

Copyright Warning & Restrictions

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted material.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One of these specified conditions is that the photocopy or reproduction is not to be “used for any purpose other than private study, scholarship, or research.” If a user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of “fair use” that user may be liable for copyright infringement,

This institution reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

Please Note: The author retains the copyright while the New Jersey Institute of Technology reserves the right to distribute this thesis or dissertation

Printing note: If you do not wish to print this page, then select “Pages from: first page # to: last page #” on the print dialog screen

The Van Houten library has removed some of the personal information and all signatures from the approval page and biographical sketches of theses and dissertations in order to protect the identity of NJIT graduates and faculty.

ABSTRACT

Title of Thesis : Prediction of Vapor and Liquid Equilibrium
Properties for 25 Organic Priority
Pollutants in Aqueous Solution

Pinchieh Pai, Master of Science, 1986

Thesis directed by : Dr. Gordon A. Lewandowski
Associate Professor of Chemical
Engineering

Dr. Dana E. Knox
Assistant Professor of Chemical
Engineering

Activity coefficients and Henry's law constants for 25 organic priority pollutants were estimated using UNIFAC thermodynamic calculations. For 6 of these compounds, the results were compared with measured values reported in the literature. This indicated errors in the UNIFAC predictions varying from 24.0 % to 95.0 %. Best results with UNIFAC were obtained using liquid-liquid equilibria, rather than vapor-liquid equilibria.

Octanol/water partition coefficients were also estimated for the same 25 organic priority pollutants using the fragment constant method. Results differed from values reported in the literature by 5 % to 170 %.

Estimated activity coefficients were also used to predict stripping rates of organic priority pollutants from aerated batch and continuous flow reactors.

Prediction of Vapor and Liquid
Equilibrium Properties for 25 Organic
Priority Pollutants in Aqueous Solution

By

Pinchieh Pai

Thesis is submitted to the faculty of the Graduate school of
the New Jersey Institute of Technology in partial fulfillment
of the requirements for the degree of Master of Science in
Chemical Engineering
1986

Blank Page

APPROVAL SHEET

Title of Thesis : Prediction of Vapor and Liquid Equilibrium
Properties for 25 Organic Priority
Pollutants in Aqueous Solution

Name of Candidate : Pinchieh Pai
Master of Science, 1986

Thesis and Abstract Approved :

5/5/86
Dr. Gordon A. Lewandowski Date
Associate Professor
Department of
Chemical Engineering and
Chemistry

5/5/86
Dr. Dana E. Knox Date
Assistant Professor
Department of
Chemical Engineering and
Chemistry

5/5/86
Dr. John E. McCormick Date
Professor
Department of
Chemical Engineering and
Chemistry

VITA

Name : Pinchieh Pai

Permanent Address :

Degree and Date to be conferred : Master of Science, 1986

Date of Birth :

Place of Birth :

Collegiate Institutions	Attended Date	Degree	Date of Degree
New Jersey Institute of Tech.	9/84-5/86	M.S.	May,1986
Tamkang University	9/76-5/80	B.S.	May,1980

Major : Chemical Engineering

ACKNOWLEDGEMENTS

The author would like to express his deep appreciation for the excellent advice given by Dr. Gordon A. Lewandowski and Dr. Dana E. Knox throughout this work.

The author also expresses his sincere appreciation to his parents and his aunt, for their help and encouragement which made this thesis possible.

TABLE OF CONTENTS

Chapter	Page
I. INTRODUCTION.....	1
II. OBJECTIVE.....	3
III. LITERATURE REVIEW.....	4
A. VAPOR PRESSURE.....	4
B. UNIFAC.....	5
C. HENRY'S LAW CONSTANT.....	7
D. OCTANOL/WATER PARTITION COEFFICIENT.....	8
E. REMOVAL MECHANISMS AND KINETICS.....	9
IV. ANALYSIS OF DATA AND RESULTS.....	13
A. VAPOR PRESSURE.....	13
B. ACTIVITY COEFFICIENTS VIA UNIFAC MODEL.....	13
C. HENRY'S LAW CONSTANT.....	17
D. OCTANOL/WATER PARTITION COEFFICIENT.....	17
E. REMOVAL MECHANISMS AND KINETICS.....	18
V. CONCLUSIONS.....	25
VI. REFERENCES.....	27
TABLES.....	33
APPENDICES.....	50

