.59	3.115	2.700
Penoxyl	26.6	25.25	3.633	2.319
Acetate	11.6	12.22	1.971	1.122
Amino	4.2	2.95	0.577	0.333
Acetamido	14.6	12.87	1.971	1.204
Nitro	6.0	6.83	1.488	0.537
Aldehydo	5.3	5.74	1.115	0.524
Acyl	9.9	9.81	1.488	0.954
Methylcarboxylate	11.4	12.03	2.026	1.066
Ethylcarboxylate	16.2	17.56	5.526	1.654
Amido	8.8	8.30	1.488	0.743
Cyano	5.2	5.85	1.115	0.539
Fluoro	-0.4	—	0.577	-0.124
Chloro	4.8	—	0.577	0.602
Bromo	7.6	—	0.577	0.992
Iodo	12.8	—	0.577	1.719

the halogens by calibrating them to molar refraction data. The use of δ^v thus permits the calculation of valance molecular connectivity index $^1\chi^v$ of the first order, by the expression

$$^1\chi^v = \sum (\delta_i^v \cdot \delta_i^v)^{-1/2}$$

These empirical δ^v values for halogens are listed in table II.7.

Table II.7: Valence Delta (δ^v) Values for Heteroatams

Group	δ^v	Group	δ^v
NH_2	3	OH	5
NH	4	O	6
$C\equiv N$	5	$C=O$	6
N	5	Furan O	6
$C=NH$	4	$O=NO$	6
Pyridine N	5	H_2O	4
Nitro N	6	H_3O^+	3
NH_3	2	F	(-) 20
NH_4^+	1	Cl	0.690
$>N<^+$	6	Br	0.254
$=NH_2^+$	3	I	0.085

to test the consistency of the halogen parameters, the ability of X and X^v to predict the boiling points of a mixed list of alkyl halides is given in table II.8. From this table it is clear that δ^v values empirically derived from molar refraction data are also useful in correlating the boiling points according to the equation;

$$BP = -69.55\ (\pm 5.17) + 19.91\ (\pm 2.41)\ X + 38.07(\pm 1.27)\ X^v$$

$r = 0.992$

$s = 4.79$

$n = 24$

A set of valance delta (δ^v) values hence can be developed for the calculation of connectivity indices for heteroatom containing molecules. Correlations with the boiling point and molar refraction for a wide range of molecules suggests the general applicability of these values. This development is considered to be an important advance in the development of graph theoretical indices because by this development molecules containing heteroatoms may now be considered with a more sophisticated molecular connectivity treatment.

Table II.8 : Boiling Points of Alkyl Halides

	Boiling Point		Connectivity Index	
Compound	Obs.	Calc.	X	X
Ethyl chloride	13.0°	17.9°	1.414	1.558
Ethyl bromide	38.0°	38.9°	1.414	2.110
Ethyl iodide	72.0°	77.8°	1.414	3.132
Propyl chloride	46.5°	46.9°	1.914	2.058
Propyl bromide	71.0°	67.9°	1.914	2.610
Propyl iodide	102.5°	106.8°	1.914	3.632
1-Methylethyl chloride	36.5°	35.4°	1.732	1.850
1-Methylethyl bromide	60.0°	54.5°	1.732	2.300
1-Methylethyl ioide	90.0°	84.3°	1.732	3.135
1-Methylpropyl chloride	69.0°	67.5°	2.270	2.414
1-Methylpropyl bromide	91.0°	88.6°	2.270	2.966
1-Methylpropyl iodide	120.0°	127.5°	2.270	3.988
1,1-Dimethylethyl chloride	51.0°	50.3°	2.000	2.102
1,1-Dimethylethyl bromide	72.5°	65.1°	2.000	2.492
1,1-Dimethylethyl iodide	98.0°	92.7°	2.000	3.215
Butyl chloride	78.0°	75.9°	2.414	2.558
Butyl bromide	101.0°	96.9°	2.414	3.110
Butyl iodide	130.0°	135.8°	2.414	4.132
1-Methylbutyl chloride	97.0°	95.5°	2.770	2.888
1-Methylbutyl bromide	117.0°	112.7°	2.770	3.338
1-Methylbutyl iodide	142.0°	144.5°	2.770	4.173
Propyl fluoride	-2.5°	8.5°	1.914	1.049
Butyl fluoride	32.5°	37.5°	2.414	1.549
Pentyl fluoride	62.8°	66.5°	2.914	2.049

II.3.3. VALANCE MOLECULAR CONNECTIVITY AND THE DEVELOPMENT OF EXTENDED CONNECTIVITY TERMS.

Molecular structures can be analyzed in terms of the number of atoms, the kind of atoms, bonding types and the adjacent environment by the molecular connectivity method. The valance molecular connectivity index, has been shown to relate to many physical and biological properties such as cavity surface area, polarizability, nonspecific local anesthetic activity, water solubility, boiling point, oil-water partition coefficient and enzyme inhibition. To explore further the fundemental nature and general applicability of valance molecular connectivity index it was proposed that any function of a molecule can be represented by a combination of terms representing various bond contributions and this statement was proved to be valid in various occasions concerning the prediction of density[86], hallugcinogenic activity[30] and enzyme inhibition studies[33].

The molecular connectivity indices are weighted counts of structural fragments and are computed by the general formula;

$$^{m}\chi_{t}^{v} = \sum (\delta_i^v \cdot \delta_j^v \ldots\ldots \delta_n^v)^{-1/2}$$

where m is the order (number of bonds), t is the type (the path in these cases) and v denotes the index is of valance form ; that is the atom δ assignments are based on the atomic valance rather than on the simple degree of adjacency. The number of deltas in the parantheses is equal to the number of bonded atoms in the fragment of order m.

The first term in the valance connectivity series, $^{0}\chi^{v}$, is derived from the summation of the square root of the reciprocal of number of valance electrons other than hydrogen on atom i;

$$^{0}\chi^{v} = \sum_{k} (\delta_i^v)_k^{-1/2}$$

and it simply is a summation of atom deltas. The second term is the index $^{1}\chi^{v}$ which is a weighted count of each bond in the molecule and is derived as a summation of δ^{v} values describing each bond in the molecule

$$^{1}\chi^{v} = \sum_{k} (\delta_i^v \cdot \delta_j^v)_k^{-1/2}$$

The following term, symbolized as $^2\chi^v$ is a summation of values describing each adjacent pair of bonds.

$$^2\chi^v = \sum_k (\delta_i^v \cdot \delta_j^v \cdot \delta_m^v)_k^{-1/2}$$

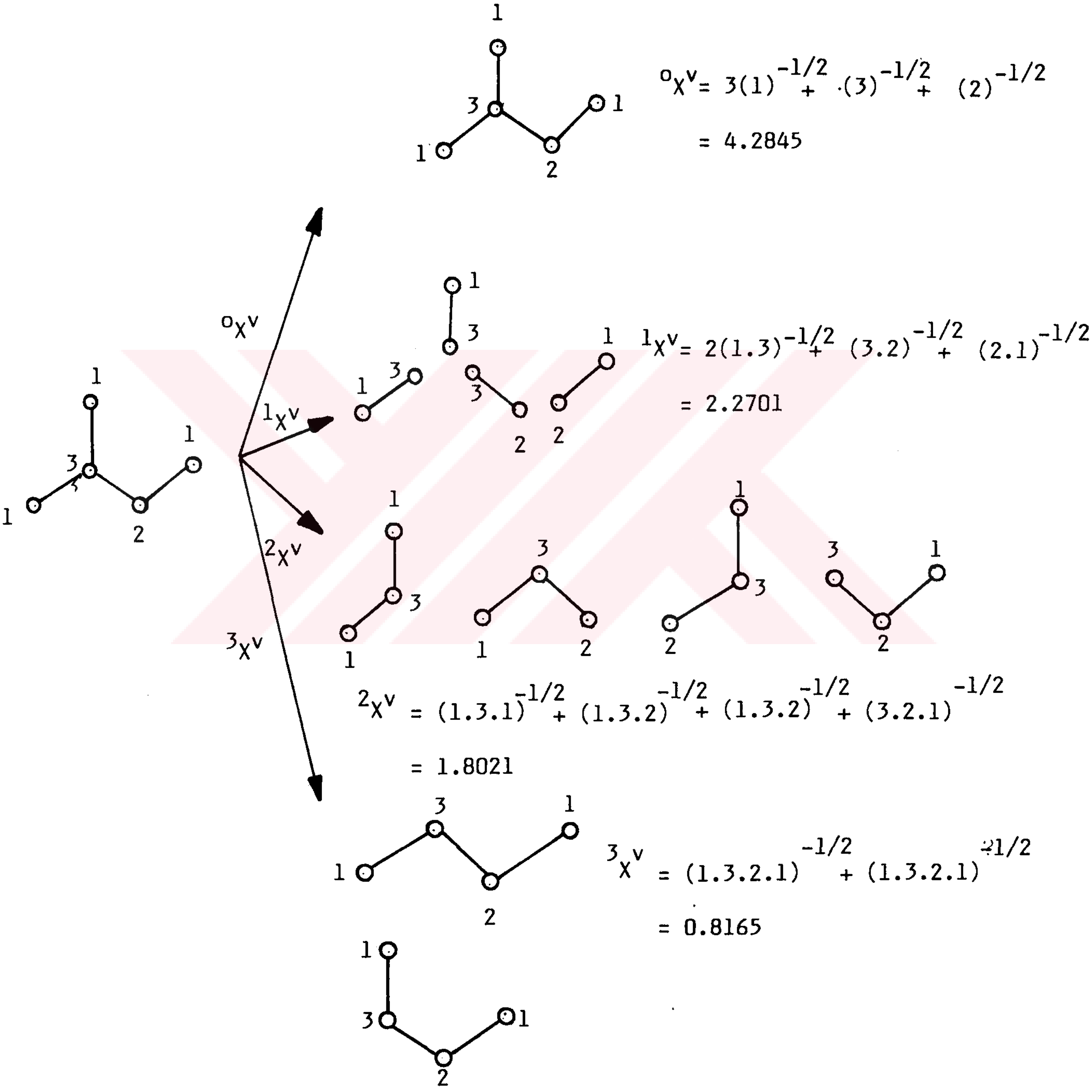
Subsequent terms in the series are calculated similarly. The specimen calculation for the first three terms in the series for benzene molecule is given below as an example.

An alternate formulation of the extended series arises from a consideration of powers of the connectivity matrix of the graph. If we take isopentane as an example and number the skeleton in any manner, the valance connectivity matrix obtained is;

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

In the upper triangle there are four unit entries corresponding to the four C_{ij} bond terms in the calculation of $^1\chi^v$.

Example: Calculation of the first four terms in the valance connectivity series for isopentane.


$^{0}\chi^{v}$
$^{1}\chi^{v}$
$^{2}\chi^{v}$
$^{3}\chi^{v}$
1
2
3

$$^{0}\chi^{v} = 3(1)^{-1/2} + (3)^{-1/2} + (2)^{-1/2}$$

$$= 4.2845$$

$$^{1}\chi^{v} = 2(1.3)^{-1/2} + (3.2)^{-1/2} + (2.1)^{-1/2}$$

$$= 2.2701$$

$$^{2}\chi^{v} = (1.3.1)^{-1/2} + (1.3.2)^{-1/2} + (1.3.2)^{-1/2} + (3.2.1)^{-1/2}$$

$$= 1.8021$$

$$^{3}\chi^{v} = (1.3.2.1)^{-1/2} + (1.3.2.1)^{-1/2}$$

$$= 0.8165$$

The square of the matrix is;

$$\begin{pmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 3 & 0 & 1 & 0 \\ 1 & 0 & 2 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix}$$

In the upper triangle, there are four unit entries corresponding to each C_{ijk} term in the calculation of $^2X^v$. The diagonal of the matrix contains the δ_i^v values of the graph.

The cube of the matrix is;

$$\begin{pmatrix} 0 & 3 & 0 & 1 & 0 \\ 3 & 0 & 4 & 0 & 3 \\ 0 & 4 & 0 & 2 & 0 \\ 1 & 0 & 2 & 0 & 1 \\ 0 & 3 & 0 & 1 & 0 \end{pmatrix}$$

Again the number of unit entries in the upper triangle corresponds to the C_{ijkl} terms used in computing $^3X^v$. The fourth power of the matrix has no unit terms and there are no C_{ijklm} terms, hence $^4X^v$ is zero.

Whatever the method of calculation is, the main question in such an analysis is , which terms in the expansion series of X^v adequately describe structural features that are manifest in influencing the experimentally observed value of the specific property under investigation. Since one has no developed intuition as to the significance of each term in the expanded series of X^v , the answer is not obvious. In this work as an approach to the answer, first three terms in the X^v expansion series, as well as combination of these terms is tested for correlation with octanol-water partition coefficients, solubilities and partial presures of certain groups of environmentally hazardous chemicals, in order to use these correlations for the prediction of compartmentalization properties of these compounds. As a result of this approach it has been shown that valance molecular connectivity indices appear to have a bright future in tracking the fate of various pollutants in the environment.

III. ECOKINETICS IN RELATION
TO VALANCE
MOLECULAR CONNECTIVITY

III. ECOKINETICS IN RELATION TO VALANCE MOLECULAR CONNECTIVITY

III.1. APPROACHES TO ENVIRONMENTAL EXPOSURE ANALYSIS

The chemical industry has long been concerned with the hazardous environmental properties of the products that are being manufactured and distributed. This increased awareness of potential problems created the need for better predictive techniques for making early decisions. Environmental hazard of a chemical is a function of its toxicity and its exposure. Bearing this in mind there is a serious need to make an initial assessment of what exposure can be expected from the introduction of a new chemical into an eco-system before the actual introduction takes place. In order to determine the environmental hazard associated with these chemicals, information on the environmental fate, as well as on production quantity, use, environmental release and toxicity is important. Knowing how a chemical behaves in the environment is particularly important in determining whether a chemical will come in contact with a critical species or men and perhaps cause a toxic effect. Because environmental fate encompasses any transport or degredation process which describe the behaviour of a chemical in the environment.

The use of compartmental analysis provides substantial information for this type of environmental exposure prediction. From such compartmental analysis key degradative mechanisms may be postulated and incorporated into the analysis for more accurate exposure concentrations.

The basic process in any hazard evaluation involving the environmental effects of chemicals is to make predictions of the expected environmental concentration (EEC) and to compare this data with the experimentally determined no-effect level for appropriate organisms. In such an approach where the prediction is based on the accessible physicochemical properties of the compounds under investigation such as water solubility (S), vapor pressure (P) and octanol-water partition coefficient (K_{ow}), the reliance is generally made on the benchmark approach in which the properties of a new chemical are predicted from similar chemical groups of known environmental distribution.

Usually it is frequently possible for ecologists to postulate variety of compartmental models of varying degrees of sophistication for characterizing the behaviour of the substance introduced to the ecosystem. Presently one of the difficult problems which is receiving considerable attention is what data should be collected and how should it be used to decide which model is most suitable for characterizing the system under consideration. The OECD Exposure Analysis Group initally considered four models for the estimation of environmental exposure.[87]

1. The Klöpffen Model by Battelle Frankfurt for the Umweltbundesamt of the Federal Republic of Germany which presumes equilibria between media[89].

2. The Neely Model based on laboratory and monitoring data for a pesticide in a pond environment[41].

3. The Mackay Fugacity Model in which fugacity capacities are used to explain various compartment relationships. This model can be used at several levels of sophistication depending on the available data[90,69].

4. The Wood Model developed for the USEPA which is an adaptation of Mackay's Fugacity Model also has several levels[88].

The Klöpffer, Mackay, and Wood models make slightly different assumptions regarding compartment sizes but if no degradation processes are considered and the chemical's distribution across the environmental media is considered to be at equilibrium, they reduce to essentially the same set of equation.

Due to the reason that it did not make provision for degradation or non-equilibrium processes Klöpffer model, and being aplied to only a specific experimental environment, Neely model was decided not be considered in the context of OECD hazard assessment. As a result, the model developed by Mackay and adapted by Wood is considered to be applicable at several levels of sophistication depending on the chemical and environmental data available.

III.1.1. ENVIRONMENTAL COMPARTMENTALIZATION

The accepted two models which are based on the concept of fugacity assumes equilibrium among a set of environmental compartments the standard dimensions of which are given in figure III.1 . In their simpler versions, where no degradation and instantaneous equilibration is assumed, both models are identical in predicting environmental compartmentalization.

The assumptions common to both models are,

1. The environment is a closed system consisting of air (A), water (W), sediment (SD), soil (S) and (aquatic) biota (B) compartments.

2. The chemical is assumed to reach thermodynamic equilibrium in the environment both with respect to interphase transfer and intraphase transport.

3. No degredation processes occur during the distribution.

As a result of these assumptions fugacities or escaping tendencies from all phases are equal so that a common fugacity (f) prevails;

$$f_A = f_W = f_{SD} = f_S = f_B = f \qquad (3.1)$$

Fugacity f_i can directly be related to the concentration C_i (mole / m^3) within different compartments (i) at low concentrations which are relevant to environmental contamination levels where the proportionality constant is the fugacity capacity Z_i (mol / m^3)

$$C_i = Z_i \cdot f_i \qquad (3.2)$$

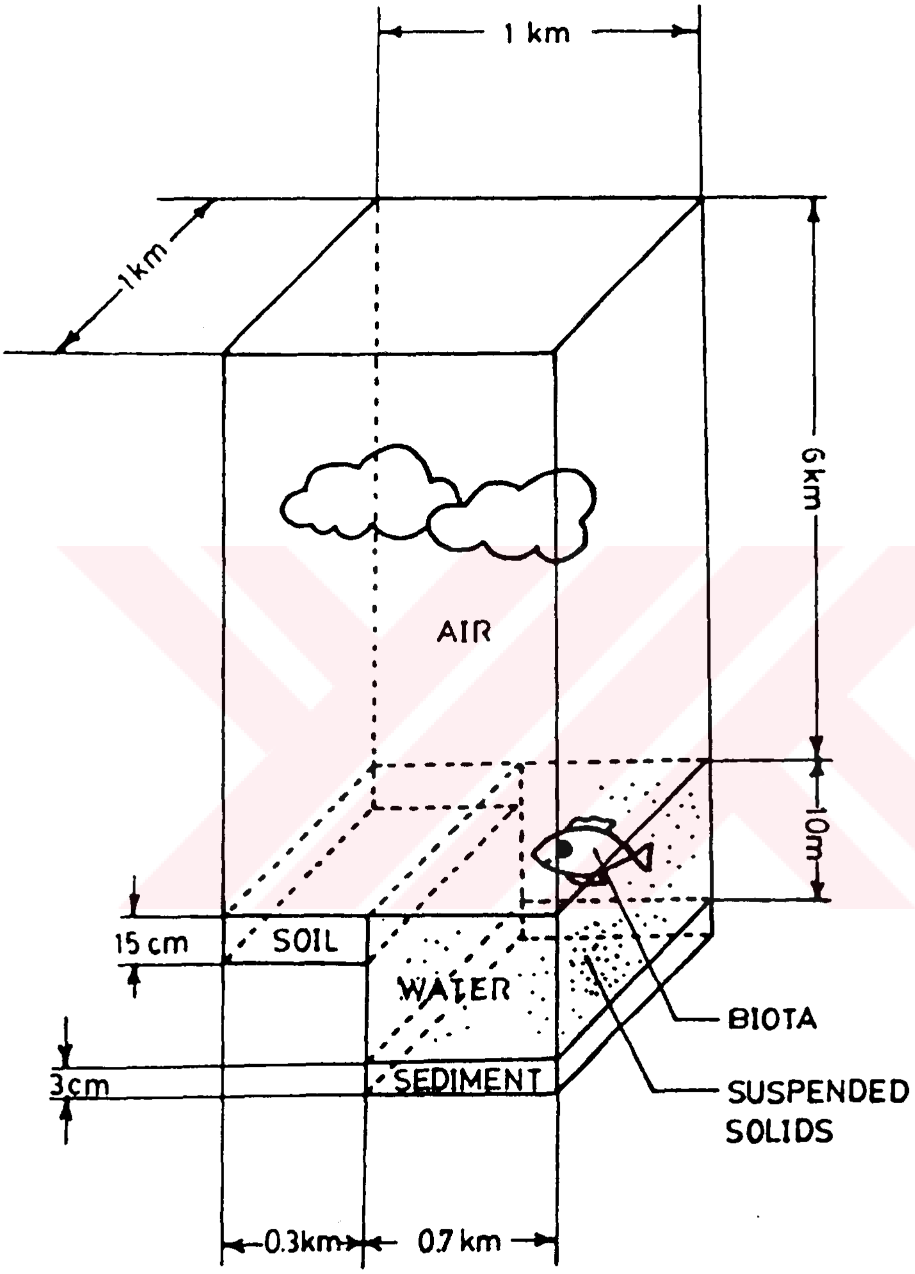

1 km
1km
6km
10m
AIR
15 cm
SOIL
WATER
3cm
SEDIMENT
BIOTA
SUSPENDED SOLIDS
0.3km
0.7 km

Figure III.1 :Unit world designed by Mackay and Neely

If each phase in equilibrium has a volume of V_i m^3 and the amount of material in each phase is M_i moles[87] then,

$$M_i = C_i \cdot V_i = f \cdot Z_i \cdot V_i \qquad (3.3)$$

Hence the total amount of material M_T is obtained as,

$$M_T = f \sum Z_i \cdot V_i \qquad (3.4)$$

and by simple transformation, mass partitioning among the compartments can be calculated as;

$$P_i = \frac{Z_i \cdot V_i}{\sum_i Z_i \cdot V_i} \qquad (3.5)$$

Where Z_i denotes compartment specific fugacity capacities for air, water, sediment, soil or biota which are given basically by Mackay[87] as

$$Z_{air} = 1/RT \qquad (3.6)$$

$$Z_{water} = 1/H \qquad (3.7)$$

$$Z_{soil\ /\ sediment} = K_D . S / H \qquad (3.8)$$

$$Z_{Biota} = K_{ow} . B / H \qquad (3.9)$$

Where R $[J / mole. K]$ is the universal gas constant, T (K^o) is the absolute temparature, H $[m^3 . P_a / mole]$ is the Henry's constant which can also be expressed as vapor press./solubility and K_D $[m^3$ water $/ 10^6$ g sorbent$]$ is the sorption coefficient which can also be expressed as;

$$K_D = K_{oc} . \frac{\%\ organic\ carbon\ content}{100} \qquad (3.6)$$

S $[g / cm^3]$, on the other hand is the sorbent density, B is the mass fraction of biota times the lipid part and K_{ow} is the n-octanol-water partition coefficient.

The aim of this work is to present a technique to estimate the distribution of chemicals in various environmental compartments mainly by making use of simple topological characteristics of molecules. The main purpose being to develop a topology dependent mathematical model as a simple and valid approach to environmental exposure analysis, Mackay's level I fugacity Model is chosen as the simplest acceptable approach for the calculations[67,68]. Although this model is quite hypothetical due to its ignorance of inputs outputs and transformations it is valuable in identifying compartments in which the bulk of a contaminant will tend to accumulate and in which the degradative processes are likely to take place. Hence, it merely represents a picture of ultimate environmental distribution in terms of both relative concentrations and relative masses providing comparative exposure information to assist priority setting.

The model chosen requires only;

- molecular weight (M_w)
- water solubility (S)
- vapor pressure (P)

- soil sorption constant (K_{OC})
- n-octanol-water partition coefficient (K_{OW})

as the necessary data. Hence, it is an adequate tool for showing the applicability of the mathematical formalism proposed. On the other hand it is generally accepted that such models should be validated by comparison with real environmental data. However, since models of this type does not describe any particular real environment, results can only be validated by general comparison of the observed environmental concentrations and of the predicted values based on direct calculation by using the observed or other semiempirical values as the data. But, since the model that is going to be developed is also based on valid physical laws the results are expected to be in broad agreement with the general environmental behaviour. Furthermore model can be extended to a higher degree of sophistication depeding on the validity of the preliminary results obtained by level I application.

III.1.2. EVALUATION OF FUGACITY CAPACITIES

The fugacity approach is used to gain insights into the likely behavour of toxic compounds. Widely used in describing chemical engineering operations, fugacity is a new and perhaps better way to quantify toxics transport and bioaccumulation in various compartments of the environment. The fugacity approach has a valuable potential for it simplifies environmental science by bringing a certain degree of order into a complex subject by assisting the elucidation of the dominant processes responsible for a substance's degradation or removal from the environment.

To apply the approach first of all a model environment to observe the distribution is conctructed in which a certain unit of typical land area with atmosphere above, soil some water, sediment and biota is considered according to set standarts (fig. III.2.). Estimating the total amount of solute likely to be present in the entire environment at any given time, one can evaluate the equilibrium distrubution of this fixed amount of toxicant in the environment.

After the necessary assumptions are made depeding on the level of the model chosen, fugacity capacities (Z_i) for the toxicant in each compartment is required to be evaluated. This implies knowing certain chemical and physical parameters and sorption characteristics defined earlier or certain relations between these parameters.

Just as temparatures (^oC) can be related to heat concentrations (cal/m^3) using a proportionality constant, obtaining heat capacity ($cal/m^3 {}^oC$),fugacities (f) can be related to concentrations using a similar fugacity capacity constant Z with units of $gmol/m^3$. atm.

$$C = Zf$$

Fugacity capacity constant Z depends on temperature, pressure, the nature of the substance and the medium in which it is present. Hence it quantifies the capacity of the phase for fugacity. So, if Z can be calculated for a substance for each environmental phase one can easily calculate how the substance will partition. Assuming the chemical is at equilibrium between all phases,

$$f_A = f_W = f_S = f_B = f$$

The following discussion describes the development of fugacities for atmosphere, water, sorped phases, biotic phases and octanol phase which is going to be used in the forgoing calculations.

III.1.2.1. FUGACITY CAPACITY FOR THE ATMOSPHERE, Z_a

In the vapor phase, the fugacity is rigorously expressed as

$$f = y \phi P_{\overline{T}} \simeq P \qquad (3.7)$$

where y is the solute's mole fraction, $P_{\overline{T}}$ is the total pressure, (atmospheric pressure) in unit of Pa, ϕ is the fugacity coefficient which is dimensionless and is introduced to account for nonideal behaviour. At atmospheric pressure, ϕ is usually close to unity and can thus be ignored. The exceptions are solutes such as carboxylic acids, that associate in the vapor phase.

The fugacity is thus equivalent, in most cases, to the partial pressure, P. It should be noted that this equation assumes the solute to be in truly gaseous form, not associated with particles. Concentration C is related to partial pressure through the general gas law

$$C = n / V = P / R T = f Z \qquad (3.8)$$

Thus Z_a for vapors is simply 1 / R T and has a value of 4.04×10^{-4} mol / (m Pa) corresponding to R of 8.31 (pa . m^3) / (mol . °K) or J / (mol °K), and a temperature of 25°C (298°K). Z_a is independent of the nature of the solute or the composition of the vapor (for nonassociating solutes and lowor atmospheric-pressure conditions) and has an obvious temperature dependence.

III.1.2.2. FUGACITY CAPACITY FOR WATER, Z_W

In aqueous solution, the fugacity is given by [69]

$$f = x\gamma P^s \qquad (3.9)$$

where x is the mole fraction; P^s is the vapor pressure of the pure liquid solute at the system temperature; and γ is the liquid-phase activity coefficient on a Raoült's Law convention. By this convention, when x is unity, γ is also unity, and f becomes the pure liquid state component vapor pressure. Generally, for nonionizing substances, γ increases to an "infinite dilution" value as x tends to zero. This relationship between x and γ is often of the form

$$\ln\gamma = K(1 - x)^2 \qquad (3.10)$$

In most environmental situations, x is quite small; thus, ln γ can be equated to K without serious error. This near constancy in γ leads to the very convenient near-linear relationship between C and f, reflected as a constant value in Z.

The relationship between f and C to give Z for infinite dilution conditions can be obtained by writing

$$Z_W = C / f = C / P = 1 / H = x / V_W f = 1 / V_W \gamma P^S \quad (3.11)$$

where V_W is the molar volume (m^3 / mol) of the solution, which is approximately equal to that of water (1.8×10^{-5} m^3/mol)

For water, Z_W is simply the reciprocal of Henry's Law constant.

III.1.2.3. FUGACITY CAPACITY FOR SORBED PHASES (SOIL, SEDIMENT OR SUSPENDED SOLIDS) Z_s , Z_{sd} , Z_{ss}

Sorption equilibria are usually exressed as equations or isotherms relating dissolved to sorbed concentrations. Examples are the Freundlich, BET, Langmuir or linear equations. For most hydrophobic compounds at concentrations well below their solubilities linear equation is adequate

$$x = K_pC \qquad (3.12)$$

where x is the sorbed concentration expressed as mol solute/10^6g sorbent(wet or dry) and Kp is a sorption coefficient with units of m^3 water/ 10^6g sorbent. The equation is often expressed in mass concentration units x in g / 10^6g or μg/g and C in g/m^3 or mg /liter in which case an identical numerical value is obtained for K_p.

If the sorbent concentration expressed as volume fraction is S and its density is ρ g / cm^3 or 10^6 g / m^3, then its concentration is S 10^6 g / m^3 or g / cm^3. The concentration of sorbed material C_s, expressed as mol / m^3 sorbent, is thus $x\rho$ mol / m^3.

At equilibrium,the fugacities of the sorbed and dissolved material must be equal, so if Z_s is the sorbed phase fugacity capacity

$$f = H\,C = C_s / Z_s \qquad (3.13)$$

then

$$Z_s = C_s / H\,C = x\rho / H\,(x / K_p) \qquad (3.14)$$

and

$$Z_s = K_p\rho / H \qquad (3.15)$$

The group $K_p\rho$ is dimensionless and is actually the partition coefficient expressed as moles per unit volume ratio.

For correlating K_p and hence Z_p for organic solutes in sediments and soils, it is very convenient to correlate the organic carbon partition coefficient, K_{oc} of Karickhoff et. al.[91] and with the octanol-water partition coefficient, K_{OW}.

The soil-water partition coefficient K_p is K_{oc} multiplied by the percent organic carbon in the soil

$$K_p = (\%\ OC)\,K_{oc} \qquad (3.16)$$

where % OC is the amount of organic carbon which is assumed 2% for soil and 4% for sediment and suspended solids. Karickhoff correlated soil organic carbon-water partition coefficient K_{oc} and n-octanol-water partition coefficient K_{OW} for a series of polycylic aromatics and chlorinated hydrocarbons ranging from 1 ppb to 1000 ppm in water solubility and obtained the following relation;

$$\log K_{oc} = -0.21 + 1.00 \log K_{OW} \qquad (3.17)$$

$$n = 10 \qquad r = 1.00$$

which leads to;

$$K_{oc} = 0.6\ K_{ow} \qquad (3.18)$$

$$n = 10 \quad r = 0.96$$

Hence from 3.17 and 3.18 K_p in equation 3.15 can be rewritten in the form

$$K_p = 0.6\ (\%\ OC\ )\ K_{ow} \qquad (3.19)$$

and the sorped phase fugacity capacity, in terms of %OC and K_{ow} becomes;

$$Z_s = 0.6 \cdot (\%\ OC) \cdot K_{ow} \cdot \rho / H \qquad (3.20)$$

III.1.2.4. FUGACITY CAPACITY FOR BIOTIC PHASES (Z_b)

For biota, a bioconcentration factor K_B is used instead of the partition coefficient. If it is expressed as a ratio of the concentrations in the biota (say fish) on a wet weight basis and in the water, it is identical to K_P. If expressed on a wet volume basis, it is analogous to the group $K_P\rho$ where ρ is the fish density.

$$Z_b = K_B \rho / H \qquad (3.21)$$

Several convenient correlations with K_{ow} also exist for K_B. Neely et. al.[59] established the first relationship between bioconcentration factor, K_B, and n-octanol-water partition coefficient, K_{ow} , of a variety of chemicals in a flowing water eco-system. An equation of the straight line of best fit was obtained as;

$$\log K_B = 0.124 + 0.542 \log K_{ow} \qquad (3.22)$$

$$n = 8 \qquad r = 0.948$$

In later years Veith et. al. worked on this correlation with 50 compounds and obtained the following correlation with a correlation coefficient, r, of 0.90

$$\log K_B = 0.85 \log K_{ow} - 0.70 \qquad (3.23)$$

Recently Mackay [34] studied the relationship between K_B and K_{ow} with the data set compiled by Veith, and he obtained a new correlation by eliminating and exchanging some of the data with new values from the recent literature. This relation which has the highest correlation coefficient is given as;

$$\log K_B = \log K_{ow} - 1.32 \qquad (3.24)$$

$$n = 59 \qquad r = 0.95$$

---

or

$$K_B = 0.048\ K_{ow} \qquad (3.25)$$

III.1.3. DESCRIPTION OF THE MODEL USED

The mathematical model developed in this work is a combination of valance molecular connectivity theory and Mackay's level I fugacity model for environmental compartmentalization analysis. In order to calculate environmental partitioning in the form of amounts in each medium the properties of the "unit world" designed by Mackay and Neèly are taken as standart for evaluative purposes (fig. III.1). The volumes and densities assumed for each compartment is given in table III.1.

This model also accepted by OECD, consists of a 1 km square with a 10 km high atmosphere; 30 % of the area is covered by soil whose depth is 3 cm and 70 % is water covering an average depth of 10 m, with 3 cm of sediment, 5 ppm by volume of suspended solids, and 0.5 ppm of biota.

The organic carbon contents are 2 % for soil and 4 % for sediment and suspended solids. A temperature of 25°C is assumed and the total amount of solute is arbitrarily taken as 100 moles.

Table III.1 : Unit World Compartment Volumes and Densities 67,68

Compartment	Volume (m^3)		Density (kg/m^3)
Air	$6x10^9$	(1 km^2 area x 6 km height)	1.19
Soil	$4.5x10^4$	(30% area x 15 cm depth)	1500
Water	$7x10^6$	(70% area X 10 m depth)	1000
Biota	7	(Water volume X 1 ppm)	1000
Suspended Solids	35	(Water volume X 5 ppm)	1500
Sediment	$2.1X10^4$	(70% area X 3 cm depth)	1500

III.2. RELATIONSHIP OF VALANCE MOLECULAR CONNECTIVITY TO PARTITION COEFFICIENT SOLUBILITY AND VAPOR PRESSURE

The molecular connectivity index is a topological index in that the calculation is fundamentally dependent on the way the constituent atoms of a molecule are attached to one another.

Seemingly encoded in the connectivity index, which results from a simple mathematical operation [35], is the molecular structure of a chemical species. Hence, it is expected that any physicochemical or biological property that is a function of the topological structure of a molecule, in this case its connectedness, is going to be related in some fashion to the connectivity index.

Since the manner in which organic groups are connected to form a molecule appears to influence molecular properties, the relationship between connectivity index and various physicochemical and biological properties was studied. As a result of these studies successful relations correlating the connectivity index (X) with these properties was reported. Recently the great utility of this simple index that could be used to predict physicochemical properties led to other studies concerning the water solubilites, boiling points, surface area, partition coefficients and many others. This simple approach was based on the calculation of molecular connectivity index (X) which is obtained from the molecular skeleton where a degree of connectivity δ_i was assigned to each vertex.

The regression equation with a correlation coefficient (r) of 0.978 and a standart error (s) of 0.455 for the correlation of connectivity index (x) with water solubility of 51 aliphatic alcohols was reported as[36]

$$\ln S = 6.702 - 2.666\ X$$

and a similar correlation with r = 0.958 and S = 0.511 was given for 18 hydocarbons as

$$\ln S = -1.505 - 2.533\ X$$

on the other hand the correlation of n-octanol water partition coefficient with molecular indices for 45 hydrocarbons, 24 esters, 9 carboxylic acids, 49 alcohols, 28 amines, 16 ketones and 12 ethers yield the regression equations given in table

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

III.2 which demonstrate that a linear relationship between log K_{OW} and the connectivity index is more than simply fortuitous[37].

Table III.2. Summary of Regression Equations, Correlation Coefficients and Standart Deviations

Class of Compounds	n	Slope	Intercept	r	s
Carboxylic acids	9	0.927 ±0.03	-1.41±0.11	0.996	0.122
Esters	24	0.996 ±0.01	-1.71±0.04	0.999	0.060
Ethers	12	0.964 ±0.07	-1.30±0.19	0.976	0.080
Alcohols	49	0.966 ±0.03	-1.53±0.09	0.997	0.151
Amines	28	0.977 ±0.04	-1.51±0.12	0.979	0.179
Ketones	16	0.982 ±0.03	-1.16±0.09	0.993	0.094
Hydrocarbons	45	0.884 ±0.03	0.406±0.09	0.975	0.160
All compounds except hydrocarbons	138	0.950 ±0.01	-1.48±0.04	0.986	0.152

Figures III.2 and III.3 illustrates this relation for solubilities and partition coefficients respectively.

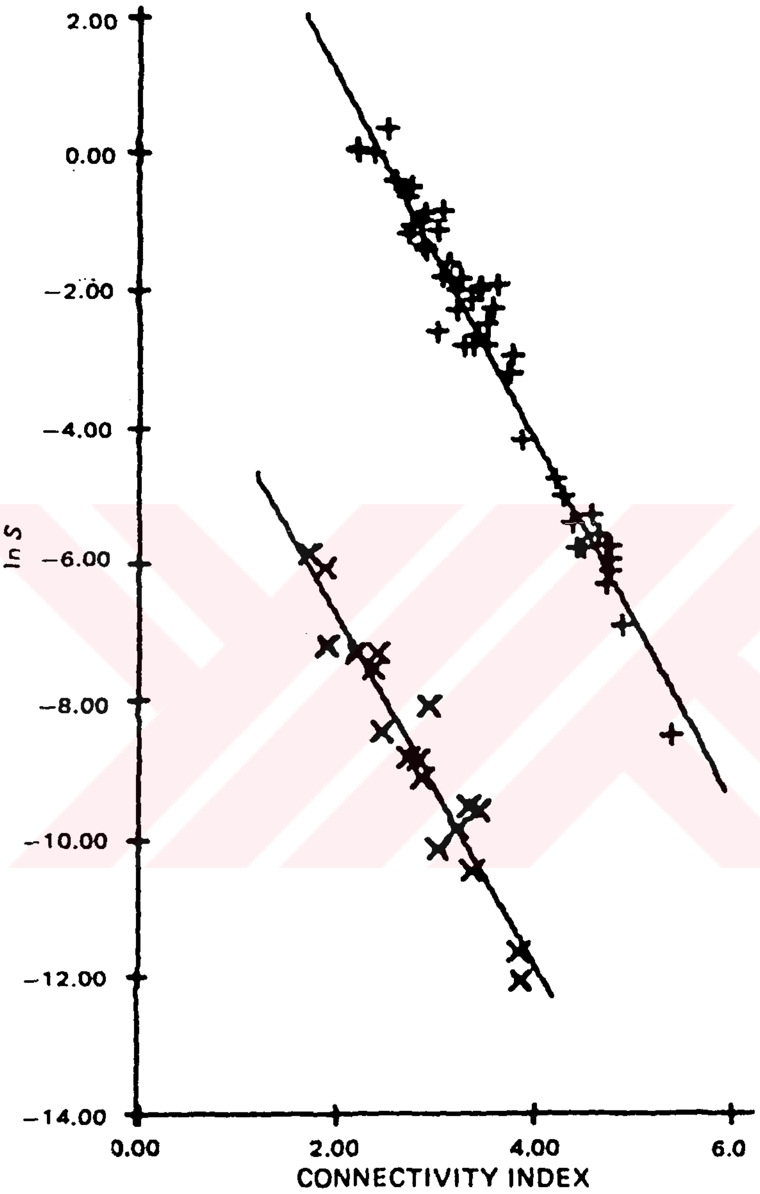


Figure III.2. : Plot of the logarithm of the partition coefficient versus the molecular connectivity index for 24 esters, nine carboxylic acids, 49 alcohols, 28 amines, 16 ketones, and 12 ethers with the corresponding regression line.

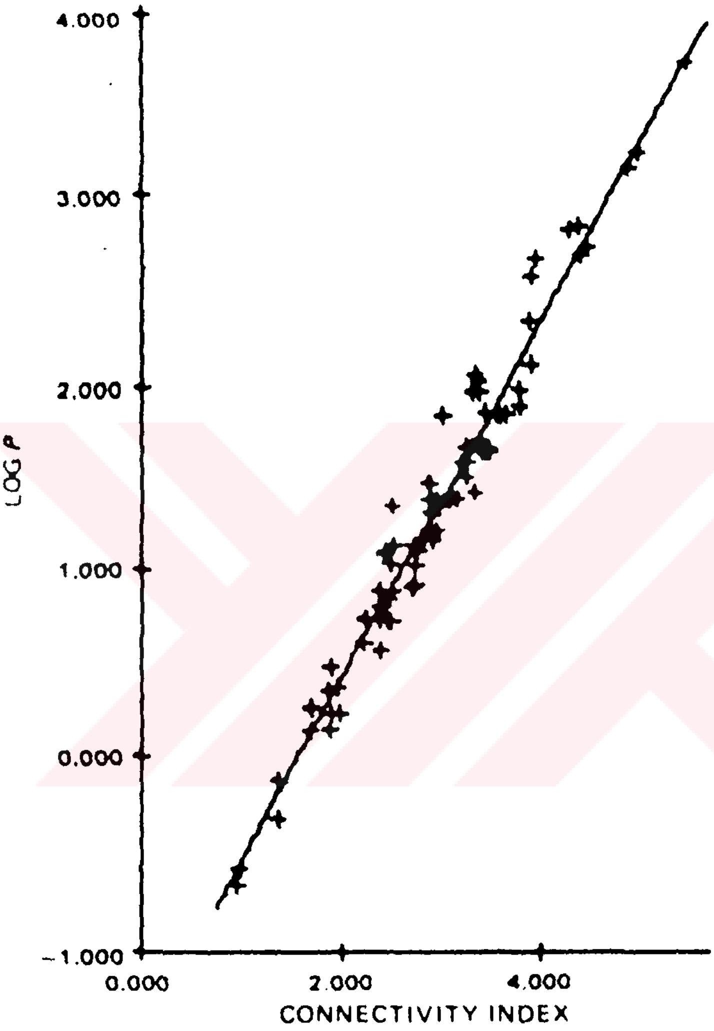


Figure III.3. : Plot of the natural logarithm of solubility versus the connectivity index for 51 alcohols (+) and 18 hydocarbons (x) with the correspoding regression lines.

YK

As can be easily observed,many of the physical parameters is directly related to the topological structure of the molecule, e.g., the number and manner that atoms are arranged in a molecule (molecular connectivity). The molecular connectivity index (X) developed and utilized by Kierr and coworkers and based on the earlier branching index put forward by Randic[37], is a nonempirical easily calculated value which seemingly encodes the shape and architecture of a molecule via the interatomic connections. However, due to the requirement to a more rational way of quantifying heteroatom content, this work uses the modified approach which is the Valance Molecular Connectivity to determine the correlations between n-octanol-water partition coefficients (K_{ow}) solubilities (S) and vapor pressures (P) of certain environmentally hazardous compounds and their molecular structures within a more sophisticated frame taking into account the indices of first three order (${}^{o}X^{v}$, ${}^{1}X^{v}$, ${}^{2}X^{v}$) in order to find the best three variable equation relating above parameters to structure. This multivariable search of valance connectivity terms is conducted in a regression analysis using a program that considers all variable combinations.

The following discussions are devoted to the development of this mathematical model which in turn leads to a simple relation for predicting the possible compartmental behaviour of certain classes of chemicals, based on the topological characteristics of compounds in question.

IV. DEVELOPMENT OF THE VALANCE CONNECTIVITY MODEL FOR THE PREDICTION OF ENVIRONMENTAL COMPARTMENTALIZATION OF VARIOUS BENZENE DERIVATIVES

YK

IV- DEVELOPMENT OF THE VALANCE CONNECTIVITY MODEL FOR THE PREDICTION OF ENVIRONMENTAL COMPARTMENTALIZATION OF VARIOUS BENZENE DERIVATIVES

IV- 1. THE VALANCE CONNECTIVITY APPROACH

The number of organic chemicals currently in use on commercial scale, amounts to several tens of thousands per year and many new ones are being introduced every passing year. Hence, experimental testing for toxic and behavioral properties both in organisms and ecosystems for each of these chemicals seems to be out of question.

However, evaluation of simple structural properties or the determination of suitable physicochemical properties, their subsequent correlation with the desired parameters determined experimentally for a limited number of congeneric compounds and the final use of this correlation for the prediction of various properties such as toxicity or compartmentalization, for the other members of the congeneric series seems to be promissing.

In the following approach the possibility of a generalization, by means of the theory of graphs, of the method of calculation of certain physicochemical properties that are functions of environmental behaviour is considered. For this specific purpose three groups of properties are chosen which can be used in combination with Mackay's level I fugacity model in order to predict compartmental partitioning of various compounds. These properties are n-octanol-water partition coefficient, (K_{OW}), solubility, (S) and vapor pressure (P).

QSAR studies, mostly concerning structure-biological activity (toxicity etc.) relations points out that, not only the congenericity of the compounds is a prerequsite but also their metabolic fate and mechanism of attack have to be identical. In the same way the prediction of environmental partitioning and other physicochemical properties from molecular structure will also require the congenericity of compounds and the physicochemical interactions they are involved in. So, in wiew of the availability of experimental data, a representative group of each congeneric series including

- polychlorinated biphenyls (PCB)
- halogen substituted benzene derivatives
- alkyl substituted benzene derivatives
- polycyclic aromatic hydrocarbons (PAH)

are selected. Concerning the structural data of these compounds, valance molecular connectivity indices, which provide a simple flexible and direct structural description independent of experimentally determined physical properties are determined.

In the foregoing sections, certain degrees of X^v indices which correlate strongly with the experimental data mentioned are sought for. And furthermore a multivariable search for the best corelation is conducted in a regression analysis.

The relevant data concerning the selected groups of compounds are given in table IV.1.

TABLE IV.1.: Compilation of Physical and Chemical Data for Various Groups of Benzene Derivatives

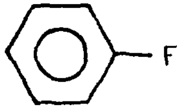
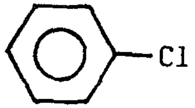
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
HALOGEN SUBSTITUTED BENZENE DERIVATIVES							
Benzene (C_6H_6)	78.114	2.13	(39,40,41)	3.2529	(42,43)	1.9776	(43)
				3.2406	(43)	1.9782	(56)
				3.2504	(44,40)	1.9779	(56)
				3.2527	(45)	2.0023	(56)
				3.2528	(47,48)	1.9779	(56)
				3.2507	(49)		
				3.2527	(49)		
				3.2430	(50)		
Fluorobenzene ($C_6H_5.F$)	96.106	2.27	(39)	3.1912	(40)	1.8838	(56)
				3.1928	(47,48)	1.9165	(56)
						1.8911	(56)
							
Chlorobenzene ($C_6H_5.Cl$)	112.56	2.84	(39)	2.4697	(45)	1.0739	(54)
		2.80	(46)	2.6812	(51)	1.0719	(46,41,51)
				2.6884	(52,53)	1.0700	(53)
				2.6739	(40)	1.0828	(56)
				2.7014	(47,48)	1.0780	(56)
				2.6513	(44)	1.0698	(56)
				2.6902	(46,41)	1.0666	(56)

TABLE IV. 1. Continued...

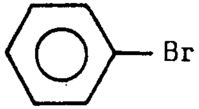
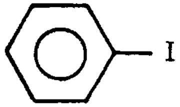
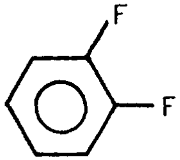
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
Bromobenzene ($C_6H_5.Br$) 	157.02	2.99 2.95 3.07	(56) (44) (56)	2.6134 2.6493 2.5529	(40) (44) (47,48)	0.5947 0.6169 0.6104 0.6262 0.6172	(56) (56) (56) (56) (54)
Iodobenzene ($C_6H_5.I$) 	204.01	3.25 3.36	(55) (47)	2.5315 2.3597 2.3027	(57,55,40) (47,48) (45)	-0.0203 -4.2×10^{-3} -0.0352 -0.0258 -5.2×10^{-3}	(56) (56) (56) (56) (54)
o-Difluorobenzene ($C_6H_4.F_2$) 	114.09	2.59	(47)	3.0572	(47,48)	1.7966	(56)

TABLE IV.1. Continued...

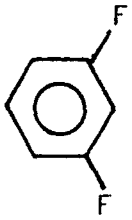
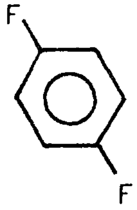
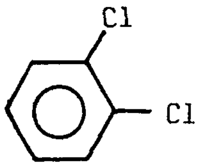
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
m-Difluorobenzene ($C_6H_4.F_2$)	114.09	2.58	(47)	3.0573	(47,48)	1.9527	(56)
							
p-Difluorobenzene ($C_6H_4.F_2$)	114.09	2.58	(47)	3.0879	(47,48)	1.8489	(56)
							
o-Dichlorobenzene ($C_6H_4.Cl_2$)	147.01	3.59	(47)	2.1761	(57)	0.1664	(54)
		3.40	(57)	2.4150	(53)	0.1072	(53)
				1.9673	(47,48)	0.1701	(56)
				2.1927	(50)	0.1252	(56)
				1.9653	(45)	0.1439	(56)

TABLE IV.1. Continued...

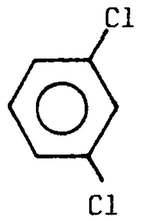
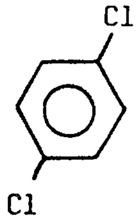
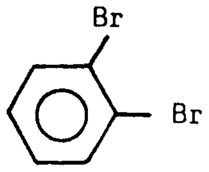
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
m-Dichlorobenzene $(C_6H_4 \cdot Cl_2)$ 	147.01	3.59	(47)	2.0792	(57)	0.3623	(54)
		3.40	(57)	2.0773	(47,48)	0.2985	(56)
				2.1255	(50)	0.2755	(56)
				2.0952	(45)	0.3509	(56)
p-Dichlorobenzene $(C_6H_4 \cdot Cl_2)$ 	147.01	3.389	(44,55)	1.8976	(58,46,51, 44,55,57)	-0.1708	(54)
		3.38	(59)	1.9574	(47,48)	0.2285	(56)
		3.40	(57)	1.8681	(50)	0.2575	(56)
				1.4896	(45)	-0.0219	(58,46)
						0.2847	(56)
o-Dibromobenzene $(C_6H_4 \cdot Br_2)$ 	235.92	4.07	(47)	1.8727	(47,48)	-0.7093	(56)
						-0.6158	(56)

Table IV.1. Continued...

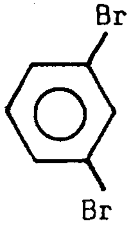
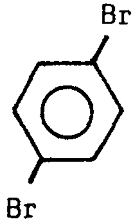
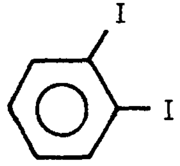
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
m-Dibromobenzene ($C_6H_4 . Br_2$)  	235.92	4.07	(47)	1.9928	(47,48)	-0.6457	(54)
p-Dibromobenzene ($C_6H_4 . Br_2$)  	235.92	4.07	(47)	1.3028	(47,48)	-0.7929 1.2807	(54) (56)
o-Diiodobenzene ($C_6H_4 . I_2$)  	329.91	4.65	(47)	1.2784	(47,48)	-2.1391	(56)

Table IV.1. Continued...

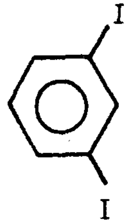
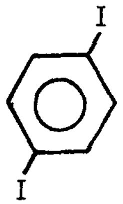
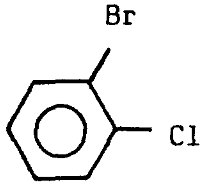
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm Hg)	Ref.
m-Diiodobenzene ($C_6H_4.I_2$) 	329.91	4.64	(47)	0.9484	(47,48)	-2.2457	(56)
p-Diiodobenzene ($C_6H_4. I_2$) 	329.91	4.64	(47)	0.2683	(47,48)	-3.1568	(56)
o-Bromochlorobenzene ($C_6H_4. BrCl$) 	191.46	3.83	(47)	2.0921	(47,48)	-0.3541	(56)

Table IV.1. Continued...

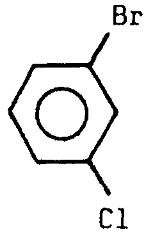
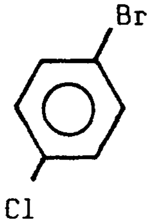
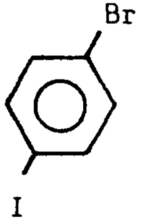
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P mm Hg	Ref.
m-Bromochlorobenzene (C_6H_4. BrCl) 	191.46	3.83	(47)	2.0737	(47,48)	-0.1894	(56)
p-Bromochlorobenzene (C_6H_4. BrCl) 	191.46	3.83	(47)	1.6521	(47,48)	-0.6155 -0.1985 -0.5877	(56) (56) (54)
p-Bromoiodobenzene (C_6H_4. BrI) 	282.91	4.36	(47)	0.8916	(47)	-2.0348	(56)

Table IV.1. Continued...

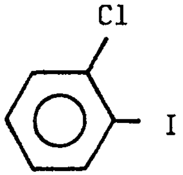
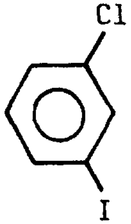
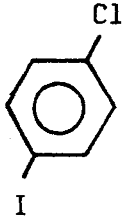
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm Hg)	Ref.
o-Chloroiodobenzene (C_6H_4. ClI) 	238.46	4.12	(47)	1.8374	(47,48)	-0.9948	(56)
m-Chloroiodobenzene (C_6H_4. ClI) 	238.46	4.12	(47)	1.8274	(47)	-0.8989	(56)
p-Chloroiodobenzene (C_6H_4. Cl I) 	238.46	4.12	(47)	1.3474	(47,48)	-1.1524	(56)

Table IV.1. Continued...

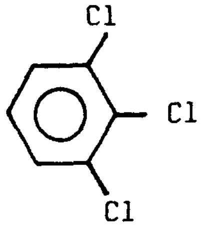
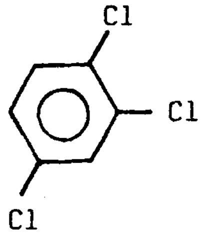
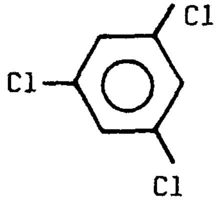
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
1,2,3-Trichlorobenzene (C_6H_3. Cl_3) 	181.46	4.27	(47)	1.4988 1.0887	(47) (45)	-0.4022 -0.6782 -0.9230	(56) (54) (56)
1,2,4-Trichlorobenzene (C_6H_3. Cl_3) 	181.46	4.18 4.27 3.93 4.02 4.12	(56) (47) (46) (46) (46)	1.4771 1.5388 1.6636	(46,58)	-0.3701 -0.5515 -0.5372 -0.3468 -	(56) (56) (56) (54)
1,3,5-Trichlorobenzene (C_6H_3. Cl_3) 	181.46	4.27	(47)	0.8188 0.6148	(47) (45)	-0.2384 -0.8133 -0.0776 -0.3010	(54) (56) (56) (46)

Table IV.1. Continued...

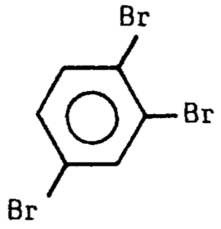
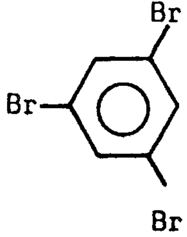
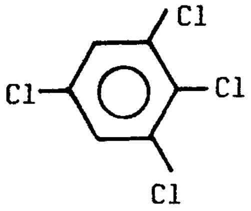
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
1,2,4-Tribromobenzene $(C_6H_3.\ Br_3)$ 	314.82	4.98	(47)	0.9980	(47)	-2.0630	(56)
1,3,5-Tribromobenzene $(C_6H_3.\ Br_3)$ 	314.82	4.98	(47)	-0.1024	(47)	-2.7472	(56)
1,2,3,5-Terachlorobenzene $(C_6H_2.\ Cl_4)$ 	215.91	5.05	(47)	0.5441 0.6038 0.6252	(47) (50) (45)	-1.1343	(54)

Table IV.1. Continued...

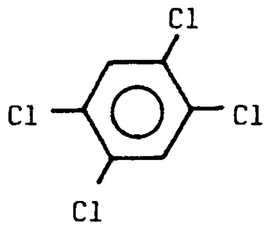
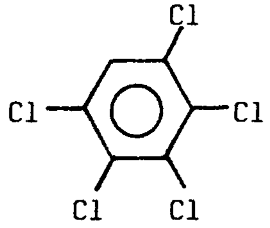
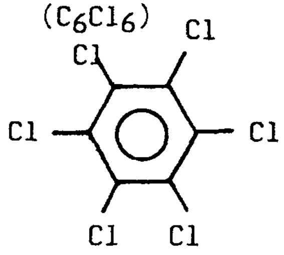
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
1,2,4,5-Tetrachlorobenzene (C_6H_2. Cl_4) 	215.91	4.67 5.05	(44) (47)	0.7782 -0.2257 0.3716	(44) (47,48) (45)	-1.0315 -2.2676	(56) (54)
Pentachlorobenzene (C_6H. Cl_5) 	250.36	5.19	(44)	-0.8697 -0.2518 0.1245 -0.0803	(44) (47,48) (50) (45)	-2.2351 -2.5229	(56) (56)
Hexachlorobenzene (C_6Cl_6) 	284.81	5.23 6.18 5.20 5.23 5.44	(44) (59) (63) (63) (63)	-1.4559 -2.3054 -2.3010 -2.3279	(44,46) (47,48) (42) (45)	-3.9586 -2.5361 -4.6778 -5.0	(56) (56) (42) (46)

Table IV.1. Continued...

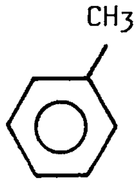
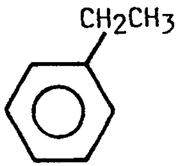
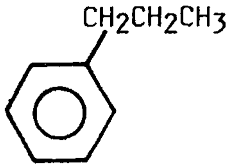
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
ALKYL SUBSTITUTED BENZENE DERIVATIVES							
Toluene 	92.14	2.69	(40,49,55)	2.7118 2.7973 2.6721 2.7243 2.7559 2.7115 2.7285 2.7055 2.7624	(40,42,53) (43) (46,58) (43) (52) (49) (49) (49) (45)	1.4544 1.4490 1.4771 1.4548 1.4541 1.4640 1.4527	(43) (54) (46,58) (53) (56) (56) (56)
Ethylbenzene 	106.17	3.15 2.832	(40,49) (41)	2.1818 2.00 2.1821 2.3181 2.2715	(40,53) (60) (49) (43) (45)	0.9823 0.9775 0.9948	(53) (43) (54)
n-Propylbenzene 	120.20	3.68	(40,49)	1.7404 1.7399	(40) (42)	0.5350	(54)

Table IV.1. Continued...

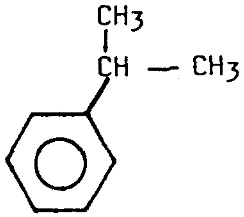
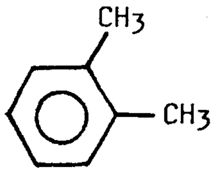
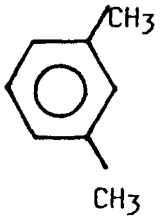
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
i-Propylbenzene 	120.20	3.66 3.323	(40,49,61) (55)	1.6990 1.6989 1.8149	(40,53) (49) (49)	0.6628	(53)
o-Xylene 	106.17	3.12 3.13	(40) (45)	2.3441 2.2430	(45) (40)	0.8153	(54)
m-Xylene 	106.17	3.20	(45)	2.2050 2.2923 2.2381	(45) (43) (43)	0.9182	(54)

Table IV.1. Continued ...

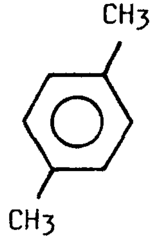
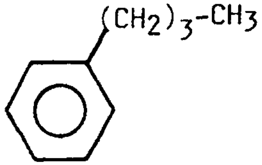
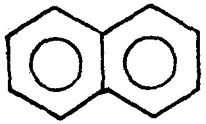
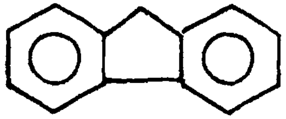
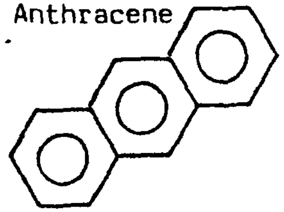
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
p-Xylene 	106.17	3.18	(45)	2.3314 2.2967 2.3010	(45) (43) (43)	0.9415	(54)
Butylbenzene 	134.22	4.11	(61)	3.6990	(53)	0.0663 0.0414	(56) (53)

Table IV.1. Continued...

COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log $P^{(*)}$ (mm/Hg)	Ref.
UNSUBSTITUTED POLYCYCLIC AROMATIC HYDROCARBONS							
Naphthalene 	128	3.37 3.36	(65) (66)	-3.4237	(65)	-1.1938 -1.3080	— (69)
Fluorene 	166	4.34	(66)			-3.2048	—
Anthracene 	178	4.63 4.54	(64) (66)	-1.3507 -1.1376 -1.3516	(65) (64) (64)	-5.2437	—

(*) Calculated according to Kistiakowsky model$^{(54)}$ (Appendix I)

Table IV.1. Continued...

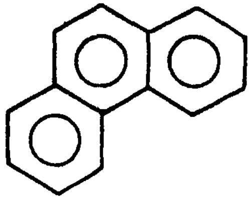
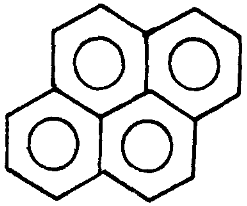
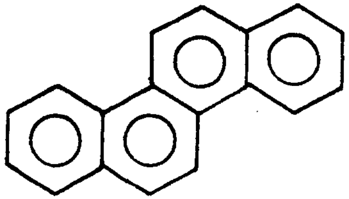
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log $P^{(*)}$ (mm/Hg)	Ref.
Phenanthrene 	178	4.46 4.57 4.63	(63) (63,66) (64)	8.68×10^{-4} 0.1104 0.0284 4.2×10^{-4}	(65) (65) (65) (65)	-4.1017	—
Pyrene 	202	5.22 5.18	(64) (66)	-0.8794 -0.8706) -0.8796 -0.8867	(65) (64) (64) (64)	-5.8960	—
Chrysene 	228	5.91	(64)	-2.7447 -2.6991 -2.7451	(65) (64,65) (64)	-8.2187	—

Table IV.1. Continued...

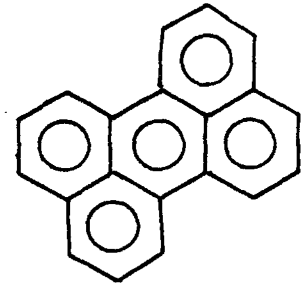
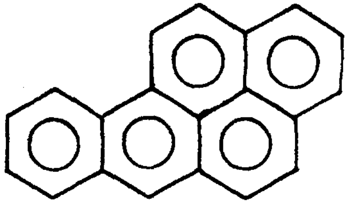
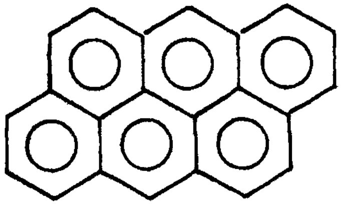
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log $P^{(*)}$ (mm/Hg)	Ref.
Perylene 	252	6.5	(64)	-3.3986	(65)	-6.6758	—
Benzo (a) pyrene 	252	6.5	(64)	-3.6990 -3.9556 -2.4206 -2.9216	(65) (64) (64) (64)		—
Anthranthene 	276	7.01	(64)	—	—		—

Table IV.1. Continued...

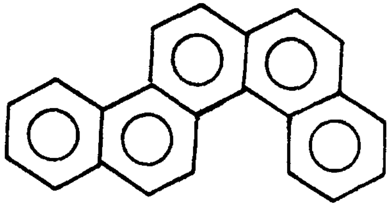
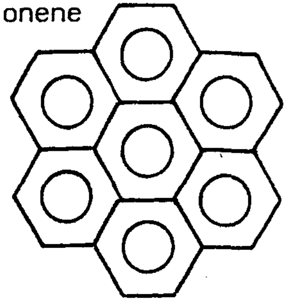
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P$^{(*)}$ (mm/Hg)	Ref.
Benz (c) chrysene 	278	7.10	(66)	—	—	—	—
Coronene 	303	7.59	(66)	—	—	-11.9667	—

TABLE IV.1 Compilation of Physical and Chemical Properties for Polychlorinated Biphenyls

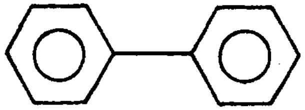
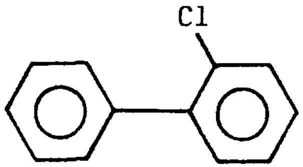
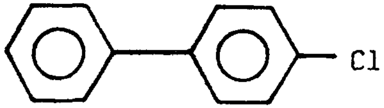
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
POLYCHLORINATED BİPHENYLS (PCB)							
Biphenyl 	154	3.76 3.88 3.95 3.98 4.04 4.09 4.17	(63) (63) (61) (61) (61) (63) (61)	0.8751	(46,58,41)	-2.00 -2.0132	(61) (46,58,41)
2-CBP 	189	4.6	(51)	0.6990	(51)	-2.0757	(51)
4-CBP 	189	4.6	(46)	0.0792 0.6990	(61) (46)	-2.3468 -2.0752	(61) (46)

Table IV.1 Continued...

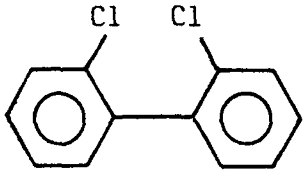
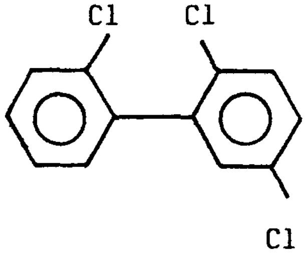
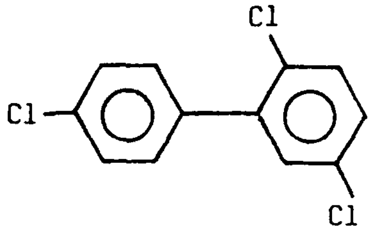
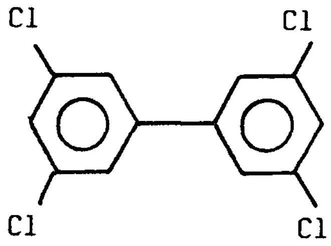
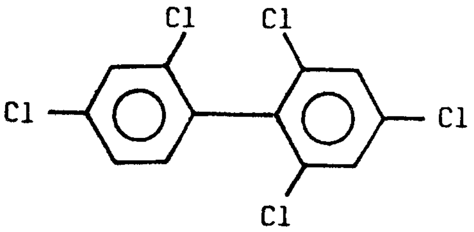
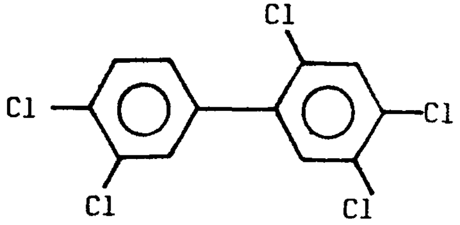
COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
2.2'- CBP 	223	4.04 4.00	(46) (61)	0.0414	(58,61)	-2.5719	(61)
2,5,2'- CBP 	257	—		-0.6198 -1.3010	(61) (46,58)	-2.6990 -2.8239	(61) (46,58)
2,5,4'- CBP 	257	4.96	(46)	-1.9586	(61)	—	—

Table IV. 1. Continued

COMPOUND	Molecular Weight g/mole	log K_{ow}	Ref.	log S (g/m^3)	Ref.	log P (mm/Hg)	Ref.
3,5,3',5'-CBP 	292	6.0	(46)	-1.5850 -1.3010	(46) (41)	-3.1079 -3.3098	(46) (41)
2,4,6,2',4'- CBP 	326	5.50 6.0	(63) (51)	-2. 0000	(41)	-4.1549	(46)
2,4,5,4',5'- CBP 	326	6.11	(62)	-2.0458 -2.0	(46) (41,62)	-5.0969 -4.1135	(62) (41)

IV.1.1. EVALUATION OF VALANCE MOLECULAR CONNECTIVITY INDICES.

Valance molecular connectivity indices from zero to second order were calculated according to Kierr and Hall[38] for 27 unsubstituted PAH's, 8 PCB's, 32 halogen substituted and 9 alkyl substituted benzene derivatives using a simple desk top calculator.

The valance molecular connectivity index ($^{n}X^{v}$) is derived from the cardinal number (δ^{v}) ennumerating the valance electrons on an atom not bonding to hydrogen ($\delta_i^{v} = Z_i^{v} - h_i$). The index is computed, as described in the previous sections, by the general formula,

$$^{m}X^{v} = \sum (\delta_i \, \delta_j \, \ldots\ldots \delta_n)^{-1/2}$$

where m is the order (number of bonds) and the number of deltas in parantheses is equal to the number of bonded atoms in the fragment of order m within the context of parameters, collectively termed as molecular connectivity related to the topological structure of organic groups, the simplest term is the zeroth order connectivity designated by ${}^{o}\chi^{v}$ and is calculated from

$${}^{o}\chi^{v} = \sum (\delta_i)^{-1/2}$$

where i is a number assigned to each nonhydrogen atom and reflects the number of atoms bonded to it. A similar term is derived for each bond by calculating the product of the numbers associated with the two atoms of the bond. These values are summed to give the first order connectivity, ${}^{1}\chi^{v}$ which is a weighted count of bonds and is calculated from

$${}^{1}\chi^{v} = \sum (\delta_i \ \delta_j)^{-1/2}$$

Similarly the product of the three adjacent delta values for each pair of adjacent bonds given the third term of the adjaceny series as

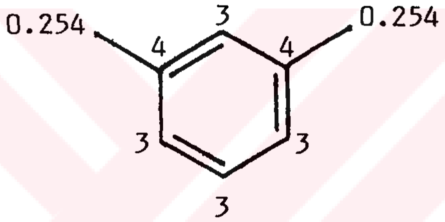
$${}^{2}\chi^{v} = \sum (\delta_i \ \delta_j \ \delta_k)^{-1/2}$$

The following example demonstrate the calculation of valance molecular connectivity indices for m-dibromobenzene.

Specimen Calculation

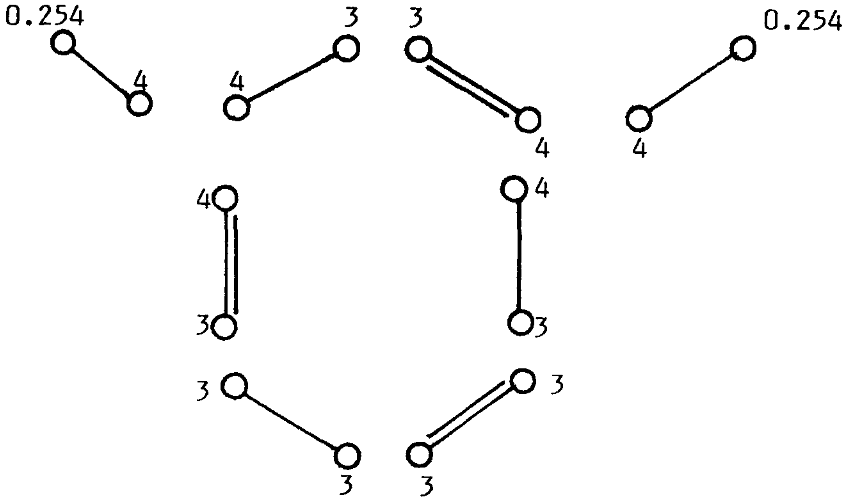
Evaluation of zeroth,first and second order valance molecular connectivity indices for m-dibromobenzene where δ^v (bromine)= 0.254*

a- Calculation of $^{o}\chi^{v}$:


0.254
3
0.254
4
4
3
3
3

$$^{o}\chi^{v} = \sum(\delta_i)^{-1/2}$$
$$= \sum 4(3)^{-1/2} + 2(4)^{-1/2} + 2(0.254)^{-1/2}$$
$$= 7.2787$$

b- Calculation of $^{1}\chi^{v}$:

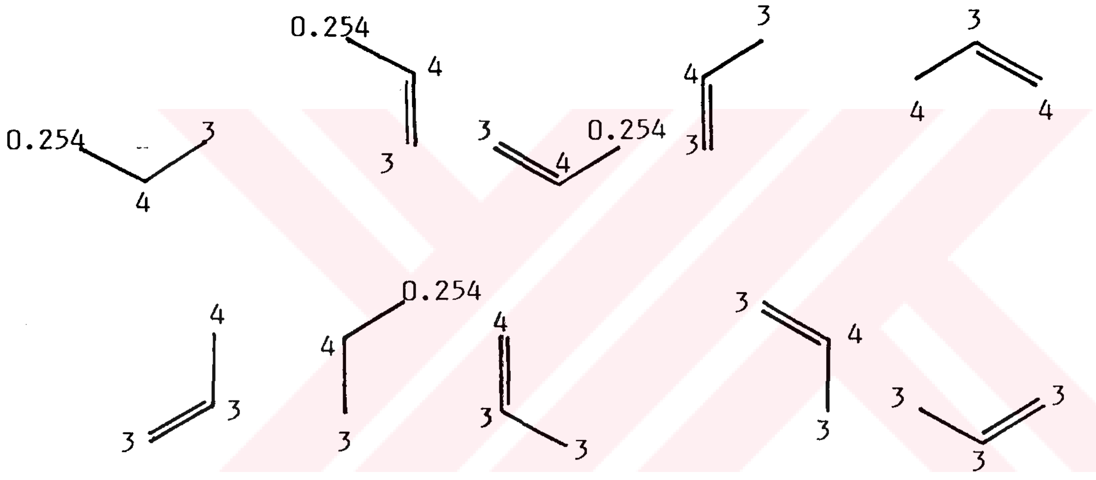

0.254
4
4
3
3
4
0.254
4
4
3
4
3
3
3
3
3

---

* Value taken from table II.7.

$$^{1}\chi^{v} = \sum(\delta_i . \delta_j)^{-1/2}$$
$$= \sum 2(3.3)^{-1/2} + 4(3.4)^{-1/2} + 2(4.0254)^{-1/2}$$
$$= 3.8056$$

c- Calculation of $^{2}\chi^{v}$:


0.254
4
3
0.254
4
3
3
4
0.254
3
4
3
3
4
4
4
3
3
0.254
4
3
4
3
3
3
4
3
3
3
3

$$^{2}\chi^{v} = \sum(\delta_i . \delta_j . \delta_k)^{-1/2}$$
$$= 4\ (4.3.0,254)^{-1/2} + 4(3.4.3)^{-1/2} + (4.4.3)^{-1/2} + (3.3.3)^{-1/}$$
$$= 3.2946$$

The results obtained for the four congeneric groups of compounds are listed in table IV.2.

Table IV.2. Calculated Valance Molecular Connectivity Indices for PAH , PCB , Halogen and Alkyl Substituted Benzene Derivatives

COMPOUND	${}^0\chi^v$	${}^1\chi^v$	${}^2\chi^v$
POLYCYCLIC AROMATIC HYDROCARBONS			
Benzene	3.4641	2.0000	1.1547
Naphthalene	5.6188	3.4047	2.3472
Acenaphtylene	6.6188	4.1488	3.1259
Acenaphthene	6.8783	4.4451	3.4324
Fluorene	7.3259	4.6118	3.4910
Phenanthrene	7.7735	4.8154	3.5078
Anthracene	7.7735	4.8094	3.5465
Fluoranthene	8.7735	5.5654	4.2549
Pyrene	8.7735	5.5594	4.2896
Triphenylene	9.9282	6.2321	4.6368
Chrysene	9.9282	6.2261	4.6685
Benz (a) anthracene	9.9282	6.2201	4.7072
Naphthacene	9.9282	6.2141	4.7459
Benz (e) pyrene	10.9282	6.9761	5.4185
Perylene	10.9282	6.9761	5.4185
Benz (b) fluoranthene	10.9282	6.9761	5.1015
Benz (k) fluoranthene	10.9282	6.9701	5.0405
Benz (a)pyrene	10.9282	6.9701	5.4537
Benz (g,h,i) perylene	11.9282	7.7201	6.2003
Antanthrene	11.9282	7.7141	5.9280
Picene	12.0829	7.6368	5.8292
Benz (c) chrysene	12.0829	7.6368	5.8322
Dibenz (a,c) anthracene	12.0829	7.6368	5.8361
Dibenz (a,j) anthracene	12.0829	7.6308	5.8679
Dibenz (a,h) anthracene	12.0829	7.6308	5.8679
Benz (b) chrysene	12.0829	7.6308	5.8679
Pentacene	12.0829	7.6188	5.9452
Coronene	12.9282	8.4641	6.9821

Table IV.2. Continued

COMPOUND	${}^0\chi^v$	${}^1\chi^v$	${}^2\chi^v$
POLYCHLORINATED BIPHENYLS			
Biphenyl	6.7735	4.0714	2.7321
4.CBP	7.9000	4.5840	3.3498
2,2'-CBP	9.0265	5.1086	3.8495
2,5,4'-CBP	10.1530	5.6152	4.5519
2,5,2'-CBP	10.1532	5.6212	4.5093
3,5,3',5'-CBP	11.2795	6.1218	5.2236
2,4,5,4',5'-CBP	12.4060	6.6524	5.5995
2,4,6,2',4'-CBP	12.4060	6.6524	5.6569
ALKYL SUBSTITUTED BENZENE DERIVATIVES			
Toluene	4.3868	2.4107	1.6548
Ethylbenzene	5.0939	2.9713	1.8392
O-xylene	5.3094	2.8274	2.0843
m-xylene	5.3094	2.8214	2.1582
p-xylene	5.3094	2.8214	2.1547
n-propyl benzene	5.8010	3.4713	2.2356
i-propylbenzene	5.9641	3.3541	2.5654
n-butylbenzene	6.5081	3.9713	4.1927
HALOGEN SUBSTITUTED BENZENE DERIVATIVES			
Fluorobenzene	3.6347	1.7867	1.2205
Chlorobenzene	4.5906	2.5126	1.7724
Bromobenzene	5.3709	2.9028	2.2229
Iodobenzene	6.8167	3.6257	3.0576
o-difluorobenzene	3.7566	2.0510	1.2478
m-difluorobenzene	3.7566	1.5734	1.2616
p-difluorobenzene	3.7566	1.5734	1.2582
o-dichlorobenzene	5.7172	3.0312	2.3039
m-dichlorobenzene	5.7172	3.0252	2.3936
p-dichlorobenzene	5.7172	3.0252	2.3901
o-dibromobenzene	7.2778	3.8115	3.1362
m-dibromobenzene	7.2778	3.8056	3.2946
p-dibromobenzene	7.2778	3.8056	3.2911
o-diiodobenzene	10.1693	5.2574	4.7022
m-diiodobenzene	10.1693	5.2513	4.9640
p-diiodobenzene	10.1693	5.2513	4.9606
o-bromochlorobenzene	6.4975	3.4214	2.7243
m-bromochlorobenzene	6.4975	3.4154	2.8442
p-bromochlorobenzene	6.4975	3.4154	2.8407

Table IV.2. Continued

COMPOUND	$^{0}\chi^{v}$	$^{1}\chi^{v}$	$^{2}\chi^{v}$
p- bromoiodobenzene	8.7236	4.5285	4.1259
o-chloroiodobenzene	7.9433	4.1443	3.5031
m-chloroiodobenzene	7.9433	4.1383	3.6789
p-chloroiodobenzene	7.9433	4.1383	3.6753
1,2,3-trichlorobenzene	6.8437	3.5498	2.8384
1,2,4-trichlorobenzene	6.8437	3.5438	2.9250
1,3,5-trichlorobenzene	6.8437	3.5378	3.0182
1,2,4-tribromobenzene	9.1846	4.7143	4.2162
1,3,5-tribromobenzene	9.1846	4.7083	4.3697
1,2,3,5-tetrachlorobenzene	7.9701	4.0624	3.4630
1,2,4,5-tetrachlorobenzene	7.9701	4.0624	3.4600
Pentachlorobenzene	9.0966	4.5870	3.8914
Hexachlorobenzene	10.2232	5.1116	4.3616

IV.1.2. CORRELATIONS

As the second step in the development of valance connectivity model for the prediction of environmental behaviour of above mentioned four group of chemical compounds, the correlation of the calculated valance molecular connectivity indices with that of relevant data is inspected.

In view of the selected data sets given in table IV.3 for n-octanol-water partition coefficients (K_{OW}), solubilities (S) and vapor pressures (p), the correlation between y=log K_{OW}, log S or log P and x= ${}^{0}\chi^{v}$ through ${}^{2}\chi^{v}$ is calculated assuming the correlation to be of linear one-parameter regression type ($y = m x + n$).

In this analysis due to the statistical reasons discussed in the following sections, only the para conformations are taken into consideration, though the results account for all three conformations.

The regression analysis is carried out according to the given program (Appendix I) using casio fx-602P programmable desk top calculator and as the main criteria for the correlation, the correlation coefficient, r, and the number data N is considered.

The results of this statistical analysis are given in table IV.3 and IV.4 where the correlation of each index with log K_{OW}, log S and log P is given both for each group and for combinations of related groups.

A closer inspection of these relations with correlation coefficients of over 0.9 which have more or less similar slopes and intercepts within interrelated groups/parameters, have led to a generalization of these values for all four groups of benzene derivatives. While going into such a generalization, It has been thought that the dispersion of data and the derivation of the lines representing each group of compounds, in the higher value connectivity index area for all three parameters (log K_{OW}, log S and log P) is due to the increasing size of the molecules. (These plots are given in figures IV.1 through IV.9)

As it has also been pointed out earlier, connectivity indices describe certain intermolecular relationships concerning the electronic structure of the molecule. Hence as the molecule gets larger and those relationships get much more complex, a single index can not account for the whole system.

We know that the individual physicochemical properties of congeneric series of compounds is sufficiently well determined by the structure of individual small sections of the molecule. Similarly a property may be divided into seperate components which constitute the contributions made by each individual bond as well as by each interaction between them. These interactions depend on the structure of the carbon chain which separates these bonds in the molecule, on the number of atoms constituting the structure and on the states of their electron shells.

Bearing in mind that these states are described by delta values constituting the valance molecular connectivity indices, the complex interrelationship between the bonded atoms as the molecule gets larger may as well be accounted for by using the higher order connectivity parameters in various combinations.

Hence, in the following section of this work, the possibility of a generalization of the method of calculation of various physicochemical properties by means of the theory of graphs is considered. For this reason a multivariable search of connectivity terms is conducted in a regression analysis using a program that considers all variable combinations.

Table IV.3. Input Data Used in Multiple Regression Analysis

					Y		
MOLECULE	MOL.WT.	${}^{0}\chi^{v}$	${}^{1}\chi^{v}$	${}^{2}\chi^{v}$	$\ln K_{ow}$	lnS	lnP
HALOGEN SUBSTITUTED BENZENES							
Benzene	78.114	3.4641	2.0000	1.1547	4.9053	7.4899	4.5543
Fluorobenzene	96.106	3.6347	1.7867	1.2205	5.2269	7.3479	4.3544
Chlorobenzene	112.56	4.5906	2.5126	1.7724	6.5367	6.1738	2.4558
p-difluorobenzene	114.09	3.7566	1.5734	1.2582	5.9487	7.1102	4.2572
m-difluorobenzene	114.09	3.7566	1.5734	1.2616	—	—	4.4960
o-difluorobenzene	114.09	3.7566	2.0510	1.2478	—	—	0.3313
p-dichlorobenzene	147.01	5.7172	3.0252	2.3901	7.8058	6.6733	0.6555
m-dichlorobenzene	147.01	5.7172	3.0252	2.3936	—	—	0.8080
o-dichlorobenzene	147.01	5.7172	3.0312	2.3039	—	—	0.3313
Bromobenzene	157.02	5.3709	2.9028	2.2229	6.8847	6.0176	1.4419
1,3,5-tirchlorobenzene	181.46	6.8437	3.5378	3.0182	—	—	-0.1788
1,2,4-trichlorobenzene	181.46	6.8437	3.5438	2.9250	—	3.4012	-0.8521
1,2,3-trichlorobenzene	181.46	6.8437	3.5498	2.8384	—	3.4510	-0.9261
p-bromochlorobenzene	191.46	6.4975	3.4154	2.8407	8.8189	3.8040	-0.4571
m-bromochlorobenzene	191.46	6.4975	3.4154	2,8442	—	—	-0.4362
o-bromochlorobenzene	191.46	6.4975	3.4214	2.7243	—	—	-0.8153

Table IV.5. Continued

MOLECULE	MOL.WT.	$^{0}\chi^{v}$	$^{1}\chi^{v}$	$^{2}\chi^{v}$	$\ln K_{ow}$	lnS	lnP
Iodobenzene	204.01	6.8167	3.6257	3.0576	7.7367	5.8290	0.0593
1,2,4,5-tetrachlorobenzene	215.91	7.9701	4.0624	3.4600	—	—	-2.3752
1,2,3,5-tetrachlorobenzene	215.91	7.9701	4.0624	3.4630	—	—	-1.5531
p-dibromobenzene	235.92	7.2778	3.8056	3.2911	9.3715	2.9997	-1.8257
m-dibromobenzene	235.92	7.2778	3.8056	3.2946	—	—	-1.4868
o-dibromobenzene	235.92	7.2778	3.8115	3.1362	—	—	-1.6332
p-chloroiodobenzene	238.46	7.9433	4.1383	3.6753	9.4867	3.1025	-2.6536
m-chloroiodobenzene	238.46	7.9433	4.1383	3.6789	—	—	-2.0698
o-chloroiodobenzene	238.46	7.9433	4.1383	3.5031	—	—	-2.2907
pentachlorobenzene	250.36	0.0966	4.5870	3.8914	11.9504	-2.0025	-5.1465
p-bromoiodobenzene	282.91	8.7236	4.5285	4.1259	10.0393	2.0531	-4.6853
Hexachlorobenzene	284.81	10.2232	5.1116	4.3616	11.9274	-5.2983	-10.7710
1,3,5-tribromobenzene	314.82	9.1846	4.7083	4.3697	—	—	-6.3255
1,2,4-tribromobenzene	314.82	9.1846	4.7143	4.2162	—	—	-4.7502
p-diiodobenzene	329.91	10.1693	5.2513	4.9606	10.6840	0.6179	-7.2687
m-diiodobenzene	329.91	10.1693	5.2513	4.9640	—	—	-5.1708
o-diiodobenzene	329.91	10.1693	5.2574	4.7022	—	—	-4.9254

Table IV.3. Continued...

MOLECULE	MOL.WT.	$^{0}\chi^{v}$	$^{1}\chi^{v}$	$^{2}\chi^{v}$	$\ln K_{ow}$	lnS	lnP
ALKYLBENZENES							
Benzene	78.114	3.4641	2.0000	1.1547	4.9053	7.4899	4.5543
Toluene	92.14	4.3868	2.4107	1.6548	6.1939	6.1527	3.3449
Ethylbenzene	106.17	5.0939	2.9713	1.8392	7.2531	5.0239	2.2618
p-xylene	106.17	5.3094	2.8214	2.1547	7.3223	5.3681	2.1679
m-xylene	106.17	5.3094	2.8214	2.1582	7.3683	5.0772	2.1143
o-xylene	106.17	5.3094	2.8274	2.0843	7.1841	5.1648	1.8773
n-propylbenzene	120.20	5.8010	3.4713	2.2356	8.4735	4.0073	1.2319
i-propylbenzene	120.20	5.9641	3.3541	2.5654	8.4275	3.9120	1.5261
n-butylbenzene	134.22	6.5081	3.9714	2.2184	4.4670	—	—
POLYCYCIC AROMATIC HYDROCARBONS							
Benzene	78.114	3.4641	2.0000	1.1547	4.9053	7.4899	4.5543
Napthalene	128	5.6188	3.4042	2.3472	7.7482	—	-2.7488
Fluorene	166	7.3259	4.6118	3.4910	9.9932	—	-7.3793
Phenanthrene	178	7.7735	4.8154	3.5078	10.5919	0.0806	-9.4445
Anthracene	178	7.7735	4.8094	3.5465	10.6610	-2.9473	-12.0741

Table IV.3. Continued...

MOLECULE	MOL.WT.	${}^0\chi^v$	${}^1\chi^v$	${}^2\chi^v$	$\ln K_{ow}$	lnS	lnP
Pyrene	202	8.7735	5.5594	4.2896	12.0195	-2.0242	-13.5760
Chrysene	228	9.9282	6.2261	4.6685	13.6083	-6.2851	-18.9243
Perylene	252	10.9282	6.9761	5.4185	14.9668	-7.8256	-15.372
Benzo (a) pyrene	252	10.9282	6.9701	5.4537	14.9668	-7.4816	___
POLYCHLORINATEDBIPHENYLS							
Benzene	78.114	3.4641	2.0000	1.1547	4.9053	7.4899	4.5543
Biphenyl	154	6.7735	4.0714	2.7321	9.1643	2.0150	-4.6204
4-CBP	189	7.9000	4.5840	3.3498	10.5919	1.6095	-5.0910
2-CBP	189	7.9000	4.5900	3.2908	10.5919	1.6095	-4.7795
2,2'-CBP	223	9.0265	5.1086	3.8495	9.2564	0.0953	-5.9220
2,5,4'-CBP	257	10.1530	5.6152	4.5519	11.4208	-4.5098	___
2,5,2'-CBP	257	10.1530	5.6212	4.5093	___	-2.2114	-6.3586
3,5,3',5'-CBP	292	11.2795	6.1218	5.2236	13.8155	-3.3226	___
2,4,5,4',5'-CBP	326	12.4060	6.6524	5.5995	14.0688	-4.7106	-10.6040

Table IV.4. Results of the Regression Analysis (y=mx + n) Showing the Correlation of Valance Molecular Connectivity Indices with log K_{ow}, log S and log P

CHEMICAL CLASS	y	X	N	n	m	R
GROUP I:						
Halogen substituted benzene derivatives	log K_{ow}	${}^{o}X_{v}$	16	0.3981	0.5121	0.9332
	log K_{ow}	${}^{1}X_{v}$	16	0.4365	0.9804	0.8873
	log K_{ow}	${}^{2}X_{v}$	16	1.0984	0.9466	0.8683
GROUP II:						
Alkyl substituted benzene derivatives	log K_{ow}	${}^{o}X_{v}$	7	-0.1007	0.6290	0.9703
	log K_{ow}	${}^{1}X_{v}$	6	0.2420	0.9812	0.9545
	log K_{ow}	${}^{2}X_{v}$	6	0.9559	1.0707	0.8922
GROUP III:						
Polycylic Aromatic Hydrocarbons (PAH)	log K_{ow}	${}^{o}X_{v}$	9	0.0679	0.5873	0.9998
	log K_{ow}	${}^{1}X_{v}$	9	0.3511	0.8825	0.9992
	log K_{ow}	${}^{2}X_{v}$	9	0.9335	1.0272	0.9947
GROUP IV:						
Polychlorinated binphenyls (PCB)	log K_{ow}	${}^{o}X_{v}$	7	0.7483	0.4354	0.9230
	log K_{ow}	${}^{1}X_{v}$	6	0.5473	0.8032	0.9287
	log K_{ow}	${}^{2}X_{v}$	6	1.3795	0.8251	0.9196

Table IV.4 Continued

CHEMICAL CLASS	Y	x	N	n	m	R
GROUPS I and IV :	log K_{ow}	$^{o}X_{v}$	22	0.7175	0.4562	0.9119
	log K_{ow}	$^{1}X_{v}$	21	0.9628	0.7949	0.8312
	log K_{ow}	$^{2}X_{v}$	21	1.2701	0.8795	0.8672
GROUPS II and III :	log K_{ow}	$^{o}X_{v}$	15	0.1133	0.5838	0.9961
	log K_{ow}	$^{1}X_{v}$	14	0.5852	0.8450	0.9940
	log K_{ow}	$^{2}X_{v}$	14	1.0680	0.9989	0.9898
GROUPS I,II,III and IV :	log K_{ow}	$^{o}X_{v}$	36	0.5607	0.4945	0.9148
	log K_{ow}	$^{1}X_{v}$	34	0.8826	0.8013	0.9023
	log K_{ow}	$^{2}X_{v}$	34	1.1800	0.9315	0.9134
GROUP I: Halogen substituted benzene derivatives	log S	$^{o}X_{v}$	17	5.3427	-0.5721	0.8645
	log S	$^{1}X_{v}$	17	5.2924	-1.0936	0.8227
	log S	$^{2}X_{v}$	17	4.4661	-1.0220	0.7852
GROUP II: Alkyl substituted benzene derivatives	log S	$^{o}X_{v}$	6	5.4057	-0.6193	0.9800
	log S	$^{1}X_{v}$	6	5.2331	-1.0936	0.9770
	log S	$^{2}X_{v}$	6	4.4798	-1.1224	0.9100

Table IV.4. Continued

CHEMICAL CLASS	y	x	N	n	m	R
GROUP III:						
Polycylic Aromatic Hydrocarbons	log S	$^{0}\chi$	5	6.6036	-0.8990	0.9784
	log S	$^{1}\chi$	5	6.1787	-1.3534	0.9762
	log S	$^{2}\chi$	5	5.2642	-1.5780	0.9663
GROUP IV:						
Polychlorinated biphenyls	log S	$^{0}\chi_{v}$	7	5.2681	-0.6141	0.9374
	log S	$^{1}\chi_{v}$	6	5.8014	-1.2110	0.9307
	log S	$^{2}\chi_{v}$	6	4.5975	-1.2584	0.9430
GROUP II and III:	log S	$^{0}\chi^{v}$	12	6.9845	-0.9323	0.9812
	log S	$^{1}\chi^{v}$	12	6.1775	-1.3493	0.9843
	log S	$^{2}\chi^{v}$	12	5.4261	-1.6032	0.9726
GROUPS I and IV:	log S	$^{0}\chi_{v}$	23	5.5858	-0.6227	0.8527
	log S	$^{1}\chi_{v}$	23	5.4286	-1.1326	0.8688
	log S	$^{2}\chi_{v}$	23	4.7023	-1.1540	0.8094
groups I,II. III and IV:	log S	$^{0}\chi_{v}$	32	5.8995	-0.6917	0.8505
	log S	$^{1}\chi_{v}$	32	5.8297	-1.2508	0.9216
	log S	$^{2}\chi_{v}$	32	4.9982	-1.3054	0.8288

Table IV.4. Continued

CHEMICAL CLASS	y	x	N	n	m	R
GROUP I:						
Halogen substituted benzene derivativis	log P	$^{o}X_{v}$	17	4.8927	-0.7897	0.9233
	log P	$^{1}X_{v}$	17	4.6191	-1.4480	0.9670
	log P	$^{2}X_{v}$	17	3.6424	-1.3923	0.9771
GROUP II:						
Alkyl substituted benzene	log P	$^{o}X_{v}$	8	4.1038	-0.6076	0.9766
	log P	$^{1}X_{v}$	8	3.6626	-0.9198	0.9491
	log P	$^{2}X_{v}$	8	3.0688	-1.0210	0.8824
GROUP IV:						
Polychlorinated biphenyls (PCB)	log P	$^{o}X_{v}$	8	3.1435	-0.6168	0.8711
	log P	$^{1}X_{v}$	8	4.0099	-1.2720	0.9347
	log P	$^{2}X_{v}$	8	2.4704	-1.2368	0.8705
GROP III:						
Polycylic Aromatic Hydrocarbons	log P	$^{o}X_{v}$	12	6.7493	-1.4012	0.9512
	log P	$^{1}X_{v}$	12	5.9886	-2.0727	0.9455
	log P	$^{2}X_{v}$	12	4.4562	-2.3388	0.9340
GROUPS I and III:	log P	$^{o}X_{v}$	18	8.4965	-1.5629	0.9284
	log P	$^{1}X_{v}$	18	7.0495	-2.2339	0.9499
	log P	$^{2}X_{v}$	18	5.5681	-2.5537	0.9378

Table IV.4 Continued

CHEMICAL CLASS	y	x	N	n	m	R
GROUPS I and IV :	log P	$^0\chi^v$	24	4.3080	-0.7187	0.9357
	log P	$^1\chi^v$	24	4.2220	-1.3335	0.9553
	log P	$^2\chi^v$	24	3.4461	-1.3861	0.9150
GROUPS I, II, III and IV:	log P	$^0\chi^v$	41	5.8969	-1.0439	0.6919
	log P	$^1\chi^v$	41	6.0695	-1.8817	0.8692
	log P	$^2\chi^v$	41	4.6886	-1.9847	0.7766

Table IV. 5. Results of the Two Variable Regression Analysis for Y=log K_{ow}

y = log K_{ow}		GR.I (HALOBENZENES)	GR.II (ALKYLBENZENES)	GR. III PAH	GR.IV PCB	GR. II and III	GR. I and IV	GR.I,II,III and IV
$^0\chi^v$	n	0.40	-0.10	0.07	0.75	0.11	0.72	0.56
	m	0.51	0.63	0.59	0.44	0.58	0.46	0.50
	R	0.93	0.97	1.0	0.92	1.0	0.91	0.92
$^1\chi^v$	n	0.44	0.24	0.35	0.55	0.59	0.96	0.88
	m	0.98	0.98	0.88	0.80	0.85	0.80	0.80
	R	0.98	0.96	1.0	0.93	0.99	0.83	0.90
$^2\chi^v$	n	1.10	0.96	0.93	1.38	1.07	1.27	1.18
	m	0.95	1.07	1.03	0.83	1.0	0.88	0.93
	R	0.87	0.89	1.0	0.92	0.99	0.87	0.91

y = log S		GR.I HALOBENZENES	GR.II ALKYLBENZENES	GR. III PAH	GR.IV PCB	GR II and III	GR.I and IV	GR I, II and IV
$^0\chi^v$	n	5.34	5.41	6.60	5.27	6.99	5.59	5.90
	m	-0.57	-0.62	-0.90	-0.61	-0.93	-0.62	-0.69
	R	0.87	0.98	0.98	0.94	0.98	0.85	0.85
$^1\chi^v$	n	5.29	5.23	6.18	5.80	6.18	5.43	5.83
	m	-1.09	-1.04	-1.35	-1.21	-1.35	-1.13	-1.25
	R	0.82	0.98	0.98	0.93	0.98	0.87	0.92
$^2\chi^v$	n	4.47	4.48	5.26	4.60	5.43	4.70	5.0
	m	-1.02	-1.12	-1.58	-1.26	-1.60	-1.15	-1.31
	R	0.79	0.91	0.97	0.94	0.97	0.81	0.83

Table IV.7. Results of the Two Variable Regression Analysis for Y=logP

y = log P		GR. I HALOBENZENES	GR. II ALKYLBENZENES	GR. III PAH	GR. IV PCB	GR II and III	GR. I and IV	Gr.I,II III and IV
$^0\chi^v$	n	4.89	4.10	6.75	3.14	7.35	4.31	5.90
	m	-0.79	-0.61	-1.40	-1.62	-1.43	-0.72	-1.04
	R	0.92	0.98	0.95	0.87	0.90	0.94	0.69
$^1\chi^v$	n	4.62	3.66	5.99	4.01	7.05	4.22	6.07
	m	-1.45	-0.92	-2.07	-1.27	-2.23	-1.33	-1.88
	R	0.97	0.95	0.95	0.94	0.95	0.96	0.87
$^2\chi^v$	n	3.64	3.07	4.46	2.47	5.57	3.45	4.69
	m	-1.39	-1.02	-2.34	-1.24	-2.55	-1.39	-1.99
	R	0.98	0.88	0.93	0.87	0.94	0.92	0.78

FIGURES IV.1–9

Results of Single Variable Regression Analysis where ${}^{0}\chi^{v}$, ${}^{1}\chi^{v}$ and ${}^{2}\chi^{v}$ are plotted versus log K_{ow}, log S and log P seperately. In these figures group I, II, III and IV represents Halobenzenes, Alkylbenzenes, Polycyclic Aromatic Hydrocarbons (PAH's) and Polychlorinated Biphenyls (PCB's) respectively. The plots on the transparent pages are the results of regression analysis carried out with electron withdrawing (groups I and IV), electron donating (groups II and III) pairs of groups and with all groups together (I, II, III and IV). On these pages [– – – – – – – – –] represents the regression equation for groups I and IV, [—— – —— –] represents the regression equation for groups II and III and [————————] represents the regression equation for groups I, II, III and IV together.

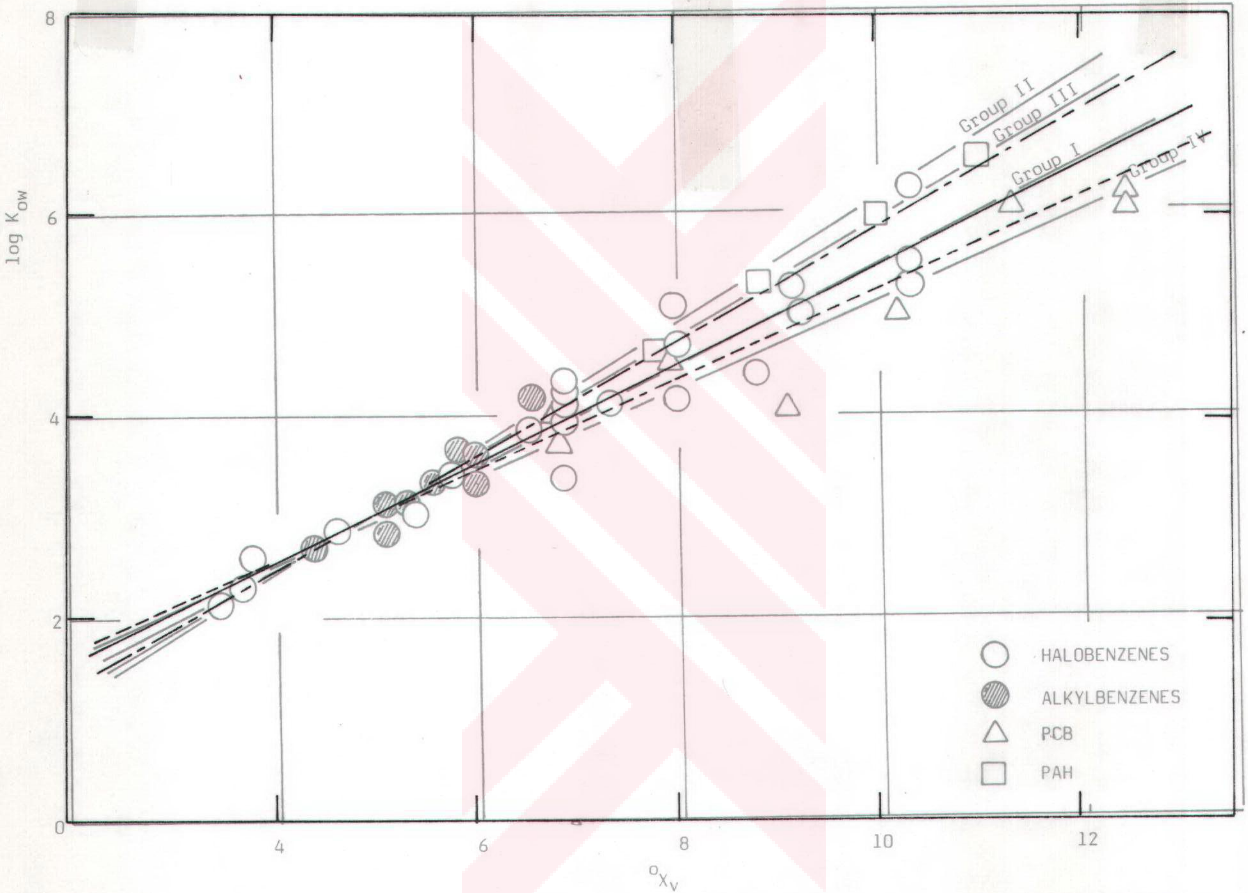


Figure IV. 1. : Plot of the logarithm of the partition coefficient versus zero order valance molecular connectivity index ($^{o}\chi^{v}$) for groups I, II, III and IV.

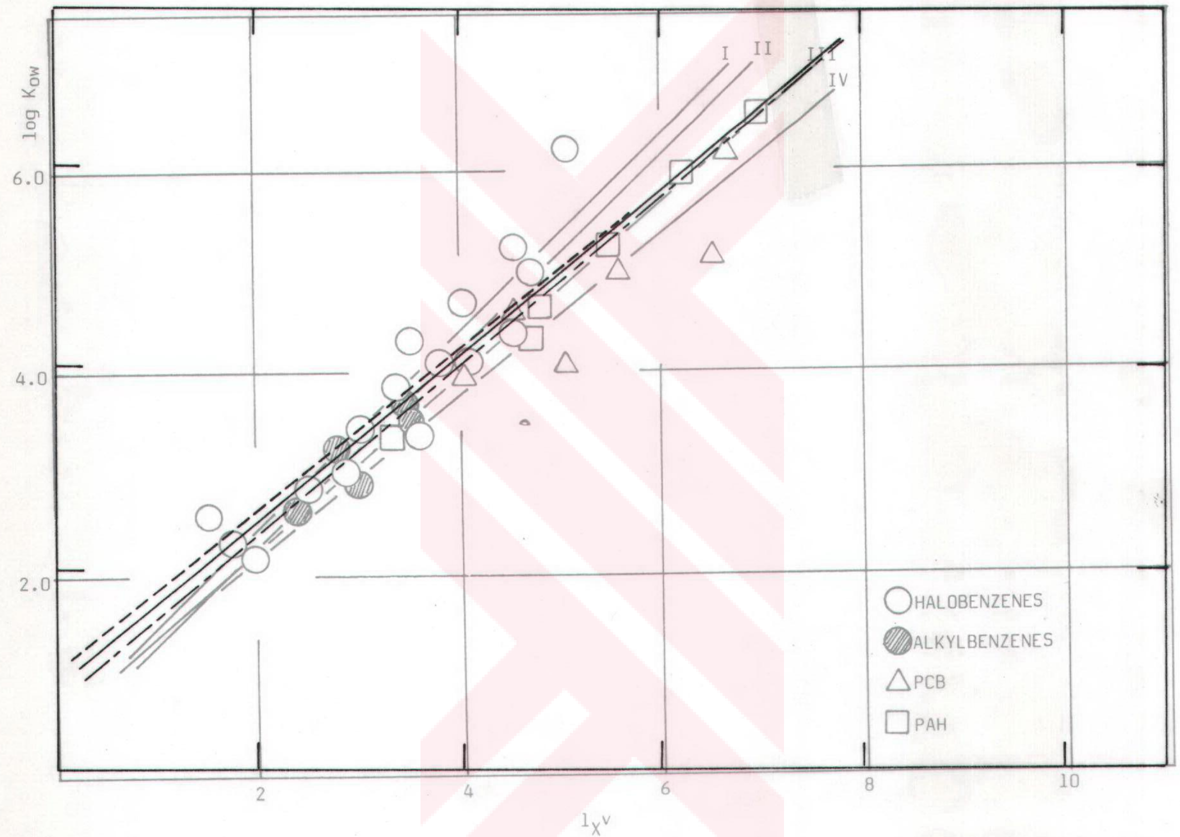


Figure IV.2. : Plot of the logarithm of the partition coefficient versus first order valance molecular connectivity index ($^1\chi^v$) for groups I, II, III and IV.

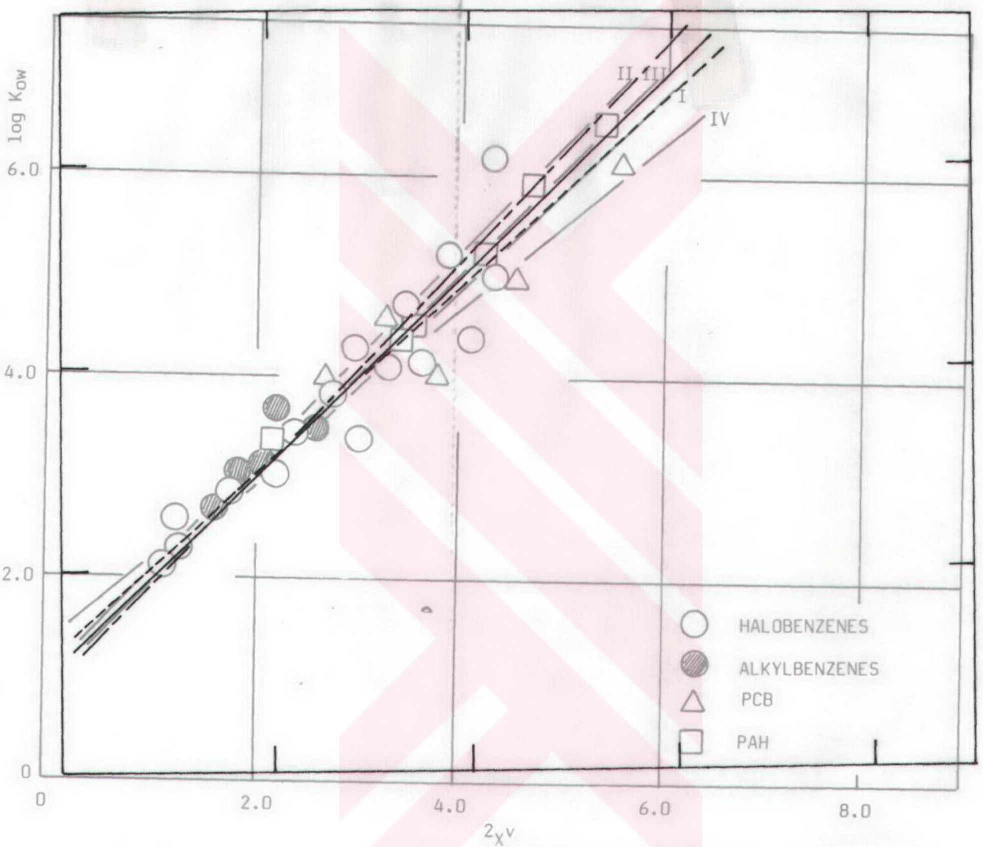
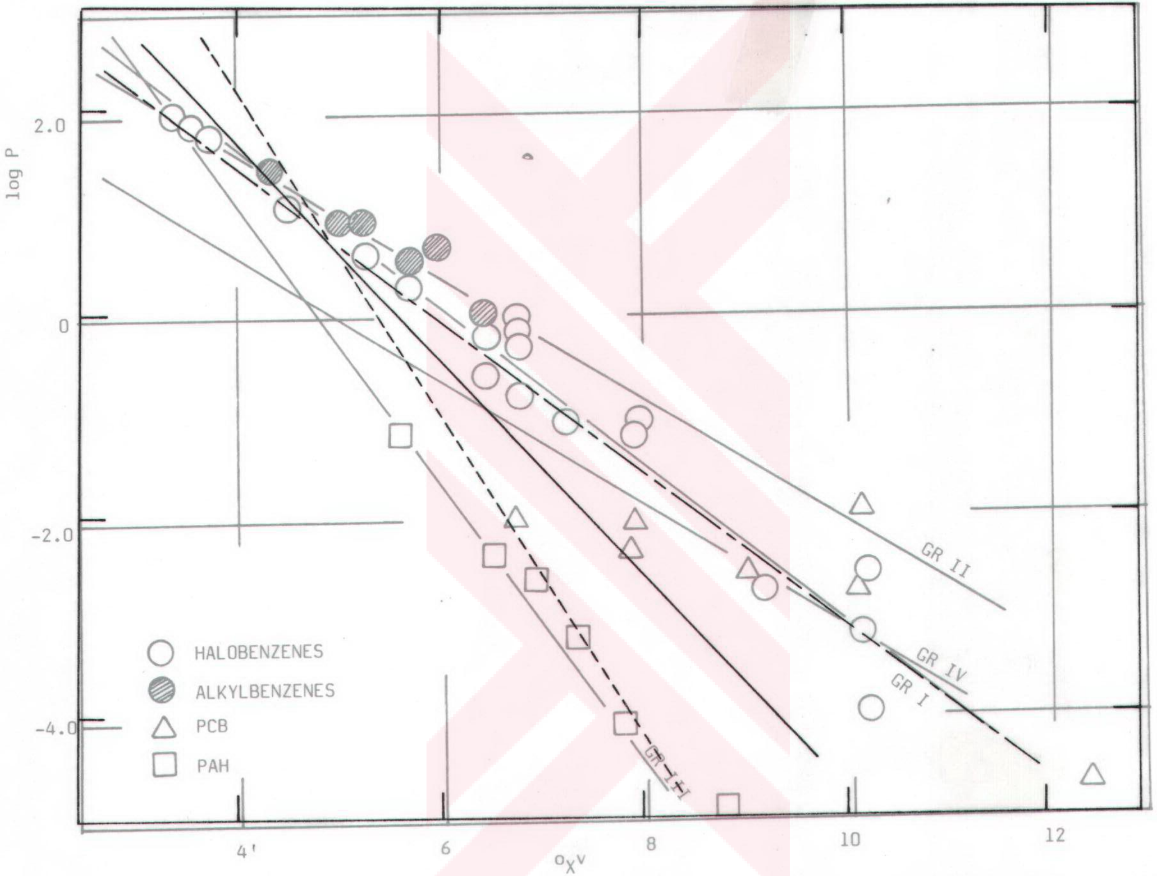


Figure IV.3. : Plot of the logarithm of the partition coefficient versus second order valance molecular connectivity index ($^2\chi^v$) for groups I, II, III and IV.



Figures IV.4. : Plot of the logarithm of vapor pressure versus zero order valance molecular connectivity index ($^o\chi^v$) for groups I, II, III and IV.

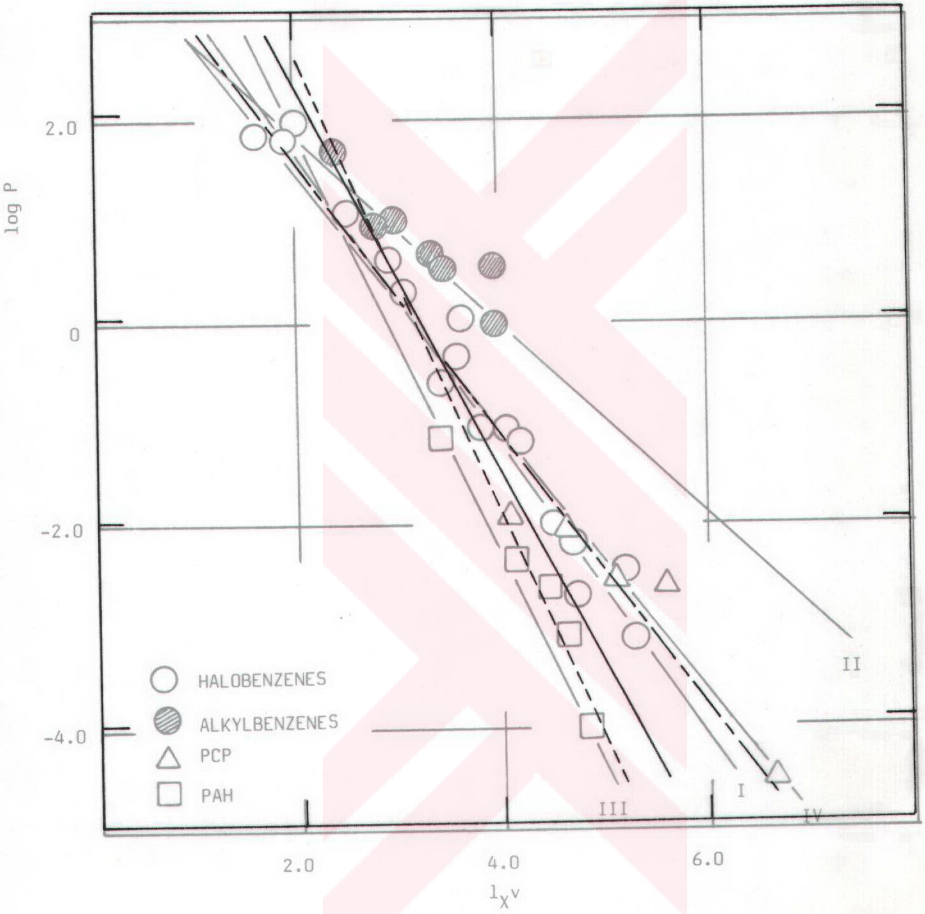


Figure IV.5 : Plot of the logarithm of vapor pressure versus first order valance molecular connectivity index ($^1\chi^v$) for groups I, II, III, and IV.

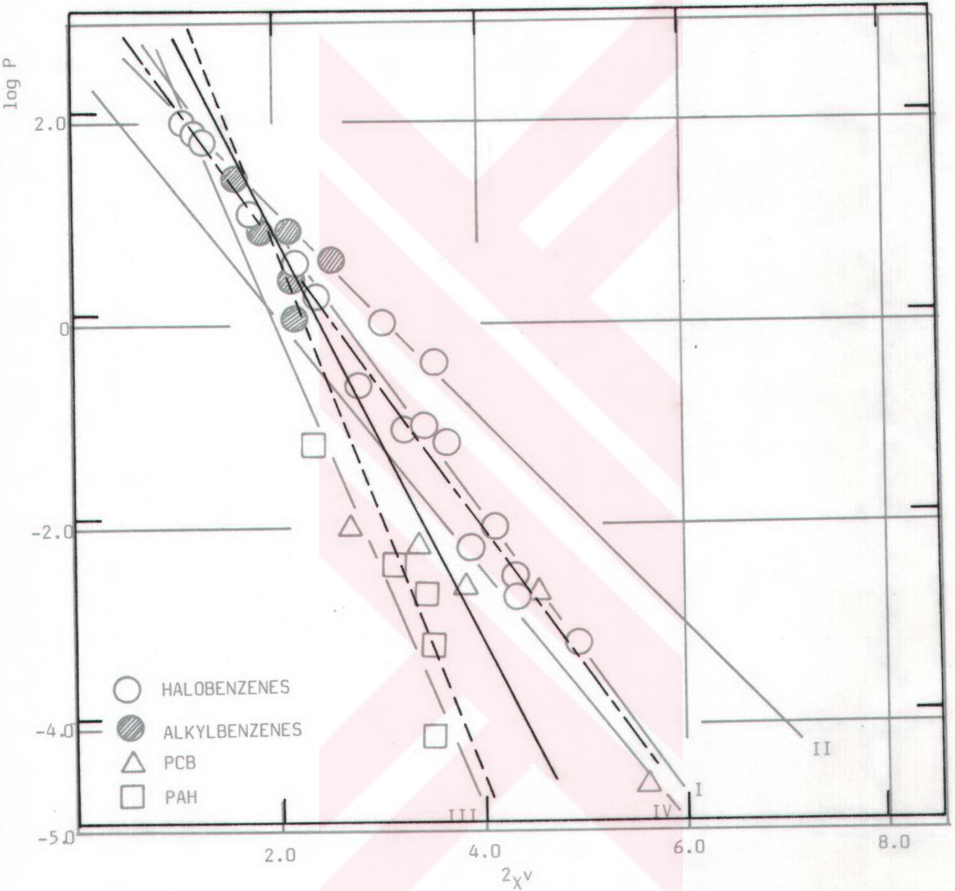


Figure IV.6. :Plot of the logarithm of vapor pressure versus second order valance molecular connectivity index ($^2\chi^v$) for groups I,II,III and IV.

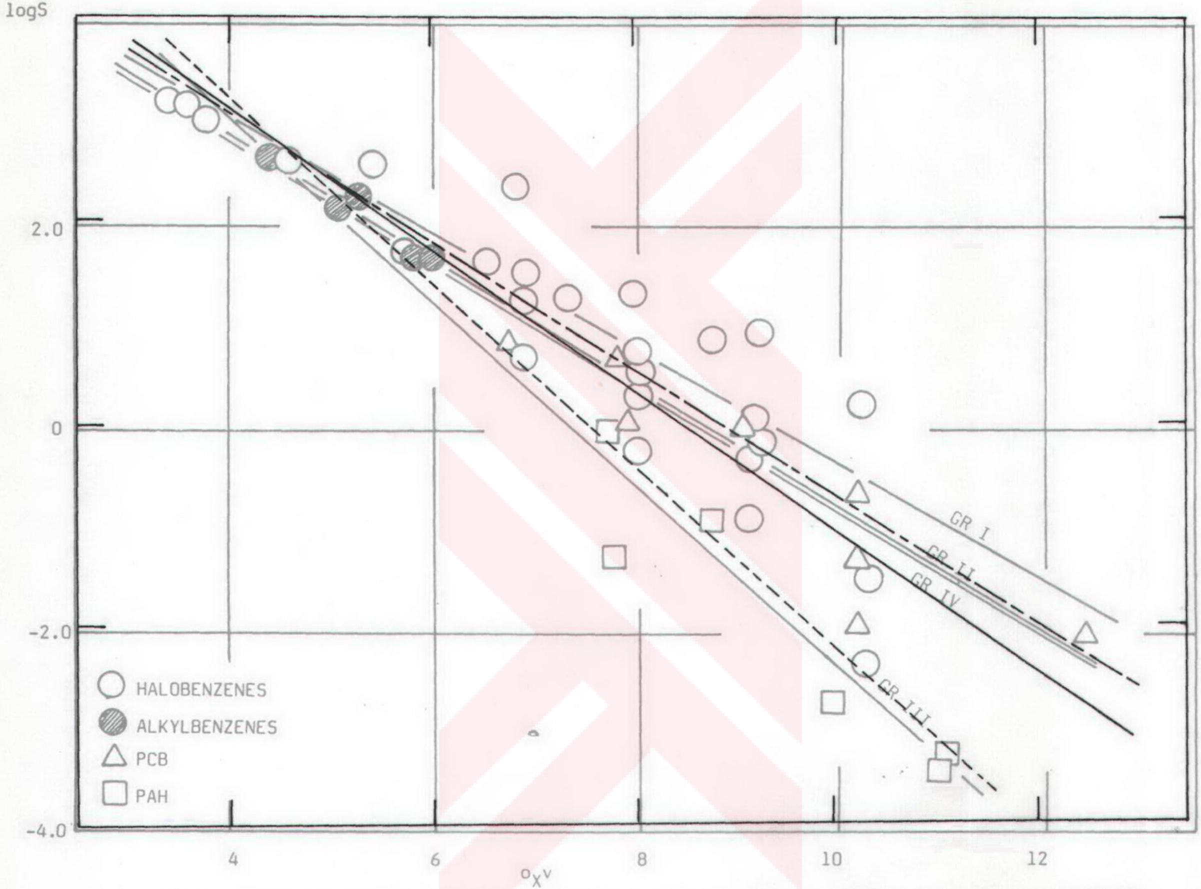


Figure IV.7. : Plot of the logarithm of solubility versus zero order valance molecular connectivity index ($^0\chi^v$) for groups I, II, III and IV.

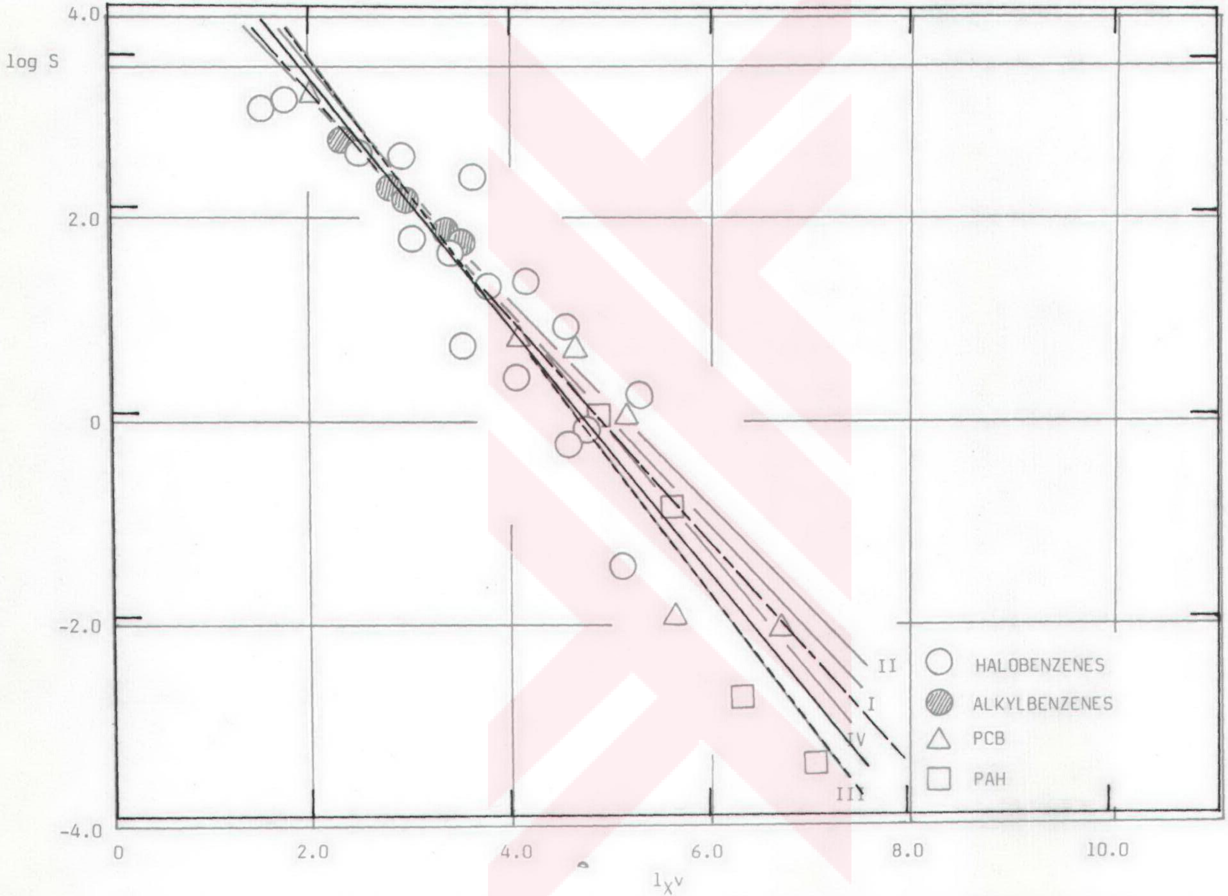


Figure IV.8. : Plot of the logarithm of solubility versus first order valance molecular connectivity index ($^1\chi^v$) for groups I, II, III and IV.

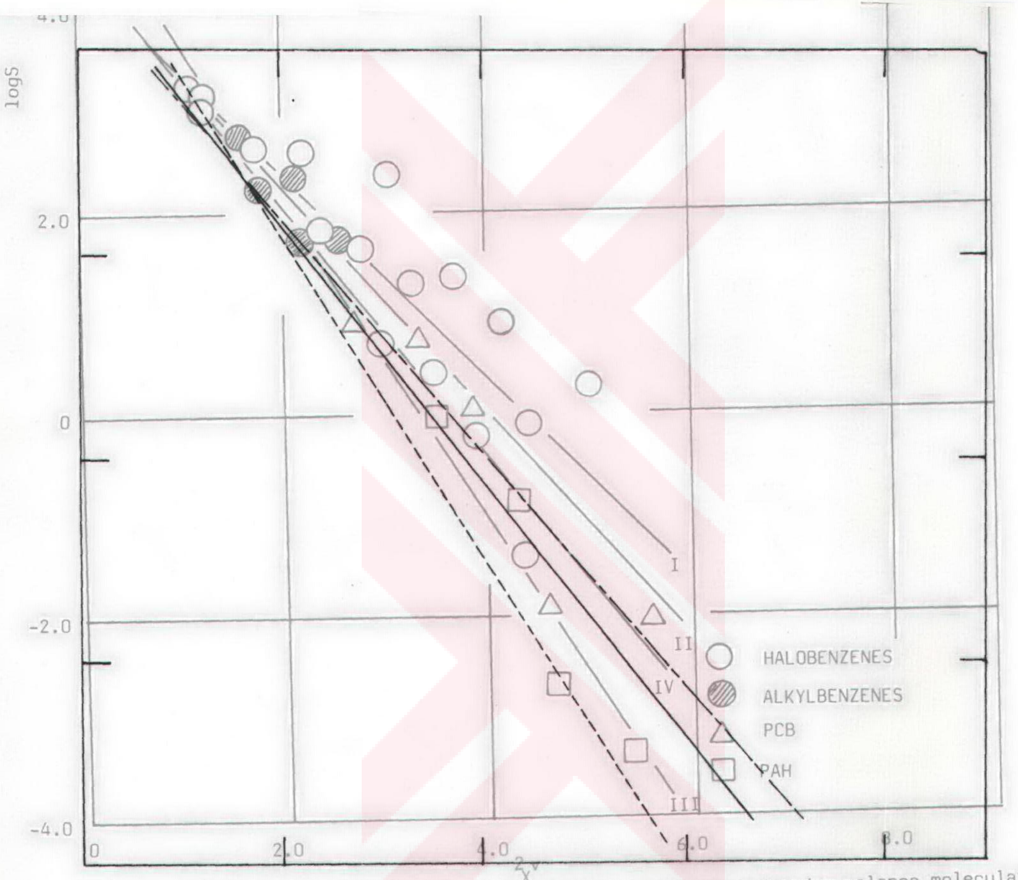


Figure IV.9 : Plot of the logarithm of solubility versus second order valance molecular connectivity index ($^2\chi^v$) for groups I, II, III and IV.

IV.1.3. RESULTS OF THE MULTIVARIABLE REGRESSION ANALYSIS

In figures V.1 to V.9, where each property under investigation is plotted versus each valance molecular connectivity index (VMCI), it can clearly be observed that, there occurs a scattering of points when one goes up to larger index values or-in other words-to larger molecules.Depending on the high correlation between these parameters and the indices, this behavior may be attributed to the inability of a single index to define the complex interrelationship between the bonds for more complex, larger molecules.

Hence, starting from this point, assuming that;

- valance molecular connectivity indices are descriptions of bond properties,
- and the physical properties under investigation, namely octanol-water partition coefficient, solubility and vapor pressure, are functions of bond properties,

it can be expected that a multivariable regression analysis would solve the problem of this scattering, when all three indices are used in combination to define the bonding relationshipswithin the molecule.

For this analysis a computer program has been developed according to the flowchart given (appendix II) with which one can play around with the type of regression equation as to the number of terms, number of parameters and the powers of the parameters.

Until the final equations for predicting ln K_{OW}, ln S and ln P, given in table V.1. are obtained, a number of equations has been tried stepwise within an upper and lower limit of highest correlation in order for the best relation to be chosen.

Examples to these equations within a logical range of correlation are given;

- for ln K_{OW} (halobenzenes) in table IV.8
- for ln S (halobenzenes) in table IV.9
- for ln P (halobenzenes) in table IV.10
- for ln K_{OW} (alkylbenzenes) in table IV.11
- for ln S (alkylbenzenes) in table IV.12
- for ln P (alkylbenzenes) in table IV.13
- for ln K_{OW}(PCB) in table IV.14
- for ln P (PCB) in table IV.15
- for ln S (PCB) in table IV.16
- for ln K_{OW} (PAH) in table IV.17
- for ln P (PAH) in table IV.18
- for ln S (PAH) in table IV.19

- for ln K_{ow} (halobenzenes and PCB's) in table IV.20
- for ln S (halobenzenes and PCB's) in table IV.21
- for ln P (halobenzenes and PCB's) in table IV.22
- for ln K_{ow} (alkylbenzenes and PAH's) in table IV.23
- for ln S (alkylbenzenes and PAH's) in table IV. 24
- for ln P (alkylbenzenes and PAH'S) in table IV.25
- for ln K_{ow}(four groups together) in table IV.26
- for ln P (four groups together) in table IV.27
- for ln S (four groups together) in table IV.28

As a result, among these multivariable regression equations, the best correlation is found out and used in the following calculations. Analysis is carried out for each of the four groups, for pairs of groups where one of the groups have electron withdrawing substituents (halobenzenes and PCB's) and the other have electron donating substituents (alkylbenzenes and PAH's) and also for all the groups together.

Table IV.8. Multiple Regression Equations for Halogen Substituted Benzenes where Y = ln Kow

HALOGEN SUBSTITUTED BENZENES

$Y = \ln Kow$, $N = 14$

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0X^v)^{5/4} + a_2({}^1X^v)^{5/4} + a_3({}^2X^v)^{5/4}$	2.3776	0.9674	-0.0643	-1.1015	0.9749
$Y = a_0 + a_1({}^0X^v) + a_2({}^1X^v) + a_3({}^2X^v)$	0.8627	2.1076	-0.3348	-1.8697	0.9784
$Y = a_0 + a_1({}^0X^v)^{-1/8} + a_2({}^1X^v)^{-1/8} + a_3({}^2X^v)^{-1/8}$	76.0911	-172.8009	6.5498	72.1474	0.9852
$Y = a_0 + a_1({}^0X^v)^{-1/4} + a_2({}^1X^v)^{-1/4} + a_3({}^2X^v)^{-1/4}$	42.7992	-110.5270	3.0455	42.1557	0.9852
$Y = a_0 + a_1({}^0X^v)^{-3/8} + a_2({}^1X^v)^{-3/8} + a_3({}^2X^v)^{-3/8}$	31.6825	-93.9332	1.8256	32.5782	0.9851
$Y = a_0 + a_1({}^0X^v)^{-1/2} + a_2({}^1X^v)^{-1/2} + a_3({}^2X^v)^{-1/2}$	26.1055	-89.4966	1.1799	28.1048	0.9849
$Y = a_0 + a_1({}^0X^v)^{-3/4} + a_2({}^1X^v)^{-3/4} + a_3({}^2X^v)^{-3/4}$	20.4863	-95.3357	0.4694	24.2736	0.9840

Table IV.9. Multiple Regression Equations for Halogen Substituted Benzene Derivatives where Y = ln S

HALOGEN SUBSTITUTED BENZENES

$Y = \text{Ln}\ S,\ N = 16$

EQUATIONS	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	12.9528	-1.4877	0.4927	2.7278	0.9852
$Y = a_0 = a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	19.2722	-6.4639	0.1984	9.3353	0.9849
$Y = a_0 + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	39.4459	-37.5441	-3.2789	39.7229	0.9867
$Y = a_0 + a_1({}^0\chi^v)^{2/5} + a_2({}^1\chi^v)^{2/5} + a_3({}^2\chi^v)^{2/5}$	49.5033	-57.7702	-5.4205	56.7490	0.9869
$Y = a_0 + a_1({}^0\chi^v)^{1/3} + a_2({}^1\chi^v)^{1/3} + a_3({}^2\chi^v)^{1/3}$	59.5080	-79.4737	-7.6292	74.1366	0.9869
$Y = a_0 + a_1({}^0\chi^v)^{1/4} + a_2({}^1\chi^v)^{1/4} + a_3({}^2\chi^v)^{1/4}$	79.4129	-125.3919	-12.1263	109.3965	0.9867

Table IV.10. Multiple Regression Equations for Halogen Substituted Benzene Derivatives where Y = ln P

HALOGEN SUBSTITUTED BENZENES

$Y = \ln P$, $N = 14$

EQUATIONS	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^{0}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	14.4772	-4.0817	-0.2613	4.3669	0.9887
$Y = a_0 + a_1({}^{0}X^{v})^{2/5} + a_2({}^{1}X^{v})^{2/5} + a_3({}^{2}X^{v})^{2/5}$	42.2544	-40.3121	-4.0352	32.2376	0.9855
$Y = a_0 + a_1({}^{0}X^{v})^{1/4} + a_2({}^{1}X^{v})^{1/4} + a_3({}^{2}X^{v})^{1/4}$	70.6325	-90.3149	-9.1819	65.8182	0.9851
$Y = a_0 = a_1({}^{0}X^{v})^{1/8} + a_2({}^{1}X^{v})^{1/8} + a_3({}^{2}X^{v})^{1/8}$	146.2996	-237.7709	-23.7092	159.0342	0.9849
$Y = a_0 + a_1({}^{0}X^{v})^{-1/8} + a_2({}^{1}X^{v})^{-1/8} + a_3({}^{2}X^{v})^{-1/8}$	-155.6715	403.9735	36.1891	-222.8848	0.9844

Table IV.11. Multiple Regression Equations for Alkylbenzenes where $Y = \ln Kow$

ALKYLBENZENES

$Y = \ln Kow$, $N = 8$

EQUATION	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^{o}X^{v})^{5/4} + a_2({}^{1}X^{v})^{5/4} + a_3({}^{2}X^{v})^{5/4}$	1.3359	0.3811	0.7110	0.1111	0.9983
$Y = a_o + a_1({}^{o}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	0.2081	0.4525	1.3497	0.4081	0.9986
$Y = a_o + a_1({}^{o}X^{v})^{-1/8} + a_2({}^{1}X^{v})^{-1/8} + a_3({}^{2}X^{v})^{-1/8}$	50.0686	46.3530	-62.2191	-28.3351	0.9987
$Y = a_o + a_1({}^{o}X^{v})^{-1/4} + a_2({}^{1}X^{v})^{-1/4} + a_3({}^{2}X^{v})^{-1/4}$	27.9054	33.3339	-37.3487	-16.6623	0.9984

Table IV.12. Multiple Regression Equations for Alkylbenzenes where $Y = \ln S$

ALKYLBENZENES

$Y = \ln S$, $N = 8$

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^{o}\chi^{v})^{5/4} + a_2({}^{1}\chi^{v})^{5/4} + a_3({}^{2}\chi^{v})^{5/4}$	10.9892	-0.3031	-0.8666	-0.0824	0.9947
$Y = a_o + a_1({}^{o}\chi^{v}) + a_2({}^{1}\chi^{v}) + a_3({}^{2}\chi^{v})$	12.1207	-0.3226	-1.5985	-0.3413	0.9953
$Y = a_o + a_1({}^{o}\chi^{v})^{1/2} + a_2({}^{1}\chi^{v})^{1/2} + a_3({}^{2}\chi^{v})^{1/2}$	17.7170	1.0108	-6.8239	-2.3308	0.9963
$Y = a_o + a_1({}^{o}\chi^{v})^{1/4} + a_2({}^{1}\chi^{v})^{1/4} + a_3({}^{2}\chi^{v})^{1/4}$	28.8508	7.0862	-19.7685	-7.2827	0.9966
$Y = a_o + a_1({}^{o}\chi^{v})^{1/8} + a_2({}^{1}\chi^{v})^{1/8} + a_3({}^{2}\chi^{v})^{1/8}$	51.0994	22.4878	-47.4761	-17.7999	0.9967

Table IV.13. Multiple Regression Equations for Alkylbenzenes where $Y = \ln P$

ALKYLBENZENES

$Y = \ln P$, $N = 8$

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^{o}X^{v})^{4/5} + a_2({}^{1}X^{v})^{4/5} + a_3({}^{2}X^{v})^{4/5}$	12.2364	-4.4985	0.7679	2.8249	0.9972
$Y = a_o + a_1({}^{o}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	10.4348	-2.7099	0.5786	2.0574	0.9976

Table IV.14. Multiple Regression Equations for PCB where Y = ln Kow

POLYCHLORINATEDBIPHENYLS

Y = ln Kow, N = 8

EQUATION	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	2.9433	-13.0361	2.6002	20.9603	0.9623
$Y = a_o + a_1({}^0\chi^v)^{3/4} + a_2({}^1\chi^v)^{3/4} + a_3({}^2\chi^v)^{3/4}$	3.9078	-7.2993	4.493	10.7432	0.9653
$Y = a_o + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	4.2085	-4.0076	3.8782	5.9164	0.9676
$Y = a_o + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	4.337	-2.1832	2.8883	3.378	0.9691
$Y = a_o + a_1({}^0\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	4.421	-1.1855	2.0256	1.9715	0.9700
$Y = a_o + a_1({}^0\chi^v)^{2} + a_2({}^1\chi^v)^{2} + a_3({}^2\chi^v)^{2}$	4.577	-0.3483	0.9194	0.6982	0.9702
$Y = a_o + a_1({}^0\chi^v)^{9/4} + a_2({}^1\chi^v)^{9/4} + a_3({}^2\chi^v)^{9/4}$	4.9531	-0.0297	0.1666	0.0932	0.9652

Table IV.15. Multiple Regression Equations for PCB where Y = ln P

POLYCHLORINATEDBIPHENYLS

$Y = \ln P$, $N = 7$

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0X^v)^{1/4} + a_2({}^1X^v)^{1/4} + a_3({}^2X^v)^{1/4}$	90.3935	-93.6390	-82.9776	135.6589	0.9914
$Y = a_0 + a_1({}^0X^v)^{1/2} + a_2({}^1X^v)^{1/2} + a_3({}^2X^v)^{1/2}$	39.5629	-23.2106	-26.5281	42.5559	0.9912
$Y = a_0 + a_1({}^0X^v)^{3/4} + a_2({}^1X^v)^{3/4} + a_3({}^2X^v)^{3/4}$	23.391	-6.597	-12.6341	17.2094	0.9910
$Y = a_0 + a_1({}^0X^v) + a_2({}^1X^v) + a_3({}^2X^v)$	15.9654	-1.6574	-7.2977	7.7202	0.9909
$Y = a_0 + a_1({}^0X^v)^{5/4} + a_2({}^1X^v)^{5/4} + a_3({}^2X^v)^{5/4}$	11.9769	-0.1932	-4.6172	3.7059	0.9906

Table IV.16. Multiple Regression Equations for PCB where Y = ln S

POLYCHLORINATED BIPHENYLS

Y = ln S, N = 9

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	12.9849	1.3632	8.8956	-19.1719	0.9722
$Y = a_0 + a_1({}^0\chi^v)^{3/4} + a_2({}^1\chi^v)^{3/4} + a_3({}^2\chi^v)^{3/4}$	10.7298	3.0428	-0.1781	-9.5702	0.9724
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	9.7755	2.2976	-2.1495	-5.1426	0.9721
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	9.2556	1.4772	-2.2229	-2.8774	0.9716

Table IV.17. Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons where Y = ln Kow

POLYCYCLIC AROMATIC HYDROCARBONS

Y = ln Kow, N = 8

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^{o}X^{v})^{1/2} + a_2({}^{1}X^{v})^{1/2} + a_3({}^{2}X^{v})^{1/2}$	-11.2669	-36.1797	82.2998	-30.7197	0.9985
$Y = a_o + a_1({}^{o}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	0.0949	0.6855	1.5883	-0.6842	0.9998
$Y = a_o + a_1({}^{o}X^{v})^{-1/2} + a_2({}^{1}X^{v})^{-1/2} + a_3({}^{2}X^{v})^{-1/2}$	36.1970	256.01	-400.4579	122.8720	0.9961

Table IV.18. Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons where Y = ln P

POLYCYCLIC AROMATIC HYDROCARBONS

$Y = \ln P$, $N = 7$

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^{0}X^{v})^{4/5} + a_2({}^{1}X^{v})^{4/5} + a_3({}^{2}X^{v})^{4/5}$	26.6685	-99.9505	176.0981	-51.6393	0.9848
$Y = a_0 + a_1({}^{0}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	19.8058	-64.1811	128.602	-42.9006	0.9870

Table IV.19. Multiple Regression Equations for Polycyclic Aromatic Hydrocarbons where Y = ln S

POLYCYCLIC AROMATIC HYDROCARBONS

Y = ln S, N = 7

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^3 + a_2({}^1\chi^v)^3 + a_3({}^2\chi^v)^3$	8.0539	-0.1595	0.7129	-0.3072	0.9796
$Y = a_0 + a_1({}^0\chi^v)^2 + a_2({}^1\chi^v)^2 + a_3({}^2\chi^v)^2$	10.7210	-1.9307	5.6930	-2.1844	0.9893
$Y = a_0 + a_1({}^0\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	12.8917	-6.1346	14.3250	-4.9320	0.9893
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	14.7242	-10.0915	20.2924	-6.2067	0.9876
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	18.0232	-15.1951	24.4080	-5.4134	0.9851
$Y = a_0 + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	40.5749	-33.2757	2.8803	23.4583	0.9804

Table IV.20. Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for $Y = \ln K_{ow}$

$Y = \ln K_{ow}$ EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	2.7319	0.7451	0.1426	-0.8174	0.9646
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	1.0983	1.6982	0.1120	-1.5302	0.9670
$Y = a_0 + a_1({}^0\chi^v)^{-1/4} + a_2({}^1\chi^v)^{-1/4} + a_3({}^2\chi^v)^{-1/4}$	44.7964	-120.1482	4.9697	45.5520	0.9656
$Y = a_0 + a_1({}^0\chi^v)^{-1/8} + a_2({}^1\chi^v)^{-1/8} + a_3({}^2\chi^v)^{-1/8}$	79.5430	-184.9892	9.1629	76.6677	0.9664
$Y = a_0 + a_1({}^0\chi^v)^{-1/10} + a_2({}^1\chi^v)^{-1/10} + a_3({}^2\chi^v)^{-1/10}$	96.9161	-219.3055	11.2101	92.5011	0.9666
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-1/4}$	1.8299	0.7954	0.3555	0.1175	0.9623
$Y = a_0 + a_1({}^0\chi^v)^{-1/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	11.1438	-11.3661	1.0871	0.2502	0.9567
$Y = a_0 + a_1({}^0\chi^v)^{-1/10} + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	27.7029	-27.9805	1.0275	0.1598	0.9572

Table IV.21. Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for Y=ln S

$Y = \ln S$

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^2 + a_2({}^1\chi^v)^2 + a_3({}^2\chi^v)^2$	9.6269	-0.3172	0.0974	0.8748	0.9667
$Y = a_0 + a_1({}^0\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	12.2968	-1.3131	0.3488	2.4346	0.9722
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	14.5100	-2.7742	0.6611	4.2332	0.9737
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	17.9058	-6.0606	1.2367	7.6363	0.9745
$Y = a_0 + a_1({}^0\chi^v)^{3/4} + a_2({}^1\chi^v)^{3/4} + a_3({}^2\chi^v)^{3/4}$	23.6439	-13.9187	2.2753	14.5267	0.9747

Table IV.22. Three Variable Regression Equations for Halobenzenes and PCB's (Groups I and IV) for Y=ln P

Y = ln P, N=22

EQUATION	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^{o}X^{v})^{5/4} + a_2({}^{1}X^{v})^{5/4} + a_3({}^{2}X^{v})^{5/4}$	9.4089	-1.2149	-0.6118	1.4745	0.9679
$Y = a_o + a_1({}^{o}X^{v}) + a_2({}^{1}X^{v}) + a_3({}^{2}X^{v})$	12.4884	-2.7830	-0.9663	2.8933	0.9717
$Y = a_o + a_1({}^{o}X^{v})^{3/4} + a_2({}^{1}X^{v})^{3/4} + a_3({}^{2}X^{v})^{3/4}$	17.7731	-6.9298	-1.5258	6.1829	0.9740
$Y = a_o + a_1({}^{o}X^{v})^{1/2} + a_2({}^{1}X^{v})^{1/2} + a_3({}^{2}X^{v})^{1/2}$	28.6130	-19.3994	-2.6457	14.8134	0.9752
$Y = a_o + a_1({}^{o}X^{v})^{1/4} + a_2({}^{1}X^{v})^{1/4} + a_3({}^{2}X^{v})^{1/4}$	61.6230	-71.1646	-6.4487	46.2285	0.9758
$Y = a_o + a_1({}^{o}X^{v})^{1/8} + a_2({}^{1}X^{v})^{1/8} + a_3({}^{2}X^{v})^{1/8}$	127.9088	-190.9253	-14.8557	114.0320	0.9760

Table IV. 23. Three Variable Regression Equations for Alkylbenezenes and PAH's (Groups II and III) where Y=ln K_{ow}

$Y = \ln K_{ow}$, N=16

EQUATION	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^o\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	-0.1773	1.5551	0.2616	-0.6863	0.9992
$Y = a_o + a_1({}^o\chi^v)^{-1/2} + a_2({}^1\chi^v)^{-1/2} + a_3({}^2\chi^v)^{-1/2}$	34.5343	-109.1279	-4.8616	33.7877	0.9818
$Y = a_o + a_1({}^o\chi^v)^{-1/4} + a_2({}^1\chi^v)^{-1/4} + a_3({}^2\chi^v)^{-1/4}$	27.3154	-135.0039	-0.8931	33.7829	0.9784
$Y = a_o + a_1({}^o\chi^v)^{-1} + a_2({}^1\chi^v)^{-1} + a_3({}^2\chi^v)^{-1}$	23.6334	-181.9107	3.5499	35.9560	0.9755
$Y = a_o + a_1({}^o\chi^v)^{-5/4} + a_2({}^1\chi^v)^{-5/4} + a_3({}^2\chi^v)^{-5/4}$	21.3395	-253.7001	9.2125	39.0508	0.9731
$Y = a_o + a_1({}^o\chi^v)^{-1/8} + a_2({}^1\chi^v)^{-1/8} + a_3({}^2\chi^v)^{-1/8}$	99.5168	-163.8370	-20.4950	64.6844	0.9877

Table IV. 24. Three Variable Regression Equations for Alkylbenzenes and PAH's (Groups II and III) for Y=ln S

Y = ln S ,N=14

EQUATION	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	13.1397	-0.6843	-1.3417	0.9429	0.9895
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	15.0086	-0.6837	-2.6987	0.6635	0.9888
$Y = a_0 + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	26.3057	1.0843	-13.6844	-0.3963	0.9841
$Y = a_0 + a_1({}^0\chi^v)^{1/3} + a_2({}^1\chi^v)^{1/3} + a_3({}^2\chi^v)^{1/3}$	39.2395	1.9032	-27.0950	0.7561	0.9812
$Y = a_0 + a_1({}^0\chi^v)^{2} + a_2({}^1\chi^v)^{2} + a_3({}^2\chi^v)^{2}$	10.2871	-0.2356	-0.2243	0.7020	0.9886
$Y = a_0 + a_1({}^0\chi^v)^{1/8} + a_2({}^1\chi^v)^{1/8} + a_3({}^2\chi^v)^{1/8}$	108.2418	-8.9520	-97.7893	17.6048	0.9767

Table IV. 25. Three Variable Regression Equations for Alkylbenzenes and PAH's (Groups I and IV) for Y=ln P

$Y = \ln P$, $N=15$

EQUATION	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^o\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	9.5343	0.2093	-2.8334	1.1584	0.9579
$Y = a_o + a_1({}^o\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	10.8750	0.9170	-4.6575	0.4279	0.9619
$Y = a_o + a_1({}^o\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	13.1823	2.7365	-8.1523	-1.0853	0.9649
$Y = a_o + a_1({}^o\chi^v)^{4/5} + a_2({}^1\chi^v)^{4/5} + a_3({}^2\chi^v)^{4/5}$	16.5118	5.9505	-13.5209	-3.1100	0.9661
$Y = a_o + a_1({}^o\chi^v)^{3/4} + a_2({}^1\chi^v)^{3/4} + a_3({}^2\chi^v)^{3/4}$	17.7054	7.1800	-15.4990	-3.7594	0.9662
$Y = a_o + a_1({}^o\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	28.1419	18.3609	-33.4176	-8.1096	0.9652

Table IV.**26**. Muptiple Regression Equations for Groups I (Halobenzenes), II (Alkylbenzenes), III (PAH) and IV (PCB) Together where Y = ln Kow

HALOGEN, ALKYL SUBSTITUTED BENZENES,
PAH'S AND PCB'S
$Y = \ln Kow$

EQUATIONS	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v)^{-1/2} + a_2({}^1\chi^v)^{-1/2} + a_3({}^2\chi^v)^{-1/2}$	26.3317	-66.6455	-6.9905	20.6669	0.9437
$Y = a_0 + a_1({}^0\chi^v)^{-1/4} + a_2({}^1\chi^v)^{-1/4} + a_3({}^2\chi^v)^{-1/4}$	-20.7794	14.3754	11.0419	-6.6539	0.9588
$Y = a_0 + a_1({}^0\chi^v)^{1/2} + a_2({}^1\chi^v)^{1/2} + a_3({}^2\chi^v)^{1/2}$	-5.4605	3.1039	4.5514	-1.4236	0.9640
$Y = a_0 + a_1({}^0\chi^v)^{3/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-4}$	1.3818	0.6054	1.3123	-0.1194	0.9698
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	1.8820	0.3429	1.3553	-0.1638	0.9699
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-2}$	2.0990	0.2709	1.3107	-0.1877	0.9699
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-3}$	2.0922	0.2724	1.3076	-0.2516	0.9699

Table IV.26. Continued

Y = ln Kow

EQUATIONS	a_0	a_1	a_2	a_3	R
$Y = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v)^{-2} + a_3({}^2\chi^v)^{-3}$	2.5078	0.9625	-1.2104	-0.5623	0.9540
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v)^{5/4} + a_3({}^2\chi^v)^{5/4}$	3.2767	0.1576	0.7984	-0.1180	0.9700
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	2.3380	0.1419	1.3775	-0.0924	0.9698
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-1/4}$	3.1570	0.1191	1.3261	-0.8150	0.9698
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-1/2}$	2.8524	0.1200	1.3219	-0.5288	0.9699
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-1}$	2.6832	0.1221	1.3163	-0.4008	0.9699
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-1/8}$	3.7461	0.1188	1.3286	-1.3960	0.9698
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-2}$	2.5783	0.1257	1.3106	-0.3840	0.9700
$Y = a_0 + a_1({}^0\chi^v)^{5/4} + a_2({}^1\chi^v) + a_3({}^2\chi^v)^{-4}$	2.5166	0.1290	1.3075	-0.5254	0.9702

Table IV.26. Continued

Y = ln Kow

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^0X^v)^{5/4} + a_2({}^1X^v) + a_3({}^2X^v)^{-6}$	2.5049	0.1299	1.3063	-0.8072	0.9701
$Y = a_o + a_1({}^0X^v)^{3/2} + a_2({}^1X^v)^{3/2} + a_3({}^2X^v)^{3/2}$	4.1949	0.0842	0.4795	-0.1066	0.9683
$Y = a_o + a_1({}^0X^v)^{2} + a_2({}^1X^v)^{2} + a_3({}^2X^v)^{2}$	5.3553	0.0285	0.1783	-0.0798	0.9601
$Y = a_o + a_1({}^0X^v)^{2} + a_2({}^1X^v) + a_3({}^2X^v)^{-2}$	3.2450	0.0145	1.3317	-0.8110	0.9700
$Y = a_o + a_1({}^0X^v)^{3} + a_2({}^1X^v) + a_3({}^2X^v)^{1/2}$	1.8590	5.64×10^{-4}	1.3723	0.9414	0.9696

Table IV.27. Muptiple Regression Equations for Groups I (Halobenzenes),
II (Alkylbenzenes), III (PAH) and IV (PCB) Together
where Y = ln P

HALOGEN, ALKYL SUBSTITUTED BENZENES,
PAH'S AND PCB'S
$Y = \ln P$, $N = 34$

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1({}^oX^v)^{5/4} + a_2({}^1X^v)^{5/4} + a_3({}^2X^v)^{5/4}$	8.2117	1.2414	-4.0102	-0.7146	0.9198
$Y = a_o + a_1({}^oX^v) + a_2({}^1X^v) + a_3({}^2X^v)$	10.6053	2.9484	-7.3222	-1.7766	0.9228
$Y = a_o + a_1({}^oX^v)^{1/2} + a_2({}^1X^v)^{1/2} + a_3({}^2X^v)^{1/2}$	23.0664	18.1535	-30.7133	-7.8235	0.9202
$Y = a_o + a_1({}^oX^v)^{-1/2} + a_2({}^1X^v)^{-1/2} + a_3({}^2X^v)^{-1/2}$	-33.6035	-45.1905	111.3624	-16.7116	0.8756

Table IV.28. Muptiple Regression Equations for Groups I (Halobenzenes), II (Alkylbenzenes), III (PAH) and IV (PCB) Together where $Y = \ln S$

HALOGEN, ALKYL SUBSTITUTED BENZENES,
PAH'S AND PCB'S
$Y = \ln S$, $N = 32$

EQUATIONS	a_o	a_1	a_2	a_3	R
$Y = a_o + a_1(^oX^v)^2 + a_2(^1X^v)^2 + a_3(^2X^v)^2$	8.9286	-0.0853	-0.3897	0.4428	0.9482
$Y = a_o + a_1(^oX^v)^{7/4} + a_2(^1X^v)^{7/4} + a_3(^2X^v)^{7/4}$	9.8276	-0.1557	-0.6425	0.6596	0.9492
$Y = a_o + a_1(^oX^v)^{3/2} + a_2(^1X^v)^{3/2} + a_3(^2X^v)^{3/2}$	11.0185	-0.2932	-1.0707	1.0065	0.9495
$Y = a_o + a_1(^oX^v)^{5/4} + a_2(^1X^v)^{5/4} + a_3(^2X^v)^{5/4}$	12.6981	-0.5869	-1.8122	1.6095	0.9473
$Y = a_o + a_1(^oX^v) + a_2(^1X^v) + a_3(^2X^v)$	15.2763	-1.2981	-3.1400	2.7856	0.9435

IV. 2. EVALUATION OF COMPARTMENTAL DISTRIBUTIONS IN TERMS OF VALANCE MOLECULAR CONNECTIVITY INDICES

In general, mass and equilibrium distributions, amounts and concentrations of chemicals in various compartments of the environment such as air, water, soil, biota, suspended solids and sediment are evaluated according to different models which are reffered in section III. 1. All these models which are accepted by OECD Exposure Analysis Group require hard-to-gether physical data such as octanol-water partition coefficients (K_{OW}), solubilities (S) and vapor pressures (P). However, such data are generally quite troublesome to find in the literature especially for larger structures which are of prime interest to environmental analysis. It is also not easy to predict and validate such properties for only a single structure using various semiempirical approaches because means of checking the results are very limited when one goes up to large and especially unknown structures.