LIST OF TABLES

Tables	Page
1. Vapor Pressure and Henry's Law Constants.....	33
2. Infinite-Dilution Activity Coefficients.....	36
3. Octanol/Water Partition Coefficients (k_{ow}).....	39
3A. Measured vs. Predicted Henry's Law Constants (H).....	42
4. Nonbiological Batch Systems.....	45
5. Biological Batch Systems.....	46
6. Kinetic Model Survey.....	47

LIST OF APPENDICES

Appendix	Page
1. Regression Equation for The Estimation of Aqueous Solubility for Alkyl Halides, Aromatics and Chlorinated Hydrocarbon, Benzene and It's Derivatives..	50
2. Leo's Fragment Method for Calculating Octanol/Water Partition Coefficients.....	53
3. Calculate The Vapor Pressure by Using Antoine's Equation.....	59
4. UNIFAC Method for Calculating Infinite-Dilution Activity Coefficients.....	60
5. Mass Balance for Nonbiological Batch System.....	64
6. Mass Balance for Biological Batch System With Zero-order and First-order Biodegradation.....	66
7. Mass Balance for Biological Continuous Flow System With Zero-order and First-order Biodegradation.....	69
8 . Mass Balance for Biological Continuous System for Monod Model [W/O Growth].....	71
9 . Sample Output of Appendix 4.....	73

I. INTRODUCTION

During the past few years a great deal of attention has been concentrated on the removal of the toxic organics or priority pollutants by wastewater treatment plants. However, a review of the literature has indicated that only limited data exist describing the fate of these priority pollutants during biological treatment. Approximately 35 % of the organic priority pollutants are known to be purgeable from mixtures with water. Therefore, the possibility exists that these chemicals may be stripped during biological treatment and become an air pollution problem.

Virtually all environmental transport models of toxic compounds require input of physical and chemical properties such as vapor pressure, Henry's law constant, aqueous solubility, octanol/water partition coefficient, chemical and microbial degradation rates, etc. An extensive survey of present data bases (see Literature Review) indicated that very little information exists regarding these properties for many priority pollutants.

It thus becomes necessary to estimate these properties using a variety of theoretical or empirical techniques. Of the 129 priority pollutants, 25 were chosen as representative of three categories of organic compounds: (i) chlorinated alkanes and alkenes, e.g. tetrachloroethane;

(ii) aromatic compounds, e.g. benzene; and (iii) polycyclic aromatic hydrocarbons, e.g. phenanthrene. All these compounds are widely used in the industrial or agricultural field as solvents, pesticides, insecticides, and other synthetic organic chemicals. The ubiquity of these chemicals in our environment is potentially hazardous because most living organisms have yet to adapt themselves to metabolize these molecules, and many may be mutagenic, carcinogenic or teratogenic (1).

In this study, estimation techniques and thermodynamic relationships were used to predict vapor pressures, activity coefficients, and octanol/water partition coefficients for 25 organic priority pollutants. These results were then used to develop material balances for batch and continuous systems, in order to predict the effluent concentration from aerated reactors.

II. OBJECTIVES

The objectives of this study were to :

1. Predict the infinite-dilution activity coefficients of 25 organic priority pollutants using UNIFAC method, coupled with vapor-liquid equilibrium and liquid-liquid equilibrium data.
2. Predict the octanol/water partition coefficients and Henry's law constants for those same compounds.
3. Compare the above results with experimental values reported in the literature.
4. Write a material balance computer program to predict the change in concentration with time for aerated batch and continuous flow reactors, with and without biomass.

III. LITERATURE REVIEW

An extensive amount of experimental and theoretical work on chemical and physical properties of the organic priority pollutants in aqueous solution have been reported. The literature search in this study concentrated on papers involving the use of activity coefficients, Henry's law constants, and octanol/water partition coefficients applied to wastewater treatment plants.

The search was conducted by using the affiliation index and the author index for the institutions, referring to authors known to be active in this field, and consulting the abstracts of the Engineering Index for the years 1972-1985.