So, being able to construct a new model that does not require any physical data for evaluation of environmental distribution of chemicals would be a remarkable advance in prediction of environmental HAZARDS that are going to be caused by UNKNOWN CHEMICALS.

As can be understood from the foregoing discussions and the statistical results obtained, the first three order valance molecular connectivity indices $^{0}\chi^{v}$, $^{1}\chi^{v}$ and $^{2}\chi^{v}$ bear a strong correlation ($R = 0.97 - 1.0$) with the physical data required for such a model to be set up.

Hence, this work proposes that by just knowing the simple molecular geometry it is possible to predict the environmental distribution of any organic compound provided that a simple statistical analysis is conducted with the known experimental values for the parameters in question for a representative group similar to the chemical group in question. In this way, the properties of well known molecules serve as a tool for predicting the properties of molecules that even do not yet exist....

IV.2.1. EVALUATION OF ln K_{OW}, ln S AND ln P IN TERMS OF VALANCE MOLECULAR CONNECTIVITY INDICES

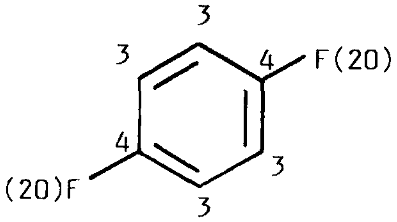
As a result of the single and multi variable regression analysis conducted the best equations defining those three parameters are chosen depending on the correlation coefficients evaluated as a part of the program used. This analysis is done for each group, for pairs of groups (I and IV, II and III) depending on the electron donating or withdrawing properties of the substituents on the phenyl ring and also for all the groups together to see whether a single set of equations be good enough to define whole aromatic systems.

The selected regression equations for ln K_{OW}, ln S and ln P are given in table IV.29 as a set of three equations for each group considered.

The evaluated results for ln K_{OW} , ln S and ln P on the other hand, are given in tables IV.30 to IV.33 where the evaluated values are compared with the values from literature.

The following example for p-difluorobenzene serves as a model for the evaluation of ln K_{OW}, ln S and ln P using the regression equations given in table IV.29.

Example:



$^0\chi^v = 3.7566$

$^1\chi^v = 1.5734$

$^2\chi^v = 1.2582$

Using the set given for halobenzene family from table IV.29;

$$\ln S = 49.5033 - 57.7702({}^{o}X^{v})^{2/5} - 5.4205({}^{1}X^{v})^{2/5} + 56.7490({}^{2}X^{v})^{2/5}$$

$$\ln S = 49.5033 - 57.7702(3.7566)^{2/5} - (5.4205)(1.5734)^{2/5} + (56.7490)(1.2582)^{2/5}$$

$$\ln S = 7.1257$$

$$\ln S_{(obs)} = 7.1102$$

$$\ln P = 14.4772 - 4.0817({}^{o}X^{v}) - 0.2613\,({}^{1}X^{v}) + 4.3669({}^{2}X^{v})$$

$$\ln P = 14.4772 - (4.0817)\,(3.7566) - (0.2613)\,(1.5734) + (4.3669)\,(1.2582)$$

$$\ln P = 4.2271$$

$$\ln P_{(obs)} = 4.2573$$

$$\ln K_{ow} = 42.7992 - 110.5270({}^{o}X^{v})^{-1/4} + 3.0455({}^{1}X^{v})^{-1/4} + 42.1557({}^{2}X^{v})^{-1/4}$$

$$\ln K_{ow} = 42.7992 - (110.5270)(3.7566)^{-1/4} + (3.0455)(1.5734)^{-1/4} + (42.1557)(1.2582)^{-1/4}$$

$$\ln K_{ow} = 5.93$$

$$\ln K_{ow}(obs) = 5.94$$

Table IV.29 Selected Regression Equations Defining ln Kow, ln S and ln P for Groups I, II, III, IV and for All Groups Together, Depending on the Correlation Coefficients.

	a_0	a_1	a_2	a_3	R
GROUP I (HALOGEN SUBSTITUTED BENZENES)					
$\ln Kow = a_0 + a_1({}^{0}\chi^{v})^{-1/4} + a_2({}^{1}\chi^{v})^{-1/4} + a_3({}^{2}\chi^{v})^{-1/4}$	42.7992	-110.5270	3.0455	42.1557	0.9852
$\ln S = a_0 + a_1({}^{0}\chi^{v})^{2/5} + a_2({}^{1}\chi^{v})^{2/5} + a_3({}^{2}\chi^{v})^{2/5}$	49.5033	-57.7702	-5.4205	56.7490	0.9869
$\ln P = a_0 + a_1({}^{0}\chi^{v}) + a_2({}^{1}\chi^{v}) + a_3({}^{2}\chi^{v})$	14.4772	-4.0817	-0.2613	4.3669	0.9887
GROUP II (ALKYLBENZENES)					
$\ln Kow = a_0 + a_1({}^{0}\chi^{v})^{-1/8} + a_2({}^{1}\chi^{v})^{-1/8} + a_3({}^{2}\chi^{v})^{-1/8}$	50.0686	46.3530	-62.2191	-28.3351	0.9987
$\ln S = a_0 + a_1({}^{0}\chi^{v})^{1/8} + a_2({}^{1}\chi^{v})^{1/8} + a_3({}^{2}\chi^{v})^{1/8}$	51.0994	22.4878	-47.4761	-17.7999	0.9967
$\ln P = a_0 + a_1({}^{0}\chi^{v}) + a_2({}^{1}\chi^{v}) + a_3({}^{2}\chi^{v})$	10.4348	-2.7099	0.5786	2.0574	0.9976

Table IV.29.Continued

	a_0	a_1	a_2	a_3	R
GROUP III (POLYCYLIC AROMATIC HYDROCARBONS)					
$\ln K_{ow} = a_0 + a_1({}^0X^v) + a_2({}^1X^v) + a_3({}^2X^v)$	0.0949	0.6855	1.5883	-0.6842	0.9998
$\ln S = a_0 + a_1({}^0X^v)^2 + a_2({}^1X^v)^2 + a_3({}^2X^v)^2$	10.7210	-1.9307	5.6930	-2.1844	0.9893
$\ln P = a_0 + a_1({}^0X^v) + a_2({}^1X^v) + a_3({}^2X^v)$	19.8058	-64.1811	128.6020	-42.9006	0.9870
GROUP IV (POLYCHLORINATED BIPHENYLS)					
$\ln K_{ow} = a_0 + a_1({}^0X^v)^2 + a_2({}^1X^v)^2 + a_3({}^2X^v)^2$	4.5770	-0.3483	0.9194	0.6982	0.9702
$\ln S = a_0 + a_1({}^0X^v)^{3/4} + a_2({}^1X^v)^{3/4} + a_3({}^2X^v)^{3/4}$	10.7298	3.0428	-0.1781	-9.5702	0.9724
$\ln P = a_0 + a_1({}^0X^v)^{3/4} + a_2({}^1X^v)^{3/4} + a_3({}^2X^v)^{3/4}$	23.3910	-6.5970	-12.6341	17.2094	0.9910

Table IV.29. Continued

	a_0	a_1	a_2	a_3	R
GROUP II and III (ELECTRON DONATING SUBSTITUENTS)					
$\ln Kow = a_0 + a_1({}^0\chi^v) + a_2({}^1\chi^v) + a_3({}^2\chi^v)$	-0.1773	1.5551	0.2616	-0.6863	0.9997
$\ln S = a_0 + a_1({}^0\chi^v)^2 + a_2({}^1\chi^v)^2 + a_3({}^2\chi^v)^2$	10.2871	-0.2356	-0.2243	0.7020	0.9886
$\ln P = a_0 + a_1({}^0\chi^v)^{3/4} + a_2({}^1\chi^v)^{3/4} + a_3({}^2\chi^v)^{3/4}$	17.7054	7.1800	-15.4990	-3.7594	-0.9660
GROUP I and IV (ELECTRON WITHDRAWING SUBSTITUENTS)					
$\ln S = a_0 + a_1({}^0\chi^v)^{3/2} + a_2({}^1\chi^v)^{3/2} + a_3({}^2\chi^v)^{3/2}$	12.2968	-1.3131	0.3488	2.4346	0.9720
$\ln P = a_0 + a_1({}^0\chi^v)^{1/8} + a_2({}^1\chi^v)^{1/8} + a_3({}^2\chi^v)^{1/8}$	127.9088	-190.9253	-14.8557	114.0320	0.9760
$\ln K_{ow} = a_0 + a_1({}^0\chi^v)^{-1/10} + a_2({}^1\chi^v)^{-1/10} + a_3({}^2\chi^v)^{-1/10}$	96.9161	-219.3055	11.2101	92.5010	0.9760

Table IV.29. Continued

	A_0	A_1	A_2	A_3	R
GROUPS I, II, III and IV TOGETHER					
$\ln Kow = A_0 + A_1({}^0X^v)^{5/4} + A_2({}^1X^v) + A_3({}^2X^v)^{-4}$	2.5166	0.1290	1.3075	-0.5254	0.9702
$\ln S = A_0 + A_1({}^0X^v)^{3/2} + A_2({}^1X^v)^{3/2} + A_3({}^2X^v)^{3/2}$	11.0185	-0.2932	-1.0707	1.0065	0.9495
$\ln P = A_0 + A_1({}^0X^v) + A_2({}^1X^v) + A_3({}^2X^v)$	10.6053	2.9484	-7.3222	-1.7766	0.9228

Table IV.30. Calculated and Observed Values for ln K_{OW}, ln S and ln P for Alkylbenzenes

	ln K_{OW}				ln S g/m^3				ln P mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
Benzene	4.87	4.94	5.45	4.91	7.47	7.50	7.35	7.49	4.58	5.68	4.12	4.55
Toluene	6.26	6.14	6.42	6.19	6.20	6.37	6.46	6.15	3.35	3.99	2.95	3.35
Ethylbenzene	7.33	7.26	7.34	7.25	5.06	4.57	4.67	5.02	2.13	1.04	0.60	2.26
p-xylene	7.30	7.34	7.22	7.32	5.17	5.12	5.54	5.37	2.11	2.39	1.77	2.17
m-xylene	7.30	7.34	7.22	7.37	5.16	5.13	5.55	5.08	2.12	2.38	1.77	2.11
o-xylene	7.20	7.39	7.23	7.19	5.23	4.90	5.37	5.17	1.97	2.50	1.85	1.88
n-propylbenzene	8.40	8.22	8.20	8.47	3.96	3.17	3.36	4.01	1.32	-1.75	-1.68	1.23
i-propylbenzene	8.48	8.21	8.09	8.43	3.96	4.00	4.31	3.91	1.49	-0.93	-0.93	1.53

Table IV.31. Calculated and Observed Values for ln K_{ow}, ln S and ln P for Unsubstituted Polycyclic Aromatic Hydrocarbons

	ln K_{ow}				ln S g/m^3				ln P mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
Benzene	4.86	4.94	5.45	4.90	7.41	7.50	7.35	7.49	5.14	5.68	4.12	4.55
Naphthalene	7.75	7.84	8.07	7.75	3.71	4.12	4.01	—	-3.73	-2.06	-1.90	-2.75
Fluorene	10.05	10.03	10.10	9.99	1.56	1.43	1.17	—	-7.06	-8.70	-7.77	-7.38
Phenanthrene	10.67	10.76	10.48	10.59	-0.82	-0.51	-0.04	0.08	-10.32	-8.89	-7.97	-9.45
Anthracene	10.64	10.74	10.48	10.66	-1.72	-0.31	0.10	-2.94	-12.75	-8.92	-7.99	-12.07
Pyrene	12.00	11.98	11.73	12.02	-2.12	-1.86	-1.72	-2.04	-12.36	-13.01	-11.86	-13.58
Chrysene	13.60	13.69	12.93	13.61	-6.51	-6.33	-4.64	-6.29	-16.99	-15.17	-14.01	-18.93
Perylene	14.96	14.92	14.20	14.97	-6.93	-8.15	-6.61	-7.83	-16.90	-19.02	-17.88	-15.37
Benzo (a) pyrene	14.93	14.90	14.19	14.97	-8.24	-7.87	-6.46	-7.48	-19.18	-19.04	-17.90	—

Table IV.32. Calculated and Observed Values for ln K_{ow}, ln S and ln P for Polychlorinated Biphenyls (PCB)

	ln K_{ow}				ln S g/m^3				ln P mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
Benzene	5.00	4.88	5.45	4.90	7.50	7.84	7.35	7.49	4.56	4.81	4.12	4.55
Biphenyl	9.05	9.19	9.24	9.16	2.66	3.01	1.60	2.02	-3.95	-3.00	-4.09	-4.62
4-CBP	9.99	10.16	10.22	10.59	0.82	1.49	0.17	1.61	-4.66	-4.64	-5.62	-5.09
2-CBP	9.77	10.30	10.22	10.59	1.13	1.10	-0.01	1.61	-5.27	-4.94	-5.56	-4.78
2,2'-CBP	10.54	11.28	11.21	9.26	-0.33	-0.90	-1.72	0.10	-6.60	-6.71	-7.03	-5.92
2,5,4'-CBP	12.13	11.91	12.20	11.42	-2.44	-1.90	-2.94	-4.51	-6.59	-7.79	-8.66	—
2,5,2'-CBP	11.92	11.98	12.20	—	-2.23	-2.22	-3.10	-2.21	-7.00	-7.96	-8.63	-6.36
3,5,3',5'-CBP	13.77	12.56	13.19	13.82	-4.27	-3.10	-4.27	-3.32	-6.92	-8.98	-10.24	—
2,4,5,4',5'-CBP	13.55	13.57	11.92	14.07	-4.73	-6.84	-6.83	-4.71	-9.91	-11.04	-11.47	-10.61

Table IV.33. Calculated and Observed Values for ln K_{ow}, ln S and ln P for Halogen Substituted Benzene Derivatives

	ln K_{ow}				ln S g/m^3				ln P mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
Benzene	5.01	4.87	5.45	4.90	7.50	7.84	7.35	7.49	4.86	4.81	4.12	4.55
Fluorobenzene	5.49	5.42	5.26	5.23	7.32	7.31	7.79	7.35	4.50	4.50	6.07	4.35
Chlorobenzene	6.24	6.19	6.62	6.54	6.74	6.52	6.25	6.17	2.82	2.74	2.59	2.46
p-difluorobenzene	5.93	5.91	5.04	5.94	7.13	6.86	8.19	7.11	4.23	4.27	7.93	4.26
m-difluorobenzene	5.90	5.89	5.04	5.94	7.19	6.87	8.20	___	4.24	4.31	7.92	___
o-difluorobenzene	5.84	5.71	5.66	5.96	6.19	7.15	7.14	___	4.06	3.61	4.45	___
p-dichlorobenzene	7.54	7.52	7.60	7.81	5.44	5.18	5.10	6.67	0.79	0.59	1.06	0.66
m-dichlorobenzene	7.52	7.50	7.60	8.27	5.49	5.20	5.10	4.79	0.80	0.61	1.06	0.81
o-dichlorobenzene	7.85	7.83	7.60	8.26	4.26	4.70	4.88	5.01	0.41	-1.39E-03	1.17	0.33
Bromobenzene	7.05	7.02	7.35	6.89	6.15	5.75	5.41	6.02	1.50	1.37	1.24	1.44
1,3,5-trichlorobenzene	8.67	8.69	8.56	___	4.11	3.88	3.92	___	-1.20	-1.39	-0.48	-0.18

Table IV.33. Calculated and Observed Values for $\ln K_{ow}$, $\ln S$ and $\ln P$ for Halogen Substituted Benzene Derivatives

	$\ln K_{ow}$				$\ln S$ g/m^3				$\ln P$ mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
1,2,4-trichloro-benzene	8.92	8.95	8.57	9.62	3.00	3.29	3.66	3.40	-1.61	-1.90	-0.36	-0.85
1,2,3-trichloro-benzene	9.16	9.20	8.58	9.83	3.42	2.76	3.42	3.45	-1.97	-2.40	-0.25	-0.93
p-bromochloro-benzene	8.28	8.29	8.31	8.82	4.68	4.41	4.22	3.80	-0.53	-0.73	-0.29	-0.46
m-bromochloro-benzene	8.27	8.28	8.31	8.82	4.73	4.43	4.23	4.78	-0.51	-0.71	-0.30	-0.43
o-bromochloro-benzene	8.62	8.60	8.32	8.82	3.25	3.76	3.91	—	-1.05	-1.35	-0.13	-0.82
Iodobenzene	8.48	8.49	8.67	7.74	4.68	4.35	3.79	5.83	-0.94	-1.11	-1.27	0.06
1,2,4,5-tetra-chlorobenzene	10.07	10.17	9.55	10.75	0.72	1.28	2.13	1.79	-3.91	-4.10	-1.77	-2.38
1,2,3,4-tetra-chlorobenzene	10.07	10.16	9.55	11.63	0.76	1.30	2.14	1.26	-3.91	-4.09	-1.77	-1.55
p-dibromobenzene	8.99	9.01	9.03	9.37	3.85	3.64	3.32	3.00	-1.83	-1.99	-1.66	-1.83

T.C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

Table IV.33. Calculated and Observed Values for ln K_{OW}, ln S and ln P for Halogen Substituted Benzene Derivatives

	ln K_{OW}				ln S g/m^3				ln P mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
p-chloroiodo-benzene	9.54	9.59	9.64	9.49	3.11	2.99	2.53	3.10	-2.99	-3.03	-2.81	-2.65
m-chloroiodo-benzene	9.54	9.59	9.65	9.49	3.15	3.02	2.54	4.21	-2.99	-3.02	-2.81	-2.07
o-chloroiodo-benzene	9.91	9.99	9.64	9.49	1.29	1.80	2.04	4.23	-3.91	-3.83	-2.53	-2.29
Pentachloro-benzene	11.25	11.43	10.55	11.95	-2.47	-1.61	0.18	-2.00	-0.05	-6.53	-3.08	-5.15
p-bromoiodo-benzene	10.15	10.24	10.37	10.04	2.22	2.23	1.58	2.05	-4.27	-4.19	-4.14	-4.69
Hexachlorobenzene	12.18	12.46	11.56	11.93	-5.02	-4.42	-1.77	-5.30	-9.54	-8.53	-4.42	-10.77
1,3,5-tribromo-benzene	10.53	10.65	10.73	13.11	1.53	1.55	1.11	—	-5.16	-4.92	-4.51	-6.33
1,2,4-tribromo-benzene	10.50	10.93	10.74	13.11	0.08	0.39	0.61	—	-5.83	-5.53	-4.34	-4.75

Table IV. **33.** Calculated and Observed Values for $\ln K_{OW}$, $\ln S$ and $\ln P$ for Halogen Substituted Benzene Derivatives

	$\ln K_{OW}$				$\ln S$ g/m^3				$\ln P$ mm.Hg			
	Calc.				Calc.				Calc.			
COMPOUND	a	b	c	obs.	a	b	c	obs.	a	b	c	obs.
m-dibromobenzene	8.98	9.00	9.03	9.37	3.89	3.66	3.33	—	-1.83	-1.98	-1.66	-1.47
o-dibromobenzene	9.36	9.41	9.04	9.37	2.1	2.63	2.88	—	-2.53	-2.79	-1.43	-1.61
p-diiodobenzene	11.17	11.32	11.72	10.68	0.58	0.81	-0.25	0.62	-6.74	-6.20	-6.68	-7.27
m-diiodobenzene	11.16	11.31	11.72	10.68	0.61	0.84	-0.24	—	-6.73	-6.19	-6.69	-5.17
o-diiodobenzene	11.54	11.74	11.73	10.71	-1.71	-1.26	-1.10	—	-7.87	-7.13	-6.26	-4.93

a) Evaluated according to regression equations obtained for each group.

b) Evaluated according to regression equations obtained for pairs of groups having electron withdrawing and electron donating substituents.

c) Evaluated according to regression equations obtained for all four groups together.

IV.2.2. EVALUATION OF FUGACITY CAPACITY CONSTANTS IN TERMS OF VALANCE MOLECULAR CONNECTIVITY INDICES

Evaluation of the fugacity capacity constants Z_i for different compartments of the environment were given in chapter III.
This work simply combines modified level I fugacity model[56] for the evaluation of compartmental distribution of chemicals with the valance molecular connectivity model as a result of which the fugacity capacity constants Z_i are expressed as functions of valance molecular connectivity indices so that, the distribution of chemicals in the environment can also be evaluated only in terms of those indices and the molecular weight.

The procedure for the calculation of fugacity capacities for different compartments of the environment proceeds as follows:

IV.2.2.1. Derivation of the Expression for the Fugacity Capacity Constant for Air

$$Z_a = 1/RT$$

IV.2.2.2. Derivation of the Expression for the Fugacity Capacity Constant for Soil

$$Z_s = Kp_s \; \rho_s \; / \; H$$

$$H = \frac{P \text{ mm Hg} \times (1 \text{ Pa} / 7.5 \times 10^{-3} \text{ mm Hg})}{S \text{ gr} / \text{m}^3 \times (1 \text{ mol} / \text{M.Wt gr.})} \text{ Pa m}^3 / \text{mole}$$

$$H = \frac{P}{S} \times \frac{\text{mol.Wt}}{0.0075} \text{ Pa m}^3 / \text{mole}$$

$$Kp_s = \%OC \times 0.6 \times K_{ow} \text{ m}^3 \text{ of water} / 10^6 \text{ gr sorbent}$$

$$Z_s = \%OC \times 0.6 \times \rho_s \times 10^{-6} \times K_{ow} \left[\frac{S}{P} \times \frac{0.0075}{\text{M.Wt}} \right]$$

let

$$Y_s = \%OC \times 0.6 \times \rho_s \times 10^{-6} \times 0.0075$$

$$Y_s = 0.02 \times 0.6 \times 1.5 \times 10^{-6} \times 10^{6} \times 0.0075$$

$$Y_s = 1.35 \times 10^{-4}$$

then

$$Z_s = Y_s \times K_{ow} \times (S / P) \times (1 / M.Wt)$$

Hence in terms of VMCI

$$Z_s = \frac{Y_s}{M.Wt} \times \left[\frac{\exp(\ln K_{ow}) \times \exp(\ln S)}{\exp(\ln P)} \right]$$

Since $e^a \times e^b = e^{a+b}$

and $e^a / e^b = e^{a-b}$

$$Z_s = \frac{Y_s}{M.Wt} \times \exp \left[\ln K_{ow} + \ln S - \ln P \right]$$

IV.2.2.3. Derivation of the Expression for the Fugacity Capacity Constant for Water

$$Z_w = 1 / H$$

$$H = \frac{M\ Wt.}{0.0075} \times (P / S)\ Pa\ m^3 / mole$$

$$Z_w = \frac{0.0075}{M\ Wt.} \times (S / P)$$

$$Z_W = \frac{0.0075}{\text{M. Wt.}} \times \exp \left[\ln S - \ln P \right]$$

IV.2.2.4. Derivation of the Expression for the Fugacity Capacity Constant for Biota

$$Z_b = K_B \rho_B / H$$

$$H = \frac{\text{M. Wt.}}{0.0075} \times (P / S) \; P_a \; m^3 / \text{mole}$$

$$\ln K_B = 0.085 \ln K_{ow} - 1.6121$$

$$K_B = \frac{\exp (0.085 \ln K_{ow})}{\exp (1.6121)} \; m^3 \text{ of water} \times \frac{1}{10^6} \text{ g biota}$$

$$Z_b = \rho_B \frac{\exp (.085 \ln K_{ow})}{5.0133 \times 10^6} \times \frac{0.0075 \times \exp (\ln S)}{\text{M Wt.} \times \exp (\ln P)}$$

let

$$Y_B = \frac{\rho_B \times 0.0075}{5.0133 \times 10^6}$$

$$Y_B = \frac{1 \times 10^6 \text{ gr}/\text{m}^3 \times 0.0075}{5.0133 \times 10^6}$$

$$Y_B = 1.4960 \times 10^{-3}$$

then

$$Z_b = \frac{Y_B}{\text{M Wt.}} \times \frac{\exp(.085 \ln K_{ow}) \times \exp(\ln S)}{\exp(\ln P)}$$

$$Z_b = \frac{Y_B}{\text{M Wt.}} \times \exp\left[(0.085 \ln K_{ow}) + \ln S - \ln P\right]$$

IV.2.2.5. Derivation of the Expression for the Fugacity Capacity Constant for Suspended Solids

$$Z_{ss} = Kp_{ss} \times \rho_{ss} / H$$

$$H = \frac{P}{S} \times \frac{M\ Wt.}{0.0075}\ P_a\ m^3 / mol$$

$$Kp_{ss} = \%OC \times 0.6 \times K_{ow}\ m^3 \text{ of water} \times \frac{1}{10^6}\ \text{g sorbent}$$

$$Z_{ss} = \frac{\%OC \times 0.6 \times 0.0075 \times \rho_{ss}}{10^6\ M\ Wt.} \times K_{ow}\ (S / P)$$

let

$$Y_{ss} = \%OC \times 0.6 \times 0.0075 \times \rho_{ss} \times 10^{-6}$$

$$Y_{ss} = 0.04 \times 0.6 \times 0.0075 \times 1.5 \times 10^6 \times 10^{-6}$$

$$Y_{ss} = 2.7 \times 10^{-4}$$

then

$$Z_{ss} = \frac{Y_{ss}}{M\ Wt.} \times \left[\frac{\exp(\ln K_{ow}) \times \exp(\ln S)}{\exp(\ln P)}\right]$$

$$Z_{ss} = \frac{Y_{ss}}{M\ Wt.} \exp\left[\ln K_{ow} + \ln S - \ln P\right]$$

IV.2.2.6. Derivation for the Expression for the Fugacity Capacity Constant for Sediment

$$Z_{sd} = Kp_{sd} \times \rho_{sd} \, / \, H$$

$$H = \frac{P}{S} \times \frac{M\ Wt.}{0.0075}$$

$$Kp_{sd} = \%OC \times 0.6 \times K_{ow}\ m^3 \text{ of water} \times \frac{1}{10^6} \text{ gr sorbent}$$

$$Z_{sd} = \frac{\%Oc \times 0.6 \times \rho_{sd} \times 0.0075}{10^6 \times M\ Wt.} \times K_{ow}\ (S/P)$$

let

$$Y_{sd} = \%OC \times 0.6 \times \rho_{sd} \times 0.0075 \times 10^{-6}$$

$$Y_{sd} = 0.04 \times 0.6 \times (1.5 \times 10^6) \times 0.0075 \times 10^{-6}$$

$$Y_{sd} = 2.7 \times 10^{-4}$$

then

$$Z_{sd} = \frac{Y_{sd}}{M\ Wt.} \exp\left[\ln K_{ow} + \ln S - \ln P\right]$$

In these calculations ln K_{OW}, ln S and ln P values are evaluated according to the regression equations obtained, in terms of valance molecular connectivity indices $^{0}\chi^{v}$, $^{1}\chi^{v}$ and $^{2}\chi^{v}$.

In order for these calculations to be carried out and compared, two computer programs (Appendix II), prepared according to the flowchart given are used. One of the programs calculates fugacity capacity constants (Z_i) and related distribution values according to level I fugacity model and the other calculates these values in terms of valance molecular connectivity indices according to the model developed in this work (VMCI). Both models use the final compartment volumes given by Mackay et. al.[68] which are given in table III.1.

IV.2.3. SPECIMEN CALCULATIONS

In the following two examples fugacity capacity constant for p-difluorobenzene are evaluated according to level I fugacity model and Valance Molecular Connectivity Model.

IV.23.1. Calculation of Fugacity Capacities According to Level I Fugacity Model

a) Calculation of Fugacity Capacity for Air

$Z_a = 1 / RT$

$T = 298^oK$

$R = 8.314 (P_a \cdot m^3)/(mol\ ^oK)$ or $8.314\ J/(mol\ ^oK)$

$$Z_a = \frac{1}{8.314 \times 298} = 4.04 \times 10^{-4}\ mol / m^3\ P_a$$

b) Calculation of Fugacity Capacity for Soil

$Z_s = Kp_s\ \rho s / H$

$\rho s = 1.5 \times 10^6\ g/m^3$

$H = P / S$

$P = 70.612\ mm\ Hg\ (1\ P_a / 7.5 \times 10^{-3}\ mm\ Hg) = 9414.93\ P_a$

$S = 1224.39\ g/m^3\ (1\ mole / 114.09\ gram) = 10.73\ mole / m^3$

$H = 9414.93 / 10.73 = 877.44\ P_a\ m^3 / mol$

$Kp_s = \%OC \times 0.6 \times K_{ow}$

$\%OC = 0.02$ for soil

$Kp_s = 0.02 \times 0.6 \times 380.19$

$Kp_s = 4.5623\ m^3$ of water $/ 10^6$ g sorbent

$Z_s = 4.5623 \times 1.5 / 877.44 = 7.80 \times 10^{-3}\ mole / m^3\ P_a$

c) Calculation of Fugacity Capacity for Water

$Z_W = 1 / H$

$H = 877.44 \ P_a \ m^3 / mole$

$Z_W = 1 / 877.44 = 1.14 \times 10^{-3} \ mole / m^3 \ P_a$

d) Calculation of Fugacity Capacity for Biota

$Z_b = K_B \rho_b / H$

$\rho_b = 1 \times 10^6 \ g/m^3$

$H = 877.44 \ P_a \ m^3 / mole$

$\log K_B = 0.85 \log K_{OW} - 0.7$

$\log K_B = 0.85 \times 2.58 - 0.7$

$\log K_B = 1.493$

$K_B = 31.12 \ m^3$ of water / 10^6 g biota

$Z_b = (31.12 \times 1) / 877.44 = 0.036 \ mole / m^3 \ P_a$

e) Calculation of Fugacity Capacity for Suspended Solids

$Z_{ss} = Kp_{ss} \rho_{ss} / H$

$\rho_{ss} = 1.5 \times 10^6 \ g/m^3$

$H = 877.44\ P_a\ m^3 / mole$

$Kp_{ss} = \%\ OC \times 0.6 \times K_{ow}$

$\%\ OC = 0.04$ for suspended solids

$Kp_{ss} = 0.04 \times 0.6 \times 380.19$

$Kp_{ss} = 9.1246\ m^3$ of water/10^6 g sorbent

$Z_{ss} = (9.1246 \times 1.5) / 877.44 = 0.016$ mole/ $m^3\ P_a$

f) Calculation of Fugacity Capacity for Sediment

$Z_{sd} = Kp_{sd} \cdot \rho_{sd} / H$

$\rho_{sd} = 1.5\ 10^6\ g/m^3$

$H = 877.44\ m^3 P_a / mole$

$Kp_{sd} = \%\ OC \times 0.6 \times K_{ow}$

$\%\ OC = 0.04$ for sediment

$Kp_{sd} = 0.04 \times 0.6 \times 380.19$

$Kp_{sd} = 9.1246\ m^3$ of water / 10^6 g sorbent

$Z_{sd} = (9.1246 \times 1.5) / 877.44 = 0.016$ mole / $m^3\ P_a$

IV.2.3.2. Calculation of Fugacity Capacity Constants According to Valance Molecular Connectivity Model

a) Calculation of Fugacity Capacity Constant for Air

$$Z_a = 1/ RT$$

$$Z_a = 1 / 8.314 \times 298$$

$$Z_a = 4.04 \times 10^{-4} \text{ mole} / m^3 \, Pa$$

b) Calculation of Fugacity Capacity for Soil

$$Z_s = \frac{Y_s}{\text{M Wt.}} \exp \left[\ln K_{ow} + \ln S - \ln P \right]$$

$${}^0\chi^v = 3.7566$$

$${}^1\chi^v = 1.5734$$

$${}^2\chi^v = 1.2587$$

$$Y_s = 1.35 \times 10^{-4}$$

From the regression equations for halobenzenes (table IV.29)

$$Z_s = \frac{1.35 \times 10^{-4}}{114.09} \exp \left[5.93 + 7.13 - 4.23 \right]$$

$Z_s = 8.09 \times 10^{-3}$ mole / $m^3 P_a$

Z_s(levelI)= 7.80×10^{-3} mole/ $m^3 P_a$

c) Calculation of Fugacity Capacity for Water

$$Z_w = \frac{0.0075}{\text{M Wt.}} \exp \left[\ln S - \ln P \right]$$

$$Z_w = \frac{0.0075}{114.09} \exp \left[7.13 - 4.23 \right]$$

$Z_w = 1.19 \times 10^{-3}$ mole / $m^3 P_a$

Z_w(level I) = 1.14×10^{-3} mole/ $m^3 P_a$

d) Calculation of Fugacity Capacity for Biota

$$Z_b = \frac{Y_B}{\text{M Wt.}} \exp \left[0.85 \ln K_{ow} + \ln S - \ln P \right]$$

$Y_B = 1.4960 \times 10^{-3}$

$$Z_b = \frac{1.4960 \times 10^{-3}}{114.09} \exp \left[(0.85 \times 5.93) + 7.13 - 4.23 \right]$$

$Z_b = 0.037$ mole / $m^3 P_a$

Z_b (levelI) = 0.036 mole/ $m^3 P_a$

e) Calculation of Fugacity Capacity for Susp. Solids.

$$Z_{ss} \frac{Y_{ss}}{M\ Wt.} \exp\left[\ln K_{ow} + \ln S - \ln P\right]$$

$Y_{ss} = 2.7 \times 10^{-4}$

$$Z_{ss} = \frac{2.7 \times 10^{-4}}{114.09} \exp\left[5.93 + 7.13 - 4.23\right]$$

$Z_{ss} = 0.016$ mole / m^3 P_a

$Z_{ss(\text{level I})} = 0.016$ mole/ m^3 P_a

d) Calculation of Fugacity Capacity for Sediment

$$Z_{sd} = \frac{Y_{sd}}{M\ Wt.} \exp\left[\ln K_{ow} + \ln S - \ln P\right]$$

$Y_{sd} = 2.7 \times 10^{-4}$

$$Z_{sd} = \frac{2.7 \times 10^{-4}}{114.09} \exp\left[5.93 + 7.13 - 4.23\right]$$

$Z_{sd} = 0.016$ mole / m^3 P_a

$Z_{sd(\text{level I})} = 0.016$ mole/ m^3 P_a

The expressions used for ln K_{ow}, ln S and ln P in these calculations are functions of valance molecular connectivity indices of first three order and are obtained as the result of regression analysis as indicated previously.

A close inspection of the procedure used in the above example shows that the fugacity capacity constants Z_i for most compartments are obtained by multiplying Y_i / M Wt. by the exponential expression exp (ln K_{ow} + ln S — ln P)which bears the same value for each compartment except biota and water. So we can further simplify these expressions by letting;

$$E = \exp(\ln K_{ow} + \ln S - \ln P)$$

so that,

$$Z_i = Y_i \times (E / M\ Wt.)$$

for compartments other than water and biota. The results of the forgoing examples are tabulated in table IV.34. for comparison.

The fugacity capacities for air, soil, water, biota, suspended solids and sediment evaluated via valance molecular connectivity approach are given in Appendix III in comparison with the

Z_i values obtained from level I fugacity calculations. In these outputs Z_i values obtained by VMCI model are the results calculated according to group specific regression equations for ln K_{ow}, ln S and ln P and i = 1,2....... 6 represent air, soil, water, biota, suspended solids and sediment compartments respectively.

Table IV.34. Fugacity Capacity Constants Evaluated by Valance Molecular Connectivity (A) and Level I Fugacity (B) Approaches for P-difluorobenzene

	Z_a	Z_s	Z_w	Z_b	Z_{ss}	$Z_{sed.}$
Level I FUGACITY APPROACH	4.04×10^{-4}	7.80×10^{-3}	1.14×10^{-3}	0.036	0.016	0.016
VMCI APPROACH	4.04×10^{-4}	8.09×10^{-3}	1.19×10^{-3}	0.037	0.016	0.016

IV.3. EVALUATION OF THE COMPARTMENTAL DISTRIBUTION IN TERMS OF VALANCE MOLECULAR CONNECTIVITY INDICES

After the evaluation of ln K_{OW}, ln S, ln P and Z_i values in terms of valance molecular connectivity indices, by the help of the computer program developed (VMCI, Appendix II) according to flow-chart given, the mass and equilibrium distributions, amounts and concentrations for the compounds are evaluated.

Under the light of assumptions made (section III.1.1) it is accepted that the fugacities for all phases areequal and a common fugacity f is calculated where,

$$f = f_A = f_W = f_S = f_B = f_{SO}$$

and the mass (P_i) and equilibrium (P_i') partitionings (%) among compartments, the amount (moles) of material in each phase (M_i) and the concentration (ppm) within different compartments (C_i) are evaluated according to,

$$P_i = Z_i V_i / \sum Z_i V_i$$

$$P_i' = Z_i / \sum Z_i$$

$$M_i = f Z_i V_i$$

and

$$C_i = f\ Z_i$$

respectively, following the mathematical procedure given in section III.1.1. As an example, two outputs for benzene are given in tables IV.35 and IV.36 for Level I Fugacity and VMCI calculations respectively.

In order to check the validity of the regression analysis done for pairs of groups having electron withdrawing and electron donating substituents and also for the whole group (groups I, II, III, and IV together), the calculations are carried out with each group of regression equations (table IV.29)

The results tabulated in table V. give the evaluated values for these three different input sets namely;

- ln K_{OW} , ln S and ln P evaluated according to the regression equations for each specific group,
- ln K_{OW}, ln S and ln P evaluated according to the regression equations for pairs of groups having electron withdrawing (halobenzene and PCB) and electron donating substituents (alkylbenzene and PAH)
- ln K_{OW}, ln S and ln P evaluated according to the regression equations for all four group together (halobenzenes, PCB's, alkylbenzenes and PAH's)

Table IV.35. Output for the Compartmental Distribution of Benzene Calculated by Level I Fugacity Model

```
NAME OF CHEMICAL:BENZENE
         ---------------

MOLECULAR WT.: 78.114
AQ. SOLUBILITY: 1789.87

VAPOR PRESSURE: 95.04

LOG OCT-WATER PART. COEFF.: 2.13

         MASS PART            EQ PART            AMOUNT            CONC

******AIR .994644299  8.49985277E-03  99.4644299  1.0881743E-03

*****SOIL 8.11475286E-05  .0924607985  8.11475286E-03  9.39075267E-06

****WATER 5.19862294E-03  .0380789649  .519862294  5.8012176E-06

****BIOTA 6.70483847E-08  .49111719  6.70483847E-06  7.48202503E-05

S. SOLIDS 1.26229489E-07  .184921597  1.26229489E-05  1.87815053E-05

*SEDIMENT 7.57376934E-05  .184921597  7.57376934E-03  1.87815053E-05
```

Table IV.36. Output for the Compartmental Distribution of Benzene Calculated by VMCI Model

```
NAME OF CHEMICAL:BENZENE
--------------------------

MOLECULAR WT: 78.114

XO= 3.4641
X1= 2
X2= 1.1547

FUGACITY CAP.CONST.

 Z1= 4.03620964E-04
 Z2= 4.85234248E-03                 OCT-WATER PART COEFF: 149.296813
 Z3= 1.80562851E-03                 SOLUBILITY: 1800.99157
 Z4= .0253774317                    VAPOR PRESSURE: 95.7669511
 Z5= 9.70468496E-03                 S/P= 18.8059821
 Z6= 9.70468496E-03                 KOW*(S/P)= 2807.67319
H= 553.823776

      MASS PART            EQ PART            AMOUNT            CONC

******AIR .994635232  7.7846378E-03  99.4635232  1.08816438E-03

*****SOIL 8.96814936E-05  .0935871326  8.96814936E-03  1.0378341E-05

****WATER 5.19117078E-03  .0348251583  .519117078  5.79290163E-06

****BIOTA 7.29599588E-08  .489454541  7.29599588E-06  8.14170603E-05

S. SOLIDS 1.39504546E-07  .187174265  1.39504546E-05  2.0756682E-05

*SEDIMENT 8.37027274E-05  .187174265  8.37027273E-03  2.0756682E-05
```

V. DISCUSSION OF THE RESULTS

V- DISCUSSION OF THE RESULTS

V.1- TABULATION OF THE RESULTS

The results obtained for the compartmental distribution of various aromatic compounds under investigation are given in the following tables (table V) for each group where (calc. a) represents the set evaluated according to the results of group specific regression, (calc. b) represents the set evaluated according to the results of regression carried out with pairs of groups having electron donating and electron withdrawing substituents and finally (calc.c) represents the set evaluated according to the results of regression analysis for all four groups together.

These three sets of results are given in comparison with the results of level I fugacity calculations which is located at the last column in each table.

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	MASS DISTRIBUTION (%) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity
HALOBENZENES				
Benzene	99.60	99.41	99.27	99.46
Fluorobenzene	99.60	99.61	99.87	99.53
Chlorobenzene	99.02	99.07	99.14	99.09
p-difluorobenzene	99.63	99.73	99.97	99.64
m-difluorobenzene	99.61	99.73	99.97	99.74
o-difluorobenzene	99.83	99.31	99.70	97.84
p-dichlorobenzene	97.85	97.99	98.81	91.42
m-dichlorobenzene	97.79	98.00	98.80	98.55
o-dichlorobenzene	98.92	97.53	99.14	97.11
Bromobenzene	98.23	98.65	98.81	98.39
1,3,5-trichlorobenzene	94.72	94.91	97.92	99.52
1,2,4-trichlorobenzene	96.88	96.46	98.56	96.47
1,2,3-trichlorobenzene	98.10	93.76	98.98	95.31

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN AIR			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	96.22	96.50	98.06	98.02
m-bromochlorobenzene	96.14	96.51	98.03	95.04
o-bromochlorobenzene	98.18	95.99	98.78	92.63
Iodobenzene	94.25	95.05	96.26	95.10
1,2,4,5-tetrachlorobenzene	93.32	87.06	97.94	93.08
1,2,3,5-tetrachlorobenzene	93.24	87.07	97.91	95.82
p-dibromobenzene	92.89	93.19	96.34	96.01
m-dibromobenzene	92.77	93.19	96.28	87.33
o-dibromobenzene	96.72	92.77	98.08	88.70
p-chloroiodobenzene	85.86	86.14	92.22	89.80
m-chloroiodobenzene	85.66	86.10	92.10	83.94
o-chloroiodobenzene	92.94	87.03	96.34	80.38
Pentachlorobenzene	88.63	79.63	97.90	93.31
p-bromoiodobenzene	74.01	74.52	83.70	71.60
Hexachlorobenzene	76.17	78.60	97.42	61.26
1,3,5-tribromobenzene	65.65	68.44	81.69	59.44
1,2,4-tribromobenzene	76.82	74.14	90.19	36.34

Table V. Continued

	MASS DISTRIBUTION (%) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
p-diiodobenzene	37.49	41.42	46.33	34.67
m-diiodobenzene	37.25	41.17	45.89	47.46
o-diiodobenzene	57.02	59.52	75.76	34.59
ALKYLBENZENES				
Toluene	99.55	99.72	99.11	99.57
Ethylbenzene	99.50	99.09	98.41	99.58
p-xylene	99.43	99.58	98.86	99.33
m-xylene	99.43	99.57	98.84	99.47
o-xylene	99.31	99.69	99.11	99.30
n-propylbenzene	99.50	95.71	95.19	99.40
i-propylbenzene	99.56	95.64	94.47	99.61
n-butylbenzene	98.33	97.53	96.92	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	69.74	88.62	90.13	-
Fluorene	18.20	4.80	13.58	-
Phenanthrene	5.41	14.06	24.73	5.70
Anthracene	1.29	11.69	22.06	7.80

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN AIR			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
Pyrene	0.89	0.36	1.23	0.23
Chrysene	0.16	0.77	0.95	0.02
Perylene	0.08	0.03	0.05	0.86
Benzo (a) pyrene	0.03	0.03	0.04	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	76.78	84.49	87.91	74.82
4-CBP	86.07	73.77	78.95	51.97
2-CBP	74.77	73.07	82.63	59.63
2,2'-CBP	67.34	62.09	73.88	88.22
2,5,4'-CBP	81.49	48.87	46.11	-
2,5,2'-CBP	74.29	51.06	50.70	-
3,5,3',5',-CBP	82.04	36.74	22.51	-
2,4,5,4',5'-CBP	32.97	56.00	30.05	12.53

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	MASS DISTRIBUTION (%) IN SOIL			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	6.75 E-03	8.66 E-03	1.86 E-02	8.11 E-03
Fluorobenzene	1.06 E-02	9.80 E-03	2.80 E-03	9.65 E-03
Chlorobenzene	5.22 E-02	4.71 E-02	6.36 E-02	6.29 E-02
p-difluorobenzene	1.50 E-02	1.08 E-02	4.42 E-04	1.44 E-02
m-difluorobenzene	1.54 E-02	1.03 E-02	4.49 E-04	1.06 E-02
o-difluorobenzene	16.10 E-02	2.26 E-02	9.29 E-03	8.95 E-02
p-dichlorobenzene	0.329	0.3033	0.189	1.57
m-dichlorobenzene	0.335	0.2986	0.192	0.350
o-dichlorobenzene	0.204	0.4595	0.138	0.694
Bromobenzene	0.189	0.1399	0.159	0.149
1,3,5-trichlorobenzene	1.54	1.5000	0.580	0.202
1,2,4-trichlorobenzene	1.01	1.81	0.402	1.41
1,2,3-trichlorobenzene	0.667	2.22	0.286	1.95

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	0.917	0.8512	0.479	0.616
m-bromochlorobenzene	0.932	0.8439	0.486	1.54
o-bromochlorobenzene	0.521	1.14	0.302	2.29
Iodobenzene	1.54	1.33	1.10	0.858
1,2,4,5-tetrachlorobenzene	2.90	5.70	0.808	3.26
1,2,3,5-tetrachlorobenzene	2.94	5.70	0.819	2.08
p-dibromobenzene	2.36	2.28	1.23	1.50
m-dibromobenzene	2.39	2.27	1.25	4.75
o-dibromobenzene	1.23	2.73	0.647	4.23
p-chloroiodobenzene	5.54	5.50	3.12	3.94
m-chloroiodobenzene	5.60	5.50	3.17	6.20
o-chloroiodobenzene	2.98	5.56	1.47	7.57
Pentachlorobenzene	5.55	10.04	0.972	3.36
p-bromoiodobenzene	11.44	11.35	7.39	12.28
Hexachlorobenzene	12.04	10.87	1.28	19.45
1,3,5-tribromobenzene	15.86	14.74	8.62	39.58
1,2,4-tribromobenzene	10.97	12.37	4.62	46.02

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SOIL			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
p-diiodobenzene	30.38	28.71	26.77	30.62
m-diiodobenzene	30.49	28.83	26.98	24.63
o-diiodobenzene	21.29	20.20	12.09	30.72
ALKYLBENZENES				
Toluene	2.5 E-02	1.35 E-02	5.54 E-02	2.2 E-02
Ethylbenzene	6.6 E-02	11.40 E-02	21.10 E-02	5.26 E-02
p-xylene	7.3 E-02	5.53 E-02	13.80 E-02	8.72 E-02
m-xylene	7.3 E-02	5.62 E-02	14.00 E-02	7.21 E-02
o-xylene	8.2 E-02	4.20 E-02	10.80 E-02	8.27 E-02
n-propylbenzene	0.129	0.01	1.12	0.159
i-propylbenzene	0.117	0.01	1.21	0.103
n-butylbenzene	0.502	0.946	1.04	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	5.34	2.13	2.12	-
Fluorene	35.46	41.07	37.72	-
Phenanthrene	44.29	40.58	34.57	43.81
Anthracene	46.06	41.59	35.77	43.13

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
Pyrene	49.85	50.08	49.27	50.20
Chrysene	51.31	51.02	50.64	51.39
Perylene	51.56	51.58	51.50	51.16
Benzo (a) pyrene	51.59	51.59	51.50	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.87	5.51	4.36	8.86
4-CBP	5.98	11.55	9.35	22.32
2-CBP	10.39	12.10	7.72	18.76
2,2'-CBP	15.09	18.55	12.73	4.27
2,5,4'-CBP	9.34	25.65	27.23	-
2,5,2'-CBP	12.90	24.60	24.92	-
3,5,3',5',-CBP	9.24	32.18	39.71	-
2,4,5,4',5'-CBP	34.44	22.61	36.04	45.05

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	MASS DISTRIBUTION (%) IN WATER			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity
HALOBENZENES				
Benzene	0.389	0.5725	0.693	0.520
Fluorobenzene	0.375	0.3762	0.125	0.448
Chlorobenzene	0.876	0.8351	0.736	0.786
p-difluorobenzene	0.344	0.2538	0.025	0.328
m-difluorobenzene	0.362	0.2474	0.025	0.241
o-difluorobenzene	0.161	0.6503	0.281	1.99
p-dichlorobenzene	1.52	1.430	0.82	5.54
m-dichlorobenzene	1.57	1.422	0.83	0.777
o-dichlorobenzene	0.689	1.585	0.596	1.54
Bromobenzene	1.41	1.080	0.885	1.32
1,3,5-trichlorobenzene	2.29	2.185	0.958	0.094
1,2,4-trichlorobenzene	1.17	2.038	0.658	0.811
1,2,3-trichlorobenzene	0.606	1.947	0.466	0.907

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	2.00	1.855	1.02	0.787
m-bromochlorobenzene	2.06	1.858	1.03	1.97
o-bromochlorobenzene	0.810	1.808	9.637	2.93
Iodobenzene	2.76	2.372	1.62	3.24
1,2,4,5-tetrachlorobenzene	1.06	1.898	0.496	0.603
1,2,3,5-tetrachlorobenzene	1.08	1.909	0.503	0.160
p-dibromobenzene	2.55	2.402	1.28	1.10
m-dibromobenzene	2.61	2.416	1.30	3.49
o-dibromobenzene	0.908	1.940	0.666	3.11
p-chloroiodobenzene	3.43	3.232	1.75	2.58
m-chloroiodobenzene	3.50	3.259	1.77	4.06
o-chloroiodobenzene	1.28	2.213	0.821	4.97
Pentachlorobenzene	0.623	0.9396	0.220	0.187
p-bromoiodobenzene	3.85	3.5148	2.00	4.63
Hexachlorobenzene	0.532	0.3661	0.106	1.11
1,3,5-tribromobenzene	3.65	3.0298	1.62	0.690
1,2,4-tribromobenzene	1.94	1.9124	0.864	0.803

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN WATER			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
p-diiodobenzene	3.72	3.0187	1.87	6.06
m-diiodobenzene	3.75	3.0475	1.89	4.88
o-diiodobenzene	1.78	1.3932	0.839	5.94
ALKYLBENZENES				
Toluene	0.406	0.252	0.781	0.388
Ethylbenzene	0.377	0.691	1.18	0.322
p-xylene	0.430	0.311	0.874	0.498
m-xylene	0.425	0.317	0.886	0.393
o-xylene	0.528	0.224	0.681	0.543
n-propylbenzene	0.252	2.342	2.66	2.288
i-propylbenzene	0.211	2.387	3.19	0.195
n-butylbenzene	0.70	0.637	1.07	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	19.92	7.254	5.76	-
Fluorene	13.19	15.705	13.42	-
Phenanthrene	8.88	7.418	8.36	9.51
Anthracene	9.57	7.821	8.72	8.74

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN WATER			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	2.64	2.722	3.42	2.61
Chrysene	0.552	0.501	1.06	0.546
Perylene	0.142	0.147	0.303	0.141
Benzo (a) pyrene	0.147	0.151	0.305	0.140
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.99	4.847	3.66	8.02
4-CBP	2.36	3.879	2.96	4.85
2-CBP	5.13	3.516	2.43	4.07
2,2'-CBP	3.45	2.020	1.49	3.52
2,5,4'-CBP	0.436	1.496	1.19	-
2,5,2'-CBP	0.741	1.333	1.08	-
3,5,3',5',-CBP	0.084	0.977	0.644	-
2,4,5,4',5'-CBP	0.388	0.250	0.208	0.302

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	MASS DISTRIBUTION (%) IN BIOTA			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	7.19 E-06	1.42 E-05	6.70 E-06
Fluorobenzene	7.98 E-06	7.50 E-06	2.19 E-06	7.6 E-06
Chlorobenzene	3.53 E-05	3.21 E-05	4.06 E-05	4.07 E-05
p-difluorobenzene	1.06 E-05	7.70 E-06	3.58 E-07	1.02 E-05
m-difluorobenzene	1.09 E-05	7.35 E-06	3.63 E-07	7.50 E-06
o-difluorobenzene	4.58 E-06	1.66 E-05	6.85 E-06	6.31 E-05
p-dichlorobenzene	1.83 E-04	1.69 E-04	1.04 E-04	8.41 E-04
m-dichlorobenzene	1.87 E-04	1.67 E-04	1.06 E-04	1.75 E-04
o-dichlorobenzene	1.08 E-04	2.45 E-04	7.59 E-05	3.46 E-04
Bromobenzene	1.13 E-04	8.41 E-05	9.09 E-05	9.16 E-05
1,3,5-trichlorobenzene	7.24 E-04	7.03 E-04	2.77 E-04	7.96 E-05
1,2,4-trichlorobenzene	4.56 E-04	8.16 E-04	1.91 E-04	5.73 E-04
1,2,3-trichlorobenzene	2.91 E-04	9.63 E-04	1.36 E-04	7.71 E-04

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	4.57 E-04	4.23 E-04	2.37 E-04	2.83 E-04
m-bromochlorobenzene	4.65 E-04	4.20 E-04	2.41 E-04	7.09 E-04
o-bromochlorobenzene	2.46 E-04	5.40 E-04	1.5 E-04	1.05 E-03
Iodobenzene	7.46 E-04	6.42 E-04	5.14 E-04	4.64 E-04
1,2,4,5-tetrachlorobenzene	1.13 E-03	2.14 E-03	3.32 E-04	1.12 E-03
1,2,3,5-tetrachlorobenzene	1.12 E-03	2.14 E-03	3.37 E-04	6.26 E-04
p-dibromobenzene	1.06 E-03	1.02 E-03	5.49 E-04	6.32 E-04
m-dibromobenzene	1.07 E-03	1.02 E-03	5.57 E-04	2.0 E-03
o-dibromobenzene	5.19 E-04	1.15 E-03	2.88 E-04	1.79 E-03
p-chloroiodobenzene	2.28 E-03	2.25 E-03	1.27 E-03	1.64 E-03
m-chloroiodobenzene	2.31 E-03	2.25 E-03	1.28 E-03	2.58 E-03
o-chloroiodobenzene	1.16 E-03	2.14 E-04	5.94 E-04	3.15 E-03
Pentachlorobenzene	1.77 E-03	3.12 E-03	3.44 E-04	9.65 E-04
p-bromoiodobenzene	4.3 E-03	4.21 E-03	2.69 E-03	4.70 E-03
Hexachlorobenzene	3.34 E-03	2.89 E-03	3.9 E-04	5.6 E-03
1,3,5-tribromobenzene	5.63 E-03	5.15 E-03	2.97 E-03	9.55 E-03
1,2,4-tribromobenzene	3.74 E-03	4.14 E-03	1.59 E-03	1.11 E-02

Table V. Continued

	MASS DISTRIBUTION (%) IN BIOTA			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	9.81 E-03	9.06 E-03	7.95 E-03	1.06 E-02
m-diiodobenzene	9.85 E-03	9.11 E-03	8.01 E-03	8.55 E-03
o-diiodobenzene	6.5 E-03	5.99 E-03	3.59 E-03	1.06 E-02
ALKYLBENZENES				
Toluene	1.65 E-05	9.28 E-06	3.64 E-05	1.5 E-05
Ethylbenzene	3.82 E-05	6.60 E-05	1.21 E-04	3.06 E-05
p-xylene	4.23 E-05	3.17 E-05	8.07 E-05	5.01 E-05
m-xylene	4.2 E-05	3.23 E-05	8.19 E-05	4.12 E-05
o-xylene	4.81 E-05	2.39 E-05	6.31 E-05	4.86 E-05
n-propylbenzene	6.32 E-05	5.05 E-04	5.62 E-04	7.71 E-05
i-propylbenzene	5.68 E-05	5.13 E-04	6.19 E-04	5.03 E-05
n-butylbenzene	2.33 E-04	3.95 E-04	4.16 E-04	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	2.88 E-03	1.13 E-03	1.09 E-03	-
Fluorene	1.35 E-02	1.57 E-02	1.43 E-02	-
Phenanthrene	1.54 E-02	1.39 E-02	1.24 E-02	1.54 E-02
Anthracene	1.61 E-02	1.43 E-02	1.28 E-02	1.50 E-02

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
Pyrene	1.42 E-02	1.43 E-02	1.46 E-02	1.43 E-02
Chrysene	1.15 E-02	1.13 E-02	1.26 E-02	1.15 E-02
Perylene	9.43 E-03	9.48 E-03	1.06 E-02	9.34 E-02
Benzo (a) pyrene	9.48 E-03	9.52 E-03	1.06 E-02	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	3.49 E-03	2.39 E-03	1.88 E-03	3.87 E-03
4-CBP	2.3 E-03	4.34 E-03	3.48 E-03	7.86 E-03
2-CBP	4.14 E-03	4.45 E-03	2.87 E-03	6.6 E-03
2,2'-CBP	5.35 E-03	5.86 E-03	4.08 E-03	1.83 E-03
2,5,4'-CBP	2.61 E-03	7.41 E-03	7.54 E-03	-
2,5,2'-CBP	3.72 E-03	7.03 E-03	6.89 E-03	-
3,5,3',5',-CBP	2.02 E-03	8.43 E-03	9.47 E-03	-
2,4,5,4',5'-CBP	7.78 E-03	5.09 E-03	7.36 E-03	9.41 E-03

Tablo V.: Results of Compartmental Distribution Values for
Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	MASS DISTRIBUTION (%) IN SUSPENDED SOLIDS			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	1.35 E-05	2.89 E-05	1.26 E-05
Fluorobenzene	1.64 E-05	1.52 E-05	4.36 E-06	1.50 E-05
Chlorobenzene	8.12 E-05	7.33 E-05	9.89 E-05	9.79 E-05
p-difluorobenzene	2.33 E-05	1.69 E-05	6.88 E-07	2.25 E-05
m-difluorobenzene	2.39 E-05	1.60 E-05	6.98 E-07	1.65 E-05
o-difluorobenzene	9.93 E-06	3.52 E-05	1.44 E-05	1.39 E-04
p-dichlorobenzene	5.11 E-04	4.72 E-04	2.94 E-04	2.45 E-03
m-dichlorobenzene	5.21 E-04	4.65 E-04	2.98 E-04	5.44 E-04
o-dichlorobenzene	3.17 E-04	7.15 E-04	2.14 E-04	1.08 E-03
Bromobenzene	2.94 E-04	2.18 E-04	2.47 E-04	2.32 E-04
1,3,5-trichlorobenzene	2.4 E-03	2.33 E-03	9.03 E-04	3.14 E-04
1,2,4-trichlorobenzene	1.57 E-03	2.82 E-03	6.25 E-04	2.19 E-03
1,2,3-trichlorobenzene	1.04 E-03	3.45 E-03	4.45 E-04	3.04 E-03

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SUSPENDED SOLIDS Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	1.43 E-03	1.32 E-03	7.44 E-04	9.58 E-04
m-bromochlorobenzene	1.45 E-03	1.31 E-03	7.56 E-04	2.4 E-03
o-bromochlorobenzene	8.11 E-04	1.77 E-03	4.70 E-04	3.57 E-03
Iodobenzene	2.40 E-03	2.07 E-03	1.70 E-03	1.34 E-03
1,2,4,5-tetrachlorobenzene	4.52 E-03	8.87 E-03	1.26 E-03	5.08 E-03
1,2,3,5-tetrachlorobenzene	4.57 E-03	8.86 E-03	1.27 E-03	3.23 E-03
p-dibromobenzene	3.67 E-03	3.55 E-03	1.92 E-03	2.33 E-03
m-dibromobenzene	3.72 E-03	3.54 E-03	1.95 E-03	7.38 E-03
o-dibromobenzene	1.91 E-03	4.25 E-03	1.001 E-03	6.58 E-03
p-chloroiodobenzene	8.61 E-03	8.55 E-03	4.85 E-03	6.12 E-03
m-chloroiodobenzene	8.72 E-03	8.55 E-03	4.93 E-03	9.64 E-03
o-chloroiodobenzene	4.65 E-03	8.65 E-03	2.28 E-03	1.18 E-02
Pentachlorobenzene	8.64 E-03	1.56 E-02	1.51 E-03	5.23 E-03
p-bromoiodobenzene	1.78 E-02	1.77 E-02	1.15 E-02	1.91 E-02
Hexachlorobenzene	1.87 E-02	1.69 E-02	1.99 E-03	3.02 E-02
1,3,5-tribromobenzene	2.47 E-02	2.29 E-02	1.34 E-02	6.16 E-02
1,2,4-tribromobenzene	1.71 E-02	1.92 E-02	7.19 E-03	7.16 E-02

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SUSPENDED SOLIDS Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
p-diiodobenzene	4.73 E-02	4.47 E-02	4.16 E-02	4.76 E-02
m-diiodobenzene	4.74 E-02	4.48 E-02	4.20 E-02	3.83 E-02
o-diiodobenzene	3.31 E-02	3.14 E-02	1.88 E-02	4.78 E-02
ALKYLBENZENES				
Toluene	3.81 E-05	2.10 E-05	8.61 E-05	3.42 E-05
Ethylbenzene	1.03 E-04	1.77 E-04	3.29 E-04	8.19 E-05
p-xylene	1.14 E-04	8.61 E-05	2.15 E-04	1.36 E-04
m-xylene	1.13 E-04	8.75 E-05	2.18 E-04	1.12 E-04
o-xylene	1.28 E-04	6.53 E-05	1.68 E-04	1.29 E-04
n-propylbenzene	2.01 E-04	1.56 E-03	1.73 E-03	2.48 E-04
i-propylbenzene	1.83 E-04	1.59 E-03	1.88 E-03	1.61 E-04
n-butylbenzene	7.80 E-04	1.47 E-03	1.61 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	8.31 E-03	3.22 E-03	3.30 E-03	-
Fluorene	5.52 E-02	6.39 E-02	5.87 E-02	-
Phenanthrene	6.89 E-02	6.31 E-02	5.38 E-02	6.81 E-02
Anthracene	7.17 E-02	6.47 E-02	5.56 E-02	6.71 E-02

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SUSPENDED SOLIDS Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity)
Pyrene	7.76 E-02	7.99 E-02	7.66 E-02	7.81 E-02
Chrysene	7.98 E-02	7.94 E-02	7.88 E-02	7.99 E-02
Perylene	8.02 E-02	8.02 E-02	8.01 E-02	7.96 E-02
Benzo (a) pyrene	8.03 E-02	8.02 E-02	8.01 E-02	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	1.22 E-02	8.57 E-03	6.78 E-03	1.38 E-02
4-CBP	9.3 E-03	1.80 E-02	1.45 E-02	3.47 E-02
2-CBP	1.62 E-02	1.88 E-02	1.20 E-02	2.92 E-02
2,2'-CBP	2.35 E-02	2.89 E-02	1.98 E-02	6.64 E-03
2,5,4'-CBP	1.45 E-02	3.99 E-02	4.24 E-02	-
2,5,2'-CBP	2.01 E-02	3.83 E-02	3.88 E-02	-
3,5,3',5',-CBP	1.44 E-02	5.01 E-02	6.18 E-02	-
2,4,5,4',5'-CBP	5.36 E-02	3.52 E-02	5.61 E-02	7.01 E-02

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	MASS DISTRIBUTION (%) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc. Fugacity
HALOBENZENES				
Benzene	-	8.08 E-03	1.74 E-02	7.57 E-03
Fluorobenzene	9.84 E-03	9.15 E-03	2.61 E-03	9.01 E-03
Chlorobenzene	4.87 E-02	4.40 E-02	5.93 E-02	5.87 E-02
p-difluorobenzene	1.40 E-02	1.01 E-02	4.13 E-04	1.35 E-02
m-difluorobenzene	1.43 E-02	9.63 E-03	4.19 E-04	9.90 E-03
o-difluorobenzene	5.96 E-03	2.11 E-02	8.67 E-03	8.35 E-02
p-dichlorobenzene	0.307	0.283	0.177	1.47
m-dichlorobenzene	0.313	0.279	0.179	0.327
o-dichlorobenzene	0.190	0.429	0.129	0.648
Bromobenzene	0.176	0.131	0.148	0.139
1,3,5-trichlorobenzene	1.44	1.400	0.542	0.188
1,2,4-trichlorobenzene	0.941	1.692	0.375	1.31
1,2,3-trichlorobenzene	0.622	2.072	0.267	1.82

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SEDIMENT Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	0.856	0.794	0.447	0.575
m-bromochlorobenzene	0.870	0.788	0.453	1.44
o-bromochlorobenzene	0.486	1.063	0.282	2.14
Iodobenzene	1.44	1.241	1.02	0.801
1,2,4,5-tetrachlorobenzene	2.71	5.324	0.754	3.05
1,2,3,5-tetrachlorobenzene	2.74	5.318	0.764	1.94
p-dibromobenzene	2.20	2.128	1.15	1.40
m-dibromobenzene	2.23	2.121	1.17	4.43
o-dibromobenzene	1.14	2.551	0.604	3.95
p-chloroiodobenzene	5.17	5.128	2.91	3.67
m-chloroiodobenzene	5.23	5.131	2.96	5.79
o-chloroiodobenzene	2.79	5.190	1.37	7.07
Pentachlorobenzene	5.18	9.371	0.907	3.14
p-bromoiodobenzene	10.68	10.594	6.90	11.46
Hexachlorobenzene	11.24	10.145	1.19	18.15
1,3,5-tribromobenzene	14.81	13.761	8.05	36.94
1,2,4-tribromobenzene	10.24	11.548	4.32	42.96

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	28.36	26.796	24.98	28.58
m-diiodobenzene	28.45	26.906	25.18	22.99
o-diiodobenzene	19.87	18.852	11.29	28.68
ALKYLBENZENES				
Toluene	0.023	0.126	0.052	0.021
Ethylbenzene	0.062	0.106	0.197	0.049
p-xylene	0.068	0.052	0.129	0.081
m-xylene	0.068	0.052	0.131	0.067
o-xylene	0.077	0.039	1.101	0.077
n-propylbenzene	0.121	0.937	1.04	0.149
i-propylbenzene	0.110	0.952	1.13	0.096
n-butylbenzene	0.468	0.883	0.986	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	4.98	1.990	1.98	-
Fluorene	33.09	38.335	35.20	-
Phenanthrene	41.34	37.870	32.27	40.89
Anthracene	42.99	38.817	33.38	40.25

Table V. Continued

Compound	MASS DISTRIBUTION (%) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	46.53	46.741	45.99	46.86
Chrysene	47.89	47.619	47.26	47.96
Perylene	48.13	48.146	48.06	47.75
Benzo (a) pyrene	48.15	48.148	48.07	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.35	5.144	4.07	8.27
4-CBP	5.58	10.779	8.72	20.83
2-CBP	9.70	11.290	7.21	17.51
2,2'-CBP	14.09	17.310	11.88	3.98
2,5,4'-CBP	8.72	23.941	25.42	-
2,5,2'-CBP	12.04	22.963	23.26	-
3,5,3',5',-CBP	8.62	30.039	37.07	-
2,4,5,4',5'-CBP	32.14	21.100	33.64	42.04

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	EQUILIBRIUM DISTRIBUTION (%) IN SUSP. SOLIDS AND SEDIMENT			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	18.44	19.65	18.49
Fluorobenzene	19.68	19.53	18.89	19.16
Chlorobenzene	21.13	21.03	21.75	21.63
p-difluorobenzene	20.51	20.44	16.31	20.52
m-difluorobenzene	20.47	20.39	16.35	20.48
o-difluorobenzene	20.21	20.15	19.96	20.66
p-dichlorobenzene	23.23	23.20	23.32	23.64
m-dichlorobenzene	23.21	23.18	23.32	24.32
o-dichlorobenzene	23.69	23.67	23.32	24.32
Bromobenzene	22.48	22.42	22.93	22.20
1,3,5-trichlorobenzene	24.91	24.94	24.76	26.51
1,2,4-trichlorobenzene	25.26	25.31	24.76	26.23
1,2,3-trichlorobenzene	25.60	25.66	24.77	26.53

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN SUSP. SOLIDS AND SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	24.35	24.35	24.39	25.12
m-bromochlorobenzene	24.33	24.34	24.39	25.12
o-bromochlorobenzene	24.84	24.81	24.40	25.12
Iodobenzene	24.64	24.65	24.91	23.53
1,2,4,5-tetrachlorobenzene	26.85	26.97	26.15	27.74
1,2,3,5-tetrachlorobenzene	26.84	26.97	26.15	28.83
p-dibromobenzene	25.36	25.40	25.42	25.90
m-dibromobenzene	25.35	25.39	25.42	25.90
o-dibromobenzene	25.89	25.95	25.43	25.90
p-chloroiodobenzene	26.14	26.21	26.28	26.06
m-chloroiodobenzene	26.13	26.20	26.28	26.06
o-chloroiodobenzene	26.64	26.74	26.27	26.06
Pentachlorobenzene	28.37	28.59	27.48	29.21
p-bromoiodobenzene	26.96	27.07	27.24	26.81
Hexachlorobenzene	29.49	29.80	28.74	29.18
1,3,5-tribromobenzene	27.46	27.60	27.72	30.53
1,2,4-tribromobenzene	27.79	27.97	27.73	30.53

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN SUSP. SOLIDS AND SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	28.26	28.45	28.95	27.65
m-diiodobenzene	28.25	28.44	28.95	27.65
o-diiodobenzene	28.73	28.96	28.96	27.68
ALKYLBENZENES				
Toluene	21.11	20.86	21.42	21.00
Ethylbenzene	22.89	22.79	22.93	22.76
p-xylene	22.84	22.89	22.73	22.88
m-xylene	22.85	22.89	22.73	22.95
o-xylene	22.70	22.96	22.74	22.66
n-propylbenzene	24.50	24.25	24.22	24.61
i-propylbenzene	24.61	24.25	24.07	24.54
n-butylbenzene	24.99	26.02	25.42	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	23.56	23.69	24.03	-
Fluorene	26.83	26.79	26.89	-
Phenanthrene	27.64	27.75	27.39	27.53
Anthracene	27.59	27.72	27.38	27.62

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN SUSP. SOLIDS AND SEDIMENT Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	29.28	29.25	28.95	29.29
Chrysene	31.05	31.14	30.33	31.06
Perylene	32.39	32.35	31.66	32.39
Benzo (a) pyrene	32.36	32.33	31.65	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	25.45	25.65	25.72	25.61
4-CBP	26.75	26.96	27.04	27.53
2-CBP	26.46	27.15	27.05	27.53
2,2'-CBP	27.47	28.41	28.32	25.74
2,5,4'-CBP	29.42	29.16	29.50	-
2,5,2'-CBP	29.18	29.25	29.51	-
3,5,3',5',-CBP	31.23	29.92	30.61	-
2,4,5,4',5'-CBP	31.00	31.02	31.68	31.53

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	EQUILIBRIUM DISTRIBUTION (%) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	49.19	48.12	49.11
Fluorobenzene	47.85	48.02	47.53	48.49
Chlorobenzene	45.89	46.05	44.68	44.94
p-difluorobenzene	46.69	46.66	42.45	46.66
m-difluorobenzene	46.78	46.72	42.53	46.57
o-difluorobenzene	46.65	47.44	47.35	46.80
p-dichlorobenzene	41.56	41.63	41.34	40.63
m-dichlorobenzene	41.61	41.67	41.34	39.01
o-dichlorobenzene	40.47	40.55	41.31	39.01
Bromobenzene	43.23	43.34	42.21	43.81
1,3,5-trichlorobenzene	37.61	37.53	37.96	33.63
1,2,4-trichlorobenzene	36.74	36.64	37.94	34.37
1,2,3-trichlorobenzene	35.90	35.79	37.91	33.64

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	38.95	38.94	38.84	37.09
m-bromochlorobenzene	38.98	38.98	38.84	37.09
o-bromochlorobenzene	37.76	37.83	38.81	37.09
Iodobenzene	38.25	38.24	37.59	40.87
1,2,4,5-tetrachlorobenzene	32.84	32.53	34.57	30.64
1,2,3,5-tetrachlorobenzene	32.86	32.56	34.57	27.92
p-dibromobenzene	36.51	36.42	36.35	35.19
m-dibromobenzene	36.54	36.45	36.35	35.19
o-dibromobenzene	35.21	35.06	36.33	35.19
p-chloroiodobenzene	34.60	34.43	34.26	34.80
m-chloroiodobenzene	34.63	34.46	34.26	34.80
o-chloroiodobenzene	33.37	33.12	34.26	34.80
Pentachlorobenzene	29.07	28.51	31.28	26.96
p-bromoiodobenzene	32.57	32.30	31.87	32.95
Hexachlorobenzene	26.28	25.49	28.13	27.03
1,3,5-tribromobenzene	31.33	30.97	30.69	23.67
1,2,4-tribromobenzene	30.50	30.07	30.67	23.67

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	29.34	28.87	27.63	30.86
m-diiodobenzene	29.35	28.89	27.63	30.86
o-diiodobenzene	28.17	27.59	27.61	30.79
ALKYLBENZENES				
Toluene	45.77	46.02	45.33	45.96
Ethylbenzene	42.24	42.50	42.23	42.50
p-xylene	42.36	42.19	42.64	42.28
m-xylene	42.34	42.20	42.64	42.11
o-xylene	42.69	42.00	42.62	42.76
n-propylbenzene	38.52	39.17	39.25	38.27
i-propylbenzene	38.24	39.19	39.62	38.42
n-butylbenzene	37.39	34.88	36.36	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	40.83	40.50	39.71	-
Fluorene	32.90	32.99	32.76	-
Phenanthrene	30.89	30.60	31.50	31.15
Anthracene	31.01	30.69	31.52	30.93

Table V. Continued

Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
	EQUILIBRIUM DISTRIBUTION (%) IN BIOTA			
Pyrene	26.80	26.88	27.61	26.76
Chrysene	22.38	22.15	24.17	22.35
Perylene	19.03	19.11	20.85	19.02
Benzo (a) pyrene	19.11	19.17	20.87	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	36.29	35.80	35.63	35.90
4-CBP	33.10	32.57	32.37	31.15
2-CBP	33.84	32.09	32.35	31.15
2,2'-CBP	31.32	28.98	29.19	35.59
2,5,4'-CBP	26.43	27.09	26.24	-
2,5,2'-CBP	27.04	26.87	26.22	-
3,5,3',5',-CBP	21.93	25.20	23.47	-
2,4,5,4',5'-CBP	22.50	22.45	20.80	21.18

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	EQUILIBRIUM DISTRIBUTION (%) IN WATER			
Compound	Calc.(a)	Calc.(h)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	3.919	2.356	3.808
Fluorobenzene	2.251	2.410	2.717	2.856
Chlorobenzene	1.140	1.198	0.809	0.868
p-difluorobenzene	1.513	1.598	2.937	1.500
m-difluorobenzene	1.551	1.572	2.937	1.497
e-difluorobenzene	1.634	1.862	1.939	1.475
p-dichlorobenzene	0.345	0.351	0.325	0.268
m-dichlorobenzene	0.349	0.355	0.325	0.174
o-dichlorobenzene	0.258	0.263	0.324	0.174
Bromobenzene	0.540	0.557	0.411	0.631
1,3,5-trichlorobenzene	0.119	0.118	0.131	0.040
1,2,4-trichlorobenzene	0.094	0.092	0.130	0.049
1,2,3-trichlorobenzene	0.075	0.072	0.130	0.040

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	0.171	0.171	0.166	0.103
m-bromochlorobenzene	0.173	0.172	0.166	0.103
o-bromochlorobenzene	0.124	0.127	0.165	0.103
Iodobenzene	0.142	0.141	0.119	0.285
1,2,4,5-tetrachlorobenzene	0.032	0.029	0.052	0.016
1,2,3,5-tetrachlorobenzene	0.032	0.029	0.052	0.007
p-dibromobenzene	0.088	0.086	0.085	0.061
m-dibromobenzene	0.089	0.087	0.085	0.061
o-dibromobenzene	0.062	0.059	0.084	0.061
p-chloroiodobenzene	0.052	0.050	0.047	0.055
m-chloroiodobenzene	0.052	0.050	0.047	0.055
o-chloroiodobenzene	0.037	0.034	0.047	0.055
Pentachlorobenzene	0.010	0.008	0.020	0.005
p-bromoiodobenzene	0.029	0.027	0.024	0.033
Hexachlorobenzene	4.19 E-03	3.23 E-03	7.64 E-03	5.36 E-03
1,3,5-tribromobenzene	0.020	0.002	0.017	0.002
1,2,4-tribromobenzene	0.016	0.0014	0.017	0.002

Table V. Continued

	EQUILIBRIUM DISTRIBUTION (%) IN WATER			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	1.11 E-02	9.61 E-03	0.65 E-02	1.76 E-02
m-diiodobenzene	1.12 E-02	9.67 E-03	0.65 E-02	1.76 E-02
o-diiodobenzene	7.73 E-03	6.42 E-03	6.46 E-03	1.72 E-02
ALKYLBENZENES				
Toluene	1.127	1.249	0.972	1.191
Ethylbenzene	0.417	0.445	0.412	0.448
p-xylene	0.431	0.413	0.462	0.420
m-xylene	0.429	0.414	0.462	0.402
o-xylene	0.469	0.394	0.460	0.478
n-propylbenzene	0.153	0.182	0.186	0.143
i-propylbenzene	0.142	0.182	0.205	0.149
n-butylbenzene	0.112	0.056	0.085	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	0.283	0.259	0.210	-
Fluorene	3.21 E-02	3.29 E-02	3.07 E-02	-
Phenanthrene	1.78 E-02	1.63 E-02	2.13 E-02	1.92 E-02
Anthracene	1.84 E-02	1.66 E-02	2.15 E-02	1.80 E-02

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	4.98 E-03	5.11 E-03	6.46 E-03	4.90 E-03
Chrysene	1.08 E-03	9.84 E-04	2.04 E-03	1.06 E-03
Perylene	2.87 E-04	2.97 E-04	5.99 E-04	2.85 E-04
Benzo (a) pyrene	2.96 E-04	3.04 E-04	6.03 E-04	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	8.31 E-02	7.25 E-02	6.93 E-02	7.45 E-02
4-CBP	3.40 E-02	2.91 E-02	2.75 E-02	1.92 E-02
2-CBP	4.20 E-02	2.54 E-02	2.73 E-02	1.92 E-02
2,2'-CBP	2.02 E-02	9.94 E-03	1.06 E-02	6.83 E-02
2,5,4'-CBP	4.42 E-03	5.47 E-03	4.14 E-03	-
2,5,2'-CBP	5.39 E-03	5.09 E-03	4.11 E-03	-
3,5,3',5',-CBP	9.07 E-04	2.92 E-03	15.94 E-04	-
2,4,5,4',5'-CBP	11.2 E-04	1.10 E-03	5.89 E-04	6.80 E-04

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	EQUILIBRIUM DISTRIBUTION (%) IN SOIL			
Compound	Calc.(a)	Calc.(h)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	9.22	9.83	9.25
Fluorobenzene	9.84	9.77	9.45	9.58
Chlorobenzene	10.57	10.52	10.88	10.81
p-difluorobenzene	10.26	10.22	8.16	10.26
m-difluorobenzene	10.23	10.19	8.17	10.24
e-difluorobenzene	10.11	10.07	9.98	10.33
p-dichlorobenzene	11.61	11.60	11.66	11.82
m-dichlorobenzene	11.60	11.59	11.66	12.16
o-dichlorobenzene	11.85	11.83	11.66	12.16
Bromobenzene	11.24	11.21	11.46	11.10
1,3,5-trichlorobenzene	12.45	12.47	12.38	13.26
1,2,4-trichlorobenzene	12.63	12.65	12.38	13.12
1,2,3-trichlorobenzene	12.80	12.83	12.39	13.26

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	12.17	12.18	12.19	12.56
m-bromochlorobenzene	12.17	12.17	12.20	12.56
o-bromochlorobenzene	12.42	12.41	12.20	12.56
Iodobenzene	12.32	12.32	12.46	11.77
1,2,4,5-tetrachlorobenzene	13.43	13.49	13.07	13.87
1,2,3,5-tetrachlorobenzene	13.42	13.48	13.07	14.41
p-dibromobenzene	12.68	12.70	12.71	12.95
m-dibromobenzene	12.67	12.69	12.71	12.95
o-dibromobenzene	12.94	12.97	12.72	12.95
p-chloroiodobenzene	13.07	13.10	13.14	13.03
m-chloroiodobenzene	13.06	13.10	13.14	13.03
o-chloroiodobenzene	13.32	13.37	13.14	13.03
Pentachlorobenzene	14.18	14.30	13.74	14.61
p-bromoiodobenzene	13.48	13.54	13.62	13.40
Hexachlorobenzene	14.74	14.90	14.37	14.59
1,3,5-tribromobenzene	13.73	13.80	13.86	15.27
1,2,4-tribromobenzene	13.90	13.98	13.86	15.27

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	14.13	14.23	14.47	13.83
m-diiodobenzene	14.13	14.22	14.47	13.83
o-diiodobenzene	14.36	14.48	14.48	13.84
ALKYLBENZENES				
Toluene	10.56	10.43	10.71	10.50
Ethylbenzene	11.44	11.39	11.46	11.38
p-xylene	11.42	11.45	11.37	11.44
m-xylene	11.42	11.45	11.37	11.47
o-xylene	11.35	11.48	11.37	11.33
n-propylbenzene	12.25	12.13	12.11	12.31
i-propylbenzene	12.31	12.12	12.04	12.27
n-butylbenzene	12.50	13.01	12.71	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	11.78	11.85	12.02	-
Fluorene	13.41	13.39	13.44	-
Phenanthrene	13.82	13.88	13.70	13.77
Anthracene	13.79	13.86	13.69	13.81

Table V. Continued

	EQUILIBRIUM DISTRIBUTION (%) IN SOIL			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	14.64	14.62	14.48	14.65
Chrysene	15.52	15.57	15.17	15.53
Perylene	16.19	16.18	15.83	16.20
Benzo (a) pyrene	16.18	16.17	15.83	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	12.73	12.83	12.86	12.80
4-CBP	13.37	13.48	13.52	13.77
2-CBP	13.22	13.58	13.53	13.77
2,2'-CBP	13.73	14.20	14.16	12.87
2,5,4'-CBP	14.71	14.58	14.75	-
2,5,2'-CBP	14.59	14.63	14.76	-
3,5,3',5',-CBP	15.61	14.96	15.31	-
2,4,5,4',5'-CBP	15.50	15.51	15.84	15.76

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	EQUILIBRIUM DISTRIBUTION (%) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	0.794	0.394	0.850
Fluorobenzene	0.697	0.745	2.53	0.741
Chlorobenzene	0.150	0.166	0.127	0.128
p-difluorobenzene	0.512	0.705	13.82	0.531
m-difluorobenzene	0.498	0.739	13.66	0.722
o-difluorobenzene	1.19	0.332	0.804	0.085
p-dichlorobenzene	2.59 E-02	2.81 E-02	4.57 E-02	5.15 E-03
m-dichlorobenzene	2.54 E-02	2.85 E-02	4.50 E-02	2.57 E-02
o-dichlorobenzene	4.31 E-02	1.88 E-02	6.29 E-02	1.28 E-02
Bromobenzene	4.39 E-02	5.93 E-02	5.36 E-02	5.49 E-02
1,3,5-trichlorobenzene	5.74 E-03	5.92 E-03	1.56 E-02	4.90 E-02
1,2,4-trichlorobenzene	9.11 E-03	4.95 E-03	2.28 E-02	6.74 E-03
1,2,3-trichlorobenzene	1.41 E-02	4.06 E-03	3.21 E-02	4.85 E-03

Table V. Continued

	EQUILIBRIUM DISTRIBUTION (%) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	9.85 E-03	1.04 E-02	1.87 E-02	1.50 E-02
m-bromochlorobenzene	9.41 E-03	1.04 E-02	1.85 E-02	5.80 E-03
o-bromochlorobenzene	1.76 E-02	7.84 E-03	2.99 E-02	3.81 E-03
Iodobenzene	5.64 E-03	6.61 E-03	8.21 E-03	9.78 E-03
1,2,4,5-tetrachlorobenzene	3.24 E-03	1.54 E-03	1.19 E-02	2.97 E-03
1,2,3,5-tetrachlorobenzene	3.20 E-03	1.55 E-03	1.72 E-02	4.99 E-03
p-dibromobenzene	3.75 E-03	3.89 E-03	7.44 E-03	6.24 E-03
m-dibromobenzene	3.69 E-03	3.90 E-03	7.33 E-03	1.79 E-03
o-dibromobenzene	7.66 E-03	3.30 E-03	1.45 E-02	2.04 E-03
p-chloroiodobenzene	1.52 E-03	1.54 E-03	2.91 E-03	2.23 E-03
m-chloroiodobenzene	1.50 E-03	1.54 E-03	2.87 E-03	1.32 E-03
o-chloroiodobenzene	3.11 E-03	1.57 E-03	6.48 E-03	1.04 E-03
Pentachlorobenzene	1.70 E-03	8.50 E-04	1.04 E-02	3.04 E-03
p-bromoiodobenzene	6.54 E-04	6.66 E-04	1.16 E-03	5.86 E-04
Hexachlorobenzene	6.99 E-04	8.08 E-04	8.21 E-03	3.45 E-04
1,3,5-tribromobenzene	4.26 E-04	4.81 E-04	9.85 E-04	6.57 E-05
1,2,4-tribromobenzene	7.30 E-04	6.29 E-04	2.03 E-03	2.52 E-05

Table V. Continued

Compound	EQUILIBRIUM DISTRIBUTION (%) IN AIR Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	1.31 E-04	1.59 E-04	1.88 E-04	1.17 E-04
m-diiodobenzene	1.29 E-04	1.52 E-04	1.85 E-04	2.0 E-04
o-diiodobenzene	2.89 E-04	3.20 E-04	6.80 E-04	1.17 E-04
ALKYLBENZENES				
Toluene	0.322	0.577	0.144	0.356
Ethylbenzene	0.129	0.075	0.04	0.162
p-xylene	0.116	0.155	0.061	0.098
m-xylene	0.117	0.152	0.060	0.119
o-xylene	0.103	0.205	0.078	0.102
n-propylbenzene	7.08 E-02	8.67 E-03	7.76 E-03	5.76 E-02
i-propylbenzene	7.83 E-02	8.53 E-03	7.06 E-03	8.87 E-02
n-butylbenzene	1.84 E-02	1.01 E-02	8.91 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	1.15 E-03	3.69 E-03	3.82 E-03	-
Fluorene	5.16 E-05	1.18 E-05	3.65 E-05	-
Phenanthrene	1.27 E-05	3.61 E-05	7.35 E-05	1.34 E-05
Anthracene	2.90 E-06	2.92 E-05	6.33 E-05	1.87 E-05

Table V. Continued

	EQUILIBRIUM DISTRIBUTION (%) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	1.95 E-06	7.99 E-07	2.72 E-06	5.13 E-07
Chrysene	3.71 E-07	1.76 E-06	2.13 E-06	4.22 E-08
Perylene	1.83 E-07	7.69 E-08	1.03 E-07	2.04 E-06
Benzo (a) pyrene	7.19 E-08	5.79 E-08	8.78 E-08	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	9.31 E-04	1.48 E-03	1.95 E-03	8.11 E-04
4-CBP	1.44 E-03	6.46 E-04	8.57 E-04	2.40 E-04
2-CBP	7.14 E-04	6.15 E-04	1.08 E-03	3.28 E-04
2,2'-CBP	4.60 E-04	3.57 E-04	6.17 E-04	2.0 E-03
2,5,4'-CBP	9.63 E-04	2.08 E-04	1.87 E-04	-
2,5,2'-CBP	6.30 E-04	2.28 E-04	2.25 E-04	-
3,5,3',5',-CBP	1.04 E-03	1.28 E-04	6.51 E-05	-
2,4,5,4',5'-CBP	1.11 E-04	2.88 E-04	9.90 E-05	3.29 E-05

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	CONCENTRATION (ppm) IN AIR			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	1.09 E-03	1.09 E-03	1.09 E-03
Fluorobenzene	1.34 E-03	1.34 E-03	1.34 E-03	1.34 E-03
Chlorobenzene	1.70 E-03	1.56 E-03	1.56 E-03	1.56 E-03
p-difluorobenzene	1.59 E-03	1.59 E-03	1.59 E-03	1.59 E-03
m-difluorobenzene	1.59 E-03	1.59 E-03	1.60 E-03	1.59 E-03
o-difluorobenzene	1.60 E-03	1.59 E-03	1.59 E-03	1.57 E-03
p-dichlorobenzene	2.02 E-03	2.02 E-03	2.03 E-03	1.88 E-03
m-dichlorobenzene	2.01 E-03	2.02 E-03	2.03 E-03	2.03 E-03
o-dichlorobenzene	2.04 E-03	2.01 E-03	2.04 E-03	2.00 E-03
Bromobenzene	2.16 E-03	2.17 E-03	2.17 E-03	2.16 E-03
1,3,5-trichlorobenzene	2.41 E-03	2.41 E-03	2.49 E-03	2.53 E-03
1,2,4-trichlorobenzene	2.46 E-03	2.40 E-03	2.51 E-03	2.45 E-03
1,2,3-trichlorobenzene	2.49 E-03	2.38 E-03	2.52 E-03	2.42 E-03

Table V. Continued

Compound	CONCENTRATION (ppm) IN AIR			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	2.58 E-03	2.00 E-03	2.63 E-03	2.63 E-03
m-bromochlorobenzene	2.58 E-03	2.59 E-03	2.63 E-03	2.55 E-03
o-bromochlorobenzene	2.63 E-03	2.57 E-03	2.65 E-03	2.48 E-03
Iodobenzene	2.69 E-03	2.72 E-03	2.75 E-03	2.72 E-03
1,2,4,5-tetrachlorobenzene	2.82 E-02	2.63 E-03	2.96 E-03	2.81 E-03
1,2,3,5-tetrachlorobenzene	2.82 E-02	2.63 E-03	2.96 E-03	2.90 E-03
p-dibromobenzene	3.07 E-03	3.08 E-03	3.18 E-03	3.17 E-03
m-dibromobenzene	3.07 E-03	3.08 E-03	3.18 E-03	2.89 E-03
o-dibromobenzene	3.20 E-03	3.07 E-03	3.24 E-03	2.93 E-03
p-chloroiodobenzene	2.87 E-03	2.88 E-03	3.08 E-03	3.0 E-03
m-chloroiodobenzene	2.86 E-03	2.88 E-03	3.08 E-03	2.80 E-03
o-chloroiodobenzene	3.10 E-03	2.91 E-03	3.22 E-03	2.68 E-03
Pentachlorobenzene	3.11 E-03	2.79 E-03	3.43 E-03	3.27 E-03
p-bromoiodobenzene	2.93 E-03	2.95 E-03	3.32 E-03	2.84 E-03
Hexachlorobenzene	3.04 E-03	3.14 E-03	3.89 E-03	2.44 E-03
1,3,5-tribromobenzene	2.90 E-03	3.02 E-03	3.60 E-03	1.00 E-03
1,2,4-tribromobenzene	3.39 E-03	3.27 E-03	3.98 E-03	0.447 E-03

Table V. Continued

Compound	CONCENTRATION (ppm) IN AİR Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	1.73 E-03	1.91 E-03	2.14 E-03	1.60 E-03
m-diiodobenzene	1.72 E-03	1.90 E-03	2.12 E-03	2.19 E-03
o-diiodobenzene	2.64 E-03	2.75 E-03	3.50 E-03	1.60 E-03
ALKYLBENZENES				
Toluene	1.29 E-03	1.29 E-03	1.28 E-03	1.29 E-03
Ethylbenzene	1.48 E-03	1.47 E-03	1.46 E-03	1.480 E-03
p-xylene	1.478 E-03	1.48 E-03	1.47 E-03	1.477 E-03
m-xylene	1.479 E-03	1.48 E-03	1.47 E-03	1.479 E-03
o-xylene	1.477 E-03	1.48 E-03	1.474 E-03	1.477 E-03
n-propylbenzene	1.675 E-03	1.61 E-03	1.60 E-03	1.673 E-03
i-propylbenzene	1.676 E-03	1.61 E-03	1.59 E-03	1.677 E-03
n-butylbenzene	1.85 E-03	1.83 E-03	1.82 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	1.25 E-03	1.59 E-03	1.62 E-03	-
Fluorene	4.23 E-04	1.12 E-04	3.16 E-04	-
Phenanthrene	1.35 E-04	3.51 E-04	6.17 E-04	1.42 E-04
Anthracene	3.22 E-05	2.92 E-04	5.50 E-04	1.94 E-04

Table V. Continued

Compound	CONCENTRATION (ppm) IN AİR Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	2.51 E-05	1.03 E-05	3.49 E-03	6.63 E-06
Chrysene	5.22 E-06	2.45 E-05	3.04 E-05	5.95 E-07
Perylene	2.75 E-06	1.15 E-06	1.58 E-06	3.03 E-05
Benzo (a) pyrene	1.08 E-06	8.69 E-07	1.34 E-06	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	1.66 E-03	1.82 E-03	1.90 E-03	1.61 E-03
4-CBP	2.28 E-03	1.95 E-03	2.09 E-03	1.38 E-03
2-CBP	1.98 E-03	1.93 E-03	2.19 E-03	1.58 E-03
2,2'-CBP	2.10 E-03	1.94 E-03	2.31 E-03	2.76 E-03
2,5,4'-CBP	2.93 E-03	1.76 E-03	1.66 E-03	-
2,5,2'-CBP	2.67 E-03	1.84 E-03	1.82 E-03	-
3,5,3',5',-CBP	3.36 E-03	1.50 E-03	0.92 E-03	-
2,4,5,4',5'-CBP	1.51 E-03	2.56 E-03	1.37 E-03	5.7 E-03

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	CONCENTRATION (ppm) IN SOIL			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	1.00 E-05	2.15 E-05	9.39 E-06
Fluorobenzene	1.50 E-05	1.40 E-05	3.99 E-06	1.37 E-05
Chlorobenzene	9.48 E-05	7.86 E-05	1.06 E-04	1.05 E-04
p-difluorobenzene	2.53 E-05	1.83 E-05	7.48 E-07	2.44 E-05
m-difluorobenzene	2.60 E-05	1.74 E-05	7.58 E-07	1.79 E-05
o-difluorobenzene	1.08 E-05	3.82 E-05	1.57 E-05	1.52 E-04
p-dichlorobenzene	7.16 E-04	6.61 E-04	4.12 E-04	3.43 E-03
m-dichlorobenzene	7.30 E-04	6.50 E-04	4.18 E-04	7.62 E-04
o-dichlorobenzene	4.44 E-04	1.00 E-03	3.00 E-04	1.51 E-03
Bromobenzene	4.39 E-04	3.25 E-04	3.69 E-04	3.47 E-04
1,3,5-trichlorobenzene	4.14 E-03	4.03 E-03	1.56 E-03	5.43 E-04
1,2,4-trichlorobenzene	2.71 E-03	4.87 E-03	1.08 E-03	3.78 E-03
1,2,3-trichlorobenzene	1.79 E-03	5.93 E-03	7.69 E-04	5.25 E-03

Table V. Continued

Compound	CONCENTRATION (ppm) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	2.60 E-03	2.41 E-03	1.36 E-03	1.75 E-03
m-bromochlorobenzene	2.65 E-03	2.39 E-03	1.38 E-03	4.38 E-03
o-bromochlorobenzene	1.48 E-03	3.23 E-03	8.57 E-04	6.50 E-03
Iodobenzene	4.67 E-03	4.02 E-03	3.31 E-03	2.60 E-03
1,2,4,5-tetrachlorobenzene	9.29 E-03	18.24 E-03	2.58 E-03	10.4 E-03
1,2,3,5-tetrachlorobenzene	9.39 E-03	18.22 E-03	2.62 E-03	6.64 E-03
p-dibromobenzene	8.24 E-03	7.97 E-03	4.31 E-03	5.23 E-03
m-dibromobenzene	8.35 E-03	7.94 E-03	4.37 E-03	1.66 E-02
o-dibromobenzene	4.28 E-03	9.55 E-03	2.26 E-03	1.48 E-02
p-chloroiodobenzene	0.0196	0.0194	0.0110	0.0139
m-chloroiodobenzene	0.0198	0.0194	0.0112	0.0219
o-chloroiodobenzene	0.0106	0.0197	0.0052	0.0268
Pentachlorobenzene	0.0206	0.0372	0.0036	0.0125
p-bromoiodobenzene	0.0480	0.0476	0.0310	0.0515
Hexachlorobenzene	0.0508	0.0459	0.0054	0.0821
1,3,5-tribromobenzene	0.0740	0.0688	0.0402	0.1846
1,2,4-tribromobenzene	0.0512	0.0577	0.0216	0.2147

Table V. Continued

Compound	CONCENTRATION (ppm) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	0.1485	0.1403	0.1308	0.1497
m-diiodobenzene	0.1490	0.1409	0.1319	0.1204
o-diiodobenzene	0.1040	0.0987	0.0591	0.1502
ALKYLBENZENES				
Toluene	3.34 E-05	1.85 E-05	7.56 E-05	3.00 E-05
Ethylbenzene	1.05 E-04	1.79 E-04	3.32 E-04	8.28 E-05
p-xylene	1.152 E-04	0.87 E-04	2.18 E-04	1.37 E-04
m-xylene	1.145 E-04	0.88 E-04	2.21 E-04	1.13 E-04
o-xylene	1.29 E-04	0.66 E-04	1.70 E-04	1.30 E-04
n-propylbenzene	2.30 E-04	1.79 E-03	1.98 E-03	2.84 E-04
i-propylbenzene	2.09 E-04	1.82 E-03	2.15 E-03	1.84 E-04
n-butylbenzene	9.97 E-04	1.88 E-03	2.06 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	0.0101	0.0040	0.0040	-
Fluorene	0.0872	0.1000	0.0928	-
Phenanthrene	0.1168	0.1070	0.0912	0.1155
Anthracene	0.1215	0.1100	0.0943	0.1137

Table V. Continued

	CONCENTRATION (ppm) IN SOIL			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	0.1492	0.1500	0.1475	0.1502
Chrysene	0.1733	0.1720	0.1710	0.1736
Perylene	0.1925	0.1930	0.1923	0.1910
Benzo (a) pyrene	0.1926	0.1930	0.1923	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	0.0180	0.0130	0.0099	0.0202
4-CBP	0.0167	0.0340	0.0262	0.0625
2-CBP	0.0291	0.0323	0.0216	0.0525
2,2'-CBP	0.0499	0.0339	0.0421	0.0141
2,5,4'-CBP	0.0356	0.0613	0.1037	-
2,5,2'-CBP	0.0491	0.0977	0.0949	-
3,5,3',5',-CBP	0.0400	0.0937	0.1718	-
2,4,5,4',5'-CBP	0.1663	0.1392	0.1741	0.2176

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	CONCENTRATION (ppm) IN WATER			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	6.39 E-06	7.73 E-06	5.80 E-06
Fluorobenzene	5.15 E-06	5.16 E-06	1.72 E-06	6.15 E-06
Chlorobenzene	1.53 E-05	1.34 E-05	1.18 E-05	1.26 E-05
p-difluorobenzene	5.60 E-06	4.14 E-06	4.04 E-07	5.35 E-06
m-difluorobenzene	5.90 E-06	4.03 E-06	4.09 E-07	5.93 E-06
o-difluorobenzene	2.62 E-06	1.06 E-05	4.57 E-06	3.26 E-05
p-dichlorobenzene	3.19 E-05	2.99 E-05	1.72 E-05	1.16 E-04
m-dichlorobenzene	3.29 E-05	2.99 E-05	1.75 E-05	1.63 E-04
o-dichlorobenzene	1.45 E-05	3.33 E-05	1.25 E-05	3.24 E-05
Bromobenzene	3.16 E-05	2.42 E-05	1.99 E-05	2.96 E-05
1,3,5-trichlorobenzene	5.94 E-05	5.66 E-05	2.48 E-05	2.43 E-06
1,2,4-trichlorobenzene	3.02 E-05	5.28 E-05	1.71 E-05	2.10 E-05
1,2,3-trichlorobenzene	1.57 E-05	5.05 E-05	1.21 E-05	2.35 E-05

Table V. Continued

	CONCENTRATION (ppm) IN WATER			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	5.48 E-05	5.08 E-05	2.78 E-05	2.15 E-05
m-bromochlorobenzene	5.63 E-05	5.08 E-05	2.82 E-05	5.40 E-05
o-bromochlorobenzene	2.22 E-05	4.95 E-05	1.74 E-05	8.01 E-05
Iodobenzene	8.05 E-05	6.91 E-05	4.73 E-05	9.44 E-05
1,2,4,5-tetrachlorobenzene	3.27 E-05	5.85 E-05	1.53 E-05	1.86 E-05
1,2,3,5-tetrachlorobenzene	3.33 E-05	5.89 E-05	1.55 E-05	0.493 E-05
p-dibromobenzene	8.60 E-05	8.09 E-05	4.30 E-05	3.71 E-05
m-dibromobenzene	8.79 E-05	8.14 E-05	4.37 E-05	11.76 E-05
o-dibromobenzene	3.06 E-05	6.54 E-05	2.24 E-05	10.49 E-05
p-chloroiodobenzene	1.17 E-04	1.09 E-04	5.95 E-05	8.79 E-05
m-chloroiodobenzene	1.19 E-04	1.11 E-04	0.604 E-04	1.38 E-04
o-chloroiodobenzene	4.36 E-05	7.54 E-05	2.79 E-05	16.92 E-05
Pentachlorobenzene	2.23 E-05	3.36 E-05	0.787 E-05	6.7 E-06
p-bromoiodobenzene	1.56 E-04	1.42 E-04	0.809 E-04	1.87 E-04
Hexachlorobenzene	2.17 E-05	1.49 E-04	0.43 E-05	4.52 E-05
1,3,5-tribromobenzene	1.64 E-04	1.36 E-04	0.73 E-04	0.31 E-04
1,2,4-tribromobenzene	8.74 E-05	8.60 E-05	3.89 E-05	3.61 E-05

Table V. Continued

Compound	CONCENTRATION (ppm) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	1.75 E-04	1.42 E-04	8.82 E-05	2.86 E-04
m-diiodobenzene	1,77 E-04	1.44 E-04	8.9 E-05	2.3 E-04
o-diiodobenzene	8.40 E-05	6.57 E-05	3.96 E-05	2.80 E-04
ALKYLBENZENES				
Toluene	5.35 E-06	3.31 E-06	1.03 E-05	5.11 E-06
Ethylbenzene	5.72 E-06	1.05 E-05	1.79 E-05	4.88 E-06
p-xylene	6.52 E-06	4.71 E-06	1.33 E-05	7.55 E-06
m-xylene	6.45 E-06	4.80 E-06	1.34 E-05	5.96 E-06
o-xylene	8.02 E-06	3.40 E-06	1.03 E-05	8.23 E-06
n-propylbenzene	4.32 E-06	4.02 E-05	4.56 E-05	4.94 E-06
i-propylbenzene	3.63 E-06	4.10 E-05	5.49 E-05	3.35 E-06
n-butylbenzene	1.34 E-05	1.22 E-05	2.06 E-05	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	3.64 E-04	1.33 E-04	1.05 E-05	-
Fluorene	3.13 E-04	3.72 E-04	3.18 E-04	
Phenanthrene	2.26 E-04	1.89 E-04	2.13 E-04	2.42 E-04
Anthracene	2.43 E-04	1.99 E-04	2.22 E-04	2.22 E-04

Table V. Continued

Compound	CONCENTRATION (ppm) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	7.61 E-05	7.85 E-05	9.87 E-05	7.54 E-05
Chrysene	1.80 E-05	1.63 E-05	3.46 E-05	1.78 E-05
Perylene	5.11 E-06	5.30 E-06	1.09 E-05	5.03 E-06
Benzo (a) pyrene	5.29 E-06	5.44 E-06	1.1 E-05	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	1.76 E-04	1.07 E-04	8.04 E-05	1.77 E-04
4-CBP	6.37 E-05	1.05 E-04	7.99 E-05	1.31 E-04
2-CBP	1.38 E-04	9.49 E-05	6.55 E-05	1.1 E-04
2,2'-CBP	1.1 E-04	6.43 E-05	4.73 E-05	1.12 E-04
2,5,4'-CBP	1.60 E-05	5.49 E-05	4.37 E-05	-
2,5,2'-CBP	2.72 E-05	4.89 E-05	3.97 E-05	-
3,5,3',5',-CBP	3.48 E-06	4.08 E-05	2.69 E-05	-
2,4,5,4',5'-CBP	1.81 E-05	1.16 E-05	0.97 E-05	1.41 E-05

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	CONCENTRATION (ppm) IN BIOTA Calc.(a)	Calc.(h)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	8.02 E-05	1.58 E-04	0.75 E-04
Fluorobenzene	1.095 E-04	1.03 E-04	3.01 E-05	1.043 E-04
Chlorobenzene	6.177 E-04	5.16 E-04	6.532 E-04	6.54 E-04
p-difluorobenzene	1.728 E-04	1.26 E-04	5.838 E-06	1.665 E-04
m-difluorobenzene	1.779 E-04	1.20 E-04	5.919 E-06	1.223 E-04
e-difluorobenzene	7.467 E-05	2.70 E-04	1.117 E-04	1.035 E-03
p-dichlorobenzene	3.884 E-03	3.56 E-03	2.191 E-03	17.65 E-03
m-dichlorobenzene	3.924 E-03	3.51 E-03	2.222 E-03	3.67 E-03
o-dichlorobenzene	2.272 E-03	5.14 E-03	1.595 E-03	7.28 E-03
Bromobenzene	2.533 E-03	1.89 E-03	2.038 E-03	2.05 E-03
1,3,5-trichlorobenzene	18.8 E-03	18.21 E-03	7.18 E-03	2.06 E-03
1,2,4-trichlorobenzene	11.8 E-03	21.16 E-03	4.6 E-03	14.86 E-03
1,2,3-trichlorobenzene	7.540 E-03	24.97 E-03	3.53 E-03	19.98 E-03

Table V. Continued

Compound	CONCENTRATION (ppm) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	12.5 E-03	11.58 E-03	6.49 E-03	7.73 E-03
m-bromochlorobenzene	12.7 E-03	11.50 E-03	6.58 E-03	19.39 E-03
o-bromochlorobenzene	6.738E-03	14.77 E-03	4.09 E-03	28.80 E-03
Iodobenzene	0.0217	0.0187	0.0150	0.0135
1,2,4,5-tetrachlorobenzene	0.0341	0.0660	0.0102	0.0346
1,2,3,5-tetrachlorobenzene	0.0345	0.0660	0.0104	0.0193
p-dibromobenzene	0.0356	0.0343	0.0185	0.0213
m-dibromobenzene	0.0361	0.0342	0.0188	0.0676
o-dibromobenzene	0.0175	0.0387	0.0097	0.0603
p-chloroiodobenzene	0.0777	0.0765	0.0431	0.0557
m-chloroiodobenzene	0.0787	0.0766	0.0438	0.0878
o-chloroiodobenzene	0.0397	0.0730	0.0203	0.1072
Pentachlorobenzene	0.0633	0.1114	0.0123	0.0345
p-bromoiodobenzene	0.1738	0.1703	0.1086	0.1898
Hexachlorobenzene	0.1358	0.1177	0.0159	0.2280
1,3,5-tribromobenzene	0.2533	0.2315	0.1336	0.4293
1,2,4-tribromobenzene	0.1685	0.1861	0.0716	0.4993

Table V. Continued

Compound	CONCENTRATION (ppm) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	0.4625	0.4272	0.3746	0.5012
m-diiodobenzene	0.4644	0.4293	0.3777	0.4030
o-diiodobenzene	0.3061	0.2821	0.1690	0.5011
ALKYLBENZENES				
Toluene	2.17 E-04	1.22 E-04	4.80 E-04	1.97 E-04
Ethylbenzene	5.79 E-04	1.00 E-03	1.84 E-03	4.64 E-04
p-xylene	6.41 E-04	4.81 E-03	1.22 E-03	7.60 E-04
m-xylene	6.37 E-04	4.89 E-03	1.24 E-03	6.25 E-04
o-xylene	7.29 E-04	3.62 E-04	9.58 E-04	7.37 E-04
n-propylbenzene	1.09 E-03	8.67 E-03	9.65 E-03	1.32 E-03
i-propylbenzene	9.75 E-04	8.81 E-03	10.62 E-03	8.64 E-04
n-butylbenzene	4.48 E-03	7.57 E-03	8.85 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	0.0526	0.0210	0.0199	-
Fluorene	0.3208	0.3730	0.3390	-
Phenanthrene	0.3917	0.3540	0.3145	0.3922
Anthracene	0.4095	0.3640	0.3257	0.3821

Table V. Continued

Compound	CONCENTRATION (ppm) IN BIOTA			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	0.4097	0.4130	0.4218	0.4117
Chrysene	0.3748	0.3680	0.4088	0.3748
Perylene	0.3394	0.3410	0.3798	0.3364
Benzo (a) pyrene	0.3412	0.3470	0.3802	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	0.0768	0.0526	0.0413	0.0850
4-CBP	0.0622	0.1172	0.0940	0.2121
2-CBP	0.1117	0.1201	0.0776	0.1783
2,2'-CBP	0.1706	0.1875	0.1300	0.0585
2,5,4'-CBP	0.0959	0.2722	0.2767	-
2,5,2'-CBP	0.1366	0.2582	0.2529	-
3,5,3',5',-CBP	0.0842	0.3518	0.3951	-
2,4,5,4',5'-CBP	0.3622	0.2371	0.3430	0.4384

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	CONCENTRATION (ppm) IN SUSP. SOLID AND SEDIMENT			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	2.00 E-05	4.30 E-05	1.88 E-05
Fluorobenzene	3.00 E-05	2.79 E-05	7.97 E-06	2.75 E-05
Chlorobenzene	1.90 E-04	1.57 E-04	2.12 E-04	2.09 E-04
p-difluorobenzene	5.06 E-05	3.67 E-05	1.50 E-06	4.88 E-05
m-difluorobenzene	5.19 E-05	3.49 E-05	1.52 E-06	3.59 E-05
o-difluorobenzene	2.16 E-05	7.65 E-05	3.14 E-05	3.05 E-04
p-dichlorobenzene	1.43 E-03	1.32 E-03	8.24 E-04	6.85 E-03
m-dichlorobenzene	1.46 E-03	1.30 E-03	8.36 E-04	1.52 E-03
o-dichlorobenzene	8.87 E-04	2.00 E-03	6.00 E-04	3.02 E-03
Bromobenzene	8.78 E-04	6.51 E-04	7.38 E-04	6.94 E-04
1,3,5-trichlorobenzene	8.29 E-03	8.07 E-03	3.12 E-03	1.09 E-03
1,2,4-trichlorobenzene	5.42 E-03	9.74 E-03	2.16 E-03	7.56 E-03
1,2,3-trichlorobenzene	3.58 E-03	11.93 E-03	1.54 E-03	10.50 E-03

Table V. Continued

Compound	CONCENTRATION (ppm) IN SUSP. SOLID AND SEDIMENT Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	5.20 E-03	4.83 E-03	2.27 E-03	3.49 E-03
m-bromochlorobenzene	5.29 E-03	4.79 E-03	2.76 E-03	8.75 E-03
o-bromochlorobenzene	2.96 E-03	6.46 E-03	1.71 E-03	13.0 E-03
Iodobenzene	9.33 E-03	8.04 E-03	6.62 E-03	5.19 E-03
1,2,4,5-tetrachlorobenzene	18.6 E-03	36.49 E-03	5.17 E-03	20.88 E-03
1,2,3,5-tetrachlorobenzene	18.8 E-03	36.45 E-03	5.24 E-03	13.28 E-03
p-dibromobenzene	16.5 E-03	15.94 E-03	8.62 E-03	10.45 E-03
m-dibromobenzene	16.7 E-03	15.89 E-03	8.76 E-03	33.17 E-03
o-dibromobenzene	8.57 E-03	19.11 E-03	4.53 E-03	29.59 E-03
p-chloroiodobenzene	0.0391	0.0388	0.0220	0.0278
m-chloroiodobenzene	0.0396	0.0388	0.0224	0.0438
o-chloroiodobenzene	0.0211	0.0393	0.0104	0.0535
Pentachlorobenzene	0.0412	0.0745	0.0072	0.0249
p-bromoiodobenzene	0.0959	0.0952	0.0619	0.1029
Hexachlorobenzene	0.1016	0.0917	0.0108	0.1641
1,3,5-tribromobenzene	0.1479	0.1375	0.0804	0.3692
1,2,4-tribromobenzene	0.1023	0.1154	0.0431	0.4293

Table V. Continued

Compound	CONCENTRATION (ppm) IN SUSP. SOLID AND SEDIMENT Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	0.2970	0.2806	0.2617	0.2994
m-diiodobenzene	0.2980	0.2818	0.2638	0.2407
o-diiodobenzene	0.2081	0.1975	0.1182	0.3003
ALKYLBENZENES				
Toluene	6.68 E-05	3.69 E-05	1.51 E-04	6.01 E-05
Ethylbenzene	2.09 E-04	3.58 E-04	6.65 E-04	1.66 E-04
p-xylene	2.30 E-04	1.74 E-04	4.35 E-04	2.74 E-04
m-xylene	2.29 E-04	1.77 E-04	4.41 E-04	2.27 E-04
o-xylene	2.58 E-04	1.32 E-04	3.41 E-04	2.60 E-04
n-propylbenzene	4.60 E-04	3.58 E-03	3.97 E-04	5.67 E-04
i-propylbenzene	4.18 E-04	3.63 E-03	4.30 E-03	3.68 E-04
n-butylbenzene	2.00 E-03	3.76 E-03	4.12 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	0.0203	0.0081	0.0081	-
Fluorene	0.1744	0.2020	0.1855	-
Phenanthrene	0.2336	0.2140	0.1823	0.2311
Anthracene	0.2429	0.2194	0.1886	0.2275

Table V. Continued

Compound	CONCENTRATION (ppm) IN SUSP. SOLID AND SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	0.2984	0.2997	0.2949	0.3005
Chrysene	0.3466	0.3447	0.3421	0.3471
Perylene	0.3850	0.3852	0.3845	0.3820
Benzo (a) pyrene	0.3852	0.3852	0.3845	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	0.0359	0.0252	0.0199	0.0405
4-CBP	0.0335	0.0647	0.0523	0.1250
2-CBP	0.0582	0.0677	0.0433	0.1050
2,2'-CBP	0.0997	0.1225	0.0841	0.0282
2,5,4'-CBP	0.0711	0.1953	0.2074	-
2,5,2'-CBP	0.0982	0.1874	0.1898	-
3,5,3',5',-CBP	0.0799	0.2785	0.3436	-
2,4,5,4',5'-CBP	0.3327	0.2184	0.3481	0.4351

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	AMOUNT (mole) IN AIR			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	99.60	99.41	99.27	99.46
Fluorobenzene	99.60	99.61	99.87	99.53
Chlorobenzene	99.02	99.07	99.14	99.09
p-difluorobenzene	99.63	99.73	99.97	99.64
m-difluorobenzene	99.61	99.73	99.97	99.74
o-difluorobenzene	99.83	99.31	99.70	97.84
p-dichlorobenzene	97.85	97.99	98.81	91.42
m-dichlorobenzene	97.79	98.00	98.80	98.55
o-dichlorobenzene	98.92	97.53	99.14	97.11
Bromobenzene	98.23	98.65	98.81	98.39
1,3,5-trichlorobenzene	94.72	94.91	97.92	99.52
1,2,4-trichlorobenzene	96.88	96.46	98.56	96.47
1,2,3-trichlorobenzene	98.10	93.76	98.98	95.31

Table V. Continued

Compound	AMOUNT (mole) IN AIR			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	96.22	96.50	98.06	98.02
m-bromochlorobenzene	96.14	96.51	98.03	95.04
o-bromochlorobenzene	98.18	95.99	98.78	92.63
Iodobenzene	94.25	95.05	96.26	95.10
1,2,4,5-tetrachlorobenzene	93.32	87.06	97.94	93.08
1,2,3,5-tetrachlorobenzene	93.24	87.07	97.91	95.82
p-dibromobenzene	92.89	93.19	96.34	96.01
m-dibromobenzene	92.77	93.19	96.28	87.33
o-dibromobenzene	96.72	92.77	98.08	88.70
p-chloroiodobenzene	85.86	86.14	92.22	89.80
m-chloroiodobenzene	85.66	86.10	92.10	83.94
o-chloroiodobenzene	92.94	87.03	96.34	80.38
Pentachlorobenzene	88.63	79.63	97.90	93.31
p-bromoiodobenzene	74.01	74.52	83.70	71.60
Hexachlorobenzene	76.17	78.60	97.42	61.26
1,3,5-tribromobenzene	65.65	68.44	81.69	59.44
1,2,4-tribromobenzene	76.82	74.14	90.19	36.34

Table V. Continued

Compound	AMOUNT (mole) IN AIR Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	37.49	41.42	46.33	34.67
m-diiodobenzene	37.25	41.17	45.89	47.46
o-diiodobenzene	57.02	59.52	75.76	34.59
ALKYLBENZENES				
Toluene	99.55	99.72	99.11	99.57
Ethylbenzene	99.50	99.09	98.41	99.58
p-xylene	99.43	99.58	98.86	99.33
m-xylene	99.43	99.57	98.84	99.47
o-xylene	99.31	99.69	99.11	99.30
n-propylbenzene	99.50	95.71	95.19	99.40
i-propylbenzene	99.56	95.64	94.47	99.61
n-butylbenzene	98.33	97.53	96.92	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	69.74	88.62	90.13	-
Fluorene	18.20	4.80	13.58	-
Phenanthrene	5.41	14.06	24.73	5.70
Anthracene	1.29	11.69	22.06	7.80

Table V. Continued

Compound	AMOUNT (mole) IN AIR Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	0.89	0.36	1.23	0.23
Chrysene	0.16	0.77	0.95	0.02
Perylene	0.08	0.03	0.05	0.86
Benzo (a) pyrene	0.03	0.03	0.04	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	76.78	84.49	87.91	74.82
4-CBP	86.07	73.77	78.95	51.97
2-CBP	74.77	73.07	82.63	59.63
2,2'-CBP	67.34	62.09	73.88	88.22
2,5,4'-CBP	81.49	48.87	46.11	-
2,5,2'-CBP	74.29	51.06	50.70	-
3,5,3',5',-CBP	82.04	36.74	22.51	-
2,4,5,4',5'-CBP	32.97	56.00	30.05	12.53

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	AMOUNT (mole) IN SOIL			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	6.75 E-03	8.66 E-03	1.86 E-02	8.11 E-03
Fluorobenzene	1.06 E-02	9.80 E-03	2.80 E-03	9.65 E-03
Chlorobenzene	5.22 E-02	4.71 E-02	6.36 E-02	6.29 E-02
p-difluorobenzene	1.50 E-02	1.08 E-02	4.42 E-04	1.44 E-02
m-difluorobenzene	1.54 E-02	1.03 E-02	4.49 E-04	1.06 E-02
θ-difluorobenzene	16.10 E-02	2.26 E-02	9.29 E-03	8.95 E-02
p-dichlorobenzene	0.329	0.3033	0.189	1.57
m-dichlorobenzene	0.335	0.2986	0.192	0.350
o-dichlorobenzene	0.204	0.4595	0.138	0.694
Bromobenzene	0.189	0.1399	0.159	0.149
1,3,5-trichlorobenzene	1.54	1.5000	0.580	0.202
1,2,4-trichlorobenzene	1.01	1.81	0.402	1.41
1,2,3-trichlorobenzene	0.667	2.22	0.286	1.95

Table V. Continued

Compound	AMOUNT (mole) IN SOIL			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	0.917	0.8512	0.479	0.616
m-bromochlorobenzene	0.932	0.8439	0.486	1.54
o-bromochlorobenzene	0.521	1.14	0.302	2.29
Iodobenzene	1.54	1.33	1.10	0.858
1,2,4,5-tetrachlorobenzene	2.90	5.70	0.808	3.26
1,2,3,5-tetrachlorobenzene	2.94	5.70	0.819	2.08
p-dibromobenzene	2.36	2.28	1.23	1.50
m-dibromobenzene	2.39	2.27	1.25	4.75
o-dibromobenzene	1.23	2.73	0.647	4.23
p-chloroiodobenzene	5.54	5.50	3.12	3.94
m-chloroiodobenzene	5.60	5.50	3.17	6.20
o-chloroiodobenzene	2.98	5.56	1.47	7.57
Pentachlorobenzene	5.55	10.04	0.972	3.36
p-bromoiodobenzene	11.44	11.35	7.39	12.28
Hexachlorobenzene	12.04	10.87	1.28	19.45
1,3,5-tribromobenzene	15.86	14.74	8.62	39.58
1,2,4-tribromobenzene	10.97	12.37	4.62	46.02

Table V. Continued

Compound	AMOUNT (mole) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	30.38	28.71	26.77	30.62
m-diiodobenzene	30.49	28.83	26.98	24.63
o-diiodobenzene	21.29	20.20	12.09	30.72
ALKYLBENZENES				
Toluene	2.5 E-02	1.35 E-02	5.54 E-02	2.2 E-02
Ethylbenzene	6.6 E-02	11.40 E-02	21.10 E-02	5.26 E-02
p-xylene	7.3 E-02	5.53 E-02	13.80 E-02	8.72 E-02
m-xylene	7.3 E-02	5.62 E-02	14.00 E-02	7.21 E-02
o-xylene	8.2 E-02	4.20 E-02	10.80 E-02	8.27 E-02
n-propylbenzene	0.129	0.01	1.12	0.159
i-propylbenzene	0.117	0.01	1.21	0.103
n-butylbenzene	0.502	0.946	1.04	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	5.34	2.13	2.12	-
Fluorene	35.46	41.07	37.72	-
Phenanthrene	44.29	40.58	34.57	43.81
Anthracene	46.06	41.59	35.77	43.13

Table V. Continued

Compound	AMOUNT (mole) IN SOIL Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	49.85	50.08	49.27	50.20
Chrysene	51.31	51.02	50.64	51.39
Perylene	51.56	51.58	51.50	51.16
Benzo (a) pyrene	51.59	51.59	51.50	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.87	5.51	4.36	8.86
4-CBP	5.98	11.55	9.35	22.32
2-CBP	10.39	12.10	7.72	18.76
2,2'-CBP	15.09	18.55	12.73	4.27
2,5,4'-CBP	9.34	25.65	27.23	-
2,5,2'-CBP	12.90	24.60	24.92	-
3,5,3',5',-CBP	9.24	32.18	39.71	-
2,4,5,4',5'-CBP	34.44	22.61	36.04	45.05

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

	AMOUNT (mole) IN WATER			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	0.389	0.5725	0.693	0.520
Fluorobenzene	0.375	0.3762	0.125	0.448
Chlorobenzene	0.876	0.8351	0.736	0.786
p-difluorobenzene	0.344	0.2538	0.025	0.328
m-difluorobenzene	0.362	0.2474	0.025	0.241
e-difluorobenzene	0.161	0.6503	0.281	1.99
p-dichlorobenzene	1.52	1.430	0.82	5.54
m-dichlorobenzene	1.57	1.422	0.83	0.777
o-dichlorobenzene	0.689	1.585	0.596	1.54
Bromobenzene	1.41	1.080	0.885	1.32
1,3,5-trichlorobenzene	2.29	2.185	0.958	0.094
1,2,4-trichlorobenzene	1.17	2.038	0.658	0.811
1,2,3-trichlorobenzene	0.606	1.947	0.466	0.907

Table V. Continued

Compound	AMOUNT (mole) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	2.00	1.855	1.02	0.787
m-bromochlorobenzene	2.06	1.858	1.03	1.97
o-bromochlorobenzene	0.810	1.808	9.637	2.93
Iodobenzene	2.76	2.372	1.62	3.24
1,2,4,5-tetrachlorobenzene	1.06	1.898	0.496	0.603
1,2,3,5-tetrachlorobenzene	1.08	1.909	0.503	0.160
p-dibromobenzene	2.55	2.402	1.28	1.10
m-dibromobenzene	2.61	2.416	1.30	3.49
o-dibromobenzene	0.908	1.940	0.666	3.11
p-chloroiodobenzene	3.43	3.232	1.75	2.58
m-chloroiodobenzene	3.50	3.259	1.77	4.06
o-chloroiodobenzene	1.28	2.213	0.821	4.97
Pentachlorobenzene	0.623	0.9396	0.220	0.187
p-bromoiodobenzene	3.85	3.5148	2.00	4.63
Hexachlorobenzene	0.532	0.3661	0.106	1.11
1,3,5-tribromobenzene	3.65	3.0298	1.62	0.690
1,2,4-tribromobenzene	1.94	1.9124	0.864	0.803

Table V. Continued

Compound	AMOUNT (mole) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	3.72	3.0187	1.87	6.06
m-diiodobenzene	3.75	3.0475	1.89	4.88
o-diiodobenzene	1.78	1.3932	0.839	5.94
ALKYLBENZENES				
Toluene	0.406	0.252	0.781	0.388
Ethylbenzene	0.377	0.691	1.18	0.322
p-xylene	0.430	0.311	0.874	0.498
m-xylene	0.425	0.317	0.886	0.393
o-xylene	0.528	0.224	0.681	0.543
n-propylbenzene	0.252	2.342	2.66	2.288
i-propylbenzene	0.211	2.387	3.19	0.195
n-butylbenzene	0.70	0.637	1.07	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	19.92	7.254	5.76	-
Fluorene	13.19	15.705	13.42	-
Phenanthrene	8.88	7.418	8.36	9.51
Anthracene	9.57	7.821	8.72	8.74

Table V. Continued

Compound	AMOUNT (mole) IN WATER Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	2.64	2.722	3.42	2.61
Chrysene	0.552	0.501	1.06	0.546
Perylene	0.142	0.147	0.303	0.141
Benzo (a) pyrene	0.147	0.151	0.305	0.140
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.99	4.847	3.66	8.02
4-CBP	2.36	3.879	2.96	4.85
2-CBP	5.13	3.516	2.43	4.07
2,2'-CBP	3.45	2.020	1.49	3.52
2,5,4'-CBP	0.436	1.496	1.19	-
2,5,2'-CBP	0.741	1.333	1.08	-
3,5,3',5',-CBP	0.084	0.977	0.644	-
2,4,5,4',5'-CBP	0.388	0.250	0.208	0.302

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	AMOUNT (mole) IN BIOTA			
	Calc.(a)	Calc.(h)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	7.19 E-06	1.42 E-05	6.70 E-06
Fluorobenzene	7.98 E-06	7.50 E-06	2.19 E-06	7.6 E-06
Chlorobenzene	3.53 E-05	3.21 E-05	4.06 E-05	4.07 E-05
p-difluorobenzene	1.06 E-05	7.70 E-06	3.58 E-07	1.02 E-05
m-difluorobenzene	1.09 E-05	7.35 E-06	3.63 E-07	7.50 E-06
o-difluorobenzene	4.58 E-06	1.66 E-05	6.85 E-06	6.31 E-05
p-dichlorobenzene	1.83 E-04	1.69 E-04	1.04 E-04	8.41 E-04
m-dichlorobenzene	1.87 E-04	1.67 E-04	1.06 E-04	1.75 E-04
o-dichlorobenzene	1.08 E-04	2.45 E-04	7.59 E-05	3.46 E-04
Bromobenzene	1.13 E-04	8.41 E-05	9.09 E-05	9.16 E-05
1,3,5-trichlorobenzene	7.24 E-04	7.03 E-04	2.77 E-04	7.96 E-05
1,2,4-trichlorobenzene	4.56 E-04	8.16 E-04	1.91 E-04	5.73 E-04
1,2,3-trichlorobenzene	2.91 E-04	9.63 E-04	1.36 E-04	7.71 E-04

Table V. Continued

Compound	AMOUNT (mole) IN BIOTA Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	4.57 E-04	4.23 E-04	2.37 E-04	2.83 E-04
m-bromochlorobenzene	4.65 E-04	4.20 E-04	2.41 E-04	7.09 E-04
o-bromochlorobenzene	2.46 E-04	5.40 E-04	1.5 E-04	1.05 E-03
Iodobenzene	7.46 E-04	6.42 E-04	5.14 E-04	4.64 E-04
1,2,4,5-tetrachlorobenzene	1.13 E-03	2.14 E-03	3.32 E-04	1.12 E-03
1,2,3,5-tetrachlorobenzene	1.12 E-03	2.14 E-03	3.37 E-04	6.26 E-04
p-dibromobenzene	1.06 E-03	1.02 E-03	5.49 E-04	6.32 E-04
m-dibromobenzene	1.07 E-03	1.02 E-03	5.57 E-04	2.0 E-03
o-dibromobenzene	5.19 E-04	1.15 E-03	2.88 E-04	1.79 E-03
p-chloroiodobenzene	2.28 E-03	2.25 E-03	1.27 E-03	1.64 E-03
m-chloroiodobenzene	2.31 E-03	2.25 E-03	1.28 E-03	2.58 E-03
o-chloroiodobenzene	1.16 E-03	2.14 E-04	5.94 E-04	3.15 E-03
Pentachlorobenzene	1.77 E-03	3.12 E-03	3.44 E-04	9.65 E-04
p-bromoiodobenzene	4.3 E-03	4.21 E-03	2.69 E-03	4.70 E-03
Hexachlorobenzene	3.34 E-03	2.89 E-03	3.9 E-04	5.6 E-03
1,3,5-tribromobenzene	5.63 E-03	5.15 E-03	2.97 E-03	9.55 E-03
1,2,4-tribromobenzene	3.74 E-03	4.14 E-03	1.59 E-03	1.11 E-02

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

Table V. Continued

Compound	AMOUNT (mole) IN BIOTA			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	9.81 E-03	9.06 E-03	7.95 E-03	1.06 E-02
m-diiodobenzene	9.85 E-03	9.11 E-03	8.01 E-03	8.55 E-03
o-diiodobenzene	6.5 E-03	5.99 E-03	3.59 E-03	1.06 E-02
ALKYLBENZENES				
Toluene	1.65 E-05	9.28 E-06	3.64 E-05	1.5 E-05
Ethylbenzene	3.82 E-05	6.60 E-05	1.21 E-04	3.06 E-05
p-xylene	4.23 E-05	3.17 E-05	8.07 E-05	5.01 E-05
m-xylene	4.2 E-05	3.23 E-05	8.19 E-05	4.12 E-05
o-xylene	4.81 E-05	2.39 E-05	6.31 E-05	4.86 E-05
n-propylbenzene	6.32 E-05	5.05 E-04	5.62 E-04	7.71 E-05
i-propylbenzene	5.68 E-05	5.13 E-04	6.19 E-04	5.03 E-05
n-butylbenzene	2.33 E-04	3.95 E-04	4.16 E-04	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	2.88 E-03	1.13 E-03	1.09 E-03	-
Fluorene	1.35 E-02	1.57 E-02	1.43 E-02	-
Phenanthrene	1.54 E-02	1.39 E-02	1.24 E-02	1.54 E-02
Anthracene	1.61 E-02	1.43 E-02	1.28 E-02	1.50 E-02

Table V. Continued

	AMOUNT (mole) IN BIOTA			
Compound	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	1.42 E-02	1.43 E-02	1.46 E-02	1.43 E-02
Chrysene	1.15 E-02	1.13 E-02	1.26 E-02	1.15 E-02
Perylene	9.43 E-03	9.48 E-03	1.06 E-02	9.34 E-02
Benzo (a) pyrene	9.48 E-03	9.52 E-03	1.06 E-02	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	3.49 E-03	2.39 E-03	1.88 E-03	3.87 E-03
4-CBP	2.3 E-03	4.34 E-03	3.48 E-03	7.86 E-03
2-CBP	4.14 E-03	4.45 E-03	2.87 E-03	6.6 E-03
2,2'-CBP	5.35 E-03	5.86 E-03	4.08 E-03	1.83 E-03
2,5,4'-CBP	2.61 E-03	7.41 E-03	7.54 E-03	-
2,5,2'-CBP	3.72 E-03	7.03 E-03	6.89 E-03	-
3,5,3',5',-CBP	2.02 E-03	8.43 E-03	9.47 E-03	-
2,4,5,4',5'-CBP	7.78 E-03	5.09 E-03	7.36 E-03	9.41 E-03

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	AMOUNT (mole) IN SUSPENDED SOLID Calc.(a)	 Calc.(h)	 Calc.(c)	 Calc.(Fugacity)
HALOBENZENES				
Benzene	-	1.35 E-05	2.89 E-05	1.26 E-05
Fluorobenzene	1.64 E-05	1.52 E-05	4.36 E-06	1.50 E-05
Chlorobenzene	8.12 E-05	7.33 E-05	9.89 E-05	9.79 E-05
p-difluorobenzene	2.33 E-05	1.69 E-05	6.88 E-07	2.25 E-05
m-difluorobenzene	2.39 E-05	1.60 E-05	6.98 E-07	1.65 E-05
e-difluorobenzene	9.93 E-06	3.52 E-05	1.44 E-05	1.39 E-04
p-dichlorobenzene	5.11 E-04	4.72 E-04	2.94 E-04	2.45 E-03
m-dichlorobenzene	5.21 E-04	4.65 E-04	2.98 E-04	5.44 E-04
o-dichlorobenzene	3.17 E-04	7.15 E-04	2.14 E-04	1.08 E-03
Bromobenzene	2.94 E-04	2.18 E-04	2.47 E-04	2.32 E-04
1,3,5-trichlorobenzene	2.4 E-03	2.33 E-03	9.03 E-04	3.14 E-04
1,2,4-trichlorobenzene	1.57 E-03	2.82 E-03	6.25 E-04	2.19 E-03
1,2,3-trichlorobenzene	1.04 E-03	3.45 E-03	4.45 E-04	3.04 E-03

Table V. Continued

Compound	AMOUNT (*mole*) IN SUSPENDED SOLID Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	1.43 E-03	1.32 E-03	7.44 E-04	9.58 E-04
m-bromochlorobenzene	1.45 E-03	1.31 E-03	7.56 E-04	2.4 E-03
o-bromochlorobenzene	8.11 E-04	1.77 E-03	4.70 E-04	3.57 E-03
Iodobenzene	2.40 E-03	2.07 E-03	1.70 E-03	1.34 E-03
1,2,4,5-tetrachlorobenzene	4.52 E-03	8.87 E-03	1.26 E-03	5.08 E-03
1,2,3,5-tetrachlorobenzene	4.57 E-03	8.86 E-03	1.27 E-03	3.23 E-03
p-dibromobenzene	3.67 E-03	3.55 E-03	1.92 E-03	2.33 E-03
m-dibromobenzene	3.72 E-03	3.54 E-03	1.95 E-03	7.38 E-03
o-dibromobenzene	1.91 E-03	4.25 E-03	1.001 E-03	6.58 E-03
p-chloroiodobenzene	8.61 E-03	8.55 E-03	4.85 E-03	6.12 E-03
m-chloroiodobenzene	8.72 E-03	8.55 E-03	4.93 E-03	9.64 E-03
o-chloroiodobenzene	4.65 E-03	8.65 E-03	2.28 E-03	1.18 E-02
Pentachlorobenzene	8.64 E-03	1.56 E-02	1.51 E-03	5.23 E-03
p-bromoiodobenzene	1.78 E-02	1.77 E-02	1.15 E-02	1.91 E-02
Hexachlorobenzene	1.87 E-02	1.69 E-02	1.99 E-03	3.02 E-02
1,3,5-tribromobenzene	2.47 E-02	2.29 E-02	1.34 E-02	6.16 E-02
1,2,4-tribromobenzene	1.71 E-02	1.92 E-02	7.19 E-03	7.16 E-02

Table V. Continued

Compound	AMOUNT (mole)IN SUSPENDED SOLID Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	4.73 E-02	4.47 E-02	4.16 E-02	4.76 E-02
m-diiodobenzene	4.74 E-02	4.48 E-02	4.20 E-02	3.83 E-02
o-diiodobenzene	3.31 E-02	3.14 E-02	1.88 E-02	4.78 E-02
ALKYLBENZENES				
Toluene	3.81 E-05	2.10 E-05	8.61 E-05	3.42 E-05
Ethylbenzene	1.03 E-04	1.77 E-04	3.29 E-04	8.19 E-05
p-xylene	1.14 E-04	8.61 E-05	2.15 E-04	1.36 E-04
m-xylene	1.13 E-04	8.75 E-05	2.18 E-04	1.12 E-04
o-xylene	1.28 E-04	6.53 E-05	1.68 E-04	1.29 E-04
n-propylbenzene	2.01 E-04	1.56 E-03	1.73 E-03	2.48 E-04
i-propylbenzene	1.83 E-04	1.59 E-03	1.88 E-03	1.61 E-04
n-butylbenzene	7.80 E-04	1.47 E-03	1.61 E-03	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	8.31 E-03	3.22 E-03	3.30 E-03	-
Fluorene	5.52 E-02	6.39 E-02	5.87 E-02	-
Phenanthrene	6.89 E-02	6.31 E-02	5.38 E-02	6.81 E-02
Anthracene	7.17 E-02	6.47 E-02	5.56 E-02	6.71 E-02

Table V. Continued

Compound	AMOUNT (mole) IN SUSPENDED SOLID			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	7.76 E-02	7.99 E-02	7.66 E-02	7.81 E-02
Chrysene	7.98 E-02	7.94 E-02	7.88 E-02	7.99 E-02
Perylene	8.02 E-02	8.02 E-02	8.01 E-02	7.96 E-02
Benzo (a) pyrene	8.03 E-02	8.02 E-02	8.01 E-02	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	1.22 E-02	8.57 E-03	6.78 E-03	1.38 E-02
4-CBP	9.3 E-03	1.80 E-02	1.45 E-02	3.47 E-02
2-CBP	1.62 E-02	1.88 E-02	1.20 E-02	2.92 E-02
2,2'-CBP	2.35 E-02	2.89 E-02	1.98 E-02	6.64 E-03
2,5,4'-CBP	1.45 E-02	3.99 E-02	4.24 E-02	-
2,5,2'-CBP	2.01 E-02	3.83 E-02	3.88 E-02	-
3,5,3',5',-CBP	1.44 E-02	5.01 E-02	6.18 E-02	-
2,4,5,4',5'-CBP	5.36 E-02	3.52 E-02	5.61 E-02	7.01 E-02

Tablo V.: Results of Compartmental Distribution Values for Various Aromatic Compounds Calculated by VMCI and Level I Fugacity Models.

Compound	AMOUNT (mole) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
HALOBENZENES				
Benzene	-	8.08 E-03	1.74 E-02	7.57 E-03
Fluorobenzene	9.84 E-03	9.15 E-03	2.61 E-03	9.01 E-03
Chlorobenzene	4.87 E-02	4.40 E-02	5.93 E-02	5.87 E-02
p-difluorobenzene	1.40 E-02	1.01 E-02	4.13 E-04	1.35 E-02
m-difluorobenzene	1.43 E-02	9.63 E-03	4.19 E-04	9.90 E-03
o-difluorobenzene	5.96 E-03	2.11 E-02	8.67 E-03	8.35 E-02
p-dichlorobenzene	0.307	0.283	0.177	1.47
m-dichlorobenzene	0.313	0.279	0.179	0.327
o-dichlorobenzene	0.190	0.429	0.129	0.648
Bromobenzene	0.176	0.131	0.148	0.139
1,3,5-trichlorobenzene	1.44	1.400	0.542	0.188
1,2,4-trichlorobenzene	0.941	1.692	0.375	1.31
1,2,3-trichlorobenzene	0.622	2.072	0.267	1.82

Table V. Continued

Compound	AMOUNT (mole) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-bromochlorobenzene	0.856	0.794	0.447	0.575
m-bromochlorobenzene	0.870	0.788	0.453	1.44
o-bromochlorobenzene	0.486	1.063	0.282	2.14
Iodobenzene	1.44	1.241	1.02	0.801
1,2,4,5-tetrachlorobenzene	2.71	5.324	0.754	3.05
1,2,3,5-tetrachlorobenzene	2.74	5.318	0.764	1.94
p-dibromobenzene	2.20	2.128	1.15	1.40
m-dibromobenzene	2.23	2.121	1.17	4.43
o-dibromobenzene	1.14	2.551	0.604	3.95
p-chloroiodobenzene	5.17	5.128	2.91	3.67
m-chloroiodobenzene	5.23	5.131	2.96	5.79
o-chloroiodobenzene	2.79	5.190	1.37	7.07
Pentachlorobenzene	5.18	9.371	0.907	3.14
p-bromoiodobenzene	10.68	10.594	6.90	11.46
Hexachlorobenzene	11.24	10.145	1.19	18.15
1,3,5-tribromobenzene	14.81	13.761	8.05	36.94
1,2,4-tribromobenzene	10.24	11.548	4.32	42.96

Table V. Continued

Compound	AMOUNT (mole) IN SEDIMENT Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
p-diiodobenzene	28.36	26.796	24.98	28.58
m-diiodobenzene	28.45	26.906	25.18	22.99
o-diiodobenzene	19.87	18.852	11.29	28.68
ALKYLBENZENES				
Toluene	0.023	0.126	0.052	0.021
Ethylbenzene	0.062	0.106	0.197	0.049
p-xylene	0.068	0.052	0.129	0.081
m-xylene	0.068	0.052	0.131	0.067
o-xylene	0.077	0.039	1.101	0.077
n-propylbenzene	0.121	0.937	1.04	0.149
i-propylbenzene	0.110	0.952	1.13	0.096
n-butylbenzene	0.468	0.883	0.986	-
POLYCYCLIC AROMATIC HYDROCARBONS				
Naphthalene	4.98	1.990	1.98	-
Fluorene	33.09	38.335	35.20	-
Phenanthrene	41.34	37.870	32.27	40.89
Anthracene	42.99	38.817	33.38	40.25

Table V. Continued

Compound	AMOUNT (mole) IN SEDIMENT			
	Calc.(a)	Calc.(b)	Calc.(c)	Calc.(Fugacity)
Pyrene	46.53	46.741	45.99	46.86
Chrysene	47.89	47.619	47.26	47.96
Perylene	48.13	48.146	48.06	47.75
Benzo (a) pyrene	48.15	48.148	48.07	-
POLYCHLORINATED BIPHENYLS				
Biphenyl	7.35	5.144	4.07	8.27
4-CBP	5.58	10.779	8.72	20.83
2-CBP	9.70	11.290	7.21	17.51
2,2'-CBP	14.09	17.310	11.88	3.98
2,5,4'-CBP	8.72	23.941	25.42	-
2,5,2'-CBP	12.04	22.963	23.26	-
3,5,3',5',-CBP	8.62	30.039	37.07	-
2,4,5,4',5'-CBP	32.14	21.100	33.64	42.04

V.2 GENERAL EVALUATION OF THE RESULTS

During the last decade concerns have been expressed as to the "best way" to assess the potential hazards posed by exposure to chemical substances. In response to these concerns the Chemicals Group of OECD initiated a Hazard Assessment Project to examine the available methods for hazard assessment of chemicals. The initial aim of this project was to determine how information on the ultimate fate and effects of a chemical can be derived from the minimum set of premarket data (MPD), how these data can be combined to give an estimate of the hazard from exposure to that chemical and how to identify indications of relevant criteria for further testing and/or assessment.