A. Vapor pressure

Reliable methods for estimating the vapor pressures of organic materials are of increasing importance as a tool in predicting the behavior and fate of chemicals that are introduced into the environment. For instance, calculation of Henry's law constants requires vapor pressure data. Numerous equations and correlations for estimating vapor pressure are presented by Lyman et al (2). Burkhard (3) has extended the group-contribution method of Macknick and Prausnitz (4) for predicting pure-component vapor pressures to include aromatic halogen groups. The error range for all of the halogenated compounds is a factor of 2

or less, which is similar to the range observed by Macknick and Prausnitz (4,5). Macknick et al (4) also suggested that extreme caution be used when no experimental data exist for the compounds of interest.

Burkhard et al (6) used eleven different methods to predict vapor pressures at 25 °C for fifteen polychlorinated biphenyls, and then compared the predicted values with experimental data. These results permitted an assessment of the predictive ability of these methods for compounds with low vapor pressures (less than 1.0 Pa). The error for the theoretically based methods was high and increased with decreasing vapor pressure. The best correlative method was based on a relationship between Gibb's free energy of vaporization and gas-liquid chromatographic retention indices. The predictive error for this method was estimated to be a factor of 1.75.

B. UNIFAC

The UNIFAC model can be used to estimate activity coefficients for organic molecules based on their chemical structure. The UNIFAC model is attractive because, while there are an ever increasing number of chemical compounds in existence, the number of functional groups which comprise these compounds is much smaller. Hence it is possible to estimate activity coefficients for a very large number of

different organic molecules from a small set of functional group properties (7).

In concept, the UNIFAC method follows the ASOG method, wherein activity coefficients in mixtures are related to interactions between structural groups. The essential features are: (a). Suitable reduction of experimentally obtained activity-coefficient data to yield parameters characterizing interactions between pairs of structural groups in nonelectrolyte systems, (b). Use of these parameters to predict activity coefficients for other systems which have not been studied experimentally but which contain the same functional groups (55).

UNIFAC divides the molecular activity coefficient into two parts: a combinatorial portion (C) which accounts for differences in the size and shape of molecules, and a residual portion (R) which takes into account the interaction energy arising between functional groups in the system. Activity coefficients are calculated by algebraic combination of the various parameters describing the functional group size, shape, and interaction energy. Grain (2) gives details of the methodology and example calculations. At present, UNIFAC energy interaction parameters can be obtained from two sources: an extensive vapor-liquid equilibria (VLE) data base (8,9), or the smaller liquid-liquid equilibria (LLE) data base (10).

UNIFAC parameters for LLE tend to be much stronger functions of temperature than those for VLE. In making LLE calculations, Anderson et al (11) assumed that the UNIFAC energy-of-interaction parameters were linearly dependent on temperature. The best data base to fit UNIFAC parameters should include both VLE and LLE data sets (where the system of interest exhibits both types of phase equilibria).

C. Henry's Law Constant

Activity coefficients can be combined with a compound's vapor pressure to give Henry's Law constant (17), which in aqueous solution may be written as:

$$H = 18 \times 10^{-6} \gamma p^{\circ}$$

where H is in $\text{m}^3\text{-atm/gmol}$, γ is activity coefficient, and p° is the vapor pressure of the pure solute in atm. Arbuckle (18) used this equation, and compared the results with his experimental observations. H values were estimated with an average absolute error of 12 %, and a maximum error of 40 %, versus values reported in the literature.

Mackay, et al (19) obtained Henry's Law constants for a number of organic solutes using a gas stripping system. A new system was also developed that is suitable for the measurement of Henry's law constants in the range of

0.0000001 to 0.00001 atm-m³/mol. The system essentially involved batch distilling a solute-water mixture.

D. Octanol/Water Partition Coefficient

In recent years the octanol/water partition coefficient (Kow) has become a key parameter in studies of the environmental fate of organic chemicals. It has been found to be related to water solubility, soil/sediment adsorption coefficients, and bioconcentration factors for aquatic life. Because of its increasing use in the estimation of these other properties, Kow is considered a required property in the study of new or problematic chemicals. Chemicals with low Kow values (less than 10) may be considered relatively hydrophilic. They tend to have high water solubilities and small soil/sediment adsorption coefficients. Conversely, chemicals with high Kow values (greater than 10,000) are very hydrophobic. An extensive discussion of the Kow data base is included in Leo and Hansch, et al. (12), along with empirical predictive equations, but the calculations are quite involved, especially for complex molecules.