One of the three working parties formed to accomplish this was the exposure Analysis Group and this group was given the task to consider environmental partitioning and the exposure from all sources to humans and the environment[87].

The exposure Analysis Working Party concluded that Potential Environmental Distribution (PED) and Potential Environmental

Concentration (PEC) should be considered when performing a first assessment of the potential hazard of a chemical based on the minimum set of premarketing data (MPD).

Both of these expressions allow the estimation of exposure potentials of chemicals within environmental compartment of major concern. As a result, the group initially considered four models which are given in chapter III and it is accepted that all of the four models as indicated previously, essentially need the following physical/chemical data

molecular weight
water solubility
vapor pressure
soil sorption constant (K_{OC})
partition coefficient (K_{OW})

Table V.2 shows some of the accepted MPD test data and the function of this data for hazard assessment.

However when we think of environmentally hazardous chemicals which generally are large molecules and rather complex system , it is unfortunately clear that the set of data proposed is hard to find in the literature and furthermore the precission of these data is generally questionable. Hence a reasonable model to get rid of those parameters would have been a remarkable advance in prediction of environmental hazards that are going to be caused by unknown chemicals irrespective of size and conformation.

In this work a new mathematical model based on the topological characteristics of molecules is developed in order to evaluate the compartmental distribution of chemicals in the environment and it has been shown that just by considering the molecular topology one can easily approach to the results obtained by one of the accepted models by OECD Exposure Analysis Group (Mackay Level I Fugacity Model) within a high accuracy.

The Valance Molecular Connectivity Index, which is the basis of this new model is known to correlate significantly with a number of physicochemical properties and by this work it is now shown to have a high degree of correlation (R=0.97—1.0) with the vapor pressures (ln P), solubilities (ln S) and octanol-water partition coefficients (ln K_{OW}) (tables IV.33).

Table V.2. MPD Test Data for Hazard Assessment Accepted by OECD Exposure Analysis Group

TEST GUIDANCE	FUNCTION FOR HAZARD ASSESSMENT
Physical/Chemical Data:	
Melting Point/Melting Range	Useful for determining physical state at ambient temperatures; measure of purity; identification.
Boiling Point/Boiling Range	Relates to vapor pressure and tendency of substance to evaporate; identification.
Density of Liquids and Solids	Used to estimate relative distribution within a medium
Vapor Pressure	Used with water solubility to determine volatility and air/water partitioning; liquid/gas and solid/gas transitions to estimate exposure as a result of inhalation.
Water Solubility	Solubility, coupled with vapor pressure, determines affinity for aqueous medium and partitioning between air and water; used to estimate exposure through aqueous media and foodstuffs.
Octanol/Water Partition Coefficient	Used to estimate bioaccumulation and soil (sediment)/water partitioning.

The importance of these parameters and also their use in structure-activity relationship studies are well known and mathematically it seems obvious that since the combination of those indices are linearly related to those parameters they should also correlate in the same fashion as P, S and K_{OW} to fugacity capacity constants and hence to various compartmental distribution values. This hypothesis is tested on four aromatic systems and is shown that the final results which are going to be presented in a graphical scheme for each group and for each compartment, compare very favourably with the results obtained by another method, namely Level I Fugacity Model.

V.2.1. VALANCE MOLECULAR CONNECTIVITY INDICES AND THE FUTURE REQUİREMENTS

In this work, the first three order of Valance Molecular Connectivity indices are evaluated and used for the four aromatic groups under investigation. It has been previously indicated that this method for describing the structure of a molecule has its roots in topology and a series of indices reflect a weighted count of subgraphs which, from simple calculations, lead to values encoding considerable structural information and it is this information that makes the evaluation of structural features influencing physical properties and related activities possible. This work considers four sets of compounds all of which are aromatic systems having electron withdrawing and donating substituents. The equations derived as a result of a detailed regression analysis defining ln K_{ow}, ln S and ln P in terms of those indices treat these sets equally well whether they are taken singly (group specific regression), in pairs (groups having electron donating and withdrawing substituents) or as a whole (four groups together). Since the correlations obtained through whole-group regression are as good as other two groups in predicting those parameters it can be easily concluded that a single set of equations are enough to discriminate between all types of molecules provided that they are aromatic. On this basis, the structural analysis derived from this admittedly limited set of aromatic compounds may have the utility as a theoretical screen for other untested aromatic compounds. Examination of additional aromatic sysytem, similarly tested, should efford a constructive challenge to this approach.

A close inspection of the evaluated indices, in the light of information given previously together with the results obtained in this work, indicates that each index is a measure or description of specific bond property. Hence, bearing in mind that the coefficients of the regression equations do not have the significance of contributions from definite pairs of C-C bond but constitute a certain linear combination of effects associated with various C-C bonds and their interactions, one can determine each of these effects seperately after assigning the suitable physical meaning to each index. Since the main purpose of this work is to develop a model to evaluate the compartmental distribution values within a certain accuracy and since such an interperetation requires a detailed statistical analysis dependent on a large variety of physical data concerning bond properties this aspect is left as another future challenge to this approach.

V.2.2. PREDICTED ENVIRONMENTAL DISTRIBUTION OF VARIOUS AROMATIC HYDROCARBONS IN COMPARISON TO THE RESULTS OBTAINED FROM LEVEL I FUGACITY CALCULATIONS

In accordance with the previously proposed procedure the mass, equilibrium distributions and concentrations of the four groups of compounds under investigation in various compartments of the environment are evaluated by VMCI model and compared with those calculated by Level I Fugacity Model. The results of those calculations are given in comparison with the accepted model in figures V.2 to V.5 for each specific group of compounds.

The evaluations, as has been done with each property (ln S, ln P ln K_{OW}, Z_i) are carried out with all three groups of regression equations to see weather all aromatic systems can be defined by a single set of equations defining ln S, ln P and ln K_{OW}. The results showed that the set of equations obtained by considering all four groups together correlated as well as the individual statistical treatment of groups, meaning that the valance molecular connectivity indices used are descriptions of specific bond properties no matter what the substituent is. This result of course has to be confirmed through a continuation of this work by considering other aromatic systems having different substituents.

The input data used in these calculation are taken from literature. However , as the result of the statistical analysis done, use of K_{OW}, S and P values for the ortho-meta, para-substituted benzene derivatives are restricted to only para conformations. Because the data available for different conformations generally are results of various empirical approaches the correlation of which are not over 90 % and which are generally group specific (may not be applicable to a certain group). The following table shows the results of the single variable regression analysis for ortho-, meta-,para-substituted benzene derivatives in comparison to the case where all three are considered together. According to this table, the para-conformation which have the highest correlation for all three parameters is selected as the input data for disubstituted halobenzenes .

In accordance with the above discussion, it can be observed from table V that the distribution values evaluated by using the input data not considered in the regression are rather off while others agree to a very high extent.

As a result it can be clearly seen from the following tables that the comparison between the two completely different methods of evaluation —one requiring the K_{OW}, S and P values

Table V.3. Comparison of ortho—, meta—, para— Substituted Benzene Derivatives in terms of Correlation of Data

Y = mx+n

	ORTHO			META			PARA			ORTHO,META, PARA		
Y =	log K_{ow}	log S	log P	log K_{ow}	log S	log P	log K_{ow}	log S	log P	log K_{ow}	log S	log P
n	0.58	-0.44	-1.07	0.44	-0.53	-1.09	0.63	-0.66	-1.28	0.56	-0.57	-1.16
m	2.10	3.28	2.72	2.51	3.44	3.01	1.89	3.55	3.24	2.13	3.49	3.00
R	0.94	0.82	0.97	0.95	0.83	0.98	0.97	0.91	0.97	0.94	0.80	0.95

and the other only requiring the GEOMETRY DEPENDENT SIMPLE INDICES— result in similar values in regard to distribution values. Hence it can be concluded that by just knowing the MOLECULAR WEIGHT and the MOLECULAR GEOMETRY it is possible to predict the compartmental distribution of any aromatic compound within a high accuracy without needing any complicated data such as octanol-water partition coefficient, solubility or vapor pressure by using VMCI model instead of the fugacity dependent models accepted by the OECD Exposure Analysis Group.

POLYCYCLIC AROMATIC HYDROCARBONS

Figure V.2. Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Level I Fugacity Approach for Polycylic Aromatic Hydrocarbons. In These Plots [●] Represents the Results Obtained Through Group Specific Regression Analysis [⬡] Represents the Results Obtained Through the Regression Carried out of Pairs of Groups having Electron Donating and Electron Withdrawing Substituents and [○] Represents the Results Obtained Through the Regression Analysis of Aromatic Groups Together.

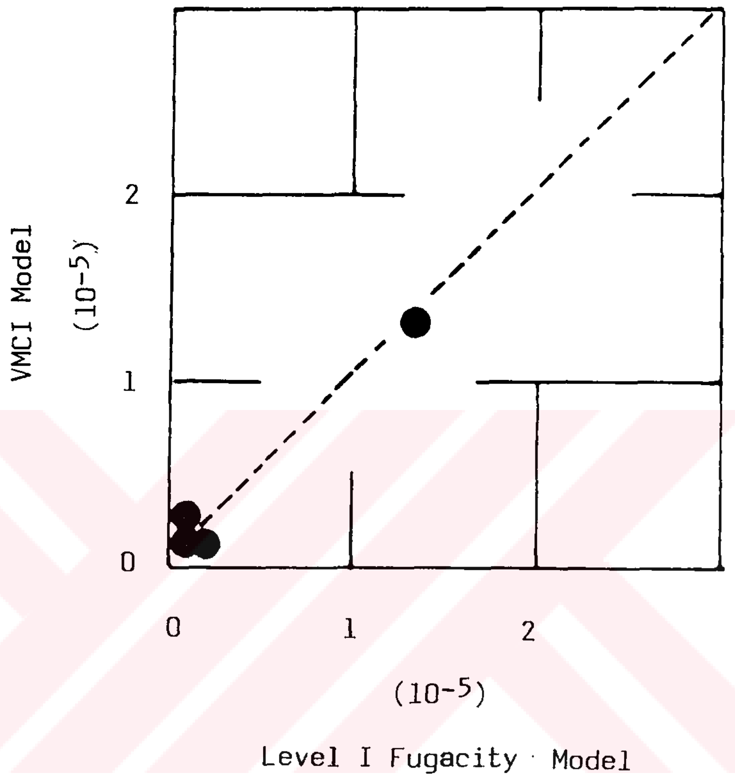


Figure V.2.1.1 Equilibrium Distribution (%) in Air

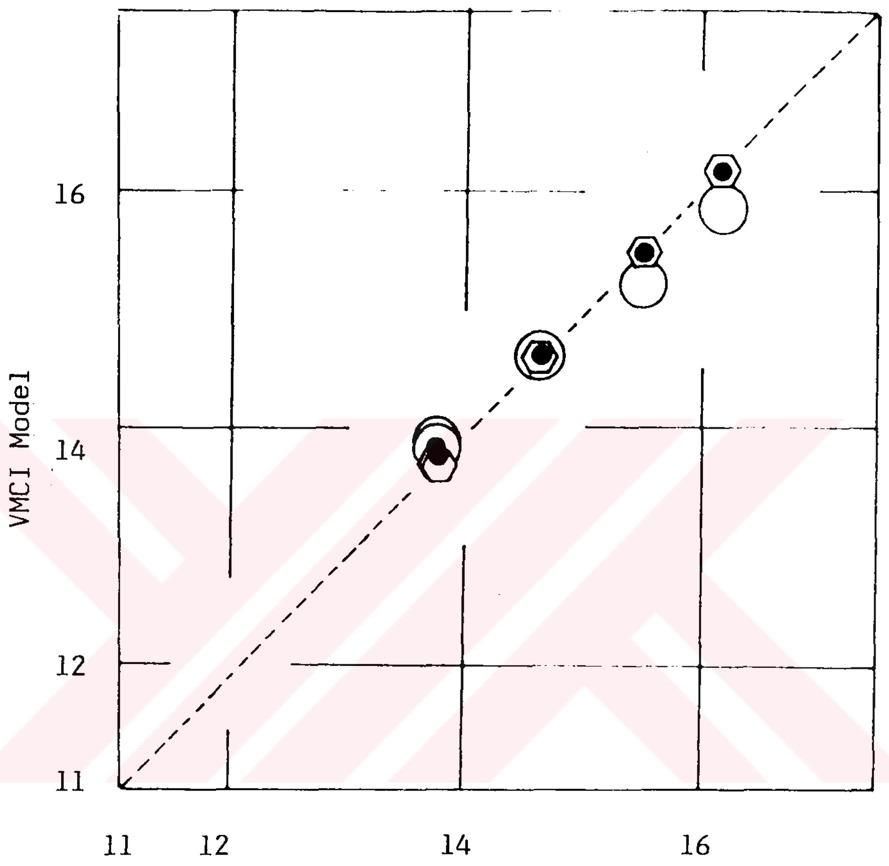


Figure V.2.1.2 Equilibrium Distribution (%) in Soil

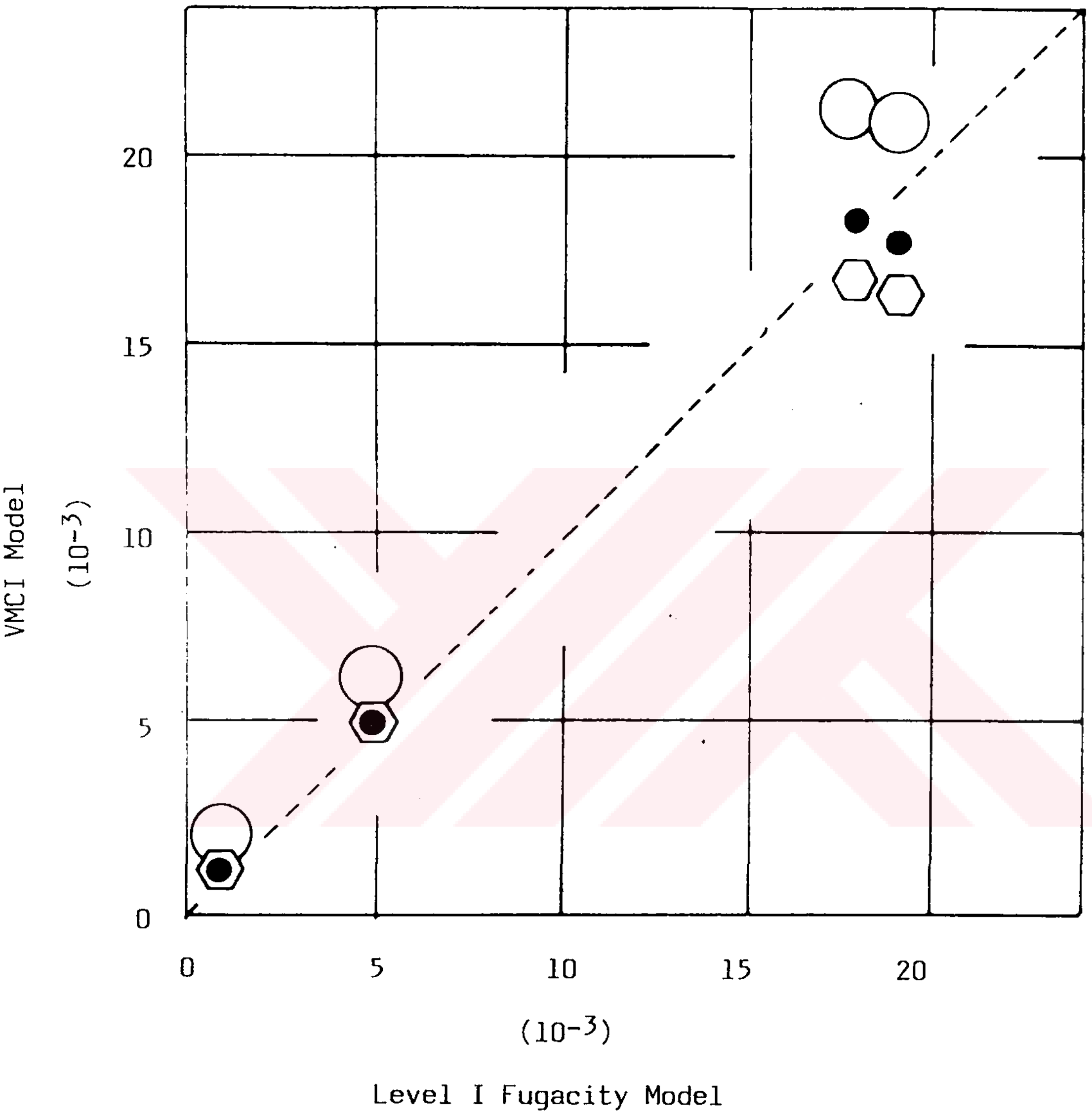


Figure V.2.1.3 Equilibrium Distribution (%) in Water

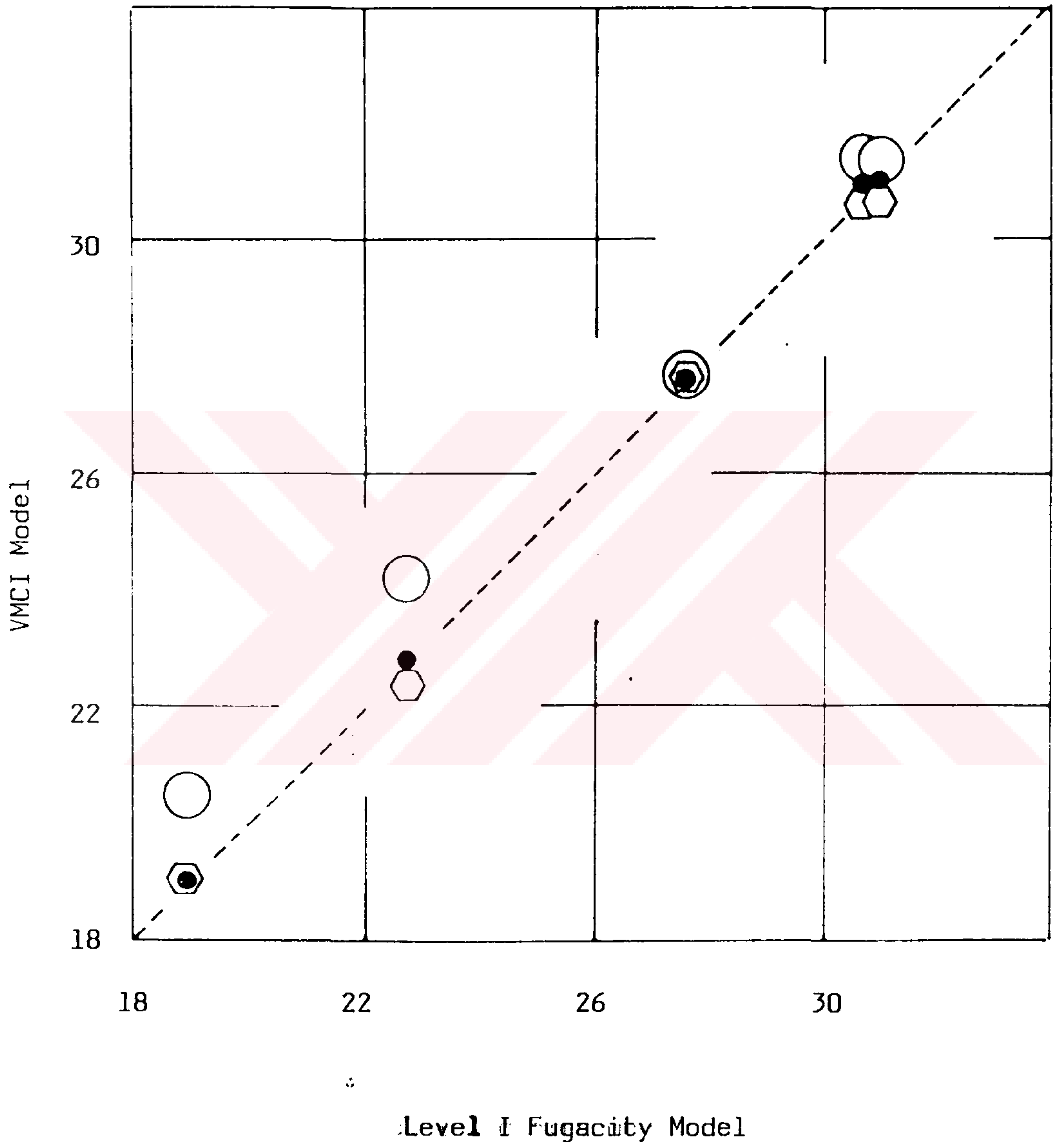


Figure V.2.1.4 Equilibrium Distribution (%) in Biota

YÖK

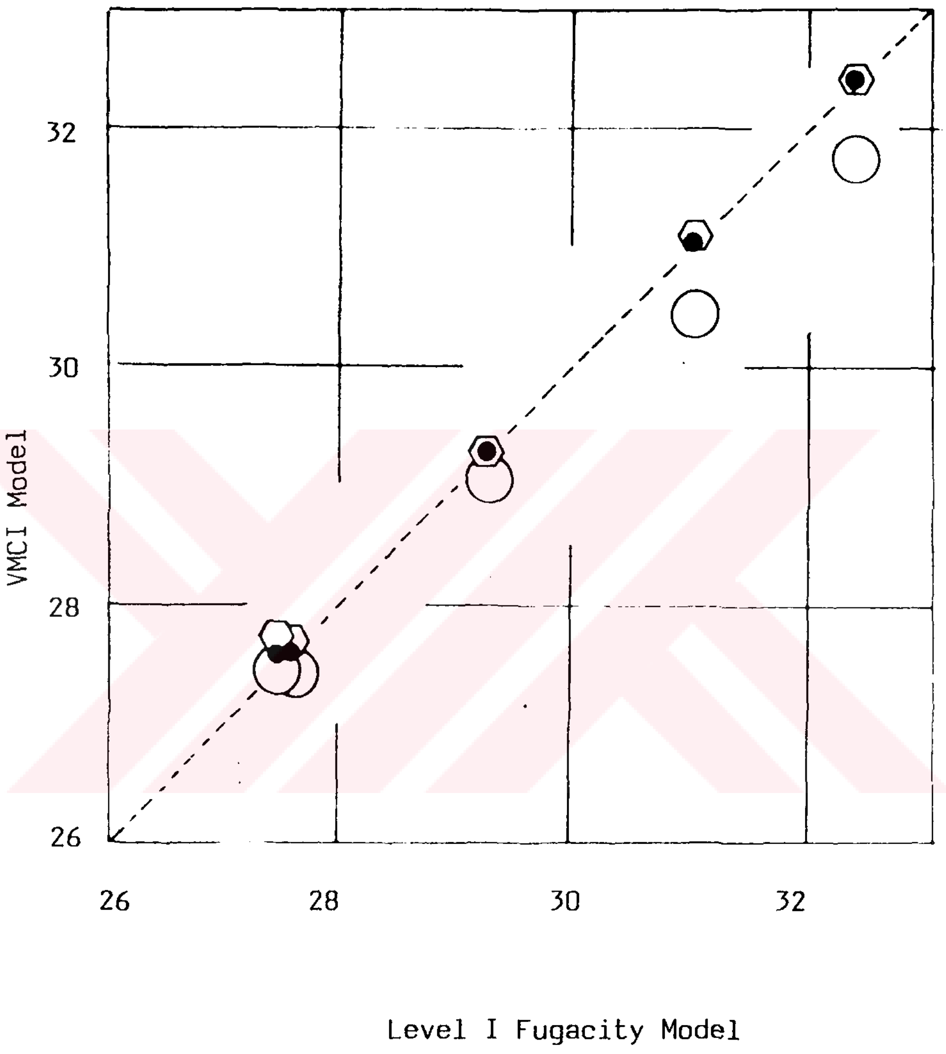


Figure V.2.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment

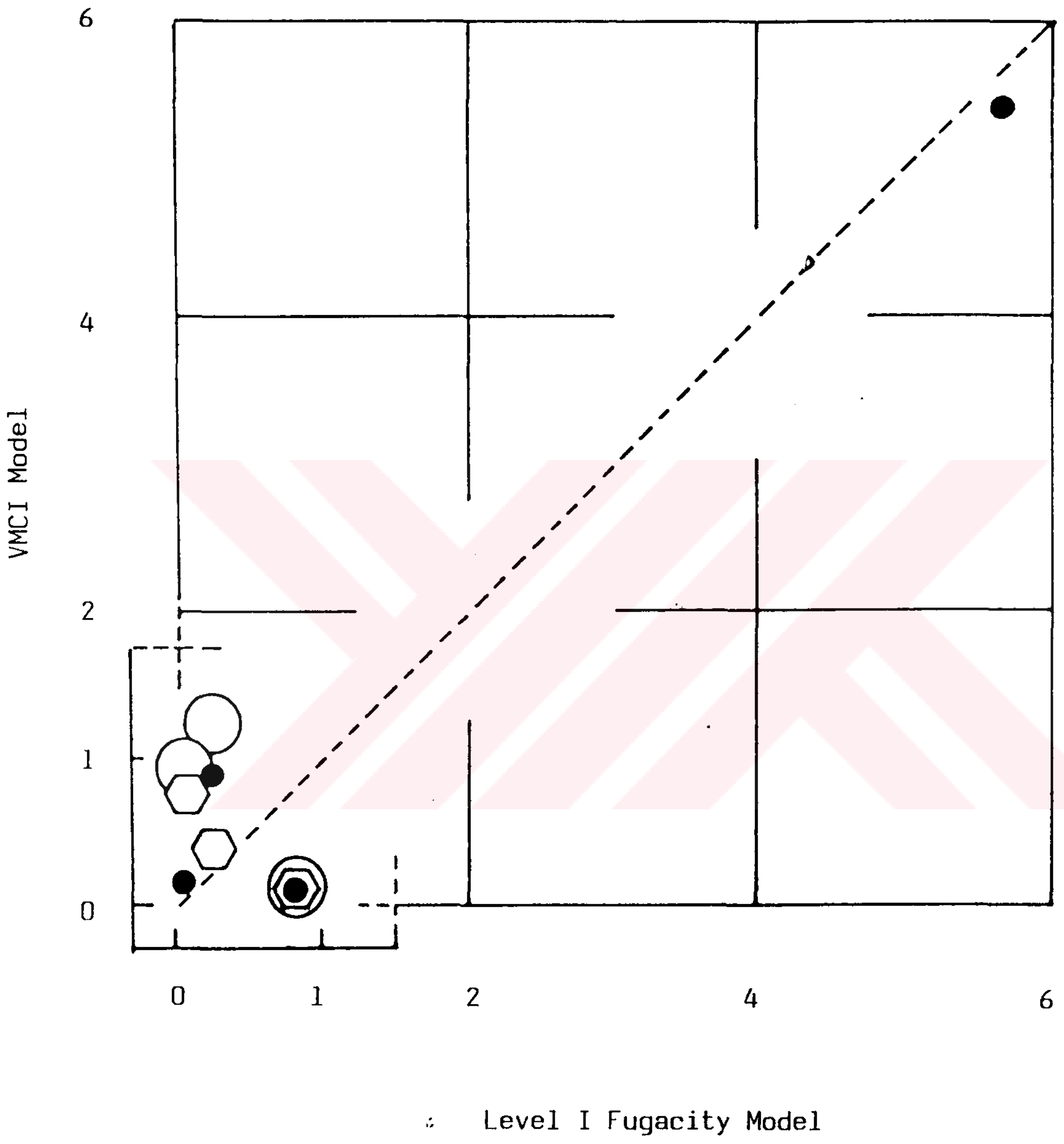


Figure V.2.2.1 Mass Distribution (%) in Air

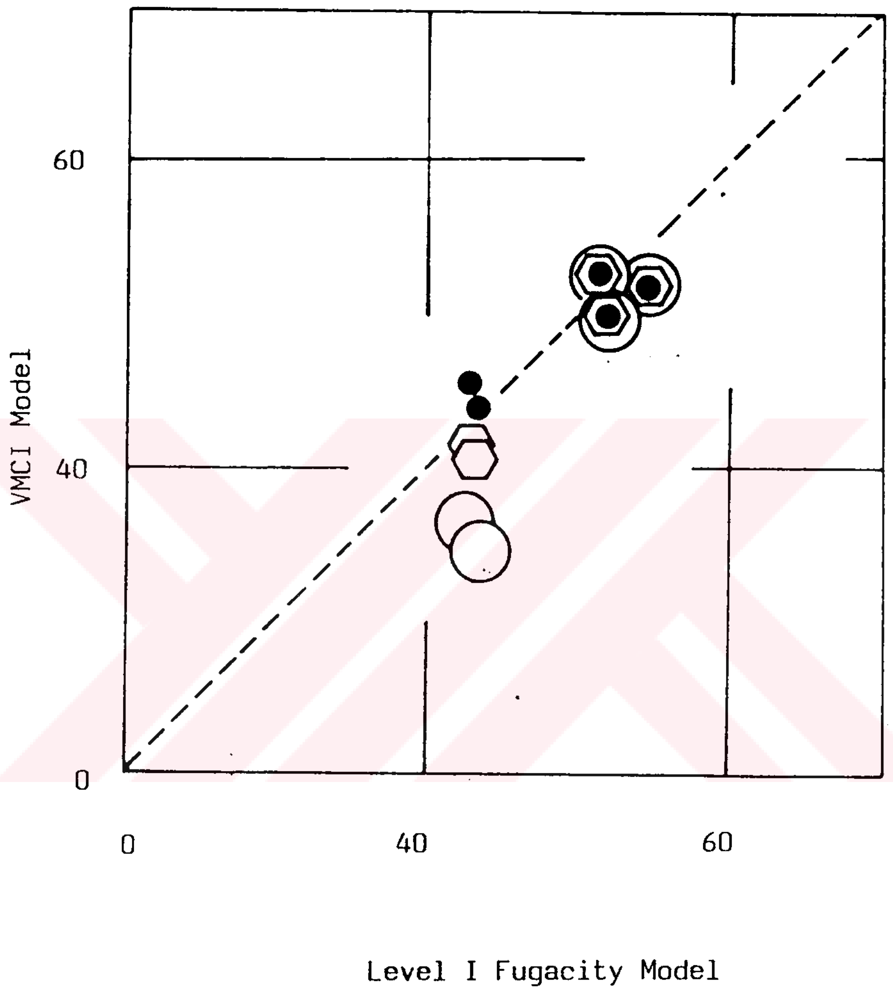


Figure V.2.2.2 Mass Distribution (%) in Soil

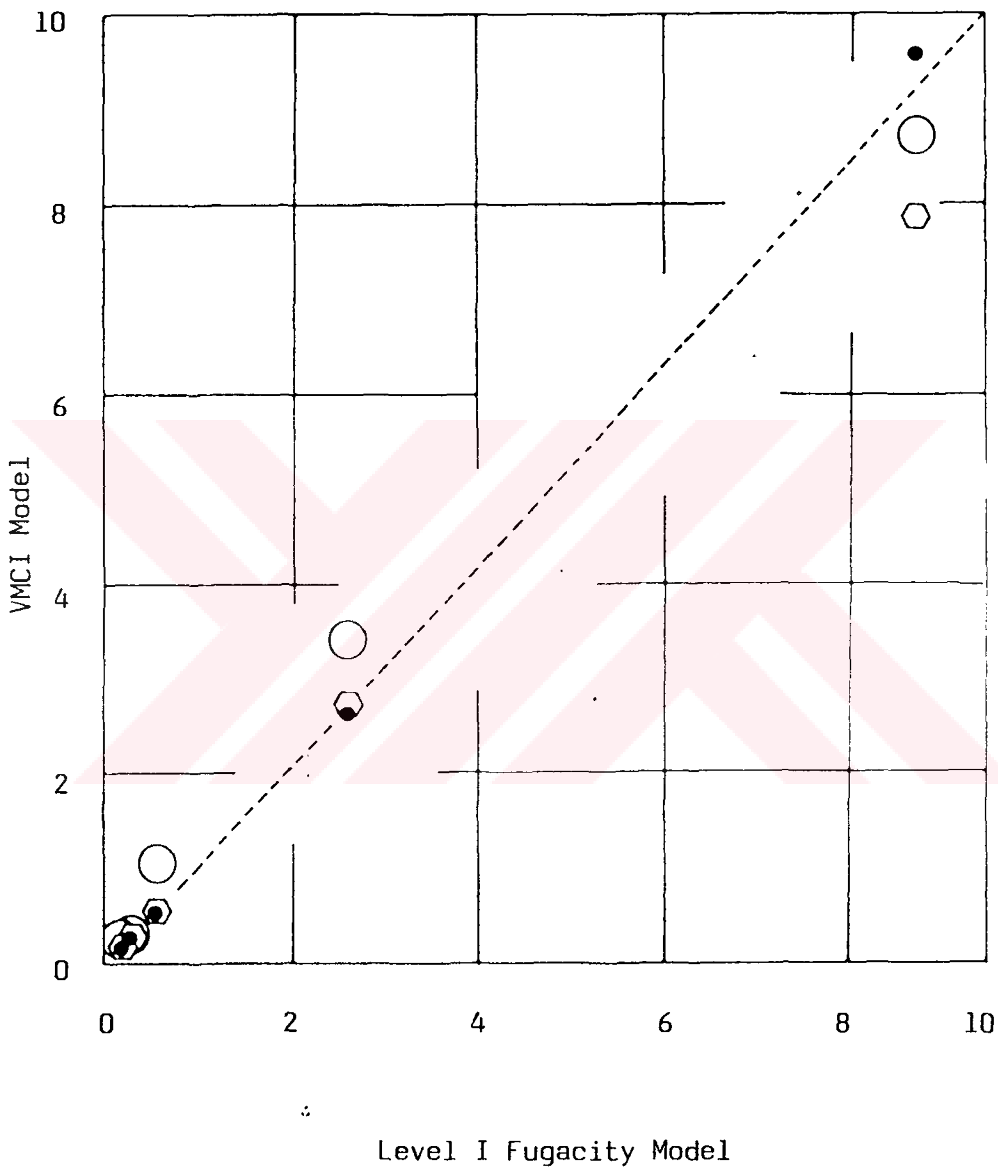


Figure V.2.2.3 Mass Distribution (%) in Water

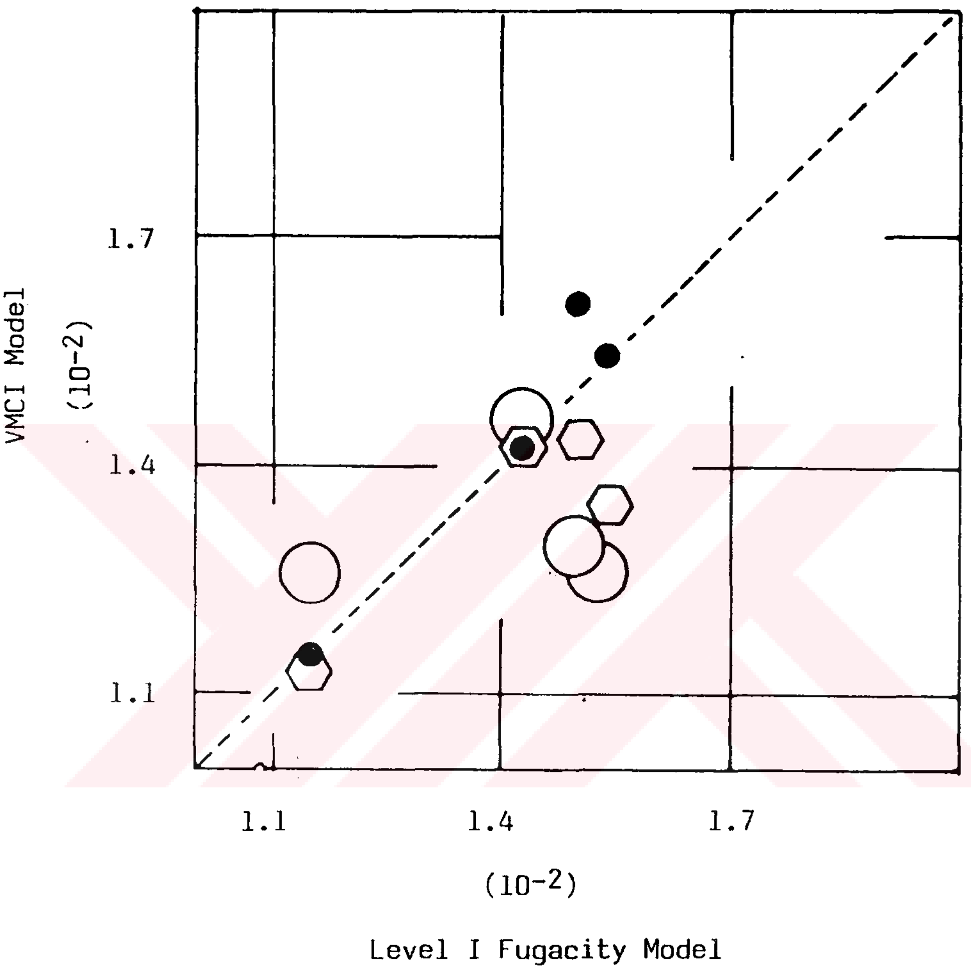


Figure V.2.2.4 Mass Distribution (%) in Biota

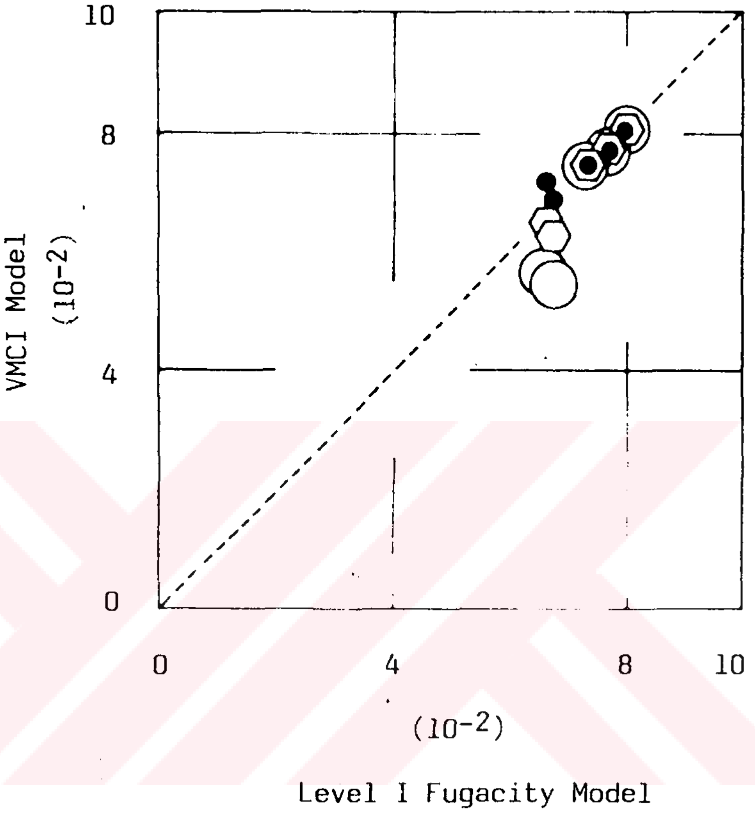


Figure V.2.2.5 Mass Distribution (%) in Suspended Solids

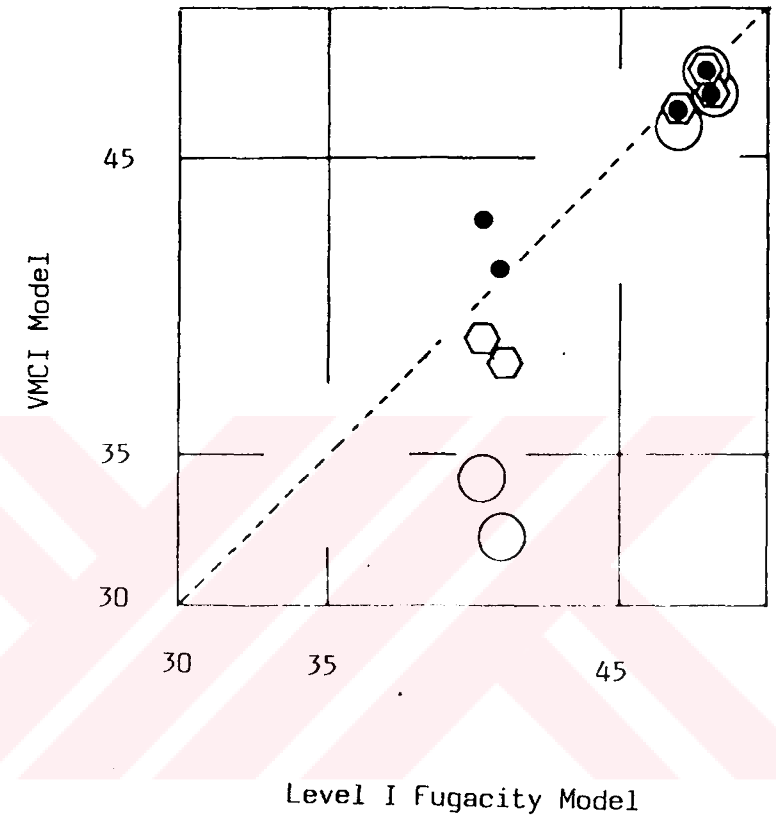


Figure V.2.2.6 Mass Distribution (%) in Sediment

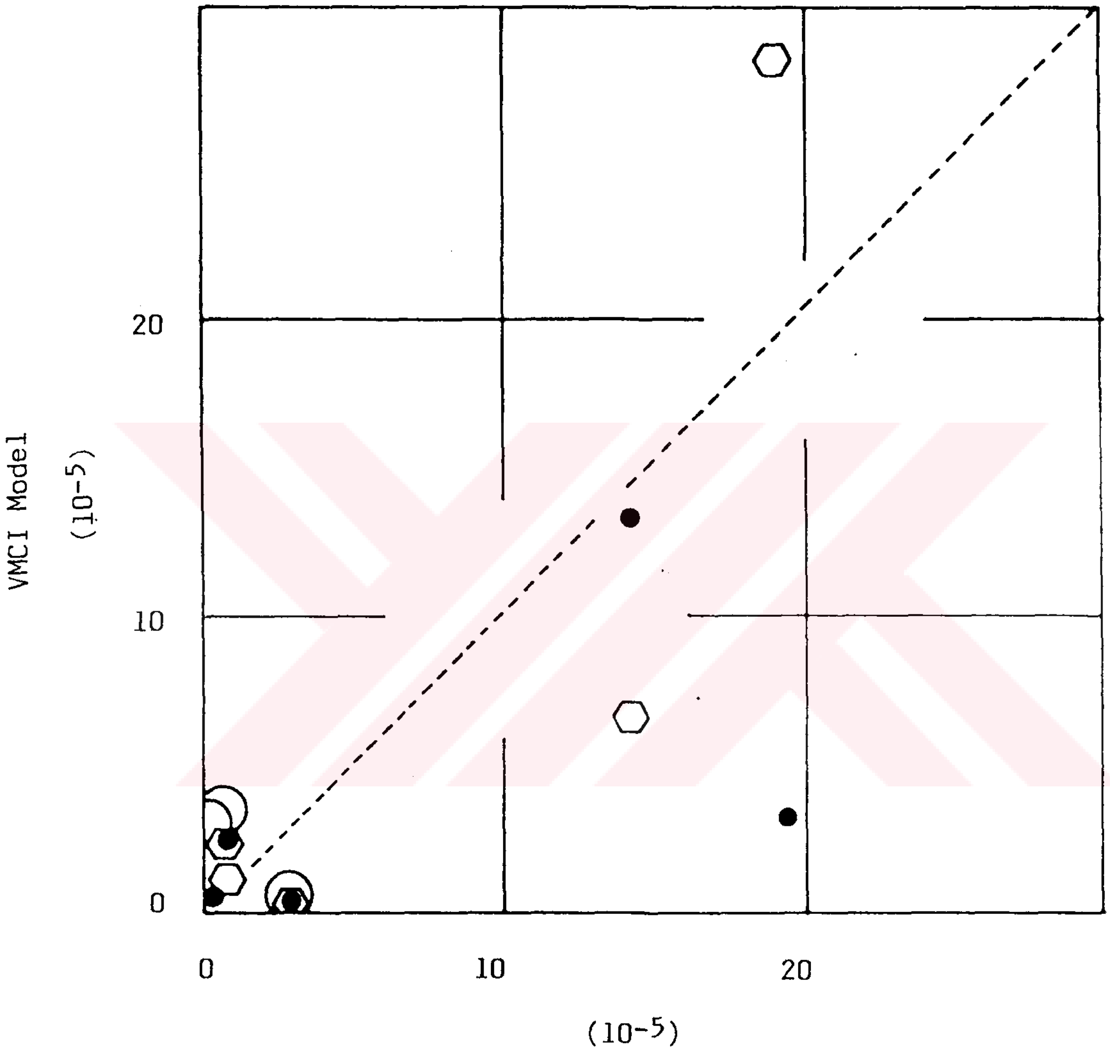


Figure V.2.3.1 Concentration (ppm) in Air

:

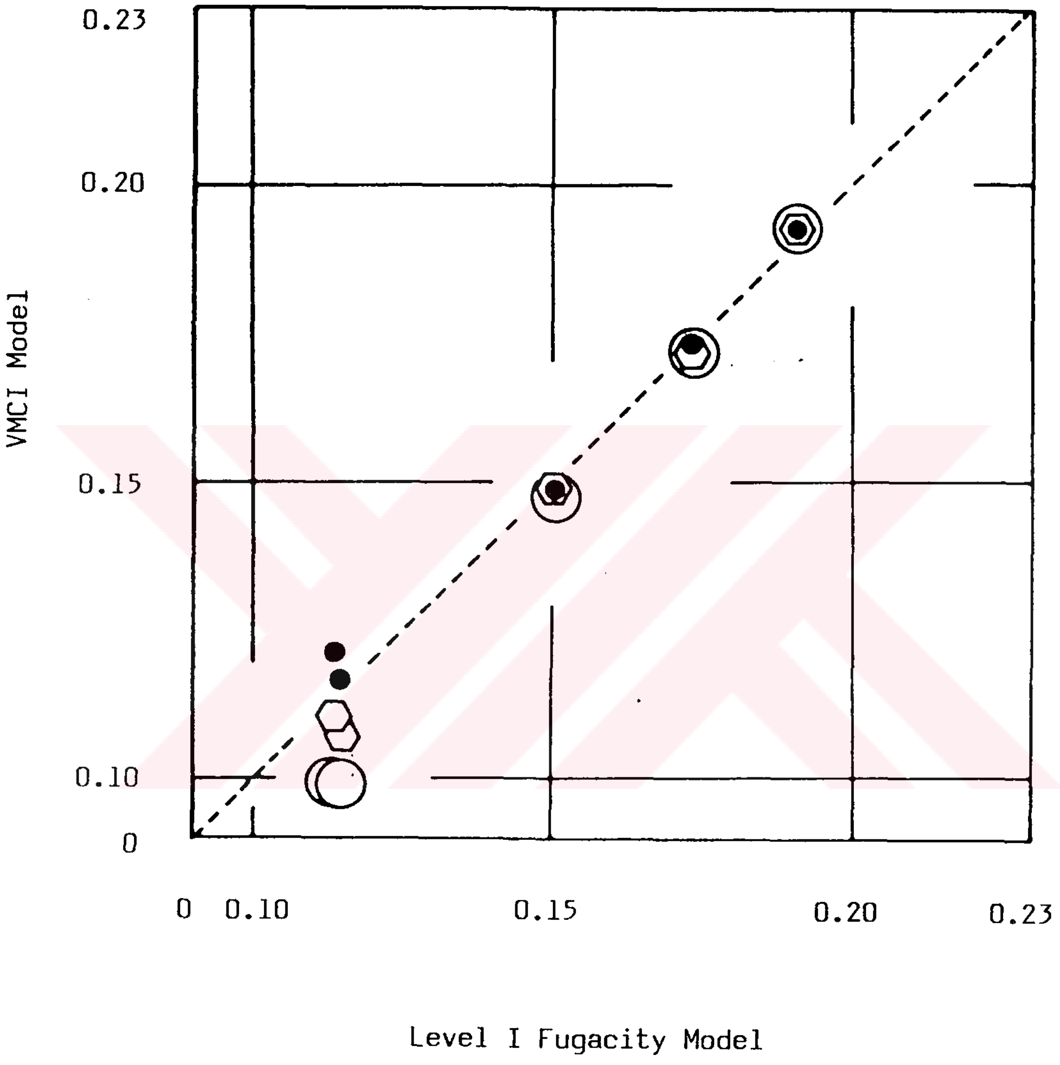


Figure V.2.3.2 Concentration (ppm) in Soil

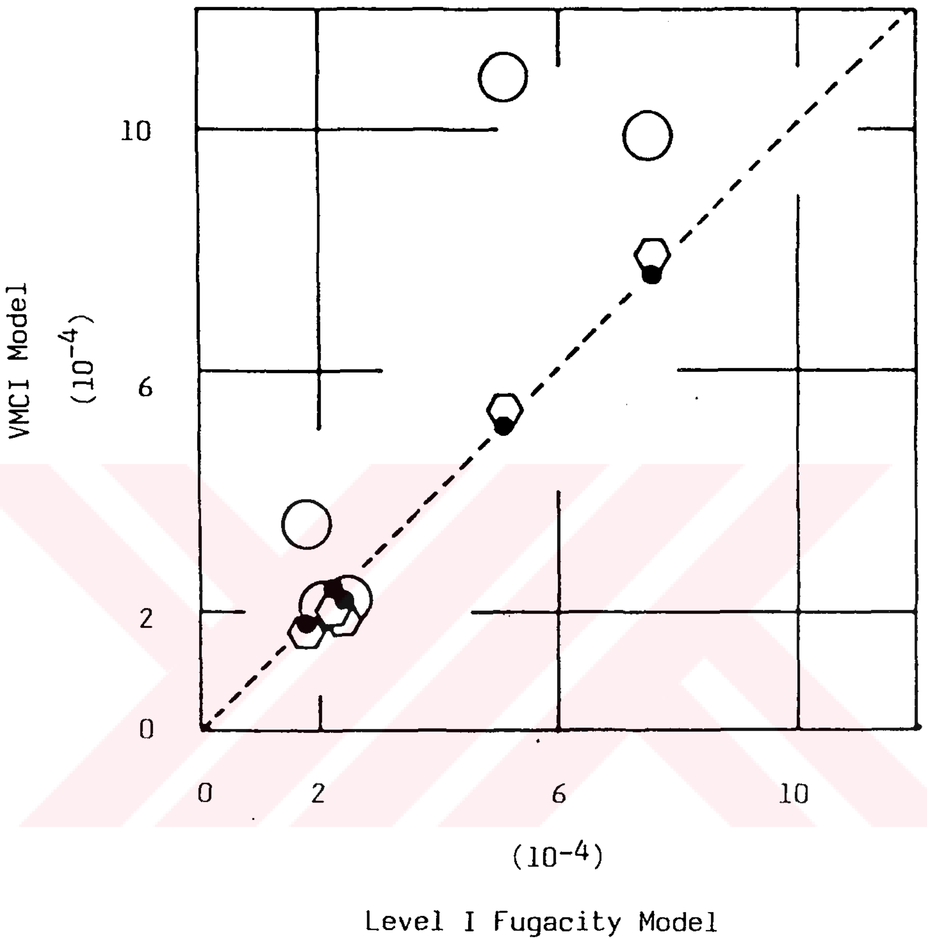
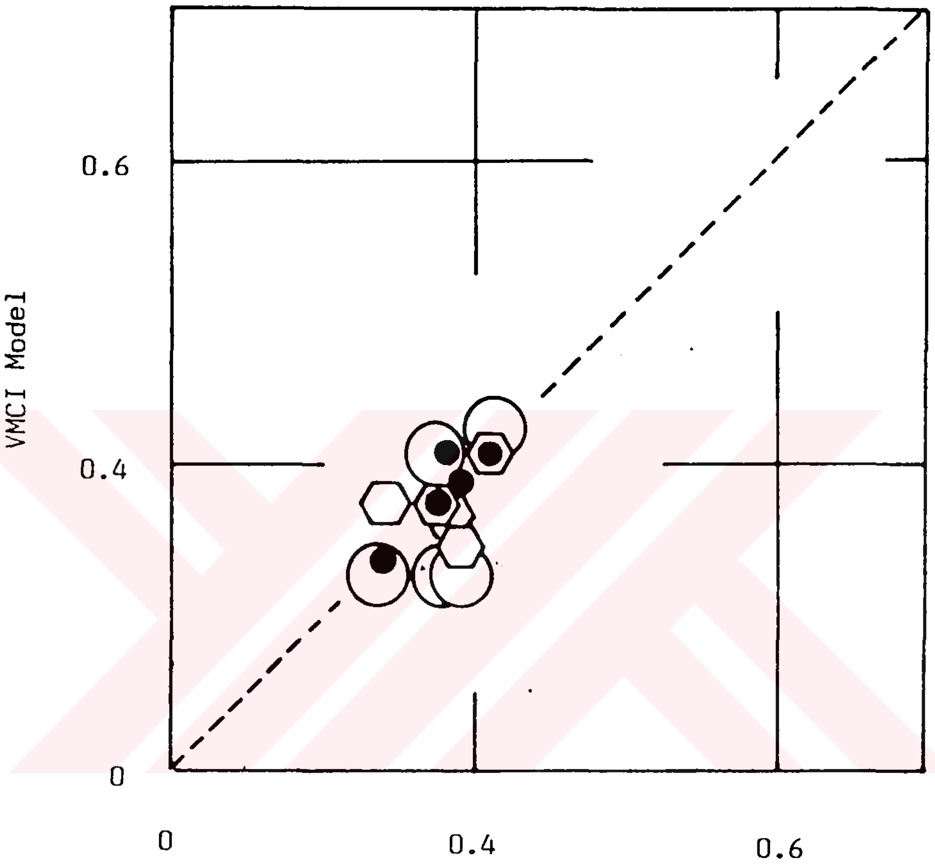


Figure V.2.3.3 Concentration (ppm) in Water



Level I Fugacity Model

Figure V.2.3.4 Concentration (ppm) in Biota

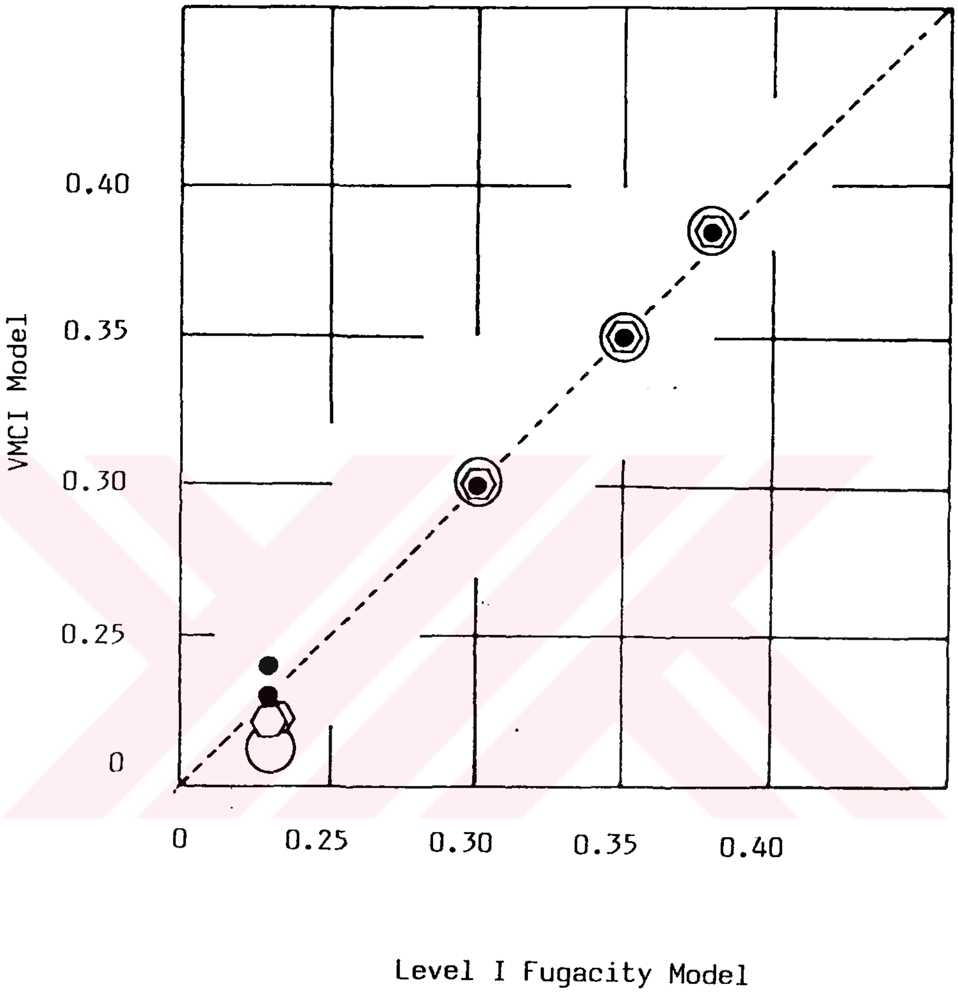
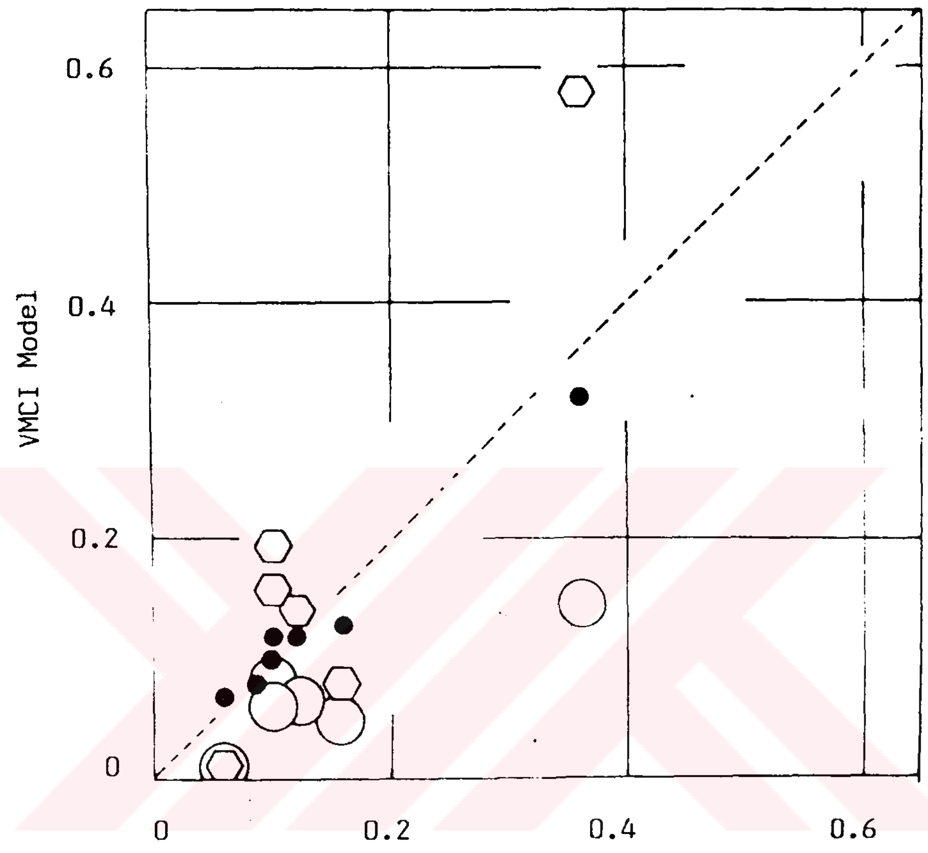


Figure V.2.3.5 Concentration (ppm) in Suspended Solids and Sediment

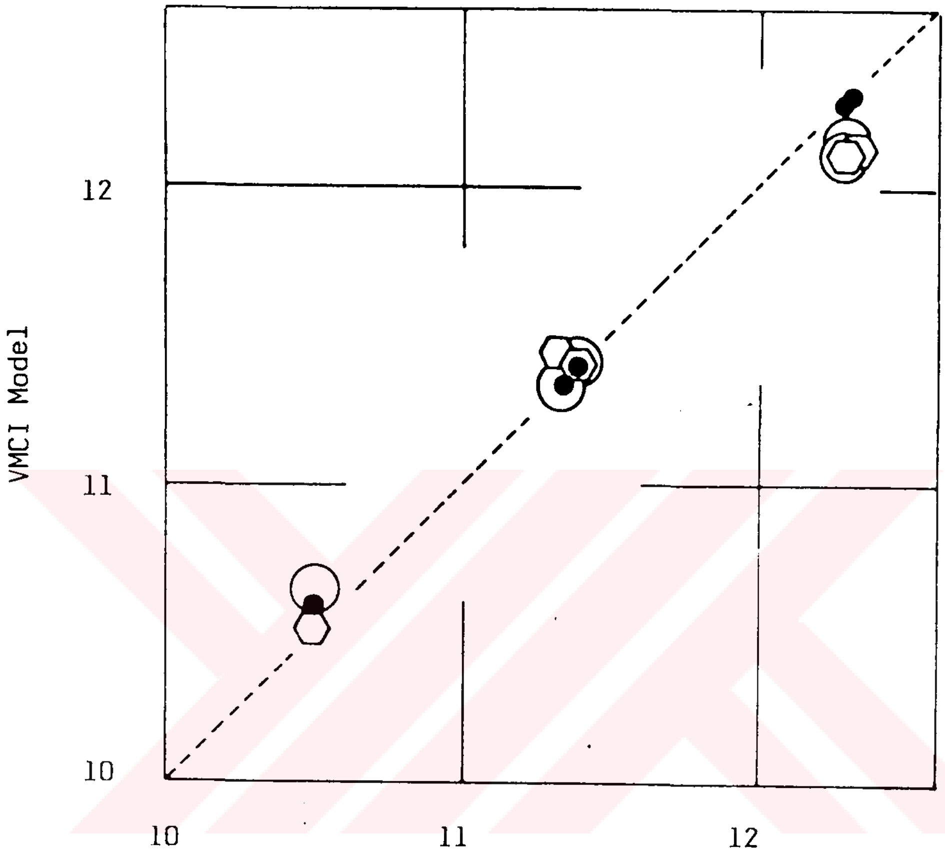
ALKYLBENZENES

Figure V.3 . Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Alkylbenzenes. In These Plots [●] Represents the Results Obtained Through Group Specific Regression Analysis [⬡] Represents the Results Obtained Through the Regression Carried out for Pairs of Groups having Electron Donating and Electron Withdrawing Substituents and [○] Represents the Results Obtained Through the Regression Analysis of Four Aromatic Groups Together.