Use of reversed-phase HPLC for estimating Kow has been adopted to an increasing extent in recent years (13,14,15) . Veith and coworkers (13) reported a correlation between Kow and retention time; however, this work did not extend beyond Kow values of 10,000,000. Sarna et al (16) have

attempted to extend this method to compounds with Kow values above 10,000,000 with the intention, firstly, of determining Kow values for a series of polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans, and secondly, of determining whether the relationship between Kow and retention time is altered by the use of columns from different manufacturers.

E. Removal Mechanisms and Kinetics

Several investigators (20-24) have become concerned with the removal of priority pollutants during biological treatment of industrial and municipal wastewaters. Strier (20), and Strier and Gallup (21) made an excellent start in developing structure-activity correlations for removal of priority pollutants.

Petrasek (25) reported the removal and partitioning of the volatile priority pollutants in conventional wastewater treatment plants consisting of a primary clarifier and a plug-flow activated sludge process. He tried to predict the behavior of organic priority pollutants based on knowledge of their structure and physical/chemical properties such as octanol/water partition coefficients and Henry's law constants. Although the results are not entirely satisfactory, higher Henry's law constants generally resulted in greater stripping rates, and higher

octanol/water partition coefficients resulted in a higher degree of adsorption to biological solids. He suggested that after obtaining a more extensive data base, an effort should be made to model the partitioning and removal of organic priority pollutants.

Gaudy and Kincannon (26) studied the effects of organic priority pollutants on the performance of activated sludge units at publicly owned treatment works. Batch and continuous flow bench-scale pilot plants were fed settled municipal sewages spiked with test compounds. Most of the test compounds were removed by either stripping, biodegradation, or attachment to the surface of the microorganisms. It was concluded that batch systems, although more easily studied, cannot be used in place of continuous systems as a means of gaining information on which to base pretreatment policy regulations. The major parameters measured were COD, suspended solids concentration, and the specific compound concentration measured by gas chromatography. However, their studies did not determine the specific removal mechanism.

Stover and Kincannon (27) studied the possibility of predicting biokinetic constants for systems containing several priority pollutants by using data obtained from systems containing a single priority pollutant. Averaging of biokinetic constants was not satisfactory. Their study

also looked at the possibility of predicting the fate and effluent concentrations of various priority pollutants. In general, they found that nitrogen compounds, phenols, and oxygenated compounds will be removed by biological degradation. Aromatics will be removed by both biological degradation and stripping, for Henry's law constants above about $0.00001 \text{ atm-m}^3 / \text{mole}$ (below that biodegradation dominates). Halogenated hydrocarbons present a special problem, some are removed by stripping, whereas others are removed by combined biodegradation and stripping. No single parameter, such as Henry's law constant or partition coefficient, was found that would predict which removal mechanism would dominate.

Pekin and Moore (28) performed pilot plant air stripping studies which verified in general the removal efficiencies predicted by Henry's law constant, provided the approach to equilibrium could be estimated.

Strier and Gallup (29) have found that compounds having Henry's law constants at the level of that of benzene or higher appear to be removed from a wastewater matrix predominantly by an air stripping mechanism, unless the compound is highly adsorptive. Their conclusions were: (i) water solubility, or octanol/water partition coefficient, is the most important property governing the removal pathway; (ii) insolubility and increasing polarity are conducive to

adsorption; (iii) insolubility and volatility enhance air stripping; (iv) intermediate solubility and increasing oxygen content facilitate biological activity.

Bishop et al (30,31) researched toxics removal in wastewater treatment plants and found that conventional primary-activated sludge treatment is generally effective in removing toxic substances, typically achieving better than 90 % removal of organics, and from 60-80 % removal of the indigenous metals. An important overall observation was that the treatment of domestic/industrial wastewaters exhibited remarkable stability over a wide range of operating conditions and produced consistent and excellent treatment of the wastewater even when spiked with high doses (up to 200 ppm) of metals or toxic organics.

Many measurements of Monod growth kinetic parameters have been made by Robinson, et al (32).

Simkins, et al (33) proposed a biodegradation kinetic model which is a function of initial substrate concentration and bacterial cell density.

Alexander (34) considered the influence of substrate concentration, and cell density on the kinetics of biodegradation. He suggested that laboratory tests using chemical concentrations greater than those found in nature may lead to erroneous conclusions about microbial transformation in nature.

IV. ANALYSIS OF DATA AND RESULTS

A. Vapor Pressure

Antoine proposed a simple vapor-pressure correlation, which has been widely used,

$$\ln p^0 = \frac{A - B}{T + C}$$

where A, B, C, are constants and T is in degrees Kelvin.

The present study tabulated values of A, B, C, (33, 34) for 25 compounds (Table 1), and calculated their vapor pressures (Appendix 5). The error varied from 0.002 to 1.87 mmHg.

The applicable temperature range corresponds in most cases to a pressure interval of about 10 to 1500 mmHg. Since wastewater treatment plants are operated within a relatively narrow temperature range (0 to 35°C), the Antoine constants listed will be valid for such applications.

B. Activity Coefficients Via UNIFAC Model

The UNIFAC model is described in detail by Fredenslund, et al (7,8,9,10). The same model is used in this work. The equations are given as follows:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$$

combinatorial residual

In UNIFAC the combinatorial part is given for a binary mixture by

$$\ln \gamma_1^C = \ln \frac{\phi_1}{x_1} + \frac{z}{2} q_1 \ln \frac{\theta_1}{\phi_1} + l_1 - \frac{\phi_1}{x_1} (x_1 l_1 + x_2 l_2)$$

and

$$\ln \gamma_2^C = \ln \frac{\phi_2}{x_2} + \frac{z}{2} q_2 \ln \frac{\theta_2}{\phi_2} + l_2 - \frac{\phi_2}{x_2} (x_1 l_1 + x_2 l_2)$$

where

$$\begin{aligned} \phi_1 &= \frac{\gamma_1 x_1}{\gamma_1 x_1 + \gamma_2 x_2} & \theta_1 &= \frac{q_1 x_1}{q_1 x_1 + q_2 x_2} \\ \phi_2 &= \frac{\gamma_2 x_2}{\gamma_1 x_1 + \gamma_2 x_2} & \theta_2 &= \frac{q_2 x_2}{q_1 x_1 + q_2 x_2} \end{aligned}$$

Note that $\phi_1 + \phi_2 = 1.0$ and $\theta_1 + \theta_2 = 1.0$

$$l_1 = z (\gamma_1 - q_1) / 2 - (\gamma_1 - 1.) ; \quad z = 10.$$

$$l_2 = z (\gamma_2 - q_2) / 2 - (\gamma_2 - 1.)$$

$$\gamma_1 = \sum_k \nu_k^{(1)} R_k \quad \gamma_2 = \sum_k \nu_k^{(2)} R_k$$

$$q_1 = \sum_k \nu_k^{(1)} Q_k \quad q_2 = \sum_k \nu_k^{(2)} Q_k$$

and where

x_1, x_2 = mole fraction of components 1 and 2

$\nu_k = 1, 2, \dots, N$ (number of groups in molecule 1 or 2)

R_k = the van der Waals volume for group k

Q_k = the van der Waals surface area for group k

k = group number

For a binary mixture, the residual part is given by:

$$\ln \gamma_1^R = \sum_k \nu_k^{(1)} [\ln \Gamma_k - \ln \Gamma_k^{(1)}]$$

$$\ln \gamma_2^R = \sum_k \nu_k^{(2)} [\ln \Gamma_k - \ln \Gamma_k^{(2)}]$$

where

$$\ln \Gamma_k = Q_k [1 - \ln \left(\sum_m \Theta_m \psi_{mk} \right) - \frac{\sum_m (\Theta_m \psi_{km})}{\sum_n \Theta_n \psi_{nm}}]$$

and m and $n = 1, 2, \dots, N$ (all groups)

$$\Theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \quad X_m = \frac{\sum_j \nu_m^{(j)} x_j}{\sum_j \sum_n \nu_n^{(j)} x_j}$$

$j = 1, 2, \dots, M$; $n = 1, 2, \dots, N$

Similar relationships hold for $\ln \Gamma_k^{(1)}$ and $\ln \Gamma_k^{(2)}$.

Note however, that these refer to the pure components.