Level I Fugacity Model

Figure V.3.1.1 Equilibrium Distribution (%) in Air



Level I Fugacity Model

Figure V.3.1.2. Equilibrium Distribution (%) in Soil

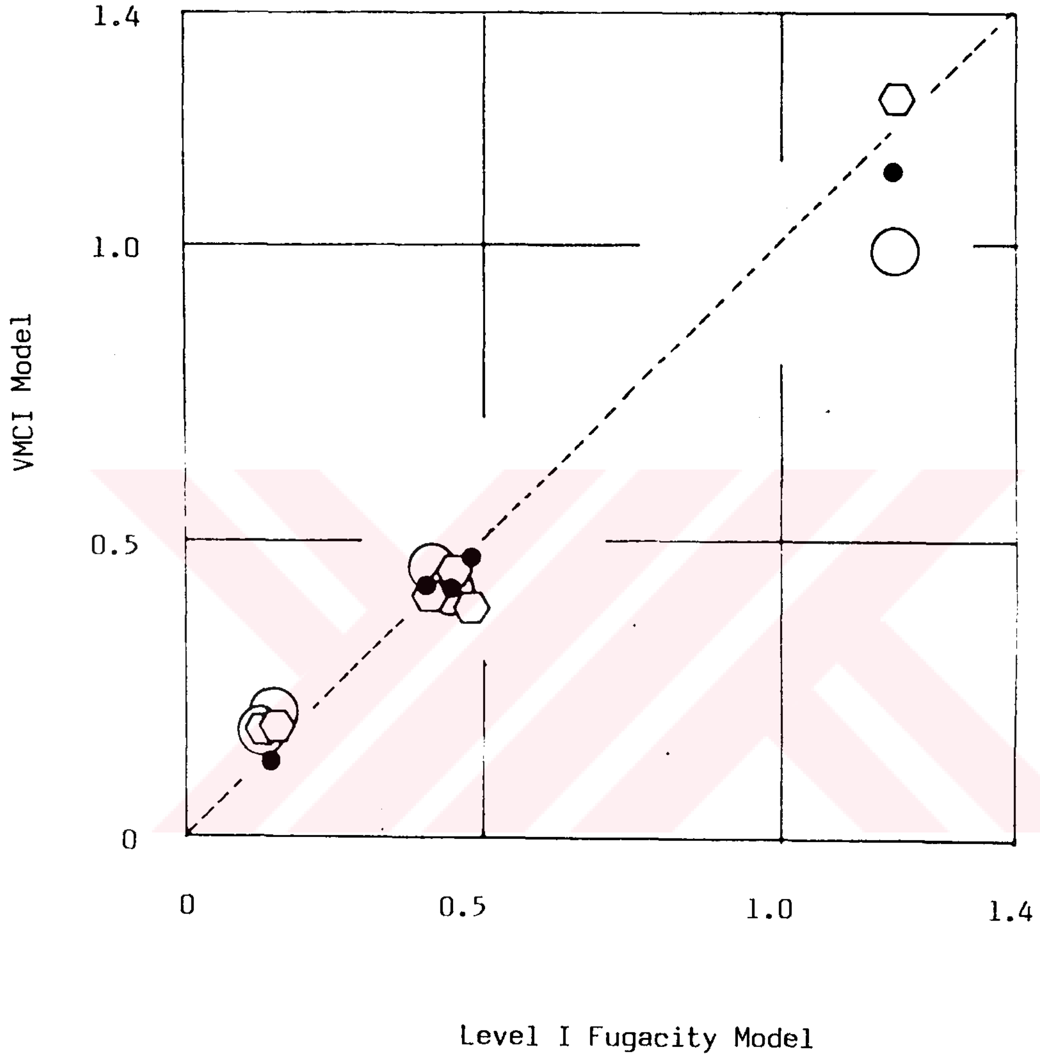


Figure V.3.1.3 Equilibrium Distribution (%) in Water

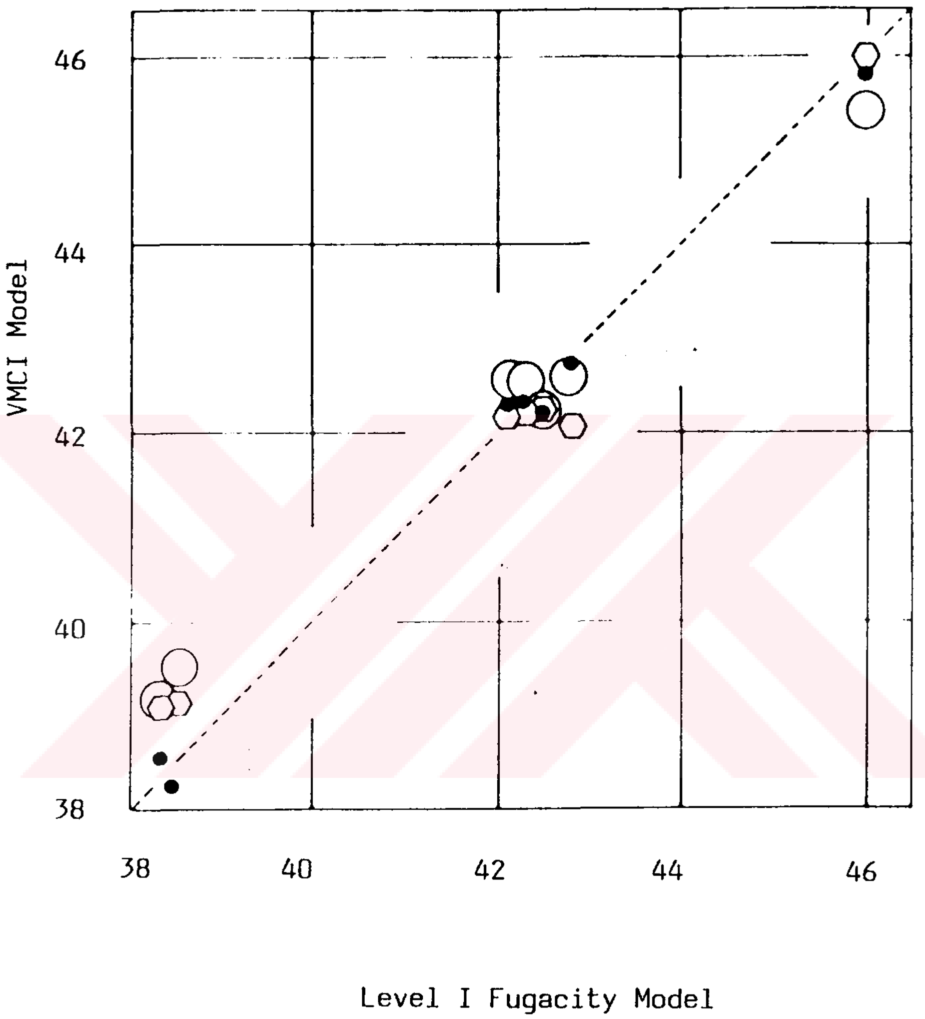


Figure V.3.1.4 Equilibrium Distribution (%) in Biota

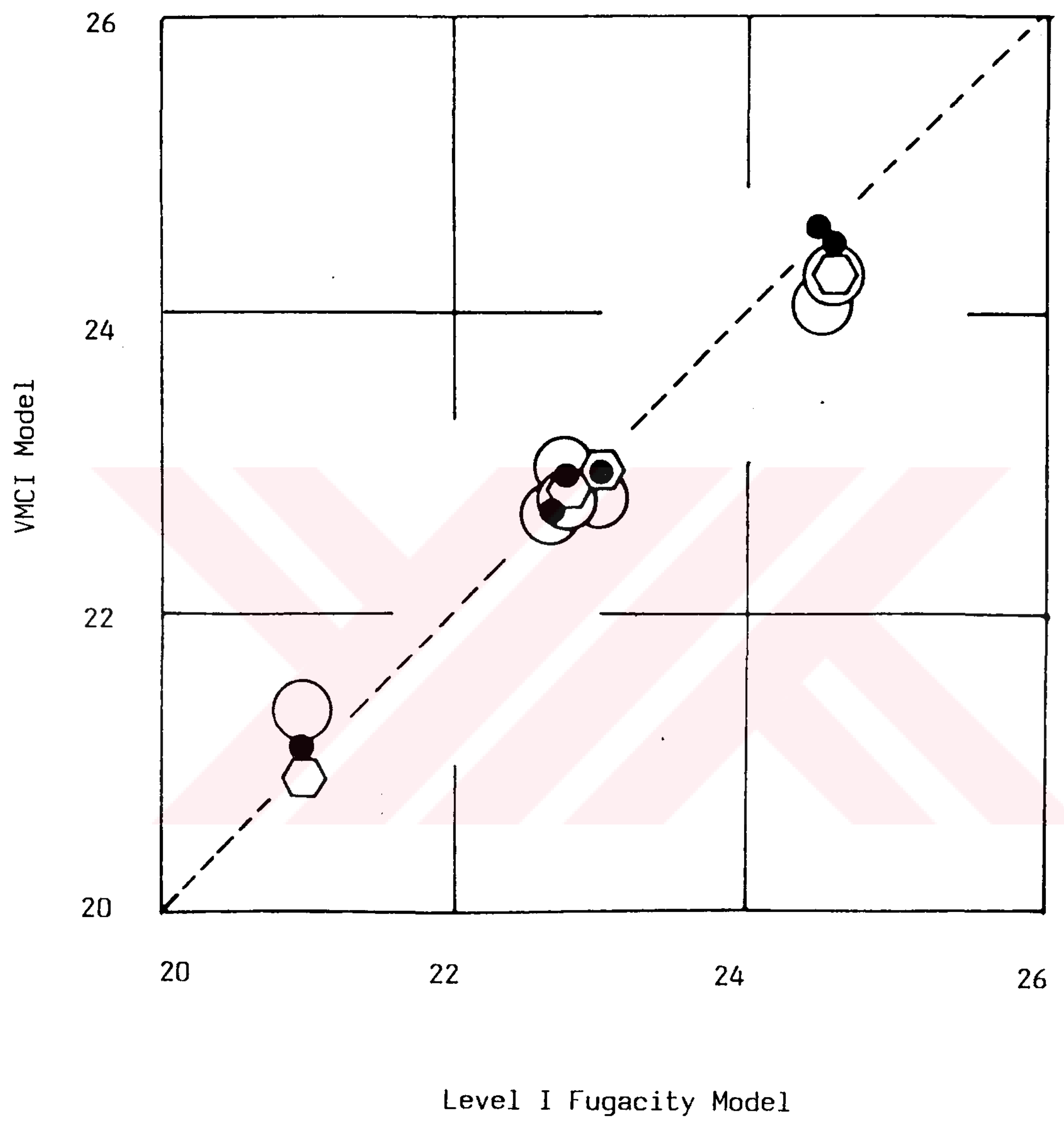


Figure V.3.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment

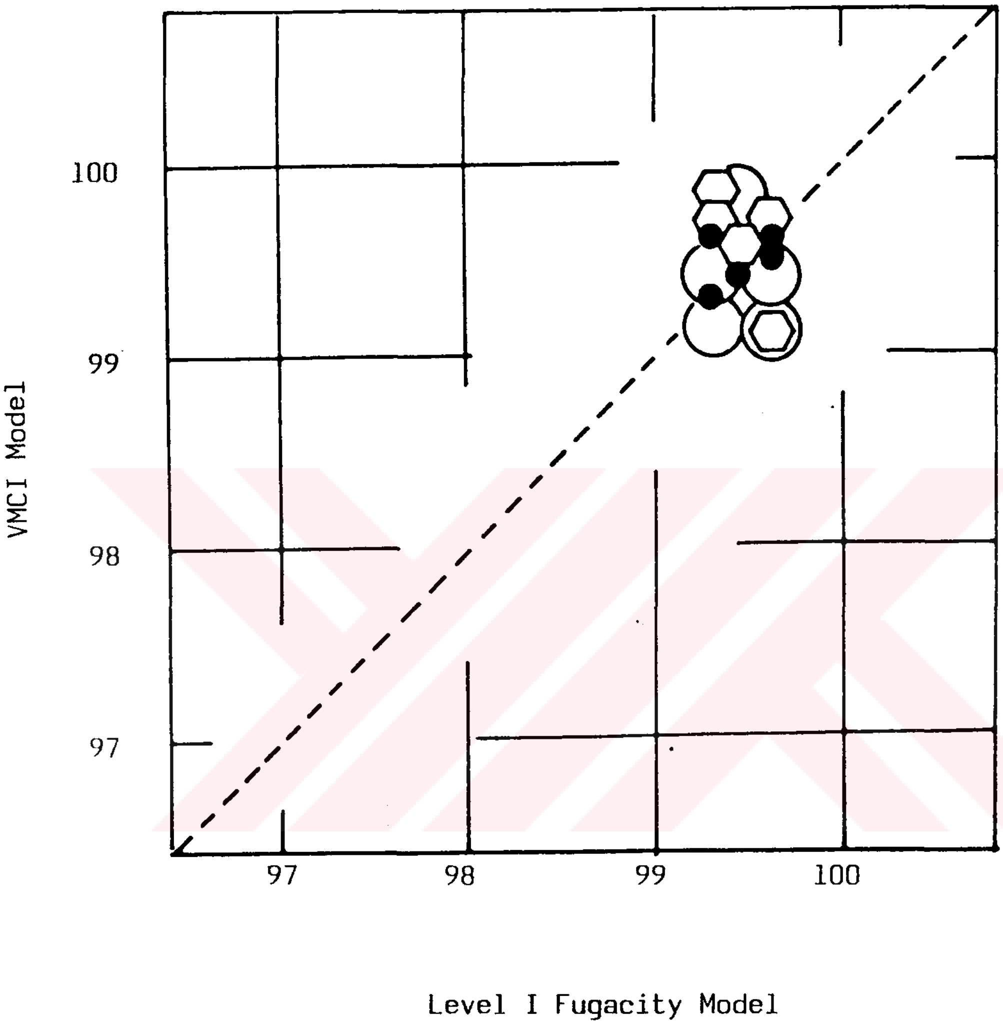


Figure V.3.2.1 Mass Distribution (%) in Air

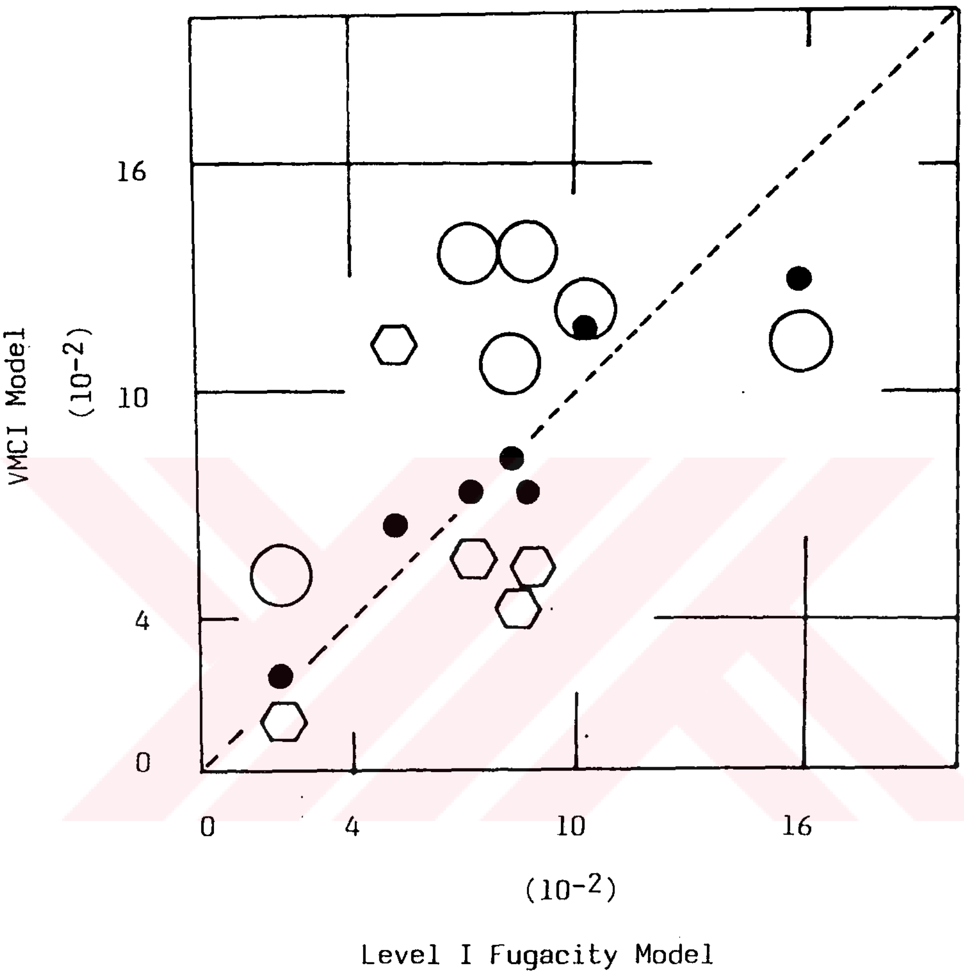


Figure V.3.2.2 Mass Distribution (%) in Soil

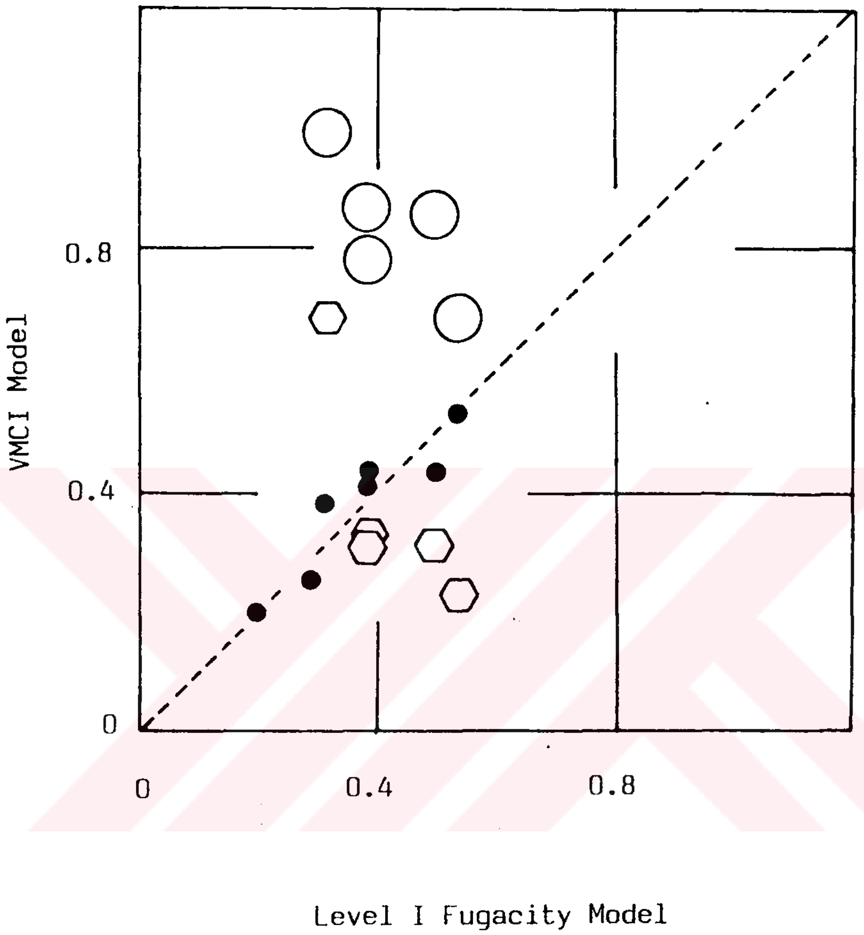


Figure V.3.2.3 Mass Distribution (%) in Water

∴

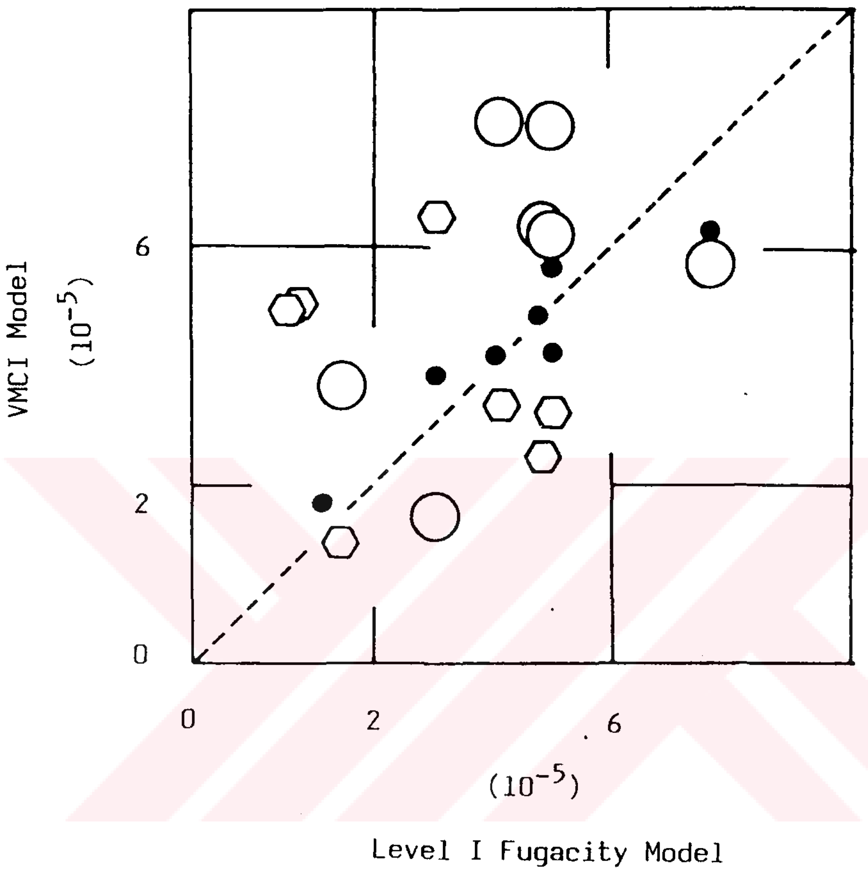


Figure V.3.2.4 Mass Distribution (%) in Biota

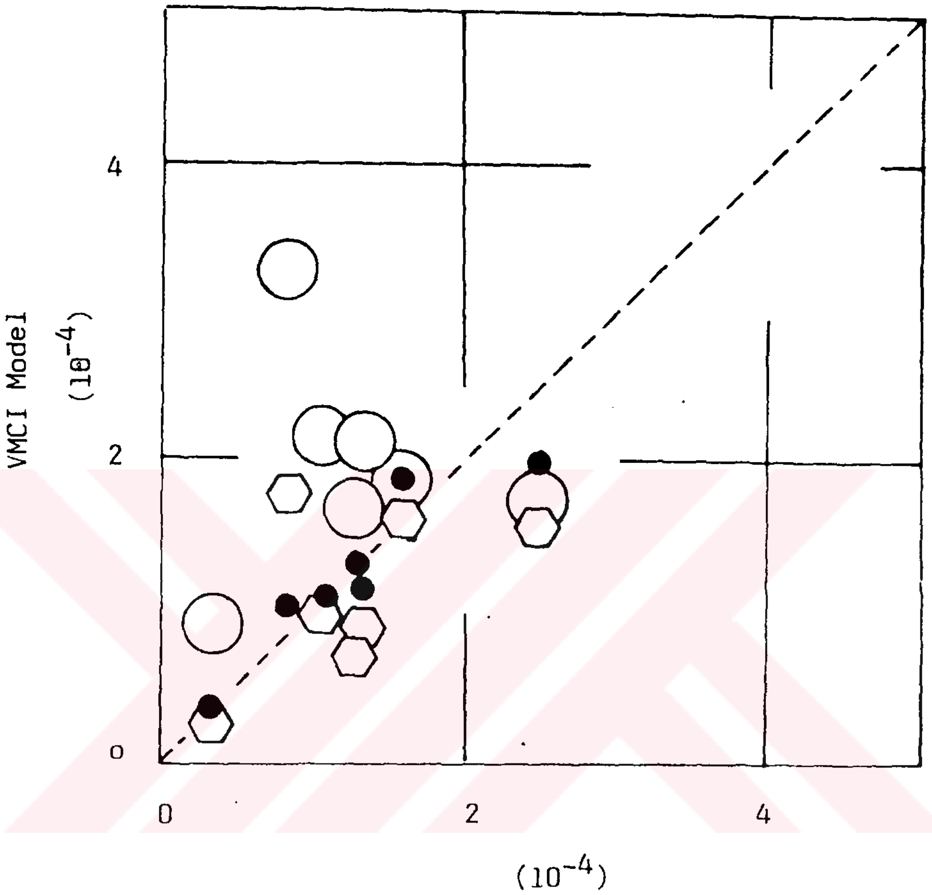


Figure V.3.2.5 Mass Distribution (%) in Suspended Solids

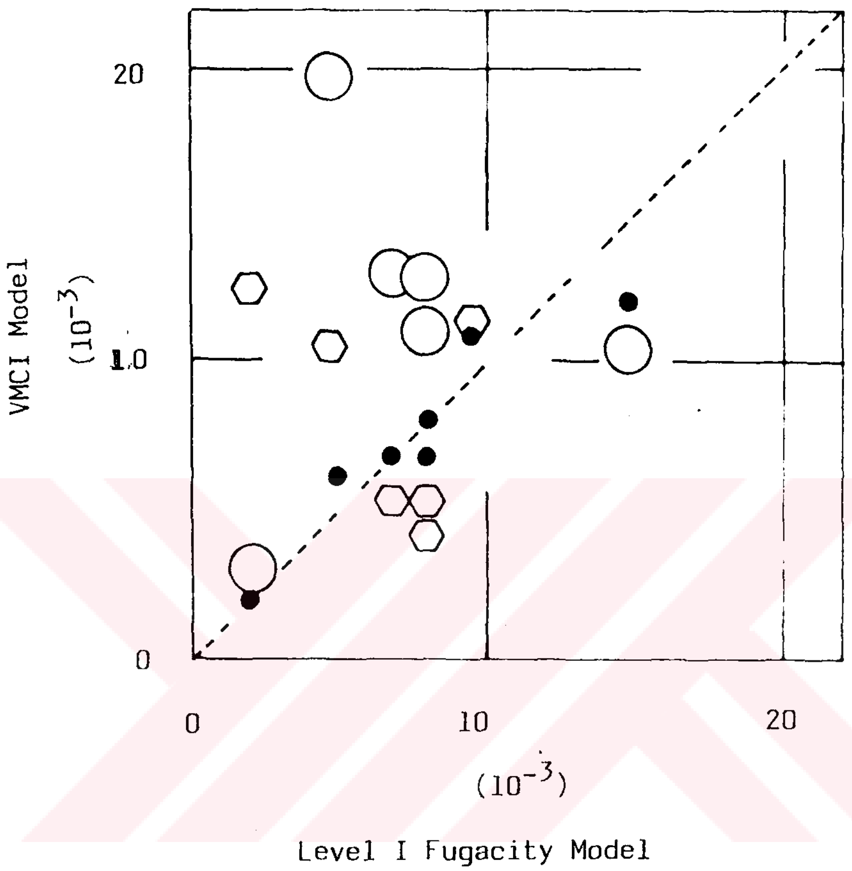


Figure V.3.2.6 Mass Distribution (%) in Sediment

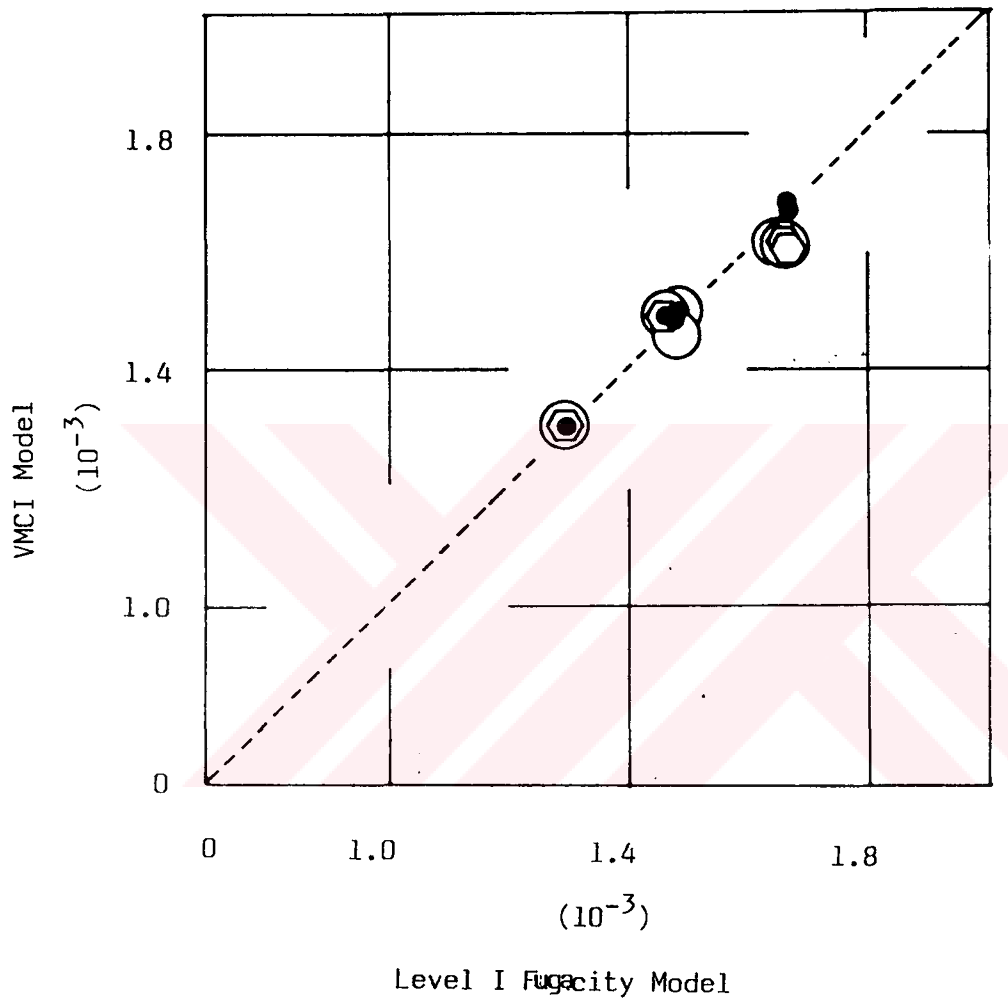


Figure V.3.3.1 Concentration (ppm) in Air

:

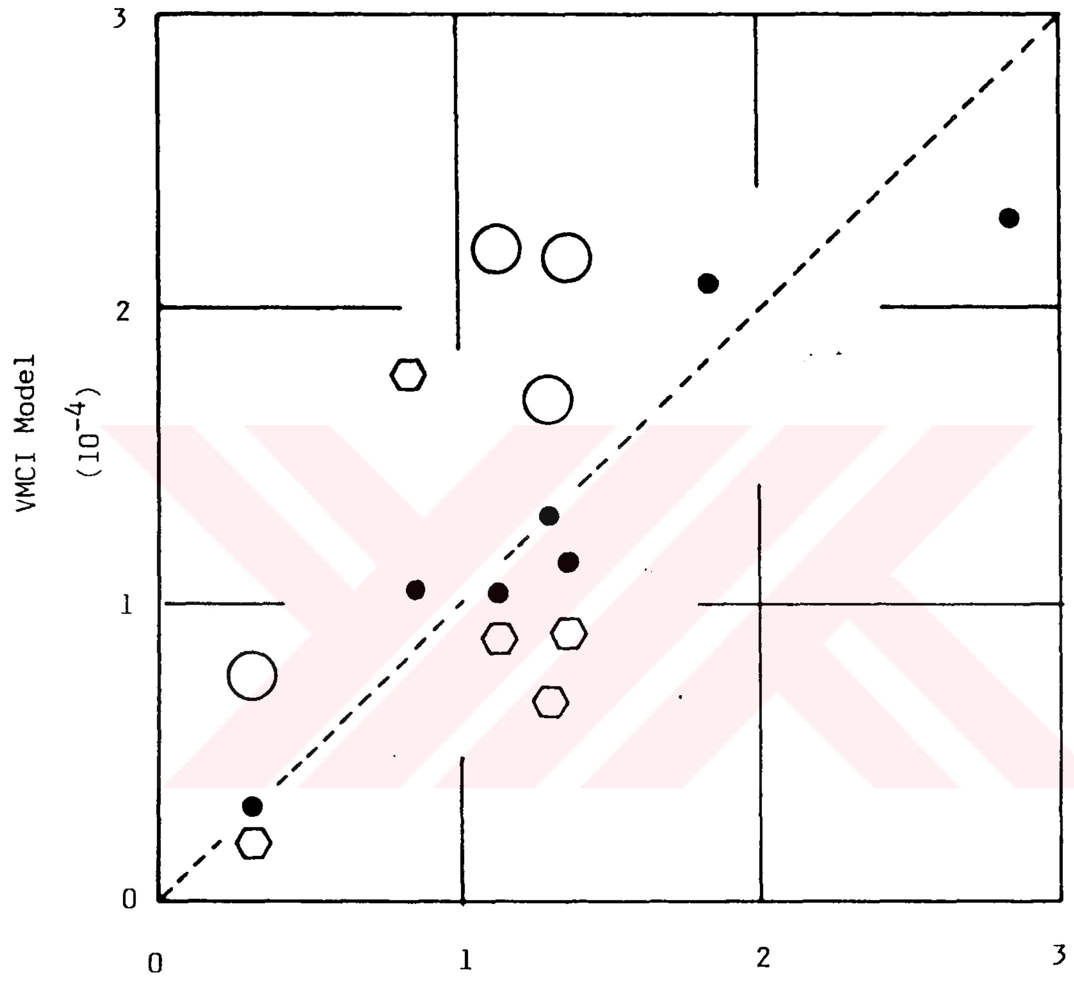


Figure V.3.3.2 Concentration (ppm) in Soil

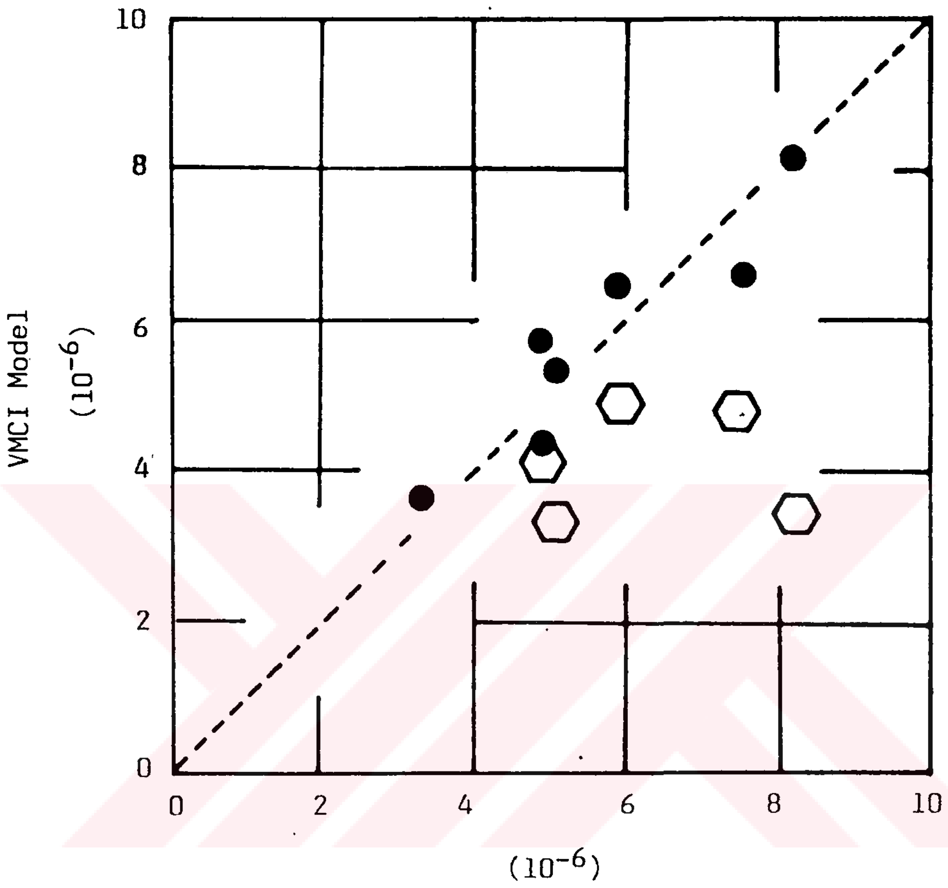


Figure V.3.3.3 Concentration (ppm) in Water

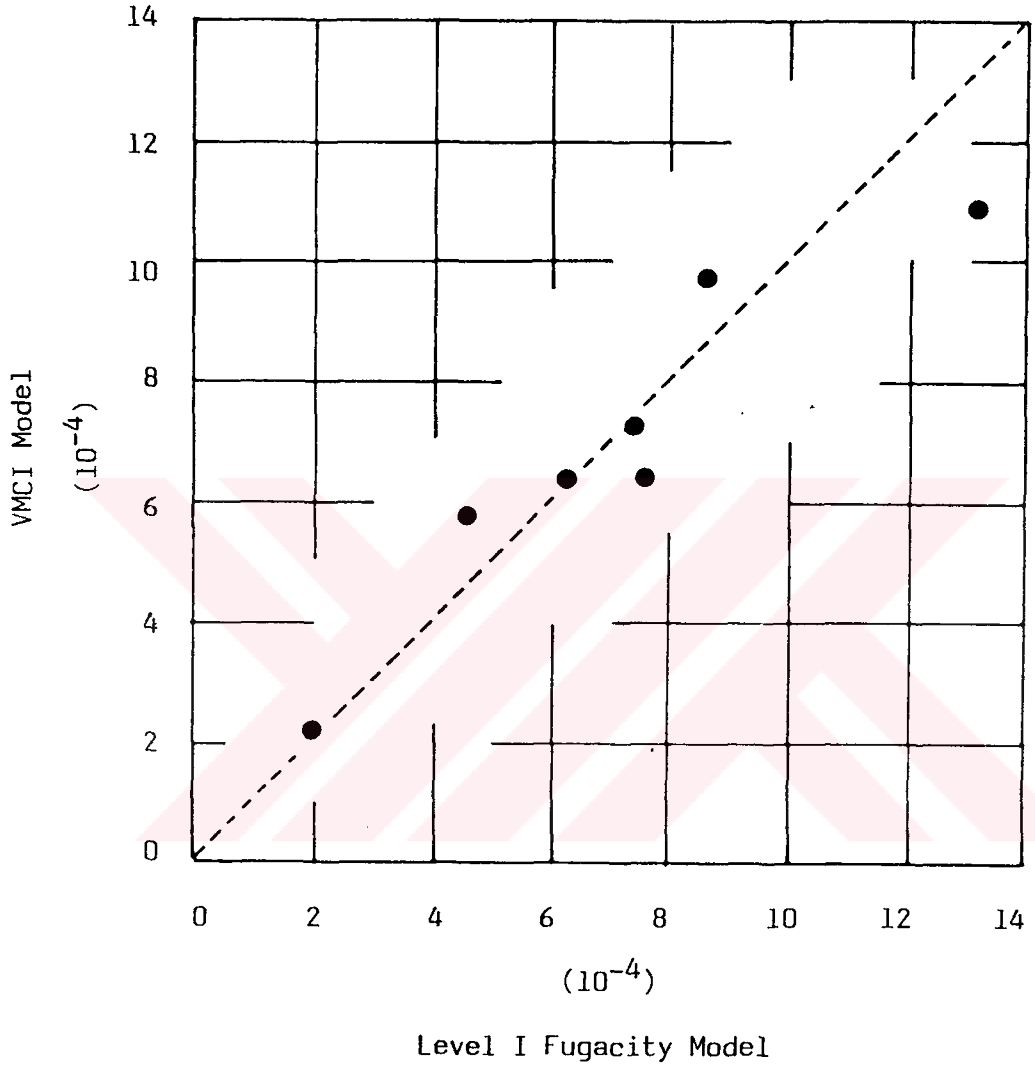


Figure V.3.3.4 Concentration (ppm) in Biota

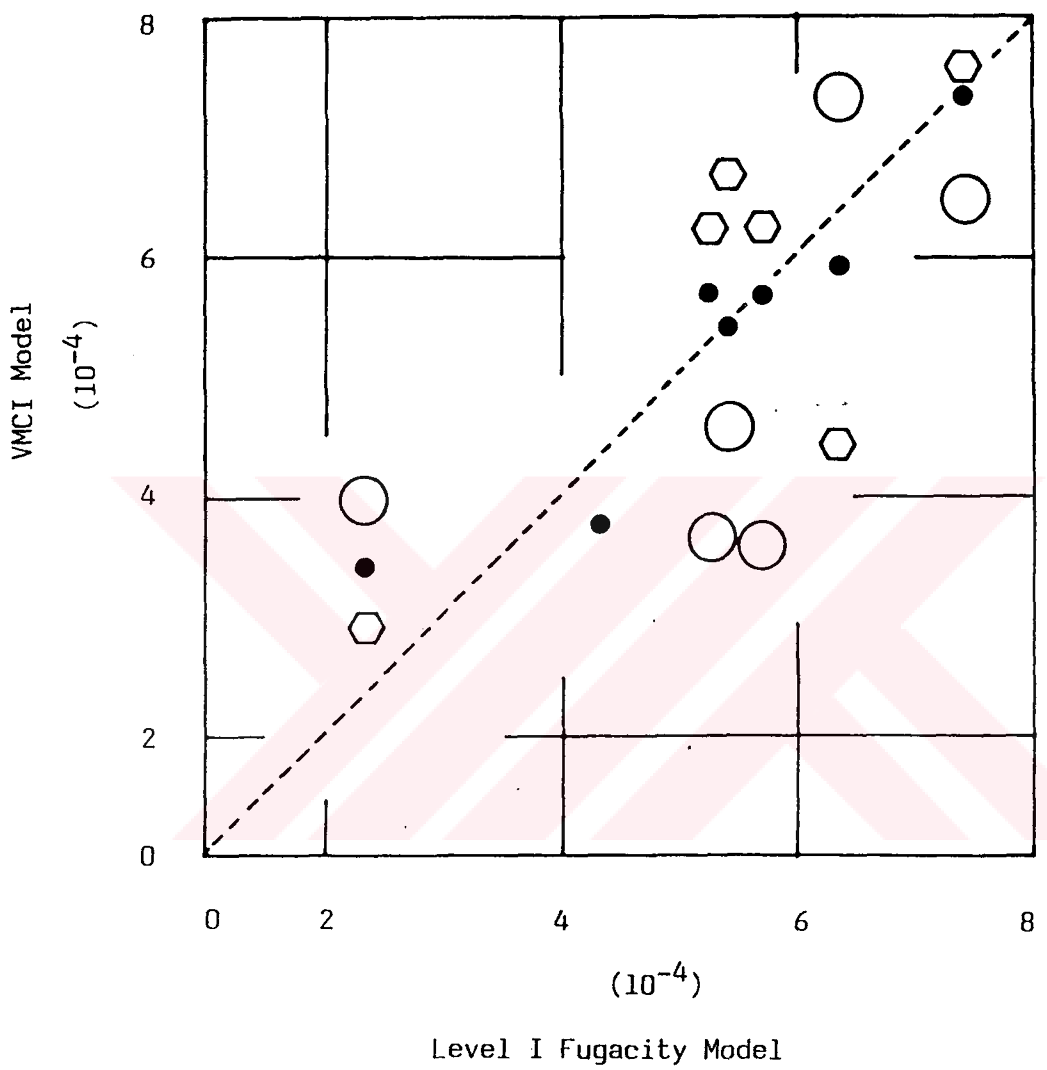


Figure V.3.3.5 Concentration (ppm) in Suspended Solids and Sediment

POLYCHLORINATED BIPHENYLS

Figure V. 4 . Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Polychlorinated Biphenyls. In These Plots [●] Represents the Results Obtained Through Group Specific Regression Analysis [⬡] Represents the Results Obtained Through the Regression Carried out for Pairs of Groups having Electron Donating and Electron Withdrawing Substituents and [○] Represents the Results Obtained Through the Regression Analysis of Four Aromatic Groups Together.

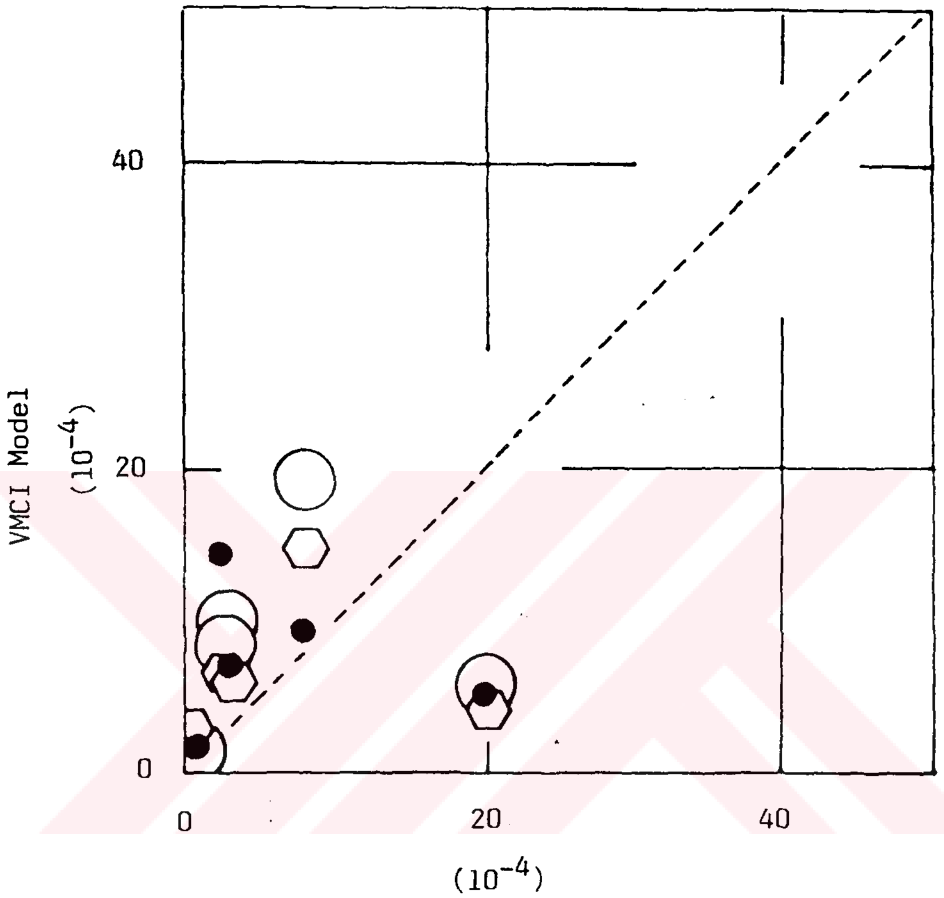


Figure V.4.1.1 Equilibrium Distribution (%) in Air

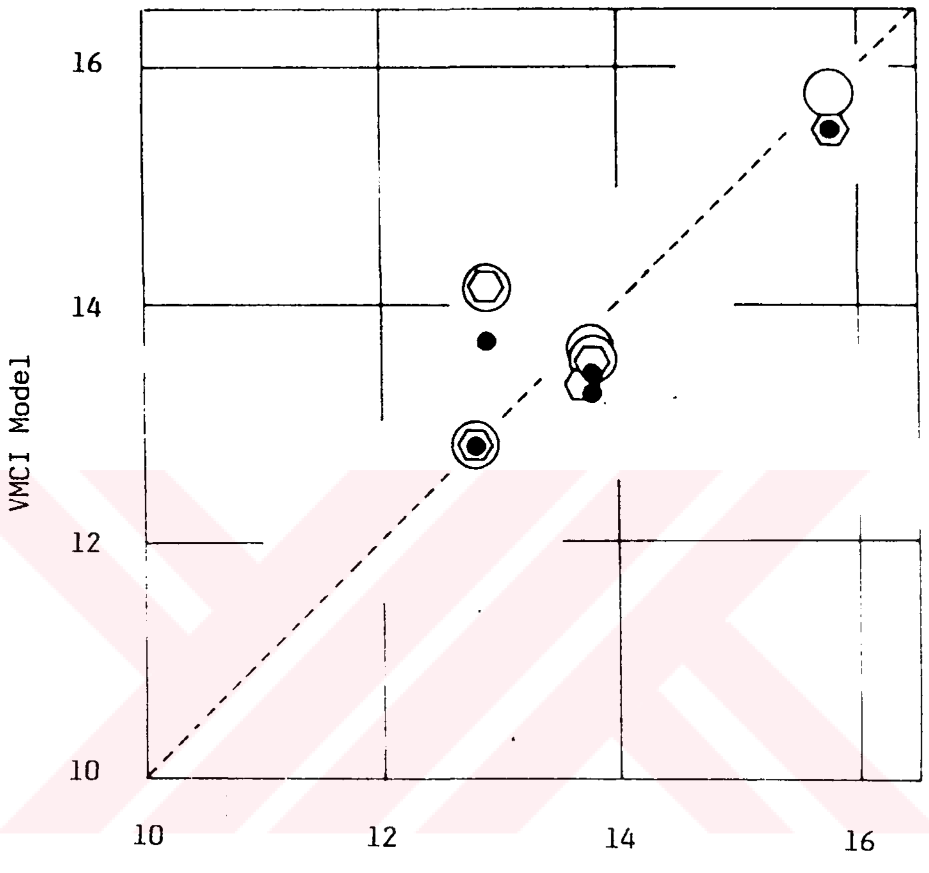
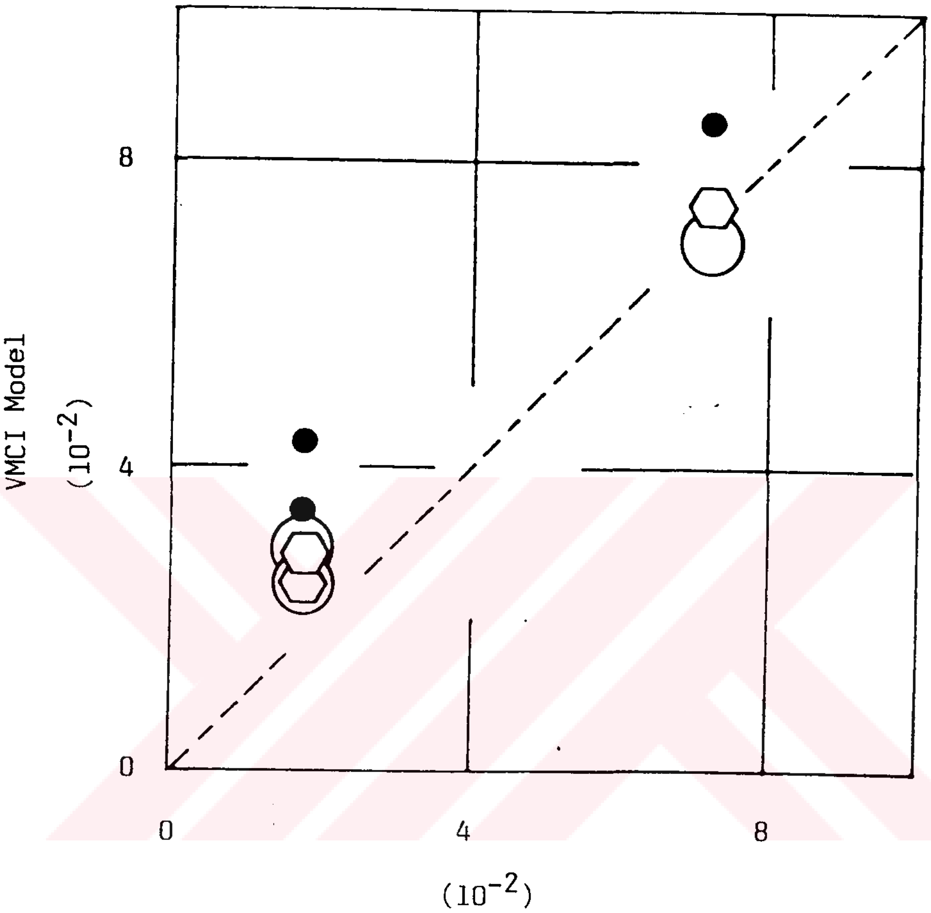


Figure V.4.1.2 Equilibrium Distribution (%) in Soil



Level I Fugacity Model

Figure V.4.1.3 Equilibrium Distribution (%) in Water

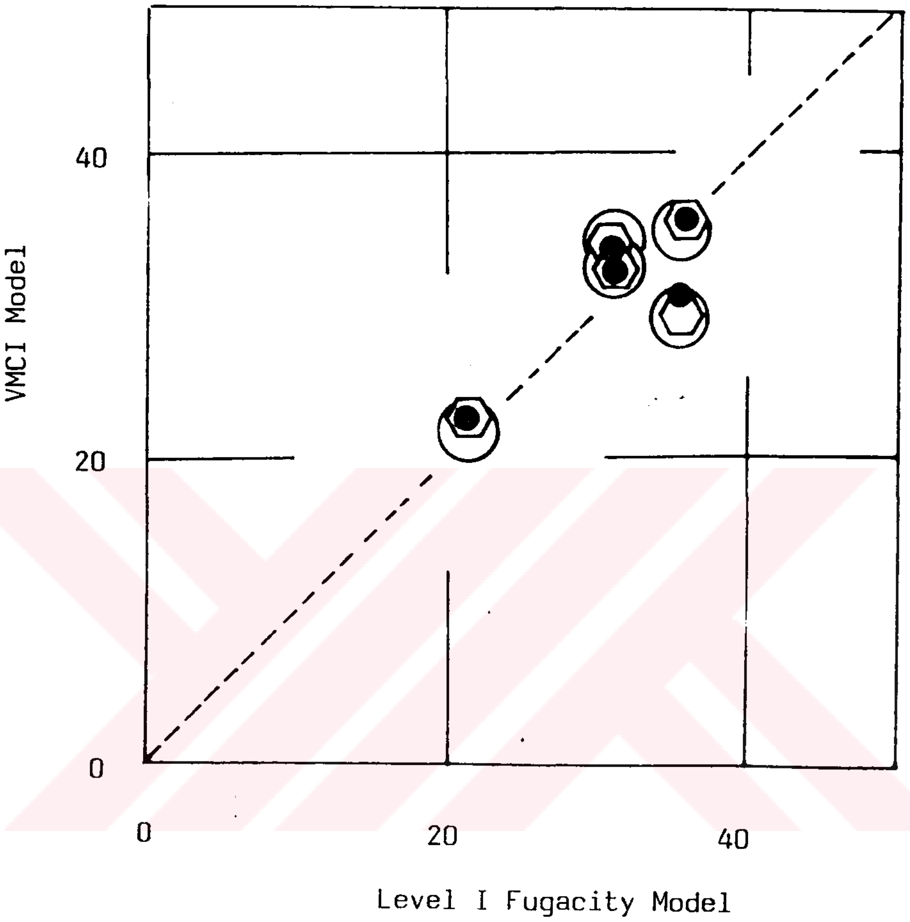


Figure V.4.1.4 Equilibrium Distribution (%) in Biota

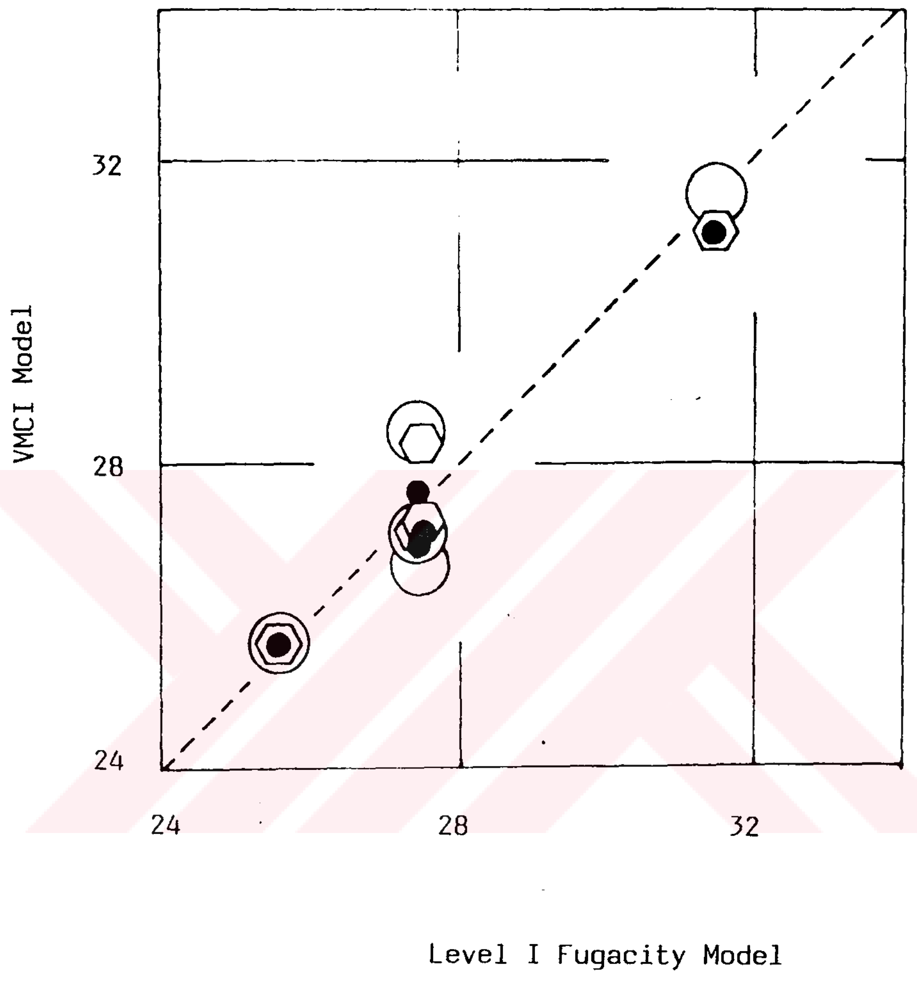


Figure V.4.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment

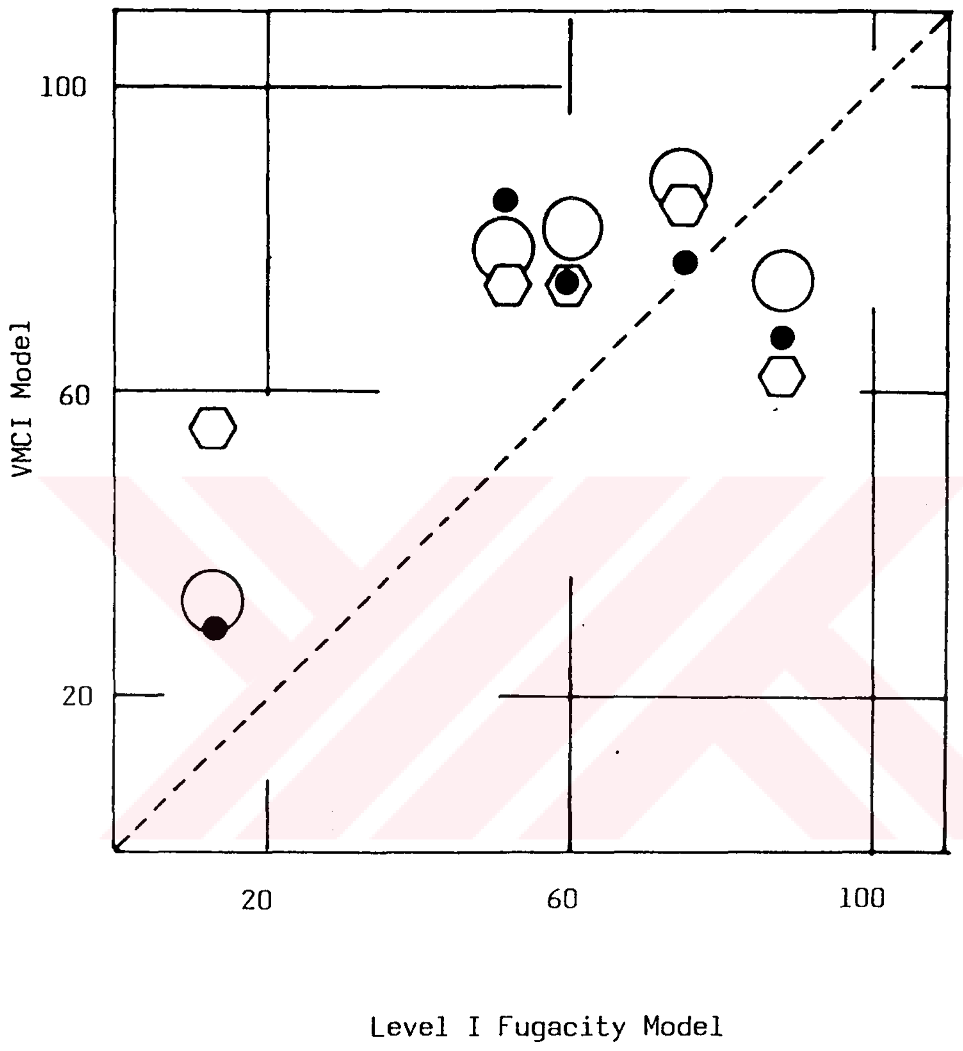


Figure V.4.2.1 Mass Distribution (%) in Air

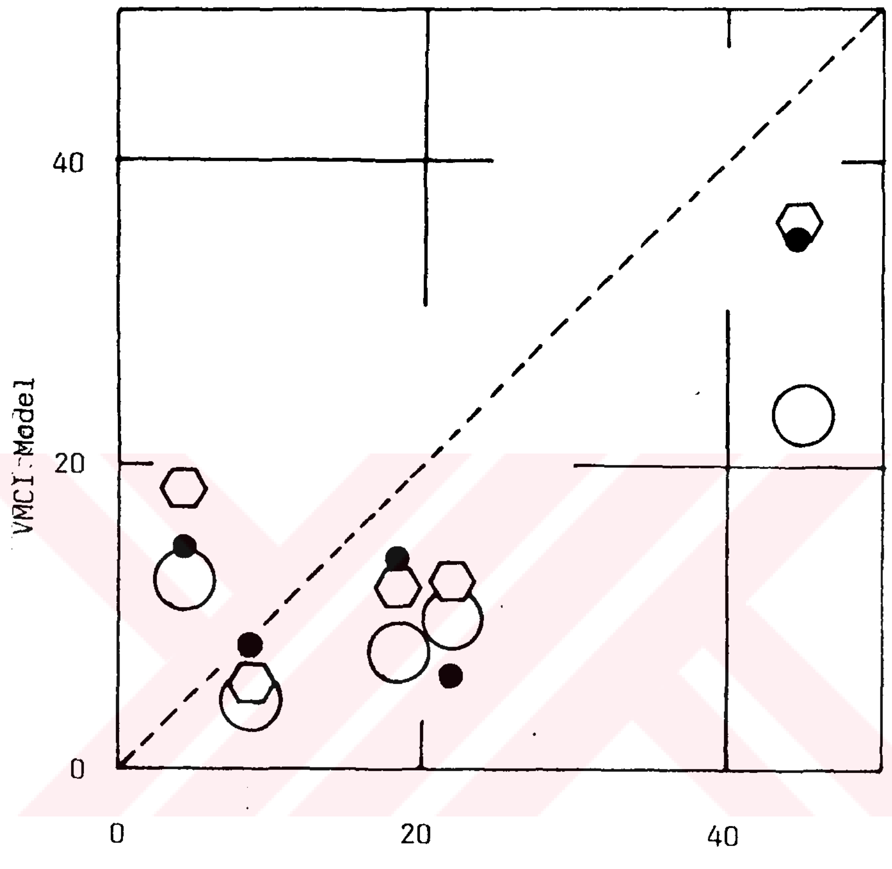
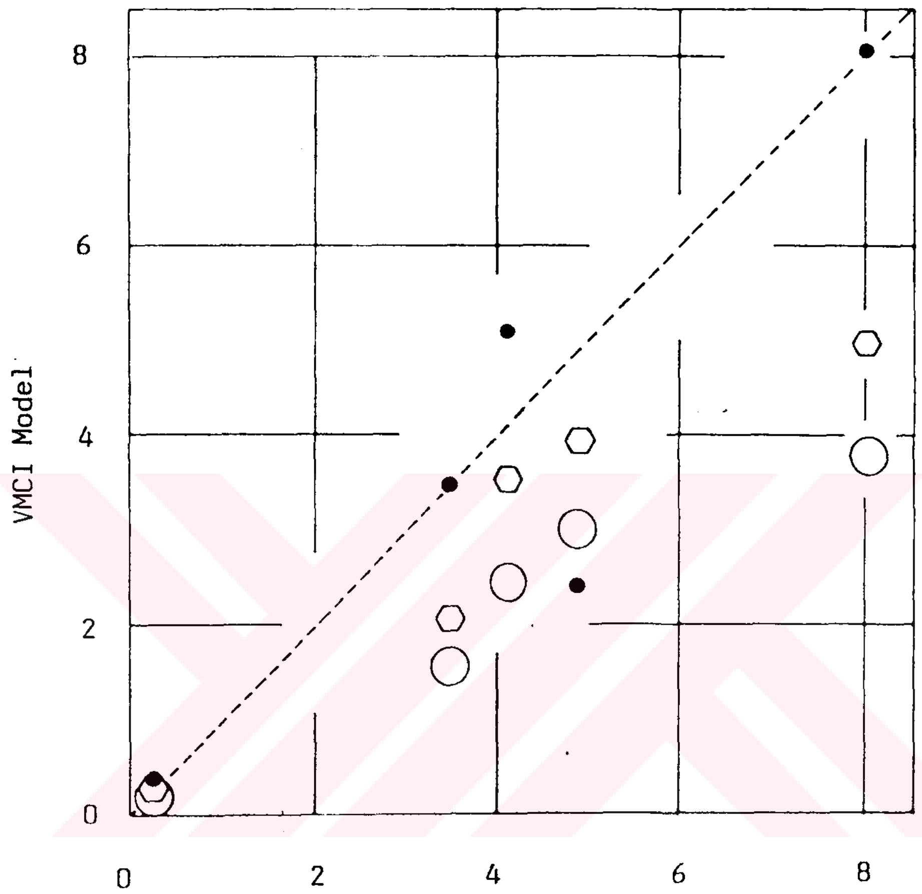


Figure V.4.2.2 Mass Distribution (%) in Soil



Level I Fugacity Model

Figure V.4.2.3 Mass Distribution (%) in Water

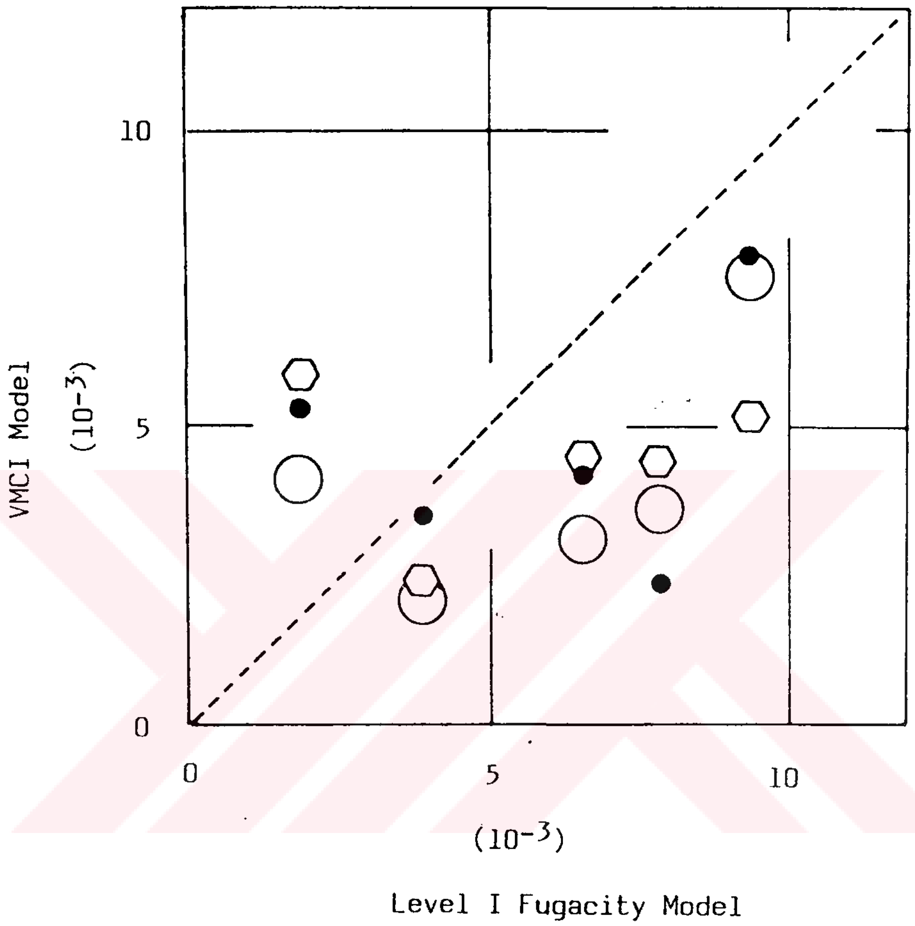


Figure V.4.2.4 Mass Distribution (%) in Biota

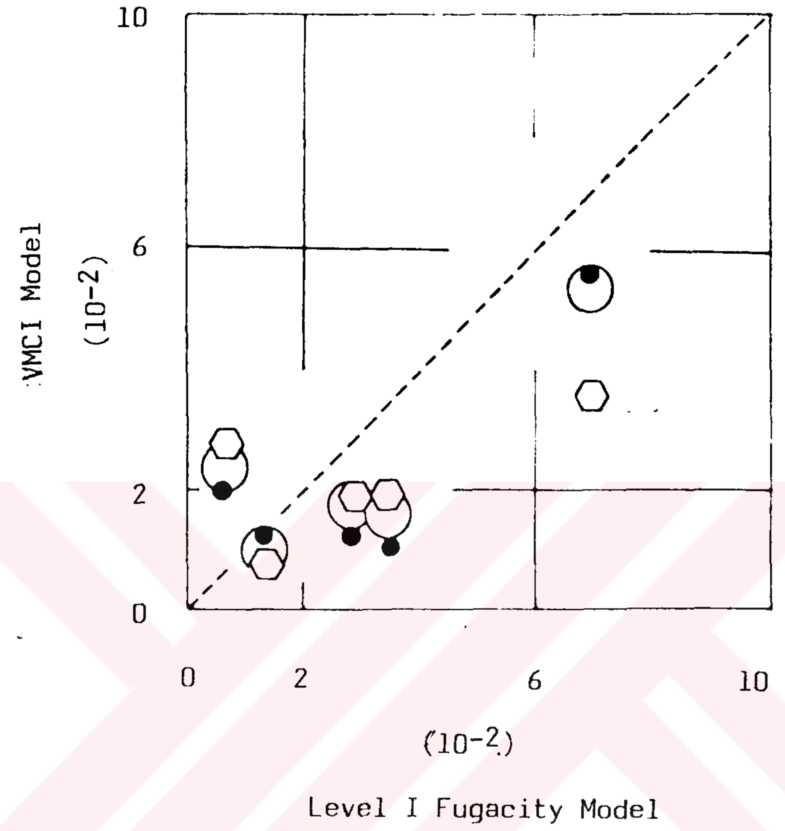


Figure V.4.2.5 Mass Distribution (%) in Suspended Solids

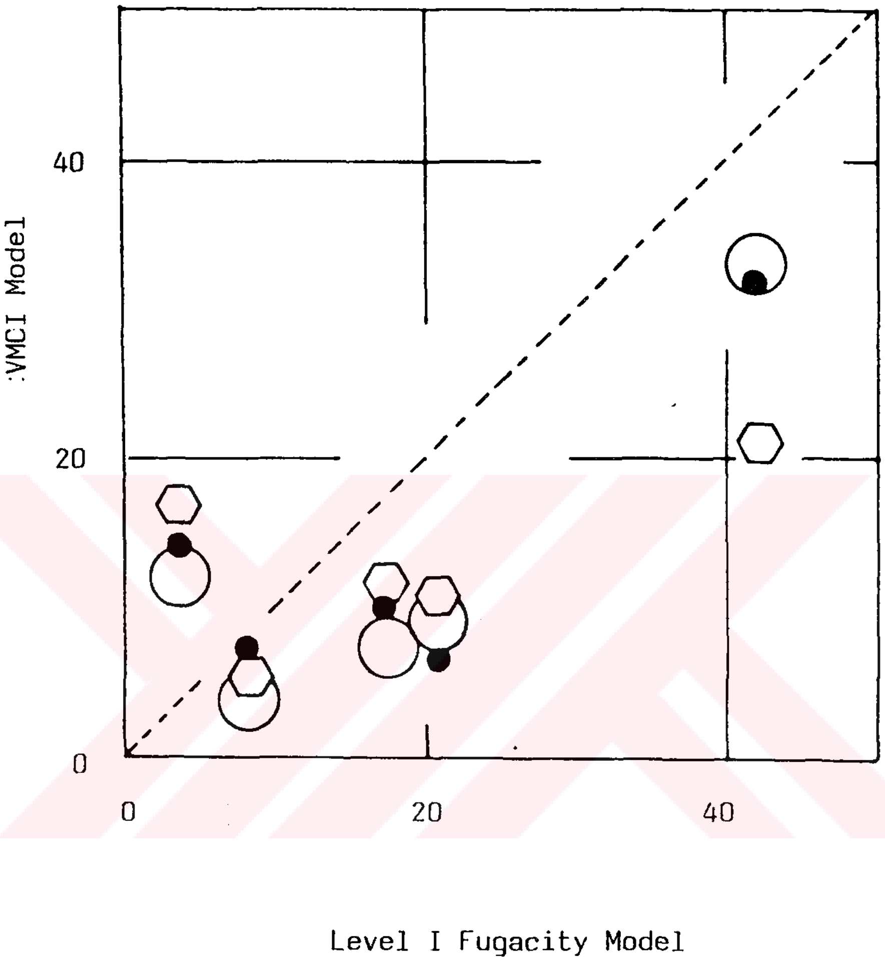


Figure V.4.2.6 Mass Distribution (%) in Sediment

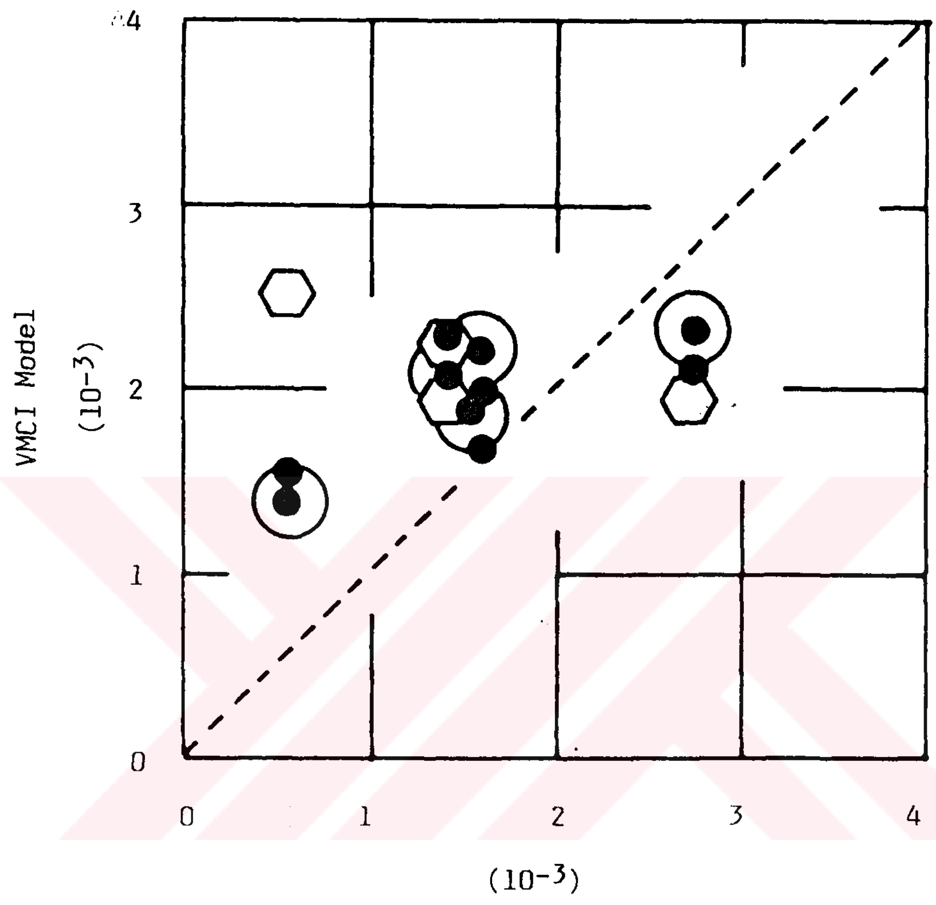


Figure V.4.3.1 Concentration (ppm) in Air

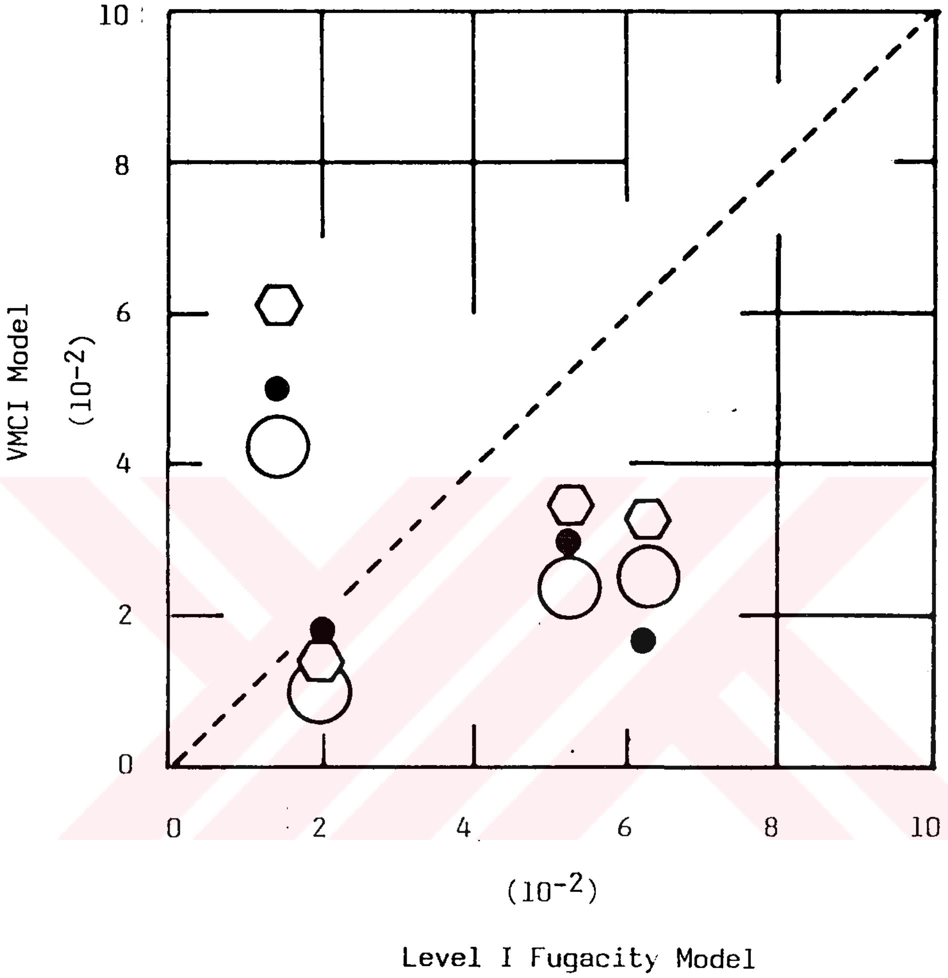


Figure V.4.3.2 Concentration (ppm) in Soil

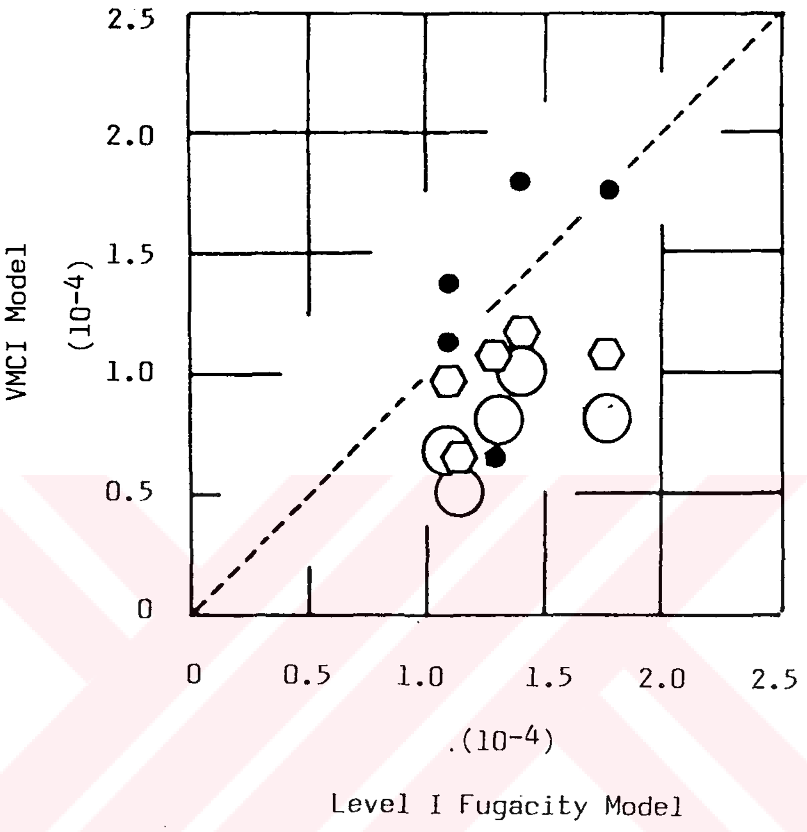


Figure V.4.3.3 Concentration (ppm) in Water

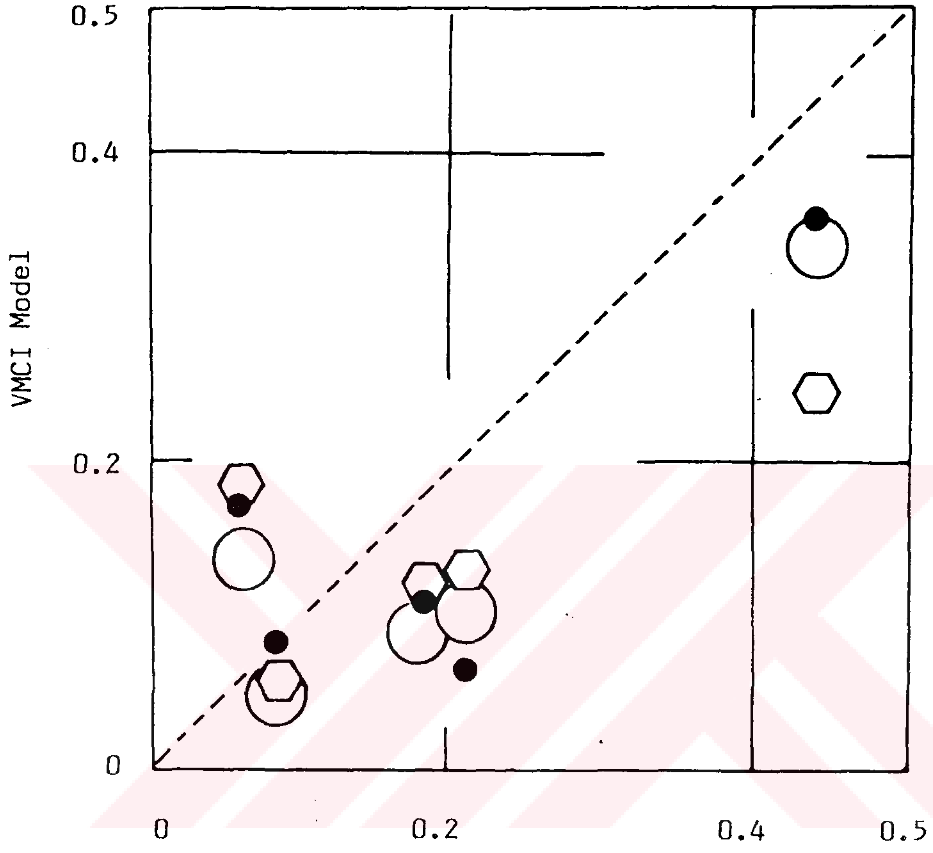


Figure V.4.3.4 Concentration (ppm) in Biota

YÖK

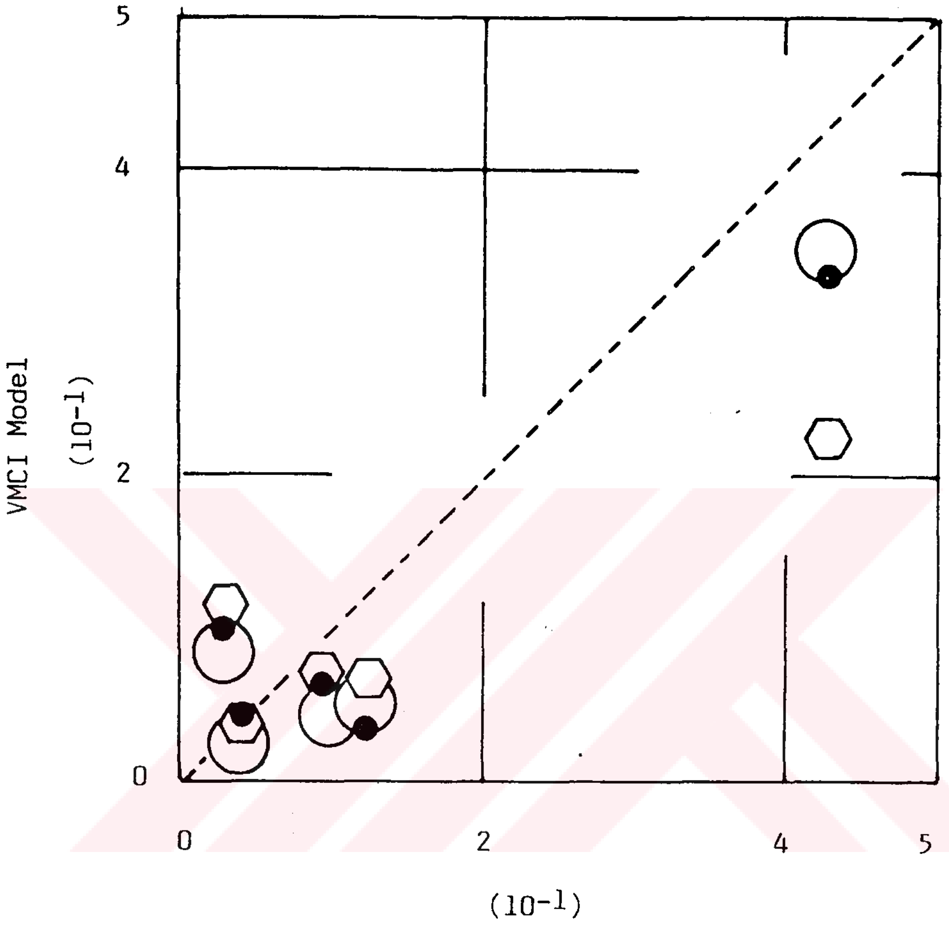


Figure V.4.3.5 Concentration (ppm) in Suspended Solids and Sediment

HALOGEN SUBSTITUTED BENZENE DERIVATIVES

Figure V. 5 . Plots of Equilibrium, Mass Partitioning (%) and Concentration (ppm) in Various Compartments of the Environment Versus Those Calculated Through Mackay's Level I Fugacity Approach for Halogen Substituted Benzene Derivatives. In These Plots [●] Represents the Results Obtained Through Group Specific Regression Analysis [⬡] Represents the Results Obtained Through the Regression Carried out for Pairs of Groups having Electron Donating and Electron Withdrawing Substituents and [○] Represents the Result Obtained Through the Regression Analysis of Four Aromatic Groups Together.