Furthermore,

j = component number

M = total number of components

n = group number

N = total groups

Θ_m = group surface area fraction

X_m = group fraction

X_j = mole fraction of molecule j in the mixture

$\nu_m^{(j)}$ = number of groups of type m in molecule j

$\psi_{nm} = \exp(-a_{nm}/T)$

T = temperature (K)

a_{nm} = group interaction parameter

In order to calculate the infinite-dilution activity coefficients,

$x_1 \rightarrow 0$, and:

$$\frac{\phi_1}{x_1} = \frac{\gamma_1}{x_1 \gamma_1 + x_2 \gamma_2} = \frac{\gamma_1}{\gamma_2}$$

$$\ln \gamma_1^C = \ln \left(\frac{\gamma_1}{\gamma_2} \right) + \frac{z}{2} q_1 \ln \frac{q_1 \gamma_2}{q_2 \gamma_1} + l_1 - \left(\frac{\delta_1}{\gamma_2} \right) l_2$$

since $x_1 \rightarrow 0$, $x_2 \rightarrow 1$. and:

$$\ln \gamma_1^C = 0$$

$$\ln \gamma_2^C = \ln \left(\frac{\gamma_2}{\gamma_1} \right) + \frac{z}{2} q_2 \ln \frac{q_2 \gamma_1}{q_1 \gamma_2} + l_2 - \left(\frac{\delta_2}{\gamma_1} \right) l_1$$

With the use of UNIFAC , activity coefficients were programmed, calculated (Appendix 4, 9), and tabulated (Table 2) for 25 organic priority pollutants.

UNIFAC does not differentiate between isomers (such as those of dichlorobenzene). Furthermore, phenanthrene and naphthalene, can be represented by more than one group contribution model. This leads to the calculation of two or three different activity coefficients for the same compound (see Appendix 9). However, only one of these values is compatible with the data of Mackay (37), Banerjee (44), and Eugene (45).

In addition, activity coefficients for 6 of the compounds studied cannot be determined because the UNIFAC interaction parameters (a_{nm}) are not available.

C. Henry's Law Constant (H)

$$H = 18 \times 10^{-6} \times P^{\circ} \times \gamma$$

where P° is in atm, γ is activity coefficient (calculated from UNIFAC), and H is in atm-m³/gmol.

As indicated in Table 3A, the average error was 50 % vs. literature values. Although both trichloroethylene and phenanthrene have very large activity coefficients, the latter has a much smaller vapor pressure than trichloroethylene. Thus, failed to predict Henry's Law constant of trichloroethylene.

D. Octanol/Water Partition Coefficient

Leo's approach (12) to the estimation of octanol/water partition coefficients uses empirically derived atomic or group fragment constants (f) and structural factors (F):

$$\log Kow = \text{sum of fragments (f)} + \text{factors (F)}$$

The only input information required for this method is the structure of the chemicals, since the fragment values and factors are known (Appendix 4). The relative error varied from 0 % to 170 %.

Kow can also be used to calculate solubilities via empirical formulae developed by Leo and Hansch (12). They found three different regression equations (a, b, c) that

correlate water solubility (S) with the octanol/water partition coefficient (Kow) for : (a) aromatics and chlorinated hydrocarbons ; (b) alkyl halides; and (c) benzene and its derivatives (12).

$$\log S = -1.37 \log Kow + 7.26 \quad (a)$$

$$\log S = -1.221 \log Kow + 0.832 \quad (b)$$

$$\log S = -0.996 \log Kow + 0.339 \quad (c)$$

Using these values of S , H can be predicted (Appendix 1) ,and tabulated (Table 3).

Since values of Kow for many of these chemicals were estimated, this affects the accuracy of S, which in turn affects the accuracy of Henry's Law constant.

E. Removal Mechanisms and Kinetics

Where ideal gas can be assumed (as in most wastewater treatment applications), the vapor-liquid equilibrium relationship can be expressed as:

$$y_i = \frac{\gamma_i x_i P_i^O}{P}$$

where γ_i : activity coefficient of component i,

x_i : mole fraction of component i in liquid phase,

y_i : mole fraction of component i in gas phase,

P : system pressure (mmHg),

P_i^O : vapor pressure of component i (mmHg).