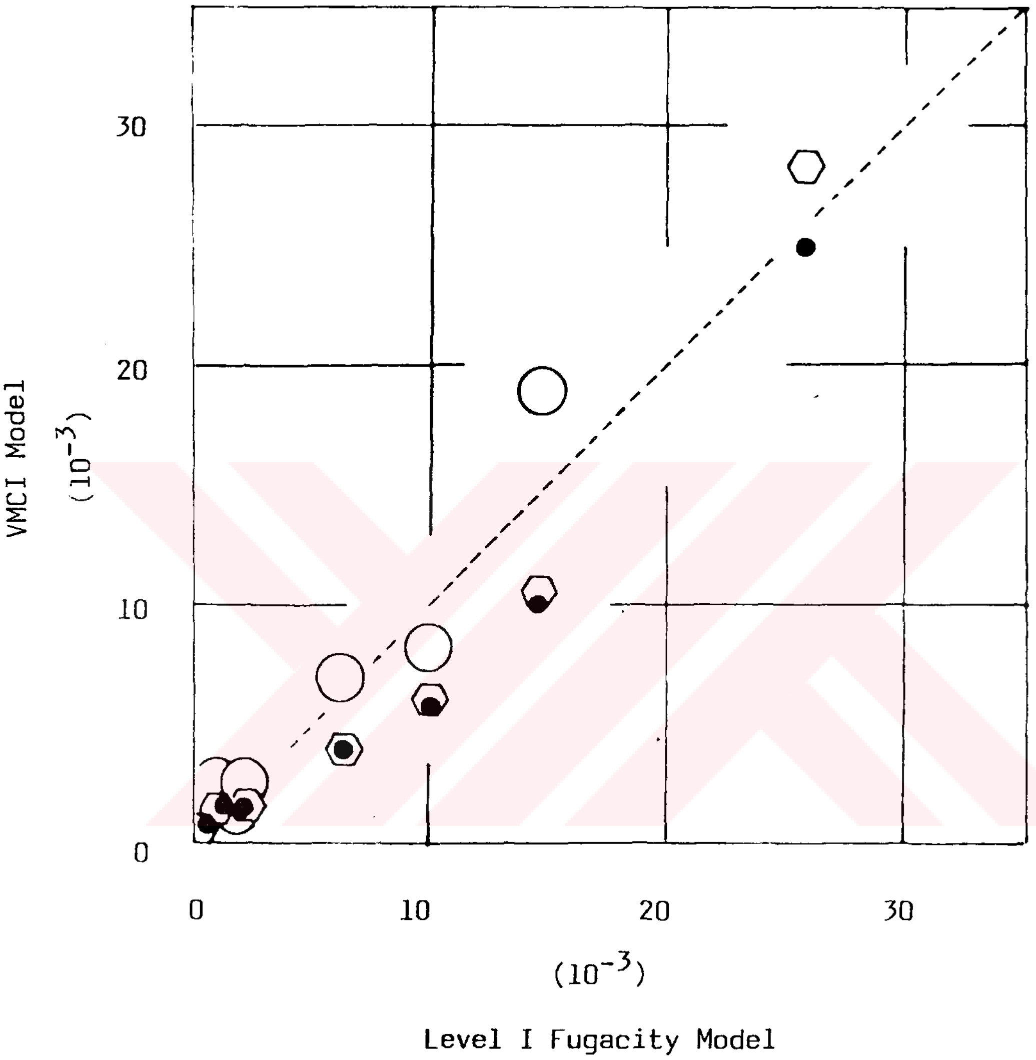
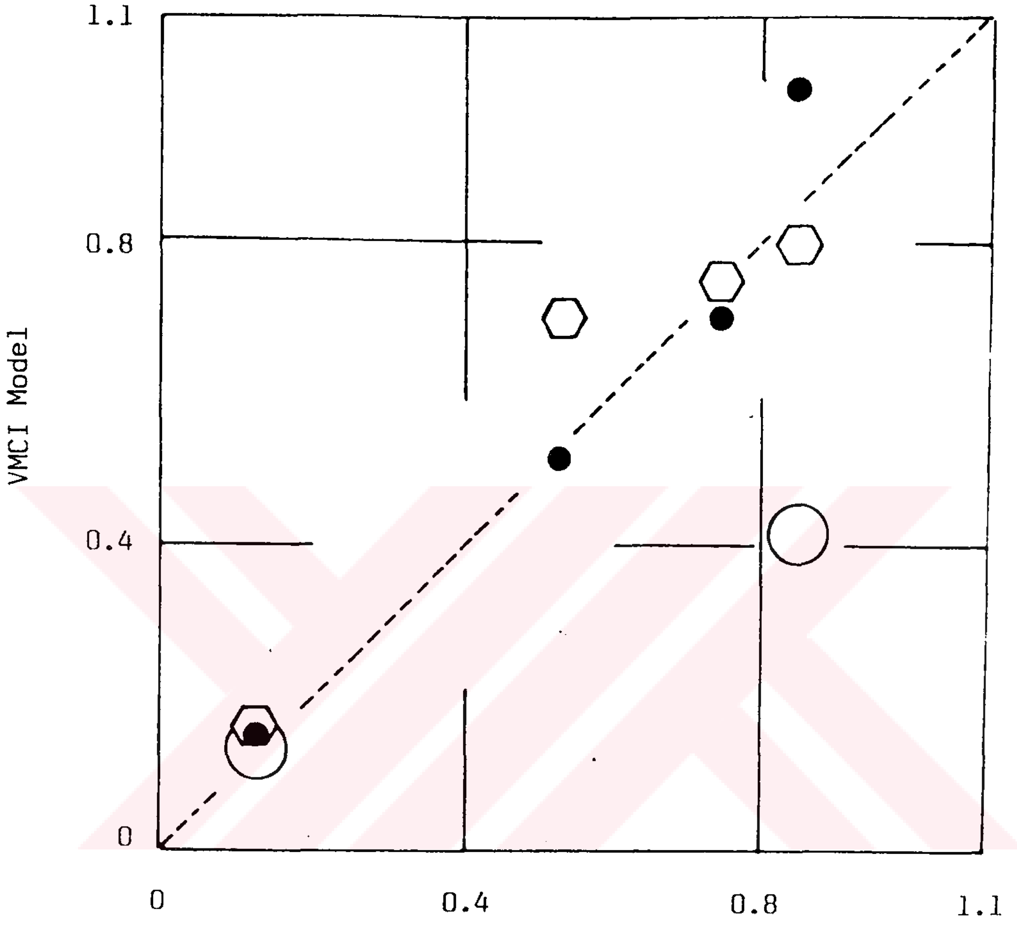


Figure V.5.1.1 Equilibrium Distribution (%) in Air Between 0-35 x 10^{-3} %



Level I Fugacity Model

Figure V.5.1.1 Equilibrium Distribution (%) in Air Between 0-1 %

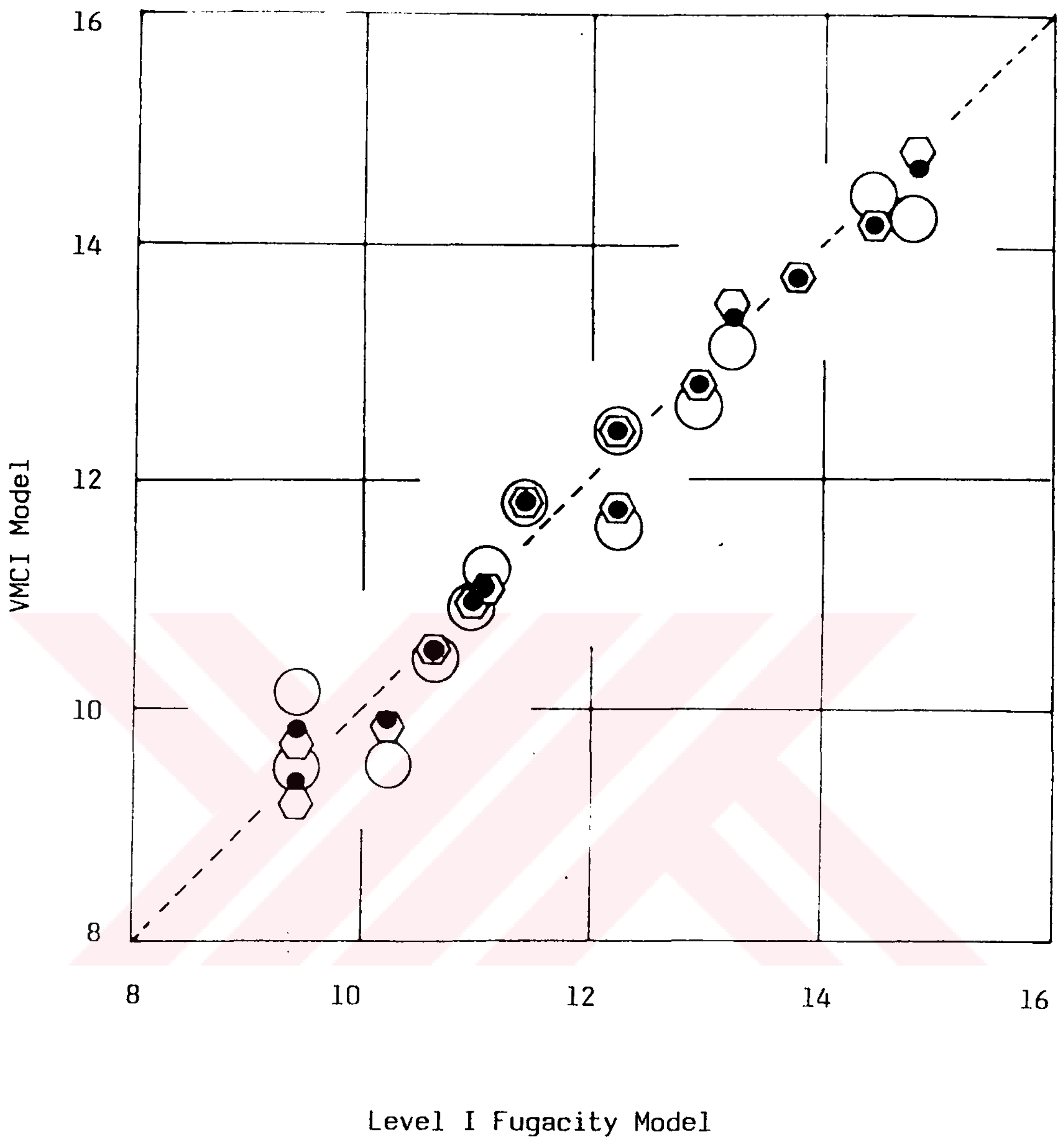
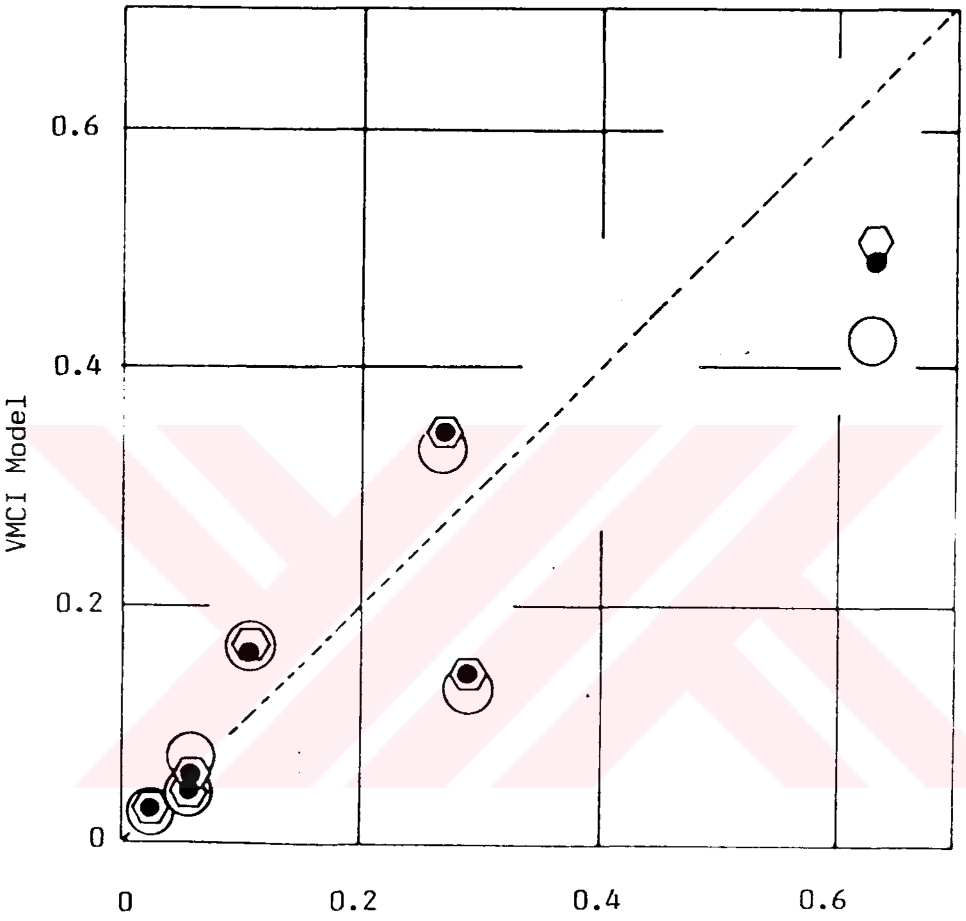


Figure V.5.1.2 Equilibrium Distribution (%) in Soil



Level I Fugacity Model

Figure V.5.1.3 Equilibrium Distribution (%) in Water Between 0-0.7 %

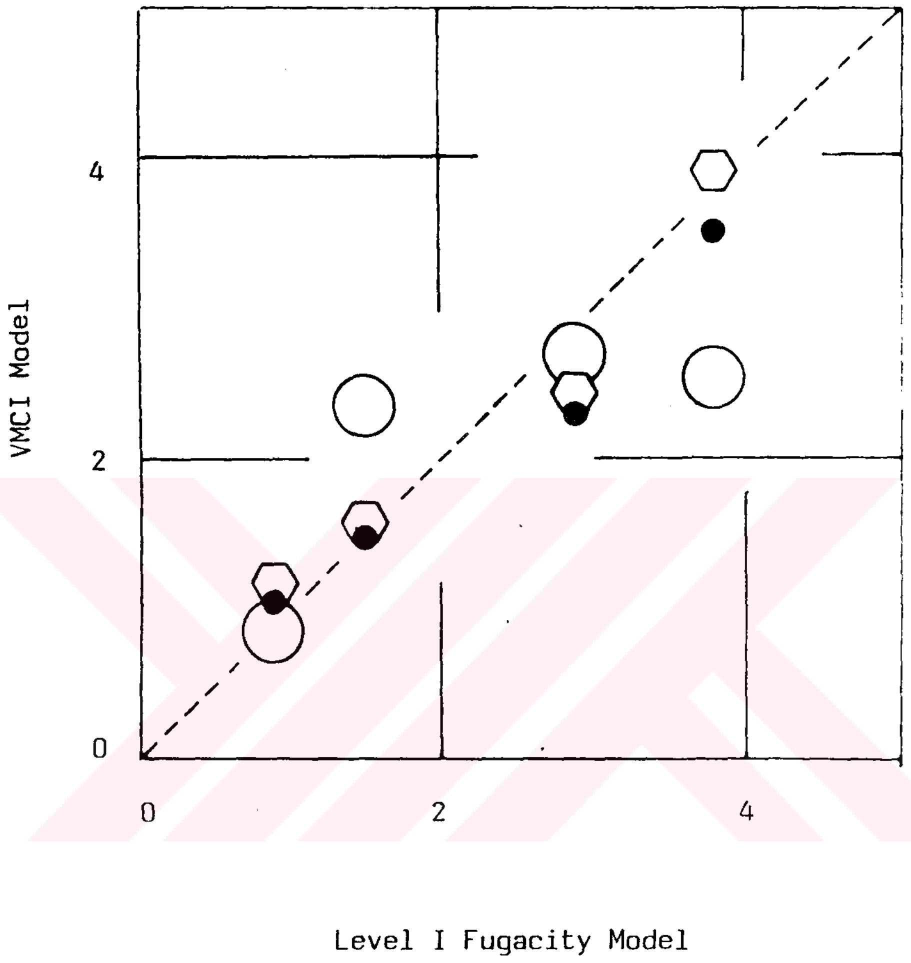


Figure V.5.1.3 Equilibrium Distribution (%) in Water Between 0-5 %

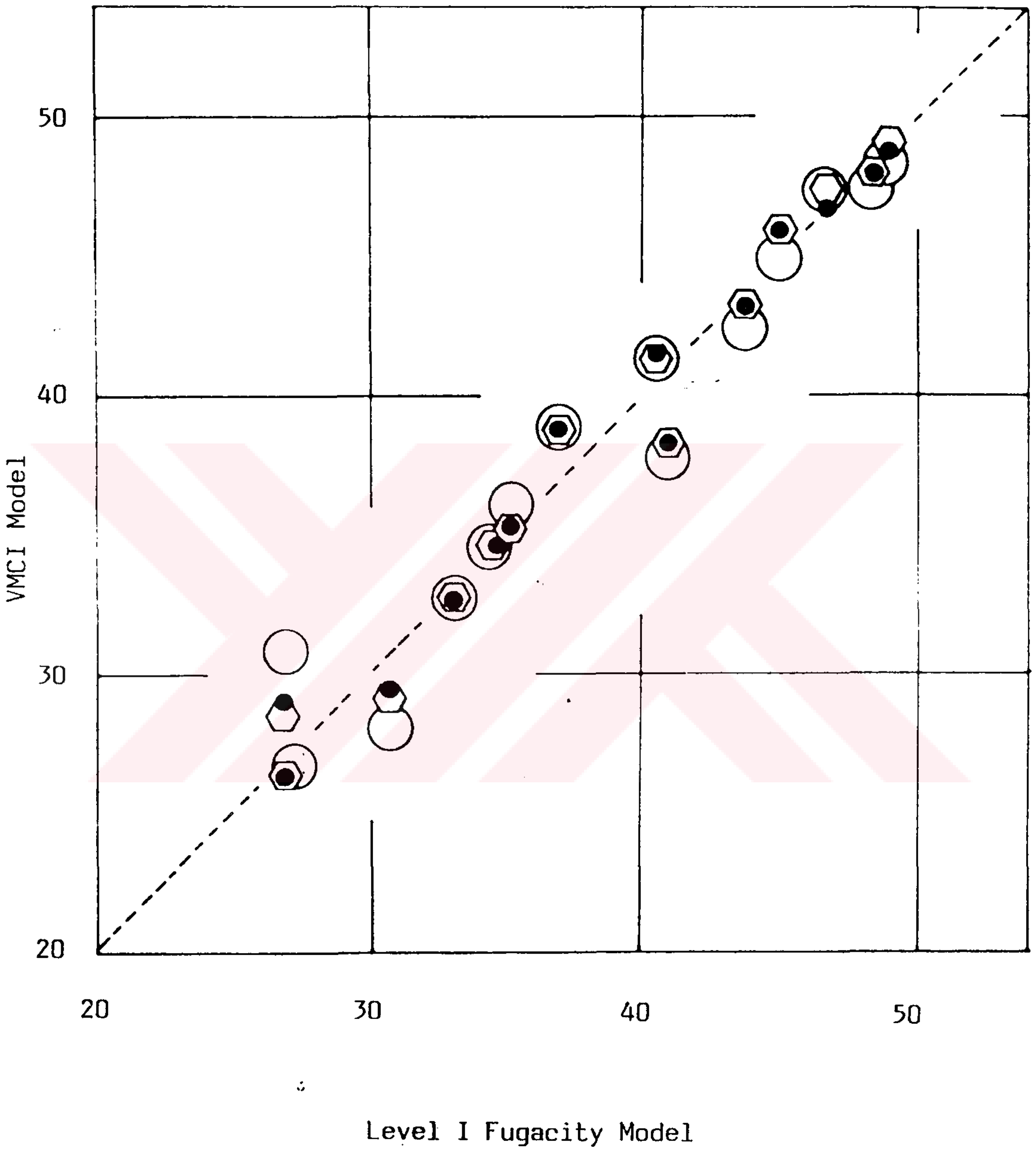


Figure V.5.1.4 Equilibrium Distribution (%) in Biota

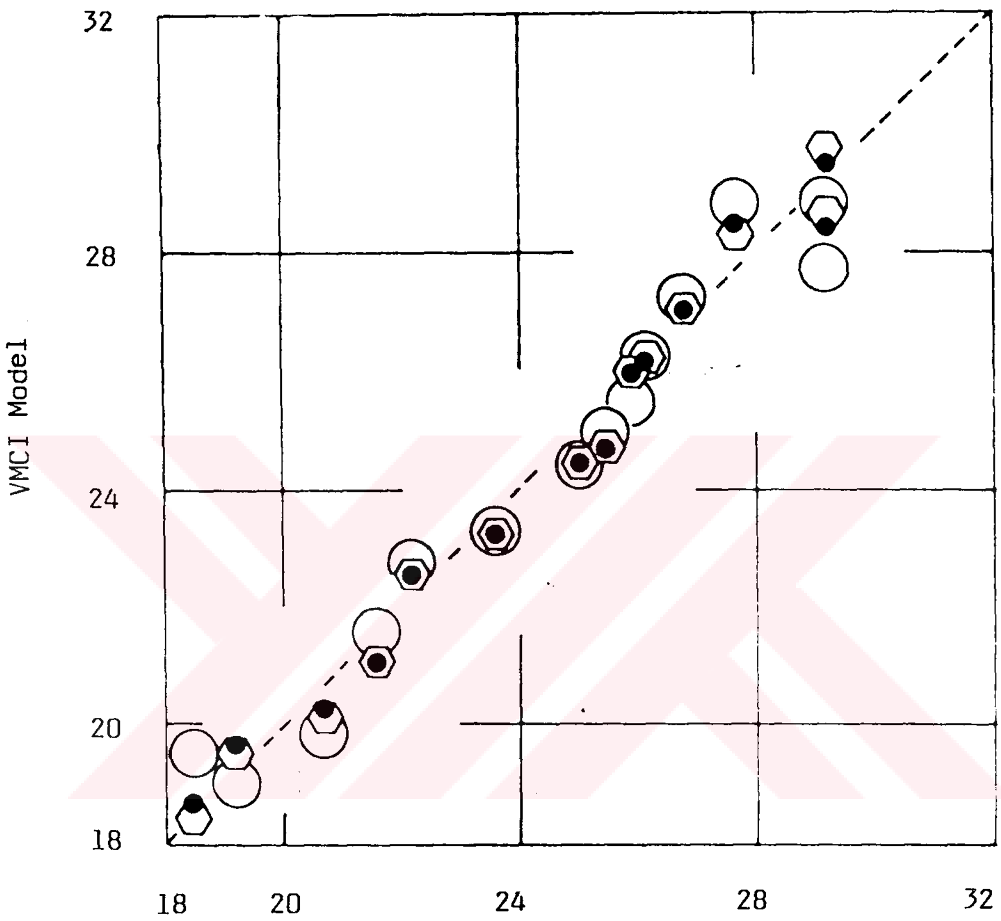


Figure V.5.1.5 Equilibrium Distribution (%) in Suspended Solids and Sediment

:

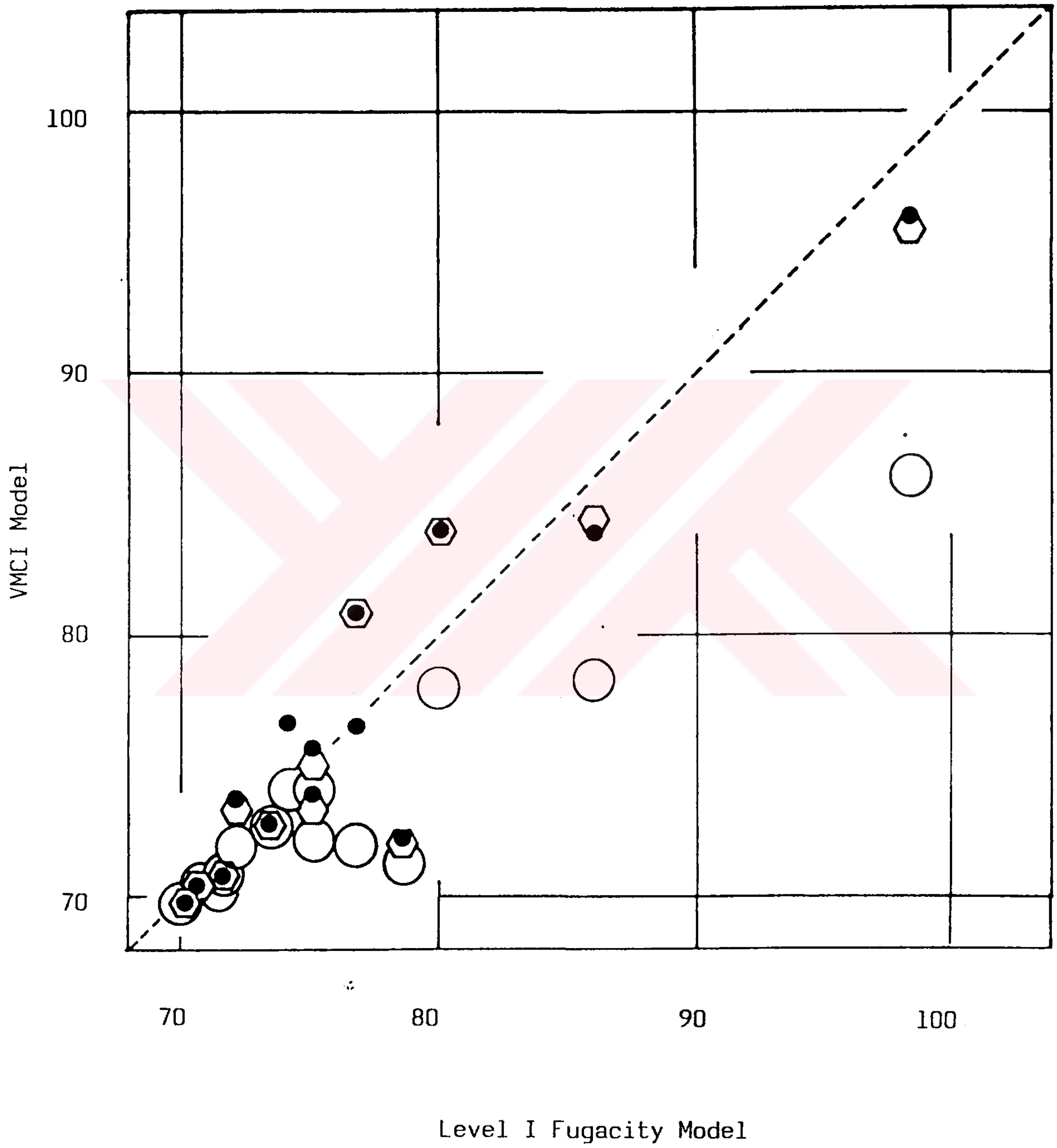


Figure V.5.2.1 Mass Distribution (%) in Air

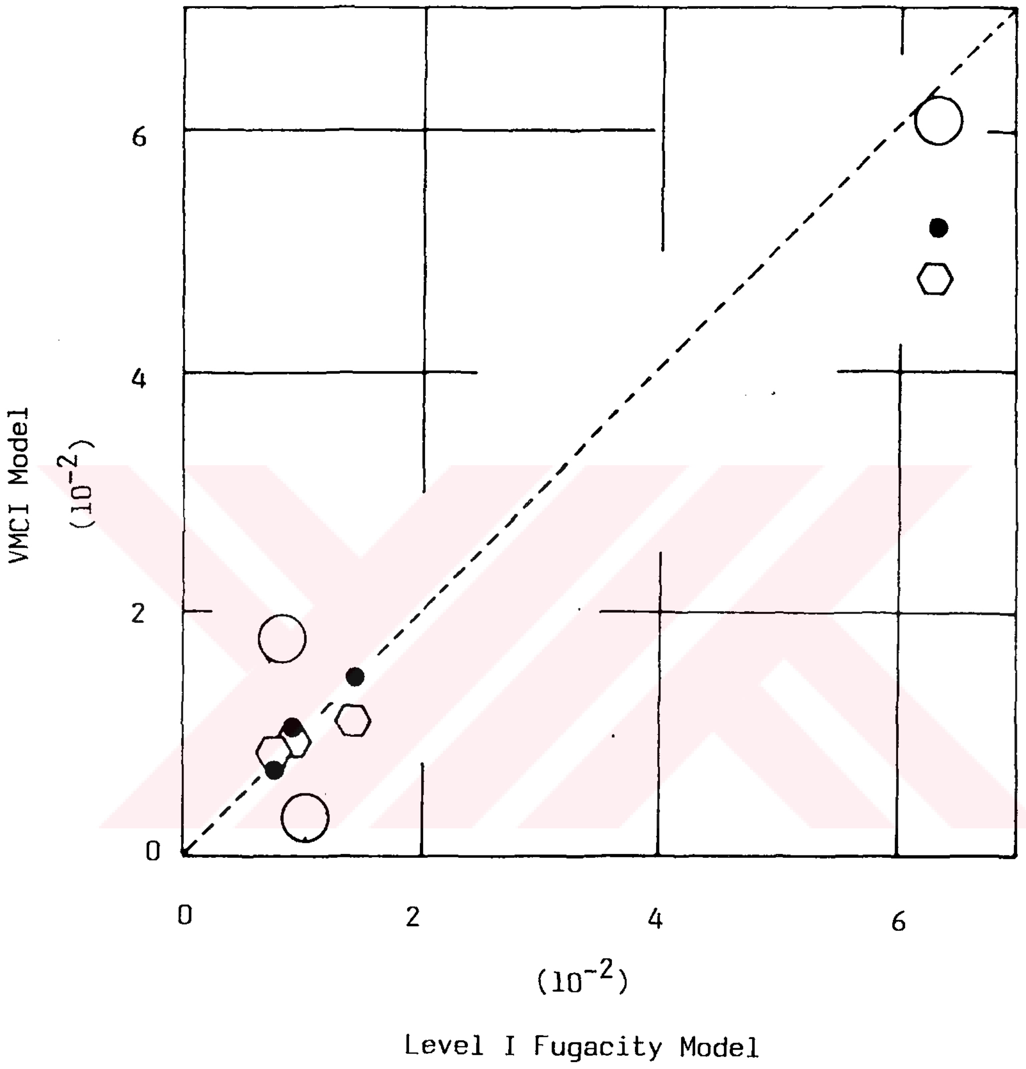
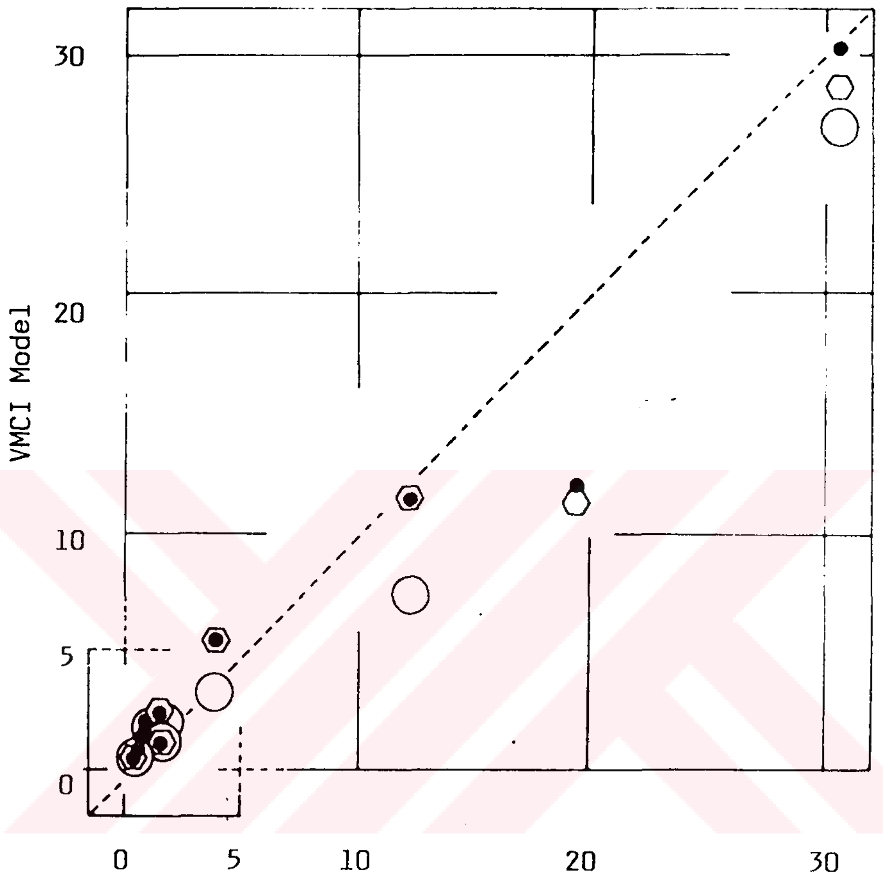


Figure V.5.2.2 Mass Distribution (%) in Soil Between 0-6 x 10^{-2} %



Level I Fugacity Model

Figure V.5.2.2 Mass Distribution (%) in Soil
Between 0-30 %

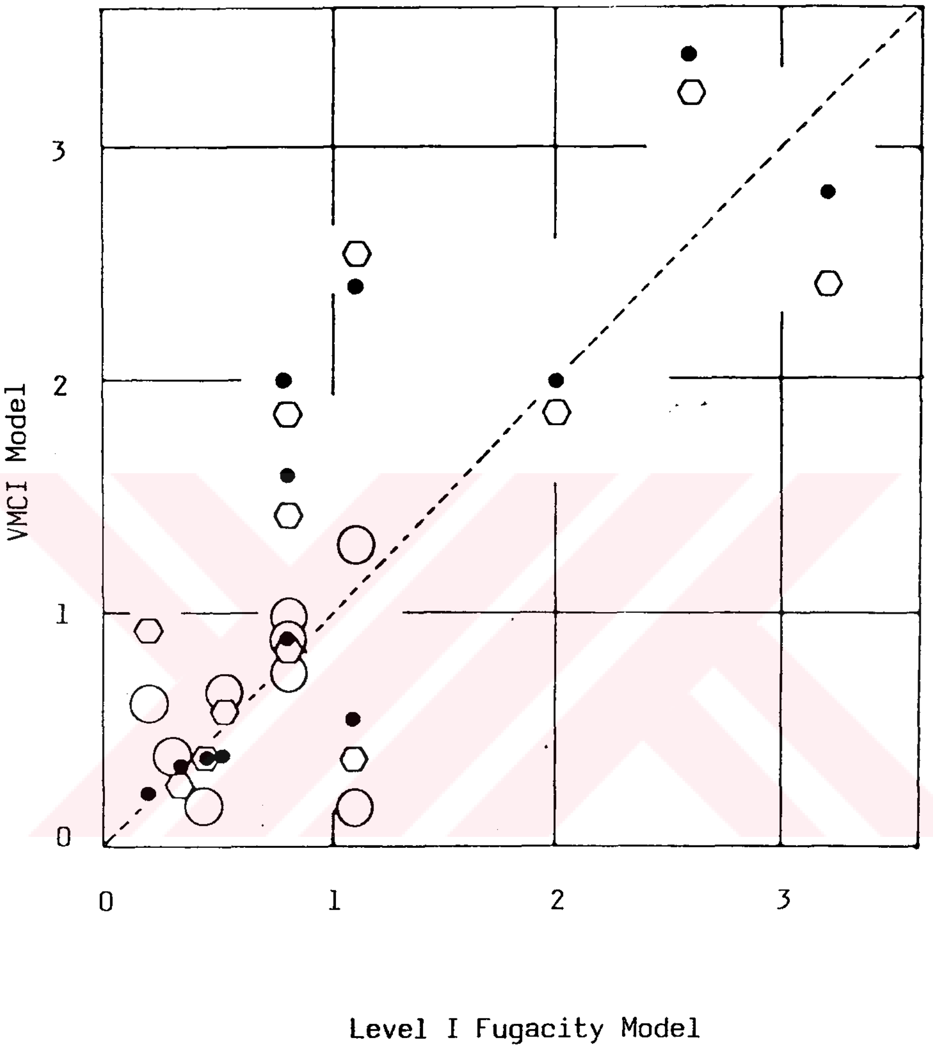


Figure V.5.2.3 Mass Distribution (%) in Water

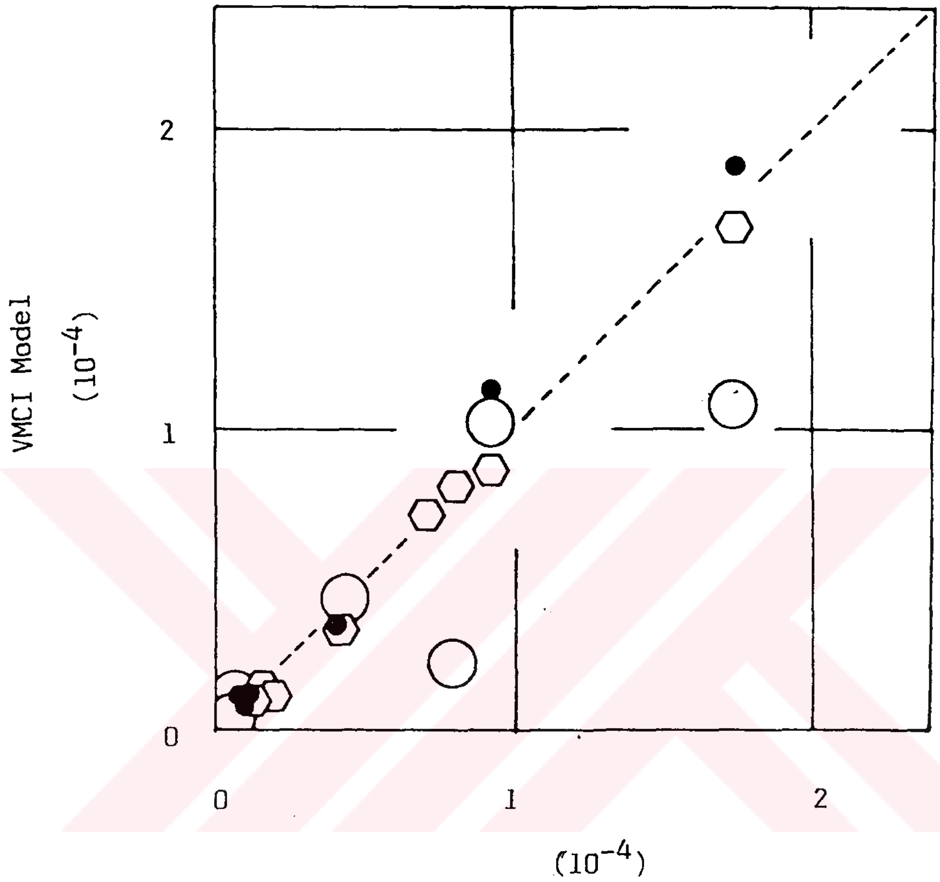


Figure V.5.2.4 Mass Distribution (%) in Biota Between 0-2 x 10^{-4} %

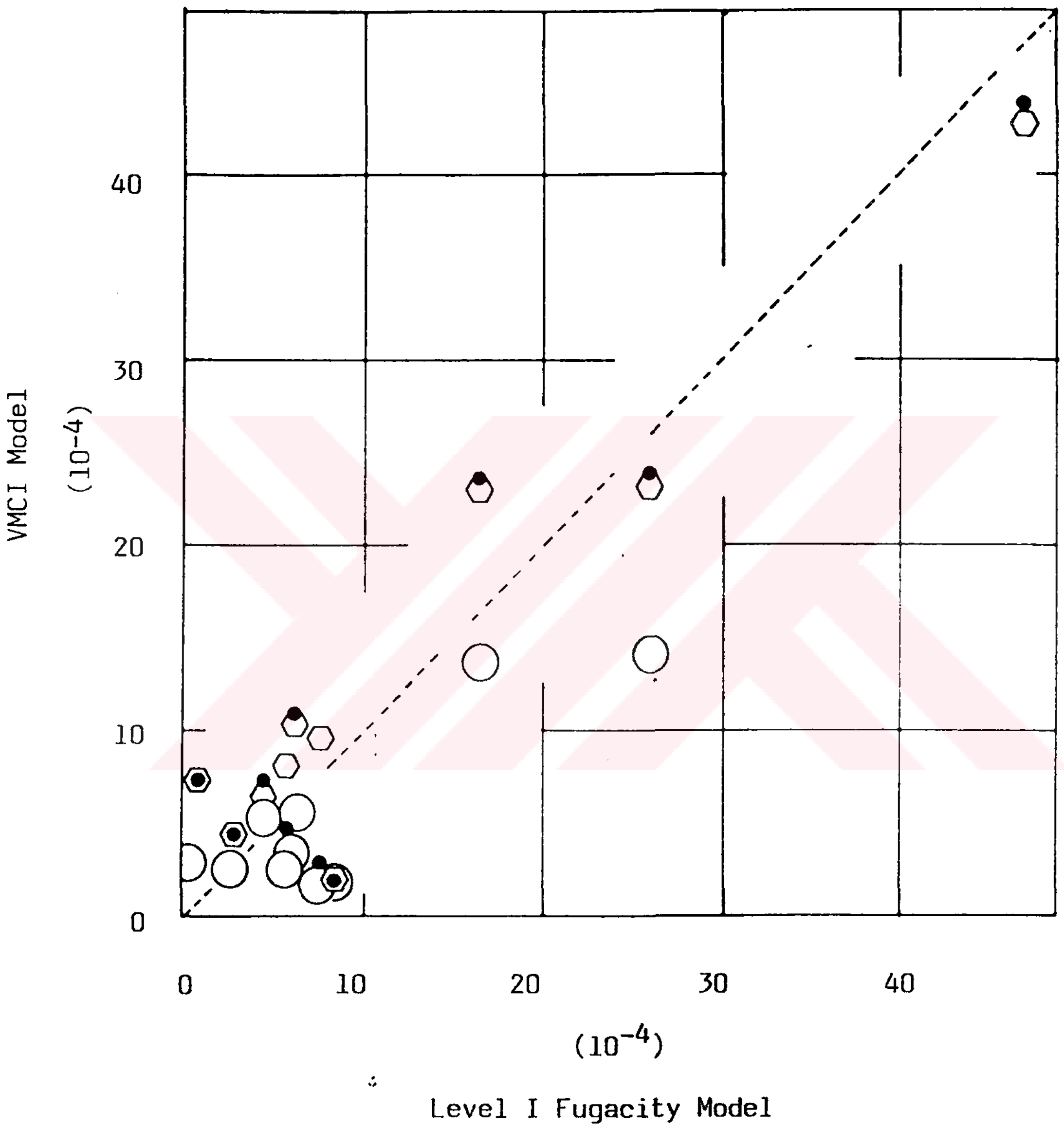


Figure V.5.2.4 Mass Distribution (%) in Biota Between 0-50 x 10^{-4} %

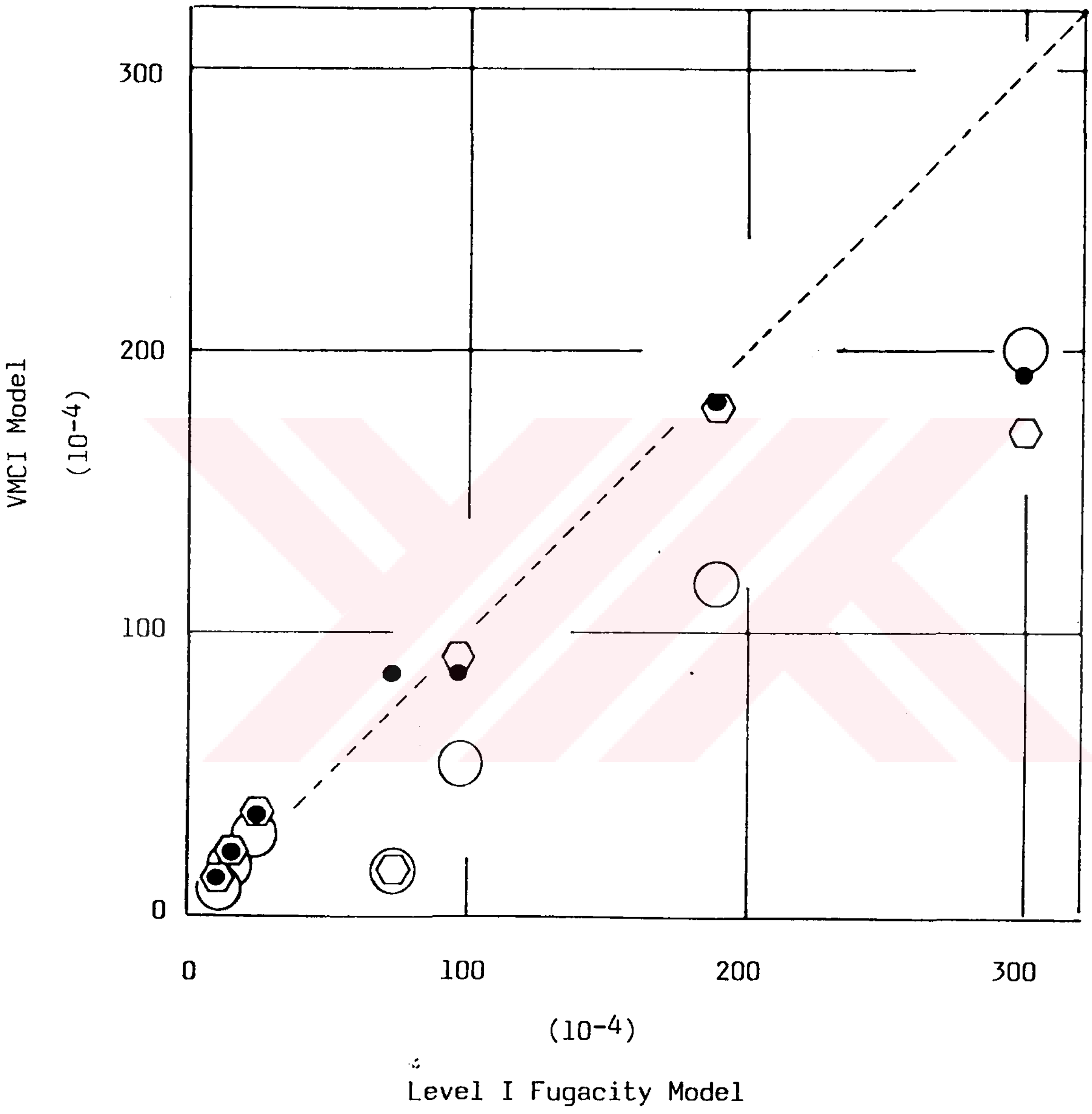


Figure V.5.2.5 Mass Distribution (%) in Suspended Solids Between 0-300 x 10^{-4} %

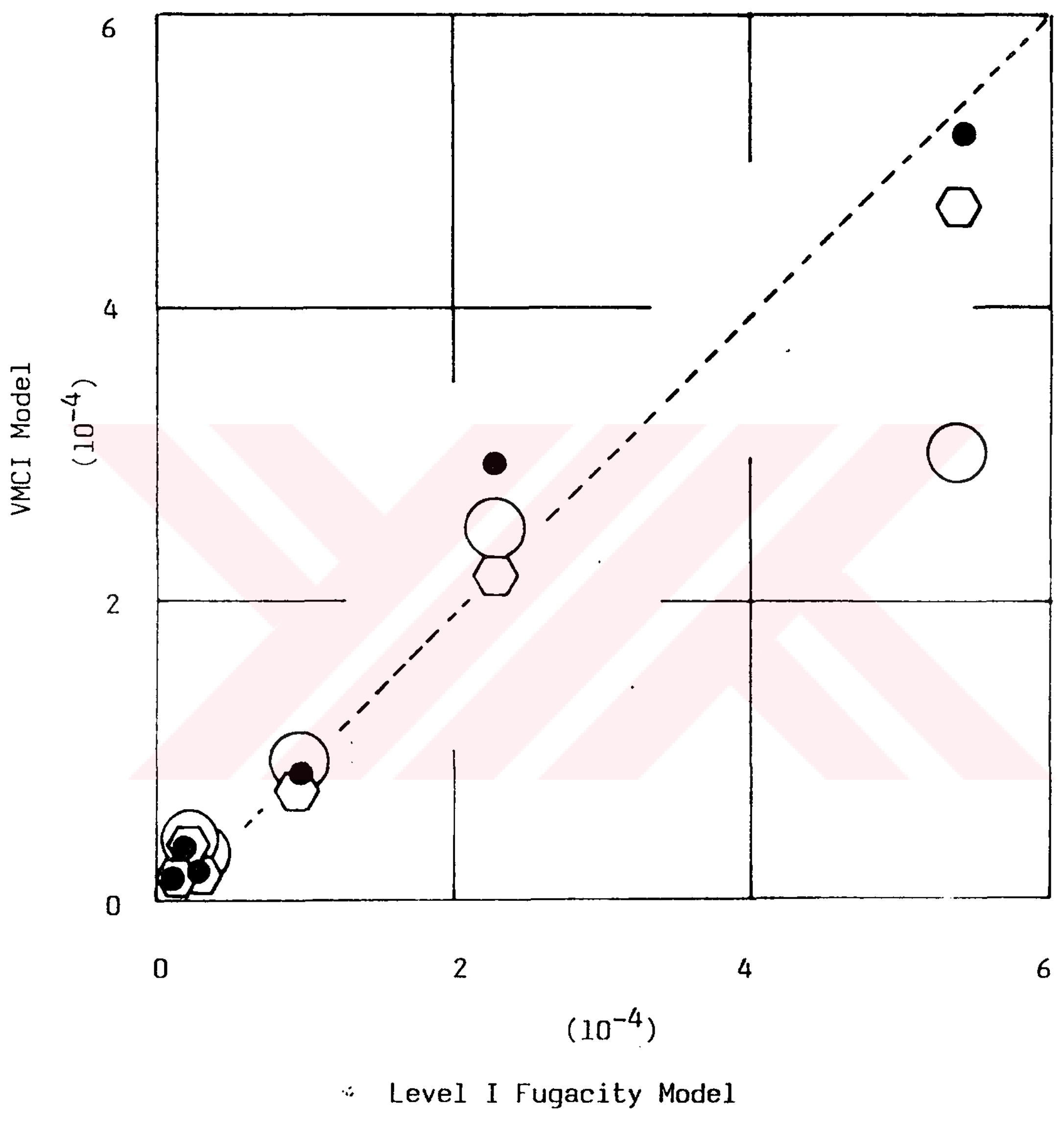


Figure V.5.2.5 Mass Distribution (%) in Suspended Solids Between 0-6 %

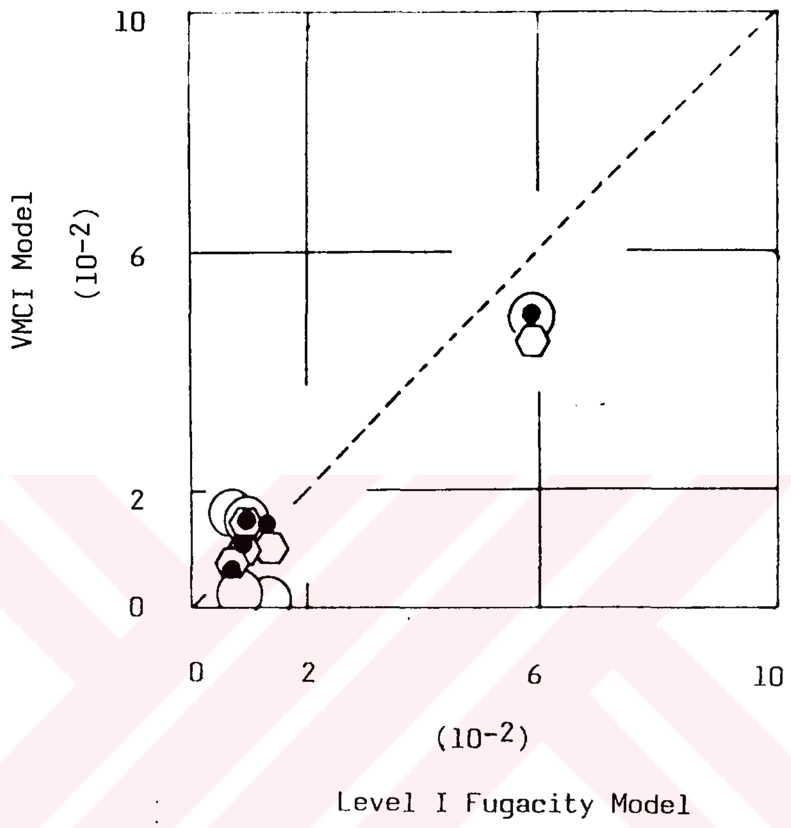


Figure V.5.2.6 Mass Distribution (%) in Sediment Between 0-10 x 10^{-2}%

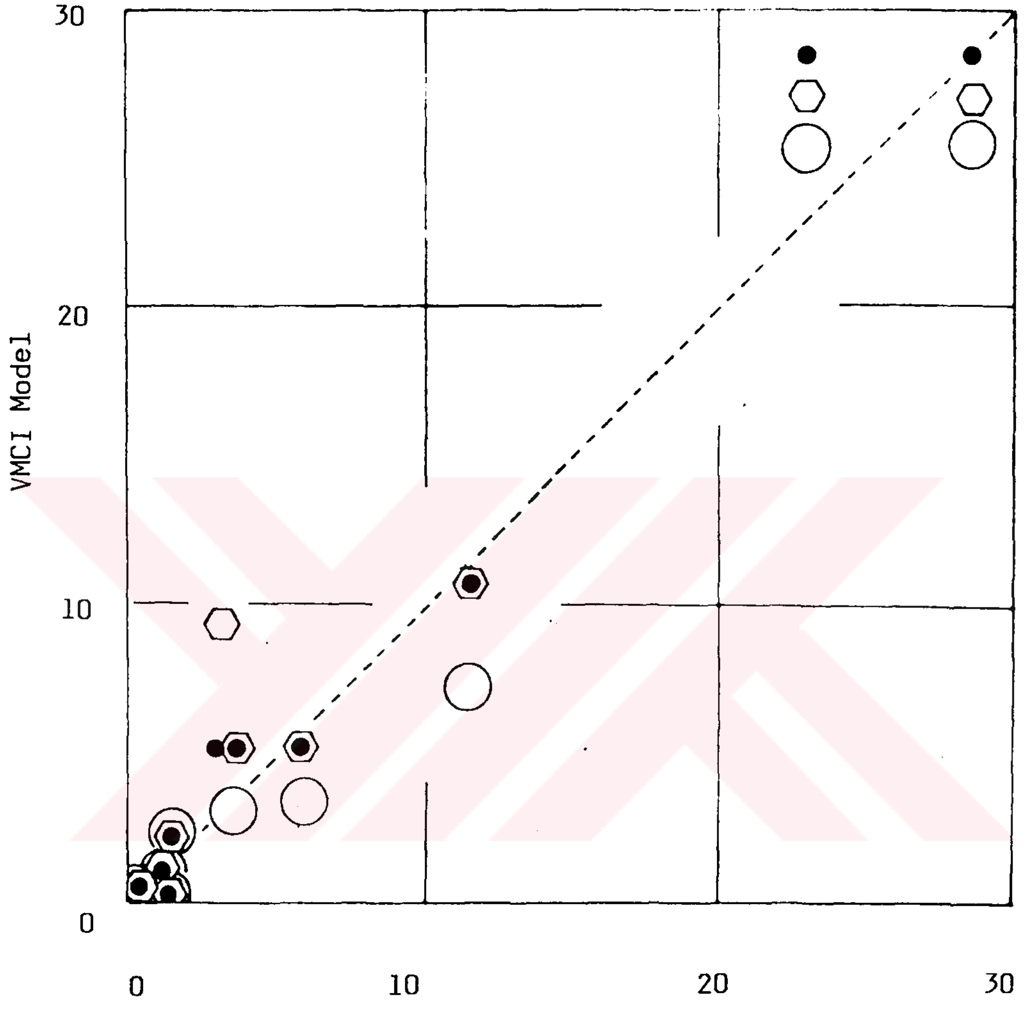


Figure V.5.2.6 Mass Distribution (%) in Sediment Between 0-30 %

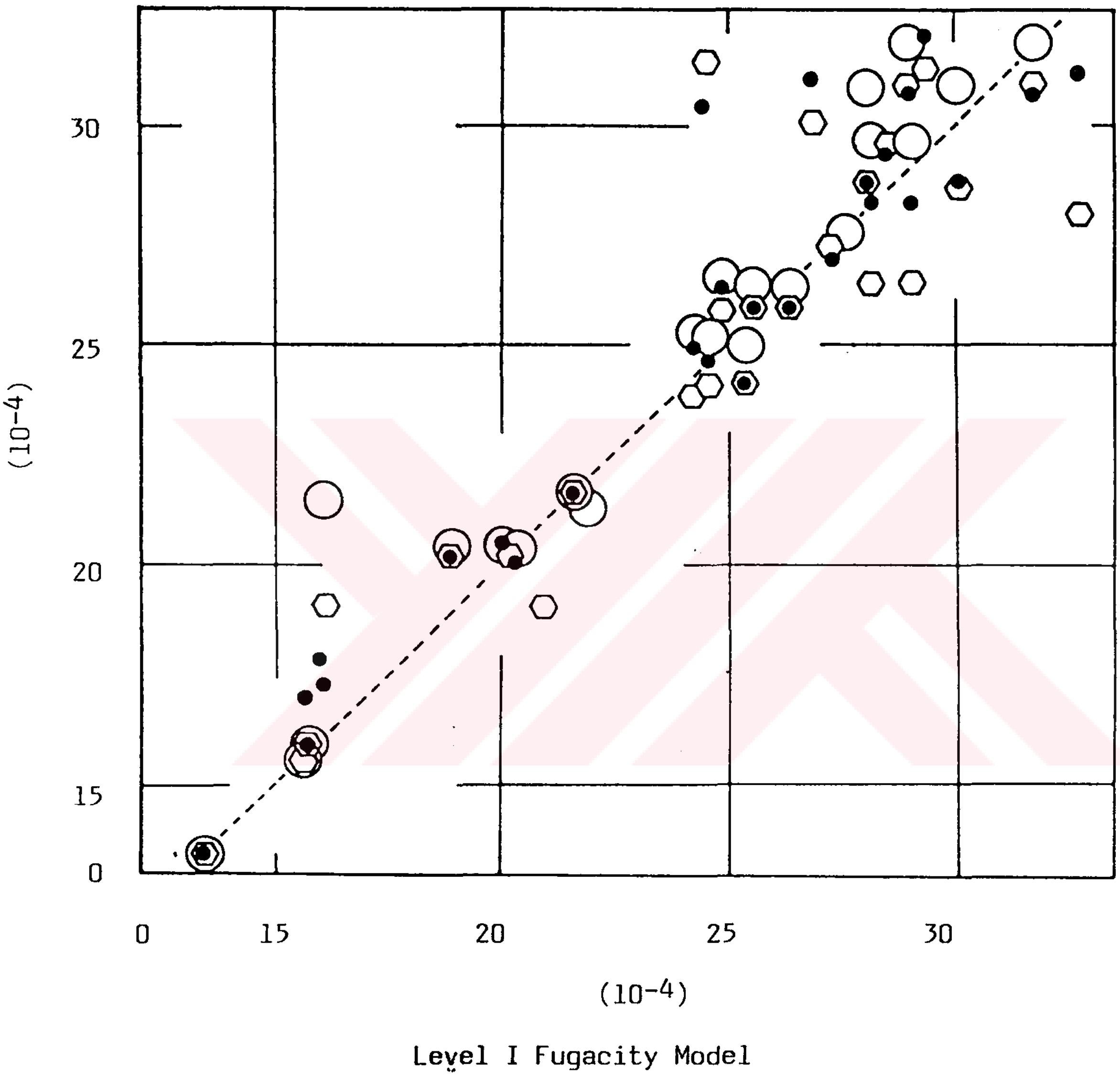


Figure V.5.3.1 Concentration (ppm) in Air

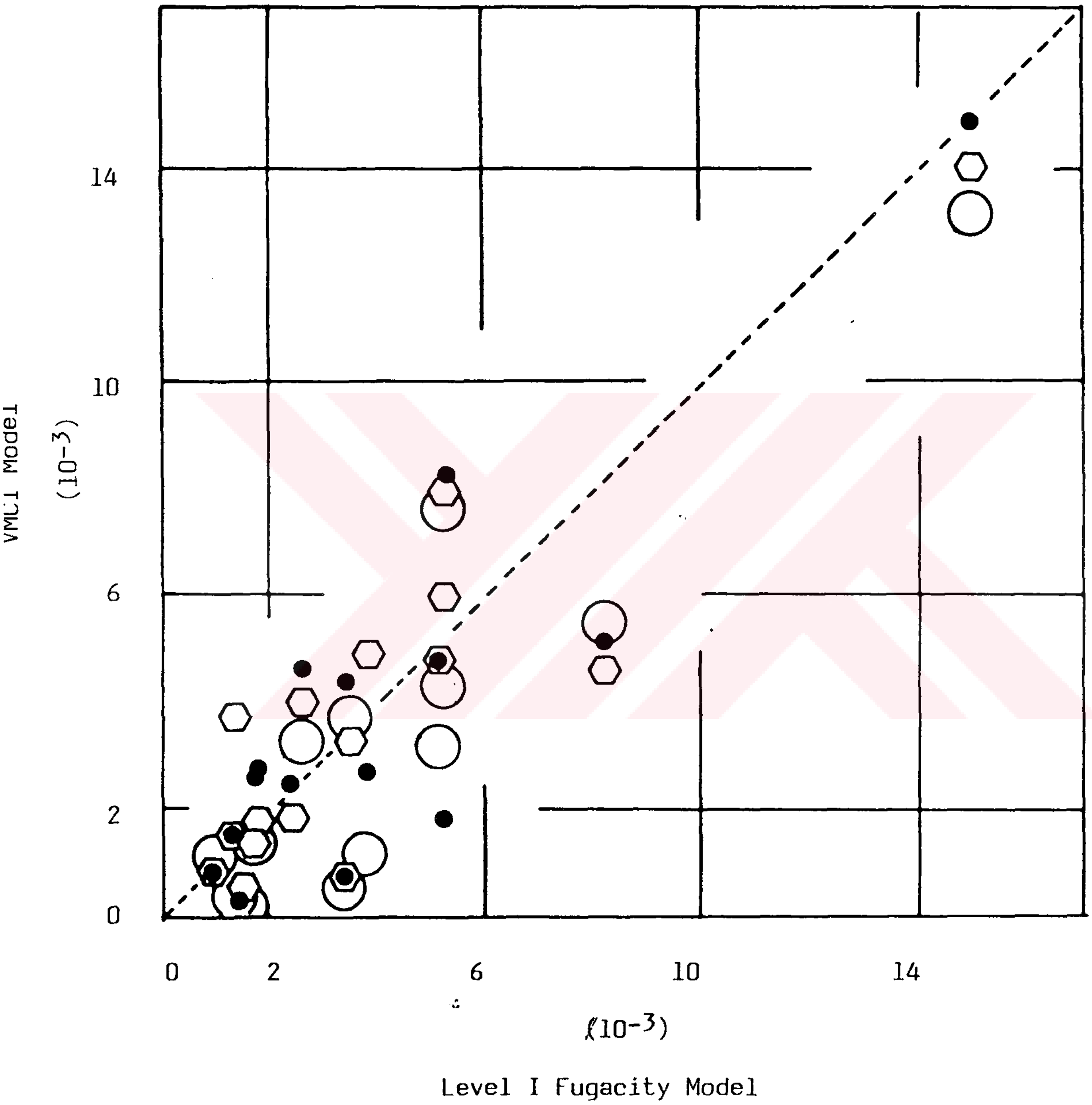


Figure V.5.3.2 Concentration (ppm) in Soil

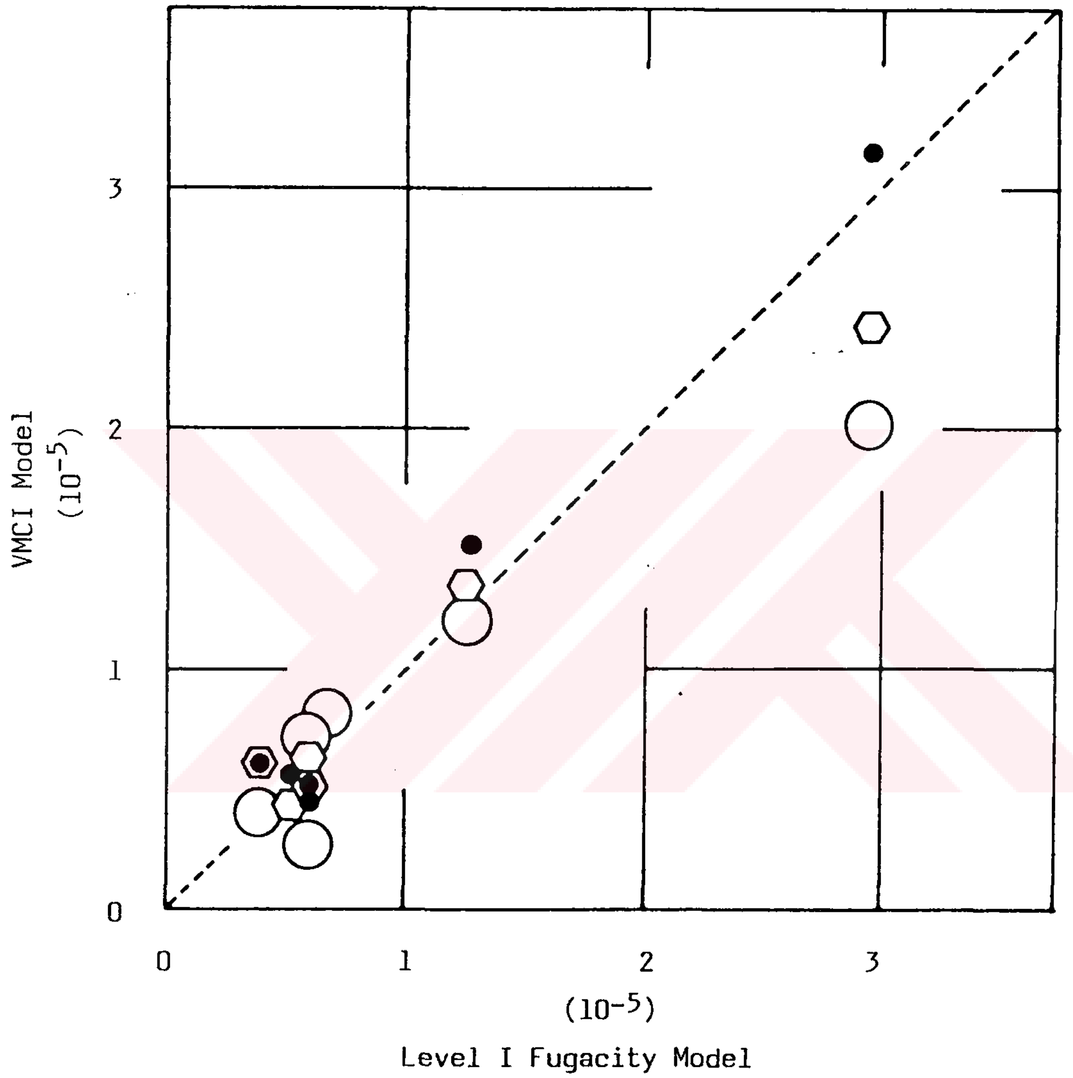


Figure V.5.3.3 Concentration (ppm) in Water Between 0-4 x 10^{-5} ppm.

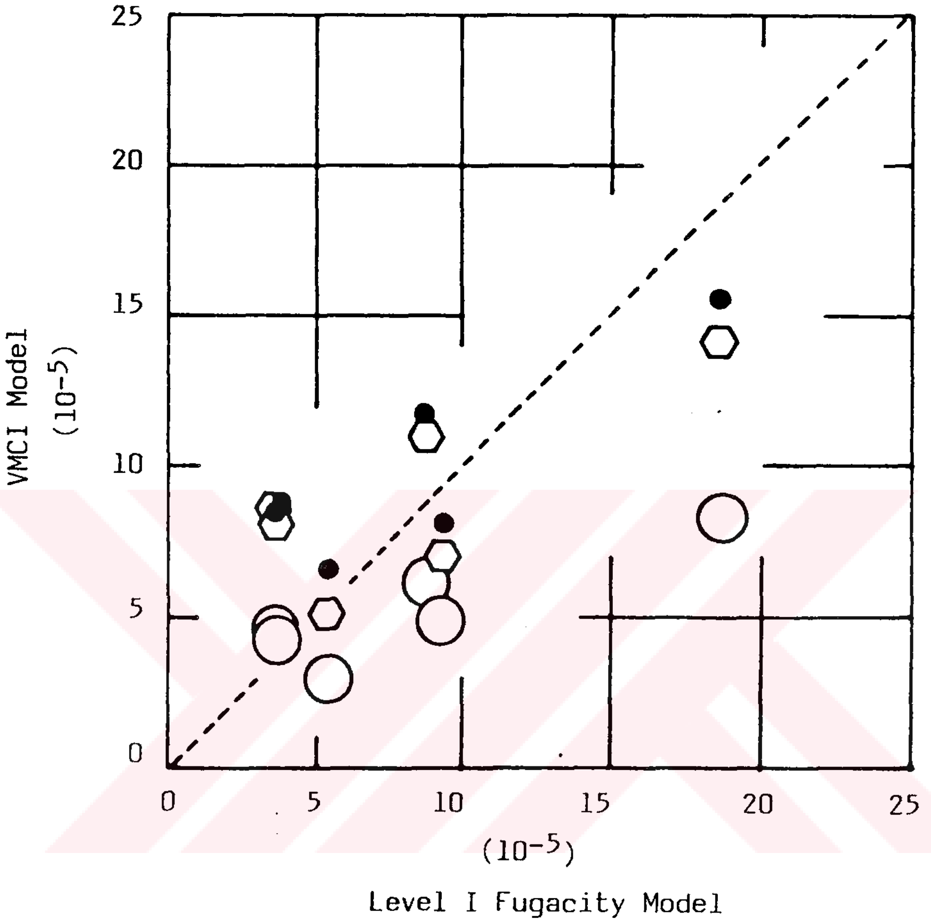


Figure V.5.3.3 Concentration (pmm) in Water Between 0-30 x 10^{-5} ppm

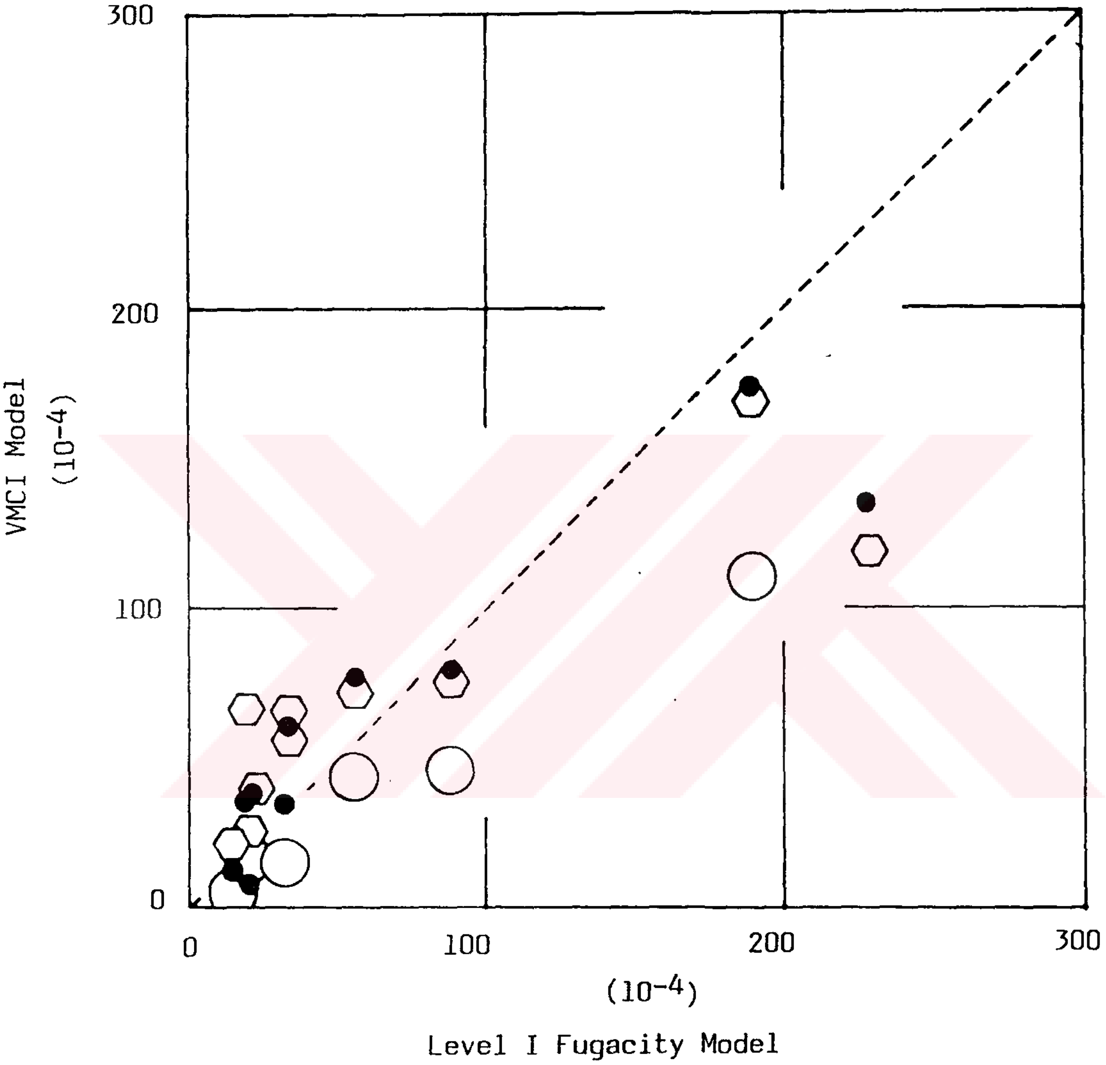


Figure V.5.3.4 Concentration (ppm) in Biota Between $0\text{-}300 \times 10^{-4}$ ppm

:

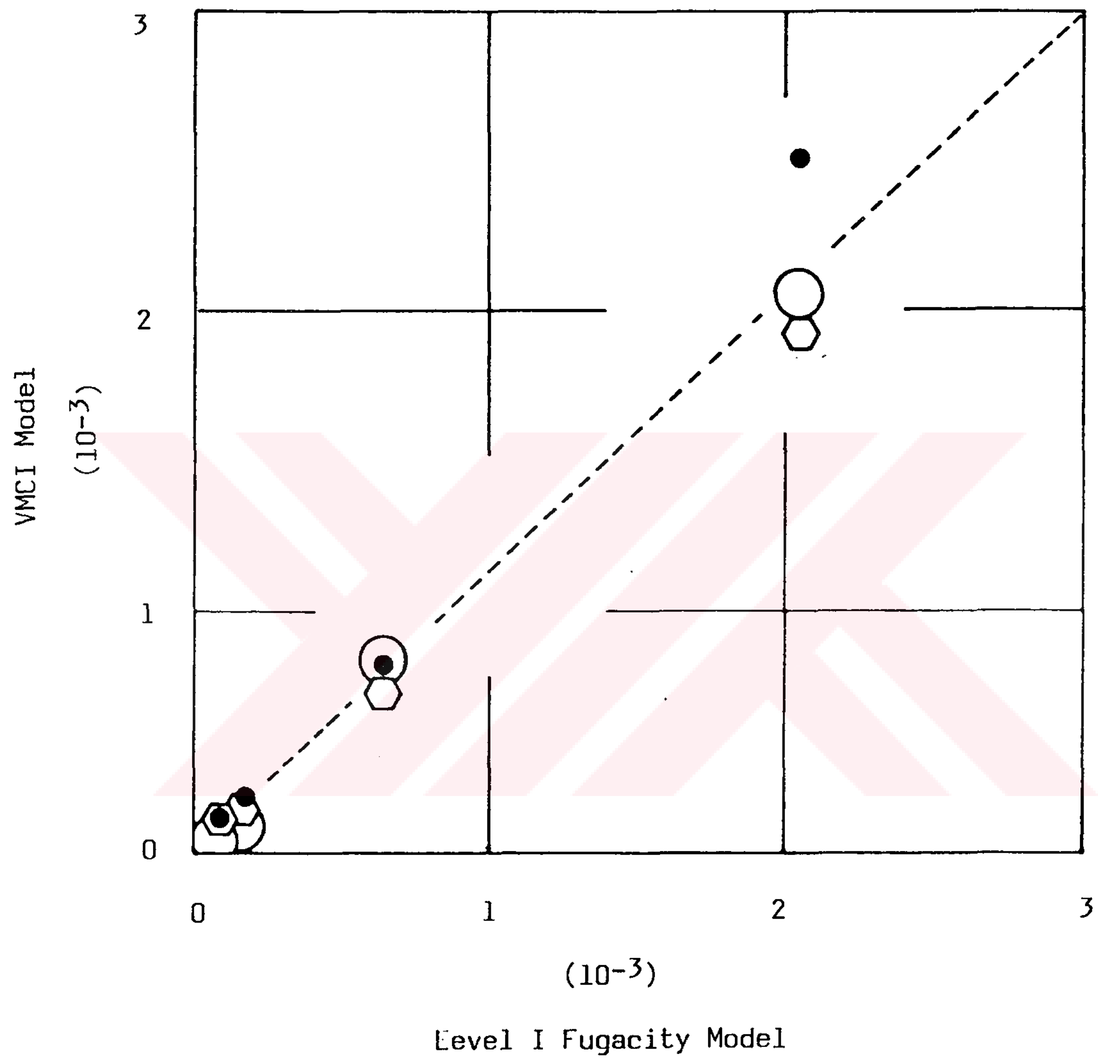


Figure V.5.3.4 Concentration (ppm) in Biota Between 0-3 x 10^{-3} ppm

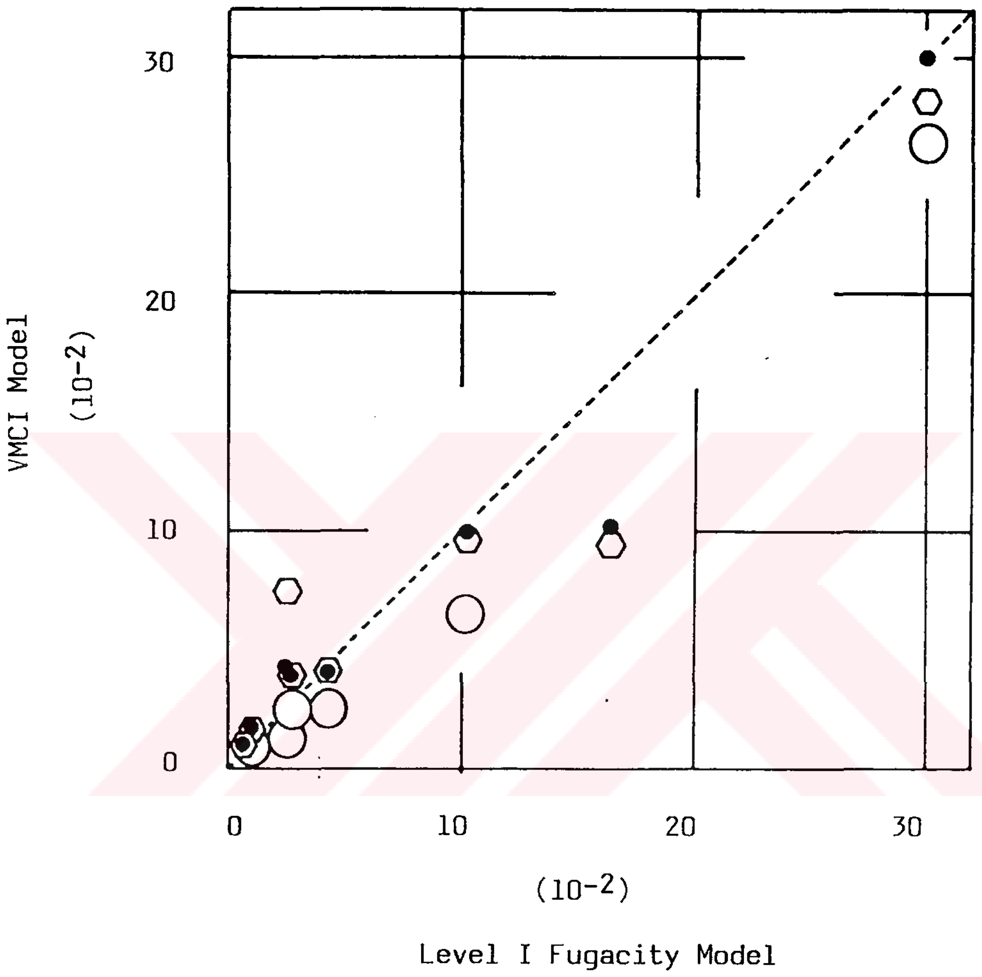


Figure V.5.3.5 Concentration (ppm) in Suspended Solids and Sediment Between 0-30 x 10^{-2} ppm

YK

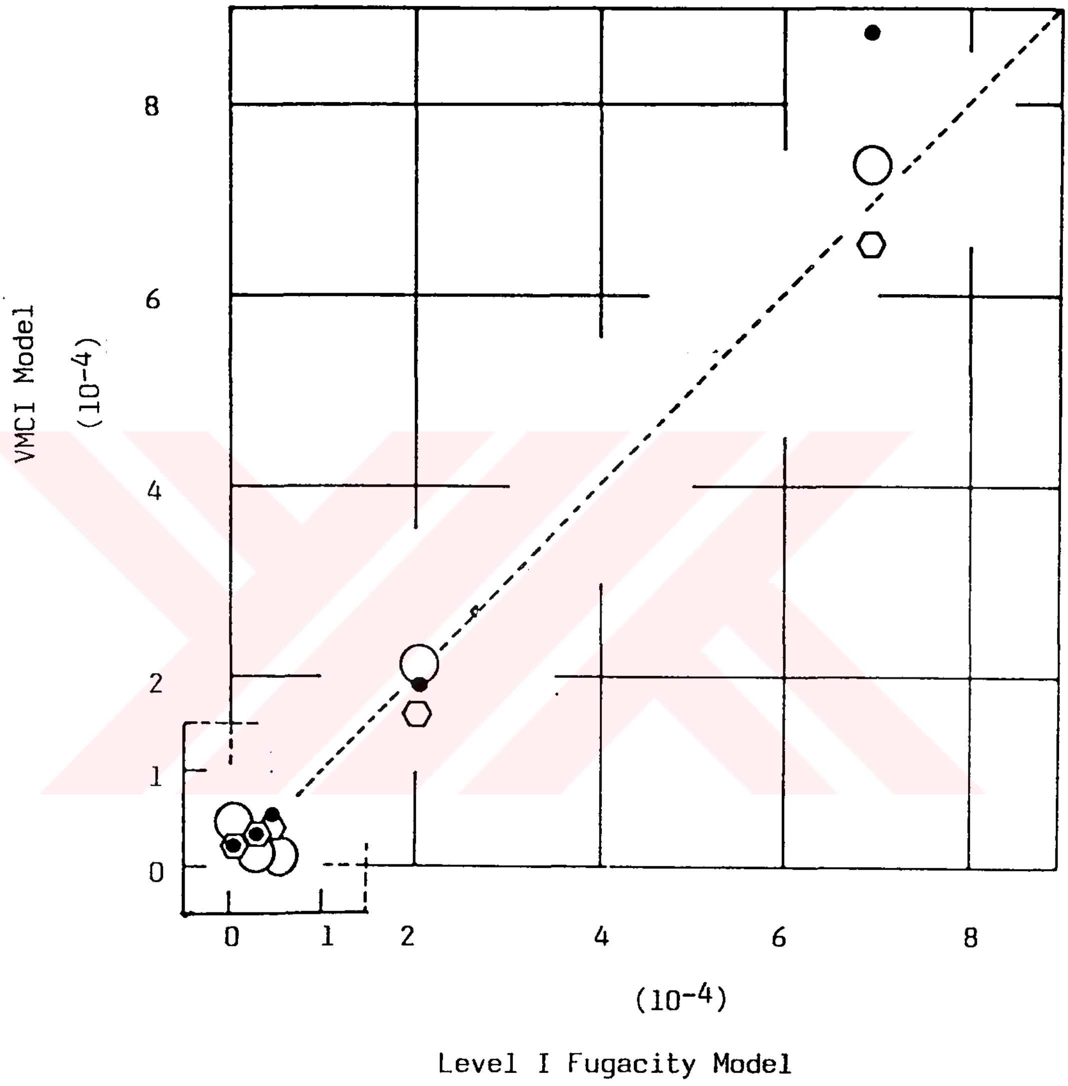


Figure V.5.3.5 Concentration (ppm) in Suspended Solids and Sediment Between 0-8 x 10^{-4} ppm

V.3. CONCLUSIONS AND THE FUTURE RESEARCH NEEDS REGARDING VMCI MODEL

As a result of this topology dependent Mathematical Model developed it has been understood that Valance Molecular Connectivity Indices which encodes information about size, conformation, branching and the heteroatom content by considering the sigma, pi and lone pair electrons on each atom is also a good measure of physical properties that are dependent on the bonding properties of the molecules such as partition coefficients, solubilities and vapor pressures. Since tendencies of molecules to partition within different phases is also a function of these properties Valance Molecular Connectivity approach is developed as a predictive model for the environmental distribution of various aromatic pollutants. Undoubtedly without further efforts to examine other aromatic systems having different substituents in a similar fashion, this model cannot be considered to be systematically validated.

However, even if at the end of such an examination the distribution values for all aromatic compounds can not be defined by a single set of equations for ln K_{OW}, ln S and ln P, to such an high accuracy, it is still clear that at least these values can be predicted precisely by using the sets obtained from a group specific regressive analysis of the available data for each congeneric group.

Another thing that can be done as a continuation of this work may be a detailed statistical evaluation of the results presented in table V.2 to V.5. Due to the high correlation between the calculated results by both models these relations are known to be of the form $y = mx$ where the intercept $(n) \sim 0$. Hence one can assign various correction factors (using the variance in slopes) to these values which at the end can be considered as a constant value that can be used in the formula used to calculate the distribution values. Or if this procedure is carried out before the evaluation of the distribution values for fugacity capacity constants these values may become constants that can be used within the formulas used to calculate the fugacity capacity constants (Z_i) and furthermore some physical significance may be assigned to them.

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

On the other hand, to further evaluate the developed model, its sensitivity to the accuracy of the input physicochemical properties need to be determined to provide an estimate of the extent to which variations in the data set will effect the predicted results. If these individual parameters are found to have a major effect-which is inevitable-it would be a good idea to reconsider the test or prediction methods for these parameters to ensure that useful results will be obtained.

These four case studies indicate that it is possible to quickly focus in on the key environmental questions that might be associated with a new product. Using the avaliable physical properties it is possible to quantitatively predict where in the environment the chemical will reside. Based on this information, by incorparating the additional data into the model a more refined estimate of exposure can be made. The only limitation is that the model is based on equilibrium situation and doesnot consider the kinetics involved in the transfer process from one medium to another. However, the model does have the ability to integrate the key properties of a chemical into a single index. So, using this approach it is possible to set priorities and to suggest new directions for the continuing investigation of potential problems associated with chemicals that have or will be introduced into the environment.

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi

APPENDICES

APPENDIX I

EVALUATION OF VAPOR PRESSURES FOR UNSUBSTITUTED POYLCYCLIC AROMATIC HYDROCARBONS

For some substances of environmental interest, especially for very low vapor pressure substances, the only vapor pressure information that may be available is the boiling point and melting point. One of the equations which can be used to calculate vapor pressures from the boiling and melting points in the absence of experimental vapor pressure data is the Kistiakowsky Linear ΔH Equation.[54]

$$\ln P = -(4.4 + \ln T_B) \left[(1.803((T_B/T) - 1) - 0.803 \ln(T_B/T) \right] -6.8((T_M/T) - 1) \quad (2.14)$$

where P is the vapor pressure in atmosphere at environmental temparature T in °K and T_B , T_M are the boiling and melting point temparatures in °K.

The third term including the melting point is neglected for liquids, i.e. when the melting point is lower than the environmental temperature. The KLH equation can be applied only to hydrocarbons and halogenated hydrocarbons that boil above 100°C. It is believed that this equation should yield predicted vapor pressures with an average error of only a factor of 1.25. The comparison between the calculated and experimental values have been shown by Mackay et al^{54} to be good.

In this study, this approach is used according to data available in table I.

Table I. : Boiling and Melting Point Data(a) for Unsubstituted Polycylic Aromatic Hydrocarbons

COMPOUND	T_M (^{o}K)	T_B (^{o}K)	ln T_B	T_B/T (b)	T_M/T (b)	ln(T_B/T) (b)
Benzene	278.66	353.26	5.8672	1.1848	0.9346	0.1696
Naphthalene (s)	353.71	491.16	6.1968	1.6473	1.1863	0.4991
Fluoranthene(s)	384.16	648.16	6.4741	2.1739	1.2884	0.7765
Fluorene (s)	389.66	567.16	6.3406	1.9022	1.3069	0.6430
Anthracene (s)	489.46	613.16	6.4186	2.0565	1.6416	0.7210
Acenaphthene(s)	369.36	552.16	6.3138	1.8519	1.2388	0.6162
Acenaphtylene(s)	365.66	543.16	6.2974	1.8217	1.2264	0.5998
Coronene (s)	712.16	798.16	6.6823	2.6770	2.3885	0.9847

Table I. Continued...

COMPOUND	T_M (^oK)	T_B (^oK)	ln T_B	T_B/T (b)	T_M/T (b)	$\ln(T_B/T)$ (b)
Phenanthrene(s)	374.16	613.16	6.4186	2.0565	1.2549	0.7210
Pyrene (s)	429.16	666.16	6.5015	2.2342	1.4394	0.8039
Chrysene (s)	528.66	721.16	6.5809	2.4187	1.7731	0.8832
Perylene (s)	551.16	648.16	6.4741	2.1739	1.8485	0.7765

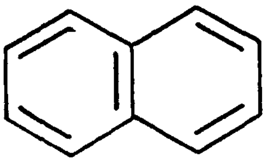
a)CRC Handbook of Chem. and Phy., 56 th. Ed.

b)T = 298.16

Specimen Calculation I:

Method : Kistiakowsky Linear ΔH Equation

Molecule : Naphtalene



Equation :

$$\ln P + -(4.4 + \ln T_B)\left[1.803\ \left[(T_{B/T}) - 1\right] - 0.803 \ln (T_{B/T})\right] -6.8\ \left[(T_{M/T}) - 1\right]$$

P : vapor pressure (atm)

T : Temperature (^{o}K)

Data :

$T_B = 491.16$

$T_M = 353.71$

$T = 298.16$

Evaluation:

$$\ln P = -(4.4 + 6.1968)\ \left[1.803\ \left[1.6473 -1\right] - 0.803\ (0.4991)\right] - 6.8\left[1.1863 - 1\right]$$

$\ln P = -10.5968\ (1.1671 - 0.4008) - 1.2668$

$\ln P = -9.3871$

$P_{calc.} = 8.38 \times 10^{-5}$ atm.

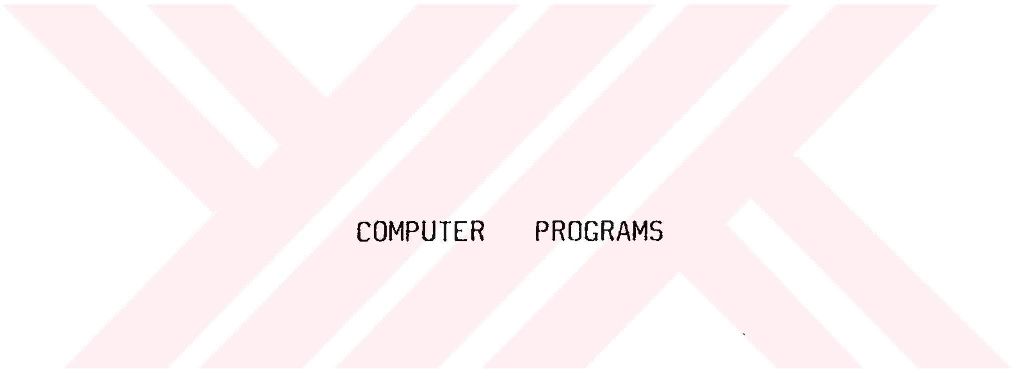
(0.0637 mm Hg)

$P_{obs.} = 0.0492$ mm Hg

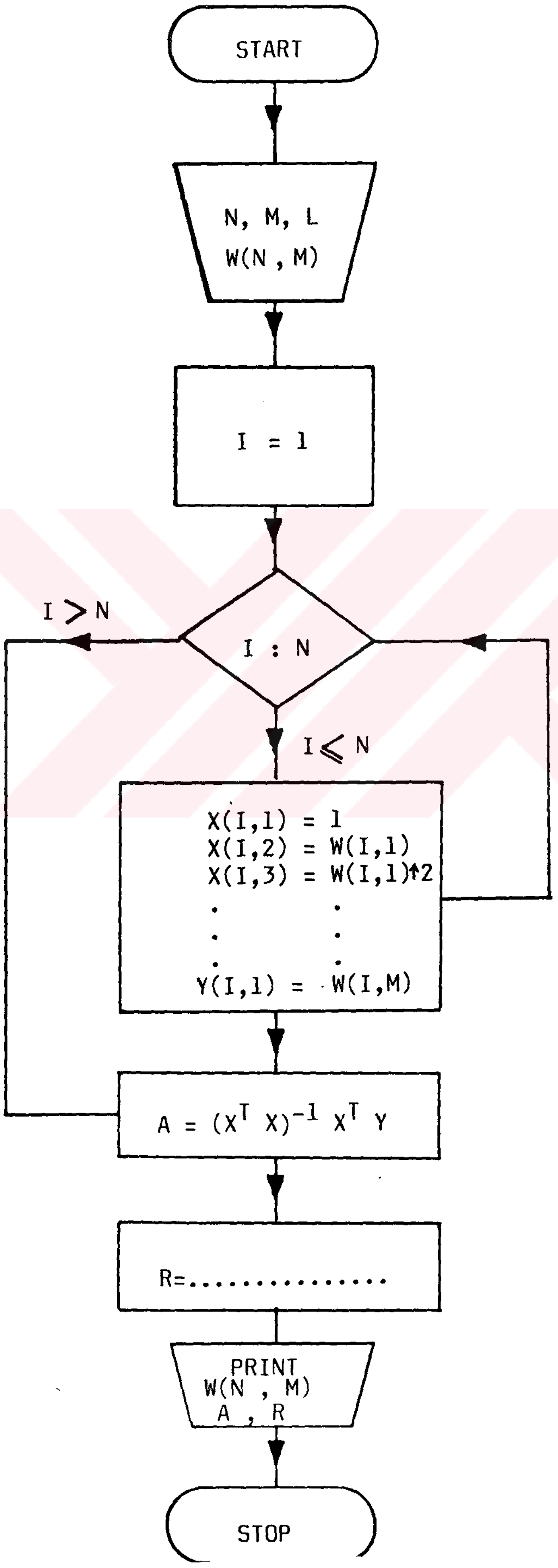
Table II Evaluated vapor Pressures of Unsubstituted Polycyclic Aromatic Hydrocarbons

COMPOUND	P(mm Hg)	log P
Benzene	100.5	2.002
Naphthalene	6.4×10^{-2}	-1.1938
Fluoranthene	9.5×10^{-6}	-5.0223
Fluorene	6.24×10^{-4}	-3.2048
Anthracene	5.71×10^{-6}	-5.2437
Acenaphtylene	3.69×10^{-3}	-2.4331
Acenaphthene	2.14×10^{-3}	-2.6689
Coronene	1.08×10^{-12}	-119667
Phenanthrene	7.91×10^{-5}	-1.017
Pyrene	1.27×10^{-6}	-5.8960
Chrysene	6.04×10^{-9}	-8.2187
Perylene	2.11×10^{-7}	-6.6758

APPENDIX II



COMPUTER PROGRAMS

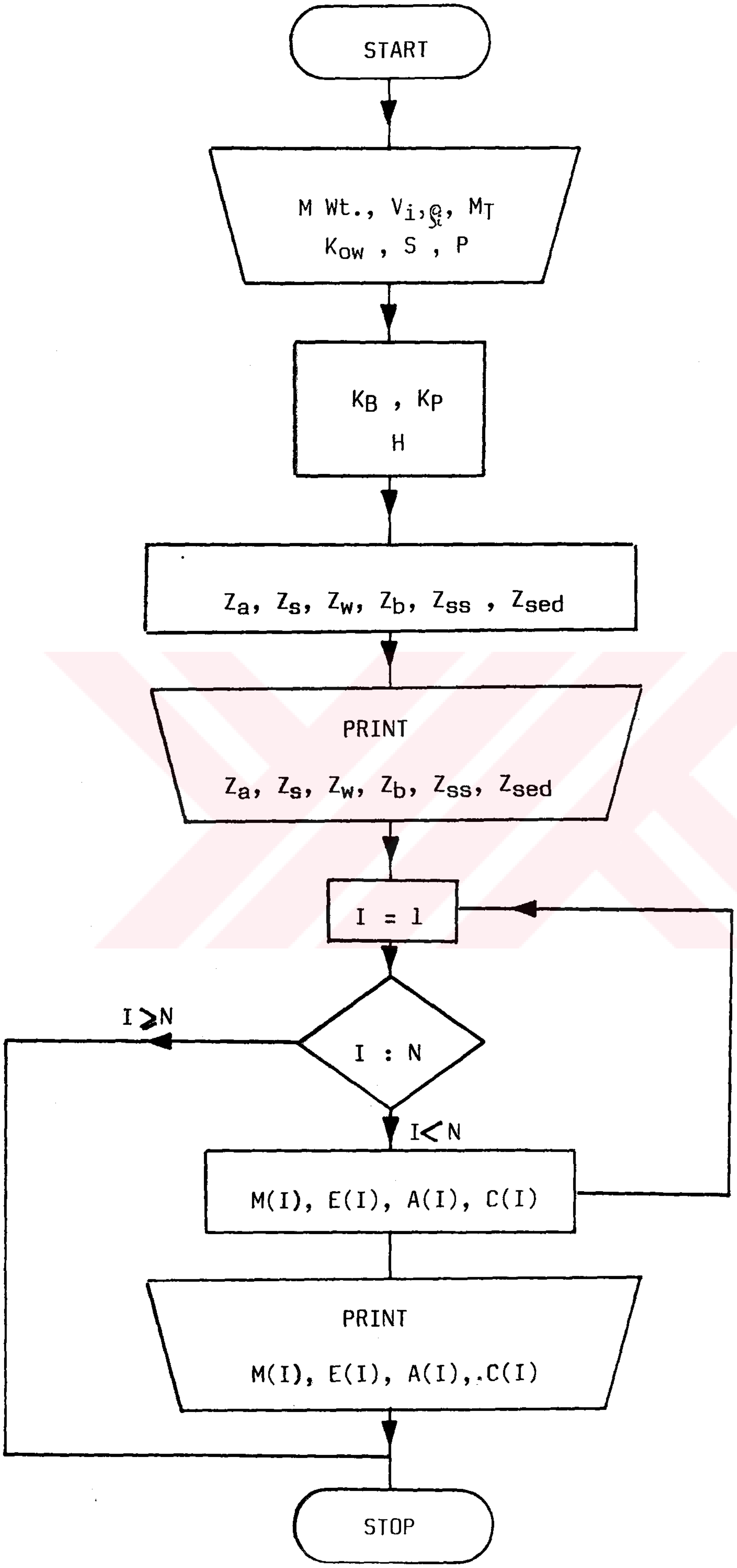

START
N, M, L
W(N , M)
I = 1
I > N
I : N
I ⩽ N
X(I,1) = 1
X(I,2) = W(I,1)
X(I,3) = W(I,1)↑2
Y(I,1) = W(I,M)
A = (X^T X)^-1 X^T Y
R=...............
PRINT
W(N , M)
A , R
STOP

```
10 REM*********************************
20 REM*                               *
30 REM* **** **** **** **** **** **** *
40 REM* *  * *    *    *  * *    *    *
50 REM* **** **** * ** **** **** **** *
60 REM* **   *    *  * **   *       * *
70 REM* * *  *    *  * * *  *       * *
80 REM* *  * **** **** *  * **** **** *
90 REM*                               *
91 REM*********************************

READY.
```

```
10 OPEN 4,4:CMD 4:LIST10-50
11 REM ----MULTIPLE REGRESSION---------
12 REM --------------------------------
13 REM --Y=LOG KOW,SOLUBILITY,VAPOR-PRESSURE -
14 REM---INDICES(X):X0,X1,X2 ---------
20 ------------------------------------
30 DIM N7(100)
31 DIM M7(10)
32 DIM L7(10)
35 READ N,M,L
40 DIM W(N,M)
41 DIM X(N,L)
42 DIM Y(N,1)
43 DIM X0(L,N),X1(L,L),X2(L,L),X3(L,1)
47 DIM Y0(N,1)
48 DIM Y1(1,N)
49 DIM A(L,1)
50 FOR I=1 TO N

READY.
READY.

51 FOR J=1 TO M
53 READ W(I,J)
54 NEXT J
55 NEXT I
60 INPUT GG
62 IF GG=1 GOTO 66
64 IF GG=0 GOTO 122
66 FOR I=1 TO N:FOR J=1 TO M
100 PRINT#4,W(I,J),
110 NEXT J
120 PRINT#4,
121 NEXT I
122 INPUT AA
124 IF AA=1 THEN 132
126 IF AA=0 THEN 141
130 NEXT I
132 FOR I=1 TO N :FOR J=1 TO M
133 W(I,J)=LOG(W(I,J))
136 PRINT#4,W(I,J);
137 NEXT J
138 PRINT#4,
139 PRINT#4,
140 NEXT I
141 FOR I=1 TO N
150 X(I,1)=1
181 X(I,2)=W(I,1)
182 X(I,3)=W(I,2)
183 X(I,4)=W(I,3)
190 Y(I,1)= W(I,M)
201 NEXT I
210 REM------MATRIX--------------------
240 FOR I=1 TO L
250 FOR J=1 TO N
260 X0(I,J)=X(J,I)
280 NEXT J
290 NEXT I
310 FOR I=1 TO L
320 FOR J=1 TO L
330 FOR K=1 TO N
340 X1(I,J)=X1(I,J)+X0(I,K)*X(K,J)
350 NEXT K
360 NEXT J
370 NEXT I
380 FOR I=1 TO L
390 X2(I,I)=1
400 NEXT I
410 FOR J=1 TO L
420 T=X1(J,J)
440 FOR K=1 TO L
450 X1(J,K)=X1(J,K)/T
460 X2(J,K)=X2(J,K)/T

READY.
```

```
70 NEXT K
80 FOR I=1 TO L
90 P=X1(I,J)
00 IF I=J THEN 550
10 FOR K=1 TO L
20 X1(I,K)=X1(I,K)-P*X1(J,K)
30 X2(I,K)=X2(I,K)-P*X2(J,K)
40 NEXT K
50 NEXT I
60 NEXT J
70 FOR I=1 TO L
80 FOR J=1 TO 1
90 FOR K=1 TO N
00 X3(I,J)=X3(I,J)+X0(I,K)*Y(K,J)
20 NEXT K
30 NEXT J
40 NEXT I
60 FOR I=1 TO L
70 FOR J=1 TO 1
80 FOR K=1 TO L
90 A(I,J)=A(I,J)+X2(I,K)*X3(K,J)
00 NEXT K
10 NEXT J
20 NEXT I
60 Y0=X3(1,1)/N
10 FOR I=1 TO N
20 FOR J= 1 TO 1
30 FOR K=1 TO L
40 Y0(I,J)=Y0(I,J)+X(I,K)*A(K,J)
50 NEXT K
60 NEXT J
70 NEXT I
80 FOR I=1 TO N
90 Y0(I,1)=Y0(I,1)-Y0
00 Y(I,1)=Y(I,1)-Y0
10 NEXT I
30 FOR I=1 TO N
40 Y1(1,I)=Y0(I,1)
50 NEXT I
70 FOR I=1 TO N
80 B=B+Y1(1,I)*Y0(I,1)
90 NEXT I
010 FOR I=1 TO N
020 Y1(1,I)=Y(I,1)
030 NEXT I
050 FOR I=1 TO N
060 C=C+Y1(1,I)*Y(I,1)
070 NEXT I
080 R=SQR(B/C)
090 REM----RESULTS--------------------
100 PRINT#4,"RESULTS"
120 PRINT#4,"--------"

EADY.
```

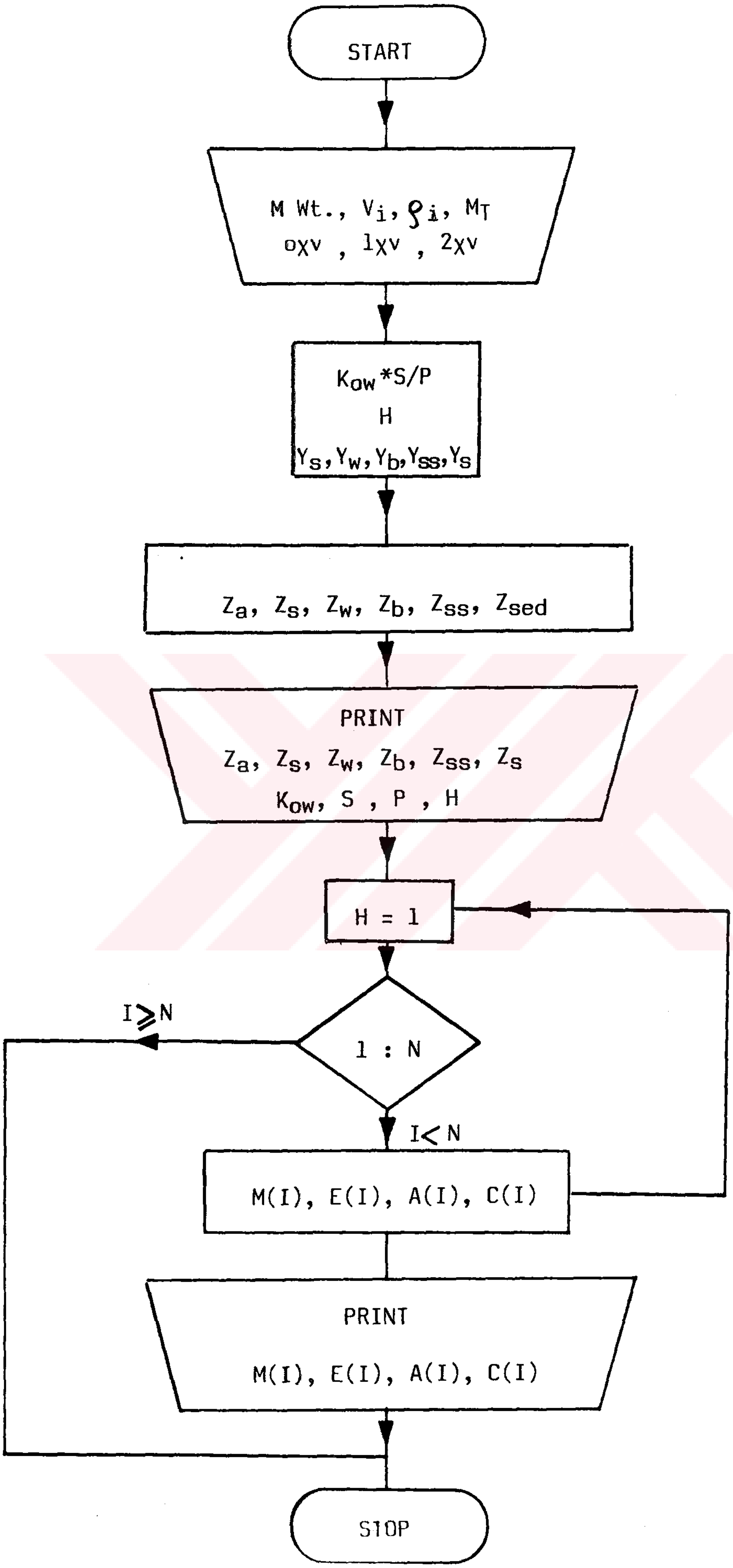
```
1170 PRINT#4,
1180 PRINT#4,"REGRESSION COEFFICIENT"
1190 PRINT#4,"------------------------"
1200 FOR I=1 TO L
1210 J=I-1
1220 PRINT#4,"A("J")="A(I,1)
1230 NEXT I
1240 PRINT#4,
1241 PRINT#4,"NUM. OF DATA="N
1242 PRINT#4,
1250 PRINT#4,"CORRELATION COEFF.="R
1251 PRINT#4,
1252 INPUTZ$:INPUT AA:INPUT BB:INPUT CC:INPUT DD
1253 INPUT S:INPUT U:INPUT V:INPUT D:INPUT E:INPUT F:INPUT GG
1254 G=AA+BB*S↑D+CC*U↑E+DD*V↑F
1255 PRINT#4,"NAME OF CHEMICAL="Z$
1256 PRINT#4,"A0="AA
1257 PRINT#4,"A1="BB
1258 PRINT#4,"A2="CC
1259 PRINT#4,"A3="DD
1260 PRINT#4,"X0="S
1261 PRINT#4,"X1="U
1262 PRINT#4,"X2="V
1263 PRINT#4,"POWER X0="D
1264 PRINT#4,"POWER X1="E
1265 PRINT#4,"POWER X2="F
1268 PRINT#4,"LOG Y="G:PRINT#4,"LOG Y(OBS)="GG
1269 INPUT H
1270 IF H=1 THEN 1272
1271 IF H=0 THEN 1279
1272 INPUT Z$
1274 GO TO 1253
1279 END

READY.
```


START
M Wt., V_i, ρ_i, M_T
K_{ow} , S , P
K_B , K_P
H
Z_a, Z_s, Z_w, Z_b, Z_{ss} , Z_{sed}
PRINT
Z_a, Z_s, Z_w, Z_b, Z_{ss}, Z_{sed}
I = 1
I ≥ N
I : N
I < N
M(I), E(I), A(I), C(I)
PRINT
M(I), E(I), A(I), C(I)
STOP

```
20 REM ********************************
30 REM *                              *
40 REM * *   * *** *** *   * *** *   **
50 REM * ** ** * * *   *  *  * *  * * *
60 REM * * * * *** *   * *   ***   *  *
70 REM * *   * * * *   **    * *   *  *
80 REM * *   * * * *   * *   * *   *  *
81 REM * *   * * * *   *  *  * *   *  *
82 REM * *   * * * *** *   * * *   *  *
83 REM *                              *
84 REM ********************************

READY.
```

```
10 OPEN 4,4:CMD 4:LIST-410
12 REM------------------------------
14 REM---MACKAY LEVEL I FUGACITY MODEL-------
15 REM-------------------------------
16 REM----LOAD "MACKAY",8 ------------
17 REM--------------------------------
140 DIM D(6)
180 DIM P(6)
190 DIM Z(6)
200 DIM M(6)
210 DIM E(6)
220 DIM A(6)
230 DIM C(6)
240 DIM T$(6)
250 T$(1)= "******AIR"
260 T$(2)= "*****SOIL"
270 T$(3)= "****WATER"
280 T$(4)= "****BIOTA"
290 T$(5)= "S. SOLIDS"
300 T$(6)= "*SEDIMENT"
310 REM ----PARAMETERS----------------
320 V(1)=6E+9
330 V(2)=45000
340 V(3)=7E+06
350 V(4)=7
360 V(5)=35
370 V(6)=21000
380 D(1)=.00119
390 D(2)=1.5
400 D(3)=1
410 D(4)=1
```

```
READY.

420 D(5)=1.5
430 D(6)=1.5
440 P(2)=2
450 P(5)=4
460 P(6)=4
470 T=298
480 R=8.314
490 REM ---------VARIABLES -------------
540 INPUT C$
560 INPUT M
580 INPUT C8
600 INPUT P5
610 P8=P5/.0075
700 INPUT L7
710 REM --FUG CAP CONST ---------
720 Z(1)=1/(R*T)
730 H=P8*M/C8
740 Z(3)=1/H
750 K8=10↑(.85*L7-.7)
760 Z(4)=K8*D(4)/H
770 K2=P(5)*.6*10↑L7/100
780 Z(5)=K2*D(5)/H
790 K3=P(2)*.6*10↑L7/100
800 Z(2)=K3*D(2)/H
810 K9=P(6)*.6*10↑L7/100
820 Z(6)=K9*D(6)/H
830 REM --DIST VALUES -------------
840 S8=0
850 S5=0
860 FOR I=1 TO 6
870 S8=S8+Z(I)
880 S5=S5+Z(I)*V(I)
890 NEXT I
900 F=100/S5
910 FOR I=1 TO 6
920 M(I)=Z(I)*V(I)/S5
930 E(I)=Z(I)/S8
940 A(I)=F*Z(I)*V(I)
950 C(I)=A(I)/V(I)*M/D(I)
960 NEXT I
991 PRINT#4,"NAME OF CHEMICAL:"C$
993 PRINT#4,"MOLECULAR WT.:"M
995 PRINT#4,"AQ. SOLUBILITY:"C8
997 PRINT#4,
998 PRINT#4,"VAPOR PRESSURE:"P5
999 PRINT#4,
1000 PRINT#4,"LOG OCT-WATER PART. COEFF.:"L7
1001 PRINT#4,
1002 REM PRINT DIST VALUES-----------
1005 PRINT#4,
1010 PRINT#4,SPC(06)"MASS PART","EQ PART";"AMOUNT","CONC"
1014 PRINT#4,
1016 FOR I=1 TO 6
1018 PRINT#4,T$(I)M(I)E(I)A(I)C(I)
1020 PRINT#4,
1021 NEXT I
1090 REM REPEAT PROCEDURE FOR NEW CHEM.
1110 INPUT AB
1120 IF AB=1 THEN 490
1121 IF AB=0 THEN 1130
1130 END

READY.
```


START
M Wt., V_i, ρ_i, M_T
$_0\chi^v$, $_1\chi^v$, $_2\chi^v$
K_{ow}*S/P
H
Y_s, Y_w, Y_b, Y_{ss}, Y_s
Z_a, Z_s, Z_w, Z_b, Z_{ss}, Z_{sed}
PRINT
Z_a, Z_s, Z_w, Z_b, Z_{ss}, Z_s
K_{ow}, S , P , H
H = 1
I ≥ N
1 : N
I < N
M(I), E(I), A(I), C(I)
PRINT
M(I), E(I), A(I), C(I)
STOP

```
10 REM ********************************
20 REM *                              *
30 REM *   *    *  *    *  *****  *   *
40 REM *   *    *  **  **  *      *   *
50 REM *   *    *  * ** *  *      *   *
60 REM *    *  *   *    *  *      *   *
70 REM *     **    *    *  *****  *   *
80 REM *                              *
90 REM ********************************

READY.
```

```
10 OPEN 4,4:CMD 4:LIST 10-410
11 REM--EVALUATION OF COMPARTMENTAL DISTRIBUTION--
12 REM HALOBEN.ALKYLBEN.PCB.PAH-------
14 REM---VALANCE MOLECULAR CONN MODEL--
15 REM--------------------------------
16 REM----LOAD "VMCI CC",8 -----------
17 REM---------------------------------
140 DIM D(6)
180 DIM P(6)
190 DIM Z(6)
200 DIM M(6)
210 DIM E(6)
220 DIM A(6)
230 DIM C(6)
240 DIM T$(6)
250 T$(1)= "******AIR"
260 T$(2)= "*****SOIL"
270 T$(3)= "****WATER"
280 T$(4)= "****BIOTA"
290 T$(5)= "S. SOLIDS"
300 T$(6)= "*SEDIMENT"
310 REM ----PARAMETERS----------------
320 V(1)=6E+9
330 V(2)=45000
340 V(3)=7E+06
350 V(4)=7
360 V(5)=35
370 V(6)=21000
380 D(1)=.00119
390 D(2)=1.5
400 D(3)=1
410 D(4)=1

READY.
```

```
420 D(5)=1.5
430 D(6)=1.5
440 P(2)=2
450 P(5)=4
460 P(6)=4
470 T=298
480 RR=8.314
490 REM --------VARIABLES ---------------
540 INPUT C$
541 INPUT M
561 REM----EVALUATION OF KOW*S/P------
562 INPUT X0:INPUT X1:INPUT X2
564 A=0.0889*(X0)↑2
565 B=.4105*(X1)↑2
566 C=0.5018*(X2)↑2
567 NS=8.8517-A-B+C
568 D=1.1769*(X0)↑(5/4)
569 E=3.8543*(X1)↑(5/4)
570 F=0.5892*(X2)↑(5/4)
571 INP=7.3442+D-E-F
572 G=0.0912*(X0)
573 H=0.2823*(X1)
574 I=1.7762*(X2)
575 LNKOW= 3.3005-G+H+I
576 P=EXP(LNKOW)
577 Q=EXP(NS)
578 R=EXP(INP)
579 SP=Q/R
580 EQN=P*SP
581 PRINT#4,"NAME OF CHEMICAL:"C$
582 PRINT#4,"X0="X0
584 PRINT#4,"X1="X1
586 PRINT#4,"X2="X2
588 PRINT#4,"OCT-WATER PART COEFF:"P
590 PRINT#4,"SOLUBILITY:"Q
592 PRINT#4,"VAPOR PRESSURE:"R
594 PRINT#4,"S/P="SP
596 PRINT#4,"KOW*(S/P)="EQN
710 REM --FUG CAP CONST ---------
720 Z(1)=1/(RR*T)
721 HH=(R*M)/(Q*.0075)
740 Z(3)=1/HH
745 K4=(P↑(.85))/5.0133
750 Z(4)=K4*D(4)/HH
780 Z(5)=P(5)*.6*P*D(5)*.01/HH
800 Z(2)=P(2)*.6*P*D(2)*.01/HH
820 Z(6)=P(6)*.6*P*D(6)*0.01/HH
821 PRINT#4,"Z1="Z(1)
822 PRINT#4,"Z2="Z(2)
823 PRINT#4,"Z3="Z(3)

READY.
```

```
824 PRINT#4,"Z4="Z(4)
825 PRINT#4,"Z5="Z(5)
826 PRINT#4,"Z6="Z(6)
827 PRINT#4,"H="HH
830 REM --DIST VALUES -------------
840 S8=0
850 S5=0
860 FOR I=1 TO 6
870 S8=S8+Z(I)
880 S5=S5+Z(I)*V(I)
890 NEXT I
900 F=100/S5
910 FOR I=1 TO 6
920 M(I)=Z(I)*V(I)/S5
930 E(I)=Z(I)/S8
940 A(I)=F*Z(I)*V(I)
950 C(I)=A(I)/V(I)*M/D(I)
960 NEXT I
993 PRINT#4,"MOLECULAR WT.:"M
1002 REM PRINT DIST VALUES------------
1005 PRINT#4,
1010 PRINT#4,SPC(06)"MASS PART","EQ PART","AMOUNT","CONC"
1014 PRINT#4,
1016 FOR I=1 TO 6
1018 PRINT#4,T$(I)M(I)E(I)A(I)C(I)
1020 PRINT#4,
1021 NEXT I
1090 REM REPEAT PROCEDURE FOR NEW CHEM
1110 INPUT AB
1120 IF AB=1 THEN 490
1121 IF AB=0 THEN 1130
1130 END

READY.
```

APPENDIX III

OUTPUTS FOR FUGACITY CAPACITY CONSTANTS CALCULATED BY LEVEL I FUGACITY AND VMCI MODELS*

(*) Given Z_i values for VMCI model are evaluated according to group specific regression equations for ln S, ln P and ln K_{ow}

.LKYLBENZENES

LEVEL I FUGACITY MODEL

VMCI MODEL

```
NAME OF CHEM:BENZENE
FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 4.39056036E-03
Z3= 1.80820409E-03
Z4= .023321015
Z5= 8.78112073E-03
Z6= 8.78112073E-03
```

```
Z1= 4.03620964E-04
Z2= 4.04363825E-03
Z3= 1.72639811E-03
Z4= .0215884903
Z5= 8.0872765E-03
Z6= 8.0872765E-03
```

```
NAME OF CHEM:TOLUENE
FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .0118922207
Z3= 1.34893324E-03
Z4= .0520583569
Z5= .0237844415
Z6= .0237844415
```

```
Z1= 4.03620964E-04
Z2= .013229083
Z3= 1.41195298E-03
Z4= .0573677732
Z5= .026458166
Z6= .026458166
```

```
NAME OF CHEM:ETHYLBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .0284389055
Z3= 1.11851129E-03
Z4= .106203877
Z5= .056877811
Z6= .056877811
```

```
Z1= 4.03620964E-04
Z2= .0359355139
Z3= 1.31054718E-03
Z4= .132650184
Z5= .0718710278
Z6= .0718710278
```

```
NAME OF CHEM:P-XYLENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .0472244404
Z3= 1.73338213E-03
Z4= .174539736
Z5= .0944488808
Z6= .0944488808
```

```
Z1= 4.03620964E-04
Z2= .0396484886
Z3= 1.4949971E-03
Z4= .147090076
Z5= .0792969772
Z6= .0792969772
```

```
NAME OF CHEM:M-XYLENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .039003776
Z3= 1.36720661E-03
Z4= .143164107
Z5= .0780075521
Z6= .0780075521
```

```
Z1= 4.03620964E-04
Z2= .0394131181
Z3= 1.47838167E-03
Z4= .146102396
Z5= .0788262363
Z6= .0788262363
```

```
NAME OF CHEM:O-XYLENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .0448530781
Z3= 1.89025218E-03
Z4= .16924652
Z5= .0897061561
Z6= .0897061561
```

```
Z1= 4.03620964E-04
Z2= .0445072192
Z3= 1.84102978E-03
Z4= .167424762
Z5= .0890144384
Z6= .0890144384
```

```
NAME OF CHEM:N-PROPYLBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .0862452894
Z3= 1.00106639E-03
Z4= .268202536
Z5= .172490579
Z6= .172490579
```

```
Z1= 4.03620964E-04
Z2= .0698896567
Z3= 8.75307808E-04
Z4= .219770689
Z5= .139779313
Z6= .139779313
```

```
NAME OF CHEM:I-PROPYLBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .0557998186
Z3= 6.78203899E-04
Z4= .174727105
Z5= .111599637
Z6= .111599637
```

```
Z1= 4.03620964E-04
Z2= .0634783905
Z3= 7.34538358E-04
Z4= .197255386
Z5= .126956781
Z6= .126956781
```

POLYCYLIC AROMATIC HYDROCARBONS

LEVEL I FUGACITY MODEL

```
NAME OF CHEM:PHENANTHRENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 413.613541
Z3= .577194578
Z4= 936.099996
Z5= 827.227081
Z6= 827.227081
```

```
NAME OF CHEM:ANTHRACENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 297.705577
Z3= .387716663
Z4= 666.828981
Z5= 595.411155
Z6= 595.411155
```

```
NAME OF CHEM:PYRENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 11531.2494
Z3= 3.86014715
Z4= 21067.0566
Z5= 23062.4989
Z6= 23062.4989
```

VMCI MODEL

```
Z1= 4.03620964E-04
Z2= 440.51413
Z3= .5674678
Z4= 984.808364
Z5= 881.028261
Z6= 881.028261
```

```
Z1= 4.03620964E-04
Z2= 1917.33412
Z3= 2.5604565
Z4= 4309.58467
Z5= 3834.66823
Z6= 3834.66823
```

```
Z1= 4.03620964E-04
Z2= 3024.96778
Z3= 1.02824584
Z4= 5537.60358
Z5= 6049.93556
Z6= 6049.93556
```

```
NAME OF CHEM:CHRYSENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 148436.324
Z3= 10.1453652
Z4= 213681.875
Z5= 296872.648
Z6= 296872.648
```

```
Z1= 4.03620964E-04
Z2= 16905.8129
Z3= 1.17044999
Z4= 24376.8877
Z5= 33811.6257
Z6= 33811.6257
```

```
NAME OF CHEM:PERYLENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 3208.36779
Z3= .0563652766
Z4= 3767.13899
Z5= 6416.73559
Z6= 6416.73559
```

```
Z1= 4.03620964E-04
Z2= 35634.3109
Z3= .630945823
Z4= 41877.582
Z5= 71268.6218
Z6= 71268.6218
```

POLYCHLORINATED BIPHENYLS

LEVEL I FUGACITY MODEL

```
NAME OF CHEM:BIPHENYL

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 6.37509386
Z3= .0370863488
Z4= 17.8736841
Z5= 12.7501877
Z6= 12.7501877
```

```
NAME OF CHEM:CBP(4)

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 23.1117431
Z3= .0322522633
Z4= 52.3070463
Z5= 46.2234862
Z6= 46.2234862
```

```
NAME OF CHEM:CBP(2)

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 16.9263253
Z3= .0236205593
Z4= 38.3080617
Z5= 33.8526506
Z6= 33.8526506
```

VMCI MODEL

```
Z1= 4.03620964E-04
Z2= 5.5157849
Z3= .0360169717
Z4= 15.7302991
Z5= 11.0315698
Z6= 11.0315698
```

```
Z1= 4.03620964E-04
Z2= 3.73824448
Z3= 9.48906689E-03
Z4= 9.25221571
Z5= 7.47648897
Z6= 7.47648897
```

```
Z1= 4.03620964E-04
Z2= 7.47700226
Z3= .0237195648
Z4= 19.1350266
Z5= 14.9540045
Z6= 14.9540045
```

```
NAME OF CHEM:CBP(22')

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 2.60207139
Z3= .0138053272
Z4= 7.1952635
Z5= 5.20414278
Z6= 5.20414278
```

```
Z1= 4.03620964E-04
Z2= 12.0625252
Z3= .0177472872
Z4= 27.5097709
Z5= 24.1250504
Z6= 24.1250504
```

```
NAME OF CHEM:CBP(2454'5')

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 193.455216
Z3= 8.34272519E-03
Z4= 259.900994
Z5= 386.910432
Z6= 386.910432
```

```
Z1= 4.03620964E-04
Z2= 56.2155086
Z3= 4.07396925E-03
Z4= 81.6159541
Z5= 112.431017
Z6= 112.431017
```

HALOGEN SUBSTITUTED BENZENES

```
LEVEL I FUGACITY MODEL                  VMCI MODEL

NAME OF CHEM:FLUOROBENZENE

FUGACITY CAP.CONST.
--------------------                    Z1= 4.03620964E-04
Z1= 4.03620964E-04                      Z2= 5.69846532E-03
Z2= 5.2196805E-03                       Z3= 1.30366904E-03
Z3= 1.55729689E-03                      Z4= .0277053731
Z4= .0264162652                         Z5= .0113969306
Z5= .010439361                          Z6= .0113969306
Z6= .010439361
```

```
NAME OF CHEM:CHLOROBENZENE

FUGACITY CAP.CONST.
--------------------                    Z1= 4.03620964E-04
Z1= 4.03620964E-04                      Z2= .0283804973
Z2= .034170429                          Z3= 3.06106308E-03
Z3= 2.74396094E-03                      Z4= .123265778
Z4= .142029293                          Z5= .0567609946
Z5= .0683408579                         Z6= .0567609946
Z6= .0683408579
```

```
NAME OF CHEM:P-DIFLUOROBENZENE

FUGACITY CAP.CONST.
--------------------                    Z1= 4.03620964E-04
Z1= 4.03620964E-04                      Z2= 8.08562543E-03
Z2= 7.80058997E-03                      Z3= 1.19296705E-03
Z3= 1.13986901E-03                      Z4= .0358062797
Z4= .0354694901                         Z5= .0161712508
Z5= .0156011799                         Z6= .0161712508
Z6= .0156011799
```

```
NAME OF CHEM:M-DIFLUOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 5.72474494E-03
Z3= 8.36534075E-04
Z4= .0260305675
Z5= .0114494899
Z6= .0114494899
```

```
Z1= 4.03620964E-04
Z2= 8.29443237E-03
Z3= 1.25707132E-03
Z4= .0379111829
Z5= .0165888647
Z6= .0165888647
```

```
NAME OF CHEM:O-DIFLUOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .0492311027
Z3= 7.03018993E-03
Z4= .223083299
Z5= .0984622053
Z6= .0984622053
```

```
Z1= 4.03620964E-04
Z2= 3.44025995E-03
Z3= 5.56322332E-04
Z4= .0156760155
Z5= 6.88051989E-03
Z6= 6.88051989E-03
```

```
NAME OF CHEM:P-DICHLOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .925730439
Z3= .0209513513
Z4= 3.18208693
Z5= 1.85146088
Z6= 1.85146088
```

```
Z1= 4.03620964E-04
Z2= .180832952
Z3= 5.36786522E-03
Z4= .647218396
Z5= .361665903
Z6= .361665903
```

```
NAME OF CHEM:M-DICHLOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= .191100324
Z3= 2.72890814E-03
Z4= .613040148
Z5= .382200647
Z6= .382200647
```

```
Z1= 4.03620964E-04
Z2= .18437465
Z3= 5.54128913E-03
Z4= .661123093
Z5= .368749301
Z6= .368749301
```

```
NAME OF CHEM:O-DICHLOROBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .384746711
Z3= 5.49417401E-03
Z4= 1.23424794
Z5= .769493422
Z6= .769493422
```

```
Z1= 4.03620964E-04
Z2= .110792705
Z3= 2.40821775E-03
Z4= .378428233
Z5= .221585409
Z6= .221585409
```

```
NAME OF CHEM:BROMOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .0815797563
Z3= 4.63777738E-03
Z4= .321965916
Z5= .163159513
Z6= .163159513
```

```
Z1= 4.03620964E-04
Z2= .103392287
Z3= 4.96507891E-03
Z4= .397739317
Z5= .206784575
Z6= .206784575
```

```
NAME OF CHEM:TRICHLOROBENZENE(135)

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .10913502
Z3= 3.25605421E-04
Z4= .276816279
Z5= .21827004
Z6= .21827004
```

```
Z1= 4.03620964E-04
Z2= .875835073
Z3= 8.37384151E-03
Z4= 2.64479717
Z5= 1.75167015
Z6= 1.75167015
```

```
NAME OF CHEM:TRICHLOROBENZENE(124)

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .784792931
Z3= 2.90725132E-03
Z4= 2.05628155
Z5= 1.56958586
Z6= 1.56958586
```

```
Z1= 4.03620964E-04
Z2= .559934522
Z3= 4.16582157E-03
Z4= 1.62842003
Z5= 1.11986904
Z6= 1.11986904
```

```
NAME OF CHEM:TRICHLOROBENZENE(123)

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 1.10280356
Z3= 3.29022543E-03
Z4= 2.79721375
Z5= 2.20560713
Z6= 2.20560713
```

```
Z1= 4.03620964E-04
Z2= .365730511
Z3= 2.1357566E-03
Z4= 1.02568607
Z5= .731461023
Z6= .731461023
```

```
NAME OF CHEM:P-BROMOCHLOROBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .337937393
Z3= 2.7769224E-03
Z4= .997846512
Z5= .675874785
Z6= .675874785
```

```
Z1= 4.03620964E-04
Z2= .513078839
Z3= 7.2068847E-03
Z4= 1.64139574
Z5= 1.02615768
Z6= 1.02615768
```

```
NAME OF CHEM:M-BROMOCHLOROBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .873775851
Z3= 7.18005106E-03
Z4= 2.58004649
Z5= 1.7475517
Z6= 1.7475517
```

```
Z1= 4.03620964E-04
Z2= .52196497
Z3= 7.40534434E-03
Z4= 1.67232861
Z5= 1.04392994
Z6= 1.04392994
```

```
NAME OF CHEM:O-BROMOCHLOROBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 1.33175982
Z3= .0109434285
Z4= 3.93236121
Z5= 2.66351964
Z6= 2.66351964
```

```
Z1= 4.03620964E-04
Z2= .285576219
Z3= 2.85386653E-03
Z4= .868107404
Z5= .571152439
Z6= .571152439
```

```
NAME OF CHEM:IODOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .485813385
Z3= .0117814019
Z4= 1.68731812
Z5= .971626769
Z6= .971626769
```

```
Z1= 4.03620964E-04
Z2= .881473302
Z3= .0101372174
Z4= 2.73659343
Z5= 1.76294661
Z6= 1.76294661
```

```
NAME OF CHEM:TETRACHLOROBENZENE(1245

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 1.88681497
Z3= 2.24107715E-03
Z4= 4.16827927
Z5= 3.77362994
Z6= 3.77362994
```

```
Z1= 4.03620964E-04
Z2= 1.67402204
Z3= 3.92797694E-03
Z4= 4.09465215
Z5= 3.34804409
Z6= 3.34804409
```

```
NAME OF CHEM:TETRACHLOROBENZENE(1235

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 1.16628354
Z3= 5.77472944E-04
Z4= 2.25960039
Z5= 2.33256709
Z6= 2.33256709
```

```
Z1= 4.03620964E-04
Z2= 1.6951314
Z3= 4.00423269E-03
Z4= 4.1504524
Z5= 3.3902628
Z6= 3.3902628
```

```
NAME OF CHEM:P-DIBROMOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= .837965934
Z3= 3.96235933E-03
Z4= 2.27747626
Z5= 1.67593187
Z6= 1.67593187
```

```
Z1= 4.03620964E-04
Z2= 1.36555633
Z3= 9.5015825E-03
Z4= 3.9316717
Z5= 2.73111267
Z6= 2.73111267
```

```
NAME OF CHEM:M-DIBROMOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 2.9243455
Z3= .0138278983
Z4= 7.94796921
Z5= 5.84869099
Z6= 5.84869099
```

```
Z1= 4.03620964E-04
Z2= 1.38655971
Z3= 9.72828685E-03
Z4= 3.99712678
Z5= 2.77311942
Z6= 2.77311942
```

```
NAME OF CHEM:O-DIBROMOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 2.56795926
Z3= .01214271
Z4= 6.97936038
Z5= 5.13591851
Z6= 5.13591851
```

```
Z1= 4.03620964E-04
Z2= .681812227
Z3= 3.24863373E-03
Z4= 1.85466236
Z5= 1.36362446
Z6= 1.36362446
```

```
NAME OF CHEM:P-CHLOROIODOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 2.35908667
Z3= 9.94194578E-03
Z4= 6.30189832
Z5= 4.71817334
Z6= 4.71817334
```

```
Z1= 4.03620964E-04
Z2= 3.47103396
Z3= .0138133043
Z4= 9.19029279
Z5= 6.94206792
Z6= 6.94206792
```

```
NAME OF CHEM:M-CHLOROIODOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 3.97450528
Z3= .0167498365
Z4= 10.6172141
Z5= 7.94901056
Z6= 7.94901056
```

```
Z1= 4.03620964E-04
Z2= 3.52081751
Z3= .0141162122
Z4= 9.33252996
Z5= 7.04163502
Z6= 7.04163502
```

```
NAME OF CHEM:O-CHLOROIODOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 5.07166589
Z3= .0213736222
Z4= 13.5480918
Z5= 10.1433318
Z6= 10.1433318
```

```
Z1= 4.03620964E-04
Z2= 1.72975604
Z3= 4.76696083E-03
Z4= 4.33429075
Z5= 3.45951207
Z6= 3.45951207
```

```
NAME OF CHEM:PENTACHLOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 1.93732284
Z3= 6.94911488E-04
Z4= 3.57626336
Z5= 3.87464568
Z6= 3.87464568
```

```
Z1= 4.03620964E-04
Z2= 3.37221003
Z3= 2.43215155E-03
Z4= 6.9106786
Z5= 6.74442006
Z6= 6.74442006
```

```
NAME OF CHEM:P-BROMOIODOBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 9.22853391
Z3= .0223800065
Z4= 22.6913434
Z5= 18.4570678
Z6= 18.4570678
```

```
Z1= 4.03620964E-04
Z2= 8.31874973
Z3= .0180035416
Z4= 20.1023912
Z5= 16.6374995
Z6= 16.6374995
```

```
NAME OF CHEM:HEXACHLOROBENZENE

FUGACITY CAP.CONST.
--------------------
Z1= 4.03620964E-04
Z2= 17.0816274
Z3= 6.26984406E-03
Z4= 31.6414764
Z5= 34.1632548
Z6= 34.1632548
```

```
Z1= 4.03620964E-04
Z2= 8.50856973
Z3= 2.41777263E-03
Z4= 15.1629979
Z5= 17.0171395
Z6= 17.0171395
```

```
NAME OF CHEM:TRIBROMOBENZENE(135)

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 93.7660271
Z3= .0105141219
Z4= 145.386142
Z5= 187.532054
Z6= 187.532054
```

```
Z1= 4.03620964E-04
Z2= 13.0033667
Z3= .019227278
Z4= 29.677669
Z5= 26.0067334
Z6= 26.0067334
```

```
NAME OF CHEM:TRIBROMOBENZENE(124)

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 244.517361
Z3= .0274180898
Z4= 379.129166
Z5= 489.034722
Z6= 489.034722
```

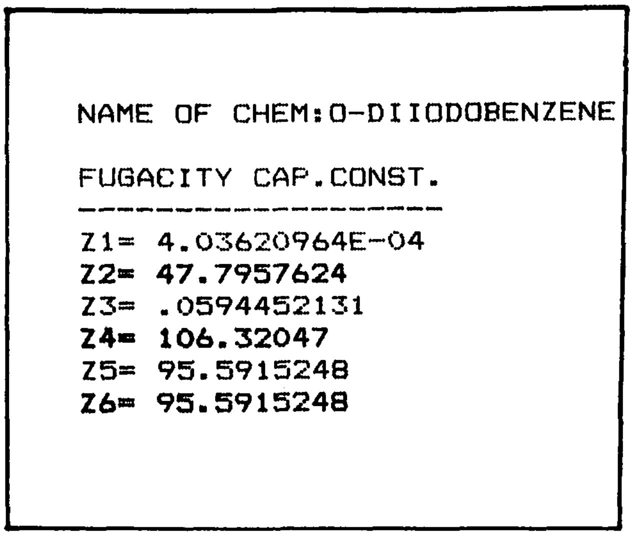
```
Z1= 4.03620964E-04
Z2= 7.68575716
Z3= 8.75229007E-03
Z4= 16.8673397
Z5= 15.3715143
Z6= 15.3715143
```

```
NAME OF CHEM:P-DIIODOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 47.5389325
Z3= .0605030014
Z4= 106.115035
Z5= 95.077865
Z6= 95.077865
```

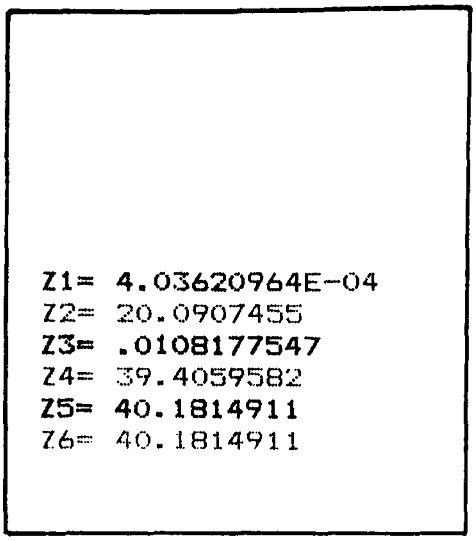
```
Z1= 4.03620964E-04
Z2= 43.6114449
Z3= .0343286413
Z4= 90.5531525
Z5= 87.2228899
Z6= 87.2228899
```

```
NAME OF CHEM:M-DIIODOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 27.9256262
Z3= .0355410631
Z4= 62.3347777
Z5= 55.8512523
Z6= 55.8512523
```

```
Z1= 4.03620964E-04
Z2= 44.0423702
Z3= .0348359748
Z4= 91.5142982
Z5= 88.0847405
Z6= 88.0847405
```



```
NAME OF CHEM:O-DIIODOBENZENE

FUGACITY CAP.CONST.
-------------------
Z1= 4.03620964E-04
Z2= 47.7957624
Z3= .0594452131
Z4= 106.32047
Z5= 95.5915248
Z6= 95.5915248
```



```
Z1= 4.03620964E-04
Z2= 20.0907455
Z3= .0108177547
Z4= 39.4059582
Z5= 40.1814911
Z6= 40.1814911
```

BIBLIOGRAPHY

1. C. Hansch, T. Fujita, J. Amer. Chem. Soc., 86, 1616 (1964)
2. R. Collander, Physiol. Plant., 7,420 (1954)
3 R. Collander, Acta. Chem. Scand., 5, 774 (1954)
4. K.S. Rogers, A. Cammarata, Biochim. Biophys. Acta, 193, 22(1969)
5. D.W. Genson, R.E. Christofferson, J. Amer. Chem. Soc.,95, 632 (1973)
6. T.K. Liu, J. Med. Chem. Chem., 17, 151 (1974)
7. R.D. Crammer, Ann. Dep. in Med. Chem., (F.H. Clarke Ed.) Academic Press (1976)
8. L.B. Kierr, L.H. Hall, "Molecular Connectivity in Chemistry and Drug Research" Academic Press, New York (1976)
9. T. DiPaolo, J. Pharm. Sci., 67, 564 (1978)
10. Ibid.,67, 566 (1978)
11. M. Bonjean and C.L. Duk, Eur. J. Med. Chem., 13,73 (1978)
12. G.R. Parker, J. Pharm. Sci., 67, 513 (1978)
13. B.K. Evans, K.C. James, and D.K. Luscombe, ibid., 68, 370 (1979)
14. J.S. Millership and A.D. Woolfson, J. Pharm. Pharmacol. 30, 483 (1978)
15. S.P. Gupta and P. Singh, Bull. Chem. Soc. Jpn., 52, 2745,(1979)
16. R.J. Gardner, Tech. Q. Master Brew. Assoc. Am., 16, 204 (1979)
17. R.J. Gardner, J. Sci.Food Agric., 31, 23 (1980)
18. L.B. Kierr, and L.H. Hall, J. Pharma. Sci.,65, 1806 (1976)
19. T.DiPaolo, L.B. Kierr, and L.H. Hall, Mol. Pharmacol. 13,31(1977)
20. L.H. Hall and L.B. Kierr, J. Pharma. Sci., 66, 642 (1977)
21. L.B. Kierr, T. DiPaolo, and L.H. Hall J. Theoret. Biol. 67, 585 (1977)
22. L.B. Kierr and L.H. Hall J. Med. Chem., 20,1631 (1977)

23. L.B. Kierr, R.J. Simons and L.H. Hall, J. Pharm. Sci., 67 725 (1978)

24. L.B. Kierr and R.A.Glennon, Life Sci., 22, 1589 (1978)

25. R.A. Glennon and L.B. Kierr, Eur. J. Med. Chem., 13, 219 (1978)

26. L.B. Kierr and L.H. Hall, J. Pharm. Sci., 67, 1408 (1978)

27. L.H. Hall and L.B. Kierr, ibid., 67, 1743 (1978)

28. L.B. Kierr and L.H. Hall, ibid., 68, 120 (1979)

29. T. Dipaolo, L.B. Kierr, and L.H. Hall ibid., 68, 39 (1979)

30. R. A. Glennon, L.B. Kierr, and A.T. Shulgin ibid, 68, 906 (1979)

31. A.J. Richard and L.B. Kierr, ibid., 69, 124 (1980)

32. D.R.Henry and J.H. Block, Eur. J.Med. Chem., 15, 133 (1980)

33. B.Vant Riet, L.B. Kierr, and H. L. Elford. J. Pharm. Sci., 69, 856 (1980)

34. Mackay, D., Environmental Science and Technology, vol. 16, no. 5, pp. 274-278, (1982)

35. L.B. Kierr, L.H. Hall, W.J. Murray, M. Randic J. Pharm. Sci., 64, 1971 (1975)

36. L.H Hall, L.B. Kierr, W.J. Murray, M. ibid., 64 (12), 1975 (1975)

37. W.J.Murray, L.H. Hall, L.B. Kierr, ibid , 64 (12), 1978 (1975)

38. L.B. Kierr, L.H. Hall, Eur. J. Med. Chem., 12,307 (1977)

39. Mackay, D., Shiu, W.Y., Sutherland, R.P., Environmental Science and Technology, Vol. 13, No. 3, pp 590-596 (1985)

40 Mackay, D., Bobra, A., Shiu, W.Y., Chemosphere, Vol. 9, pp.710-711 (1980)

41. Neely, W.B., "Chemicals in the Environment, Distribution, Transport, Fate Analysis", Marcel Dekker, New York (1980)

42. Scheele, B., Chemosphere, Vol.9, pp 293-309 (1980)

43. Bohon, L., Claussen, W.F., Journal of American Chemical Society, Vol.73, pp. 1571- 1578 (1951)

44. Keenaga, E.E., Goring, C.A.I., American Society for testing and Materials Special Technical Publication No. 707, pp. 78-115 (1980)
45. Miller, M.M., Wasik, S.P., Environmental Science and technology, Vol. 19, No. 6, pp.522-529 (1985)
46. Neely, W.B., ,International Journal of Environmental Studies, Vol.13, pp 101-108 (1979)
47. Yalkowsky, S.H., Orr, R.J., Valvani, S.C., Industrial Engineering and Chemical Fundamentals, Vol. 18, No. 4, pp. 351-353 (1979)
48. Lande, S.S., BanerJee, S., Chemosphere, Vol. 10, No. 7 pp. 751-759 (1981)
50. BanerJee, S., Yalkowsky, S.H., Valvani, S.C., Environmental Science and Technology, Vol. 14, No. 10,pp. 1227-1229 (1980)
51. Neely, W.B., Environmental Toxicology and Chemistry, Vol. 1, pp. 259-266 (1982)
52. Gross, P.M., Saylor, J.H.,Journal of American Chemical Society, Vol. 53, pp. 1744-1751 (1931)
53. Riddick, J.a., Bunger, W.B., "Organic Solvents: Physical Properties and Methods of Purification, 3rd Ed.", Techniques of Chemistry, Vol. 2, Wiley-Interscience, New York (1970)
54. Mackay, D., Bobra, A., Chan, D.W., Shiu, W.Y., Environmental Science and Technology, Vol. 16, No. 10, pp.645-649 (1982)
55. Chiou, C.T., Freed, V.H., Schmedding, D.W., Kohnert, R.L., Environmental Science and Technology, Vol.11, No. 5 pp. 475-478 (1977)

56. R. İşeri, M.Sc. Thesis, Boğaziçi University (1986)
57. Strier, M.P., Environmental Science and Technology, Vol. 14, No. 1, pp. 28-31 (1980)
58. Neely W.B., Chemical Technology, Vol.11 pp. 249-251(1981)
59. Neely, W.B., Branson, D.R., Blau, G.L., Environmental Science and Technology, Vol. 8, No. 13, pp.1113-1115 (1974)
60. Dean, J.A., Lange's Handbook of Chemistry, 11 th Ed., pp. 7.54-7.393, Mc Graw-Hill Book Company, New York (1973)
61. Rekker, R.F., "The Hydrophobic Fragmental Constant" Pharmacochemistry Library, Vol. 2, Elsevier Scientific Publishing Company New York (1977)
62. W.B. Neely, An Integrated Approach to Assessing the Potantial Impact of Organic Chemicals in the Environment
63. H. Geyer, G. Politzki, D. Freitag, Chemosphere, 13 (2), 269 (1984)
64. G.B. Whitehouse, R.C. Cooke, Chemosphere, 11(8), 689 (1982)
65. B.J. Eadie, P.F. Landrum, W. Faust, Chemosphere, 11 (9), 847 (1982)
66. H. Govers, C. Ruepert, H. Aiking, Chemosphere, 13 (2), 227 (1984)
67. Mackay, D., Paterson, S., Environmental Science and Technology Vol.16, No.12 pp. 654A-660A (1982)
68. Addison, R.F., Paterson, S., Mackay, D., Chemosphere, Vol. 12, No. 6, pp. 827-834 (1983)
69. Mackay, D., Paterson, S., Environmental Science and Technology Vol. 15, No.9, pp. 1006-1014 (1981)
70. A.M. Butlerov, Z. Chemie, 549 (1861)
71. R.H. Penny, J. Chem. Docum., 5, 113 (1965)

72. R. Fugmann et.al., Angew. Chem., 82, 611(1970)

73. L. Spialter, J. Chem. Docum., 4, 261,(1964)

74. J. Lederberg, NASA Report CR-57029, (1964)

75. A.M. Duffield et al., J. Amer.Chem. Soc., 91,2977 (1969)

76. A. Grovac et.al., Theoret. Chim. Acta. (Berl.) 26,67, (1972)

77. H.Hosoya et.al., Theoret. Chim. Acta (Berl.) 25,215 (1972)

78. L.B. Kierr, L.H. Hall, J. Pharm. Sciences, 70 (6) 583 (1981)

79. J.L. Spialterl J. Amer. Chem. Soc.,85, 2012 (1963)

80. L. Spialter, J. Chem. Doc. 4, 261 (1964)

81. H.Hosoya, Bull. Chem. Soc. of Japan, 44, 2332 (1971)

82. E.A. Smolenskii, Russ. J. Phy. Chem., 38, 700 (1964)

83. Y. İnel, F. Menemenli, H. Beker, Boğaziçi Üniv. Dergisi

84. M. Randic, J. Amer. Chem. Soc., 97, 6609 (1975)

85. W.J. Murray, L.H. Hall, L.B. Kierr, J. Pharm. Sci., 64 , 1978 (1975)

86. L.B. Kierr et al., ibid, 65 (8) 1226 (1976)

87. Hushon, J.M., Klein, A.W., Stratchan, W.J.M., Schmidt-Bleek, F.,-Chemosphere, Vol. 12, No. 6, pp. 887-911 (1983)

88. W.P. Wood, OECD Chemicals group, Working Party of Exposure analysis (EXPO) Room Doc. 80. 21(1981)

89. Frische R., Klöpffer W., Schönborn W. 1979. Bewertung von organisch-chemischen Stoffen und Produkten in Bezug auf ihr Umweltverhalten-chemische, biologische und wirtschaftliche Aspekte. Battelle,Institut e. V. Frankfurt, Germany, under contract of the UMWELTBUNDESAMT:BF-R-63,560-1

90. Mackay, D., Environmental Science and Technology, Vol.13 No. 10. pp.1218-1223 (1979)

91. Karickhoff, S.W., Brown, D.S., Scott, T.a., Water Research Vol. 13, pp.241-248 (1979)

92. D.H. Rouvray, R.I.C Reviews, 173 (1971)

T. C.
Yükseköğretim Kurulu
Dokümantasyon Merkezi