For a nonbiological batch system, the substrate material

balance (on a mole basis) is:

$$\begin{aligned} \frac{d (x_i V D_l)}{d t} &= - A y_i D_g & (i) \\ &= \frac{-A P_1^0 \gamma_i x_i D_g}{P} \end{aligned}$$

where A : air flowrate (liters/hr),
 D_l : density of liquid phase (mol/liter),
 D_g : density of gas phase (mol/liter),
 V : reaction volume (liters),

Assuming the liquid volume is constant and

$$D_l = 1000 / 18 = 55.6 \text{ gmol/liter (for water)}$$

$$D_g = \frac{n}{V} = \frac{P}{R T} = \frac{1.}{.082 \times 298.15} = 0.0408 \text{ gmol/liter}$$

For constant reactor volume, and assuming that γ is independent of x for dilute solutions, equation (i) becomes:

$$V \frac{d x_i}{d t} = - \frac{A P_1^0 x_i \gamma_i D_g}{P D_l}$$

which after integration yields:

$$\begin{aligned} \ln \frac{x_0}{x} &= \frac{A D_g \gamma_i P_1^0 t}{P V D_l} \\ x &= \frac{\text{mole of solute}}{\text{mole of solute} + \text{mole of solvent}} \end{aligned}$$

For dilute solutions:

$$\frac{x_0}{x} \approx \frac{\text{ppm}_0}{\text{ppm}}$$

where subscript $_0$ denotes the initial condition.

For a biological batch system:

$$\frac{d}{dt} (x_i V D_l) = -A y_i D_g + r_B V$$

or
$$\frac{dx_i}{dt} = - \frac{A P_i^0 x_i Y_i D_g}{P V D_l} + \frac{r_B}{D_l} \quad (ii)$$

where r_B = biodegradation rate (ppm/ hr),

Now consider the following three biodegradation kinetic equations:

(1) zero-order biological reaction

$$r_B = -K_0$$

(2) first-order biological reaction

$$r_B = -K_1 (x) D_l$$

(3 a) Monod model without growth

$$r_B = \frac{-K_1 (x) D_l}{K_2 + (x) D_l}$$

(3 b) Monod model with growth

$$r_B = \frac{-K_1 (x) D_l [B_0 + Y (x_0 - x) D_l]}{K_2 + (x) D_l}$$

where K_0, K_1, K_2 : constants,

B_0 : initial biomass concentration ,

Y : yield coefficient

Substituting the above three equations into equation

(ii) and integrating, yields:

(4) zero-order

$$x = \left(\frac{K_0}{a D_1} + x_0 \right) \exp (- a t) - \frac{K_0}{a D_1}$$

where

$$a = \frac{A P_1^0 \gamma_i D_g}{P V D_1}$$

(5) first-order

$$x = x_0 \exp [(- a + K_1) t]$$

where

$$a = \frac{A P_1^0 \gamma_i D_g}{P V D_1}$$

(6 a) Monod model without growth

$$\begin{aligned} & \left(D_1 - \frac{2 K_2 a}{b} \right) \ln \left[\left(\frac{a x_0 + b}{a x + b} \right) \left(\frac{x}{x_0} \right) \right] + \\ & + D_1 \ln \left[\frac{a x_0^2 + b x}{a x^2 + b} \right] = 2 a t \end{aligned}$$

where

$$a = \frac{A P_1^0 \gamma_i D_g}{P V}$$

$$b = \frac{A P_1^0 \gamma_i D_g K_2}{P V D_1} + K_1$$

(6 b) Monod model with growth

$$\begin{aligned} & \left(D_1 - \frac{2 K_2 a}{b} \right) \ln \left[\left(\frac{a x_0 + b}{a x + b} \right) \left(\frac{x}{x_0} \right) \right] + \\ & + D_1 \ln \left[\frac{a x_0^2 + b x_0}{a x^2 + b} \right] = 2 a t \end{aligned}$$

where

$$a = \left[\frac{A P_1^0 \gamma_i D_g}{P V D_1} + K_1 Y \right] D_1$$

$$b = \frac{A P_1^0 Y_i Dg K_2}{P V D_l} + K_1 B_0 + K_1 Y x_0 D_l$$

For a non-biological continuous flow system, the substrate material balance is:

$$\frac{d}{dt} (x V D_l) = -A y Dg + F D_l x_0 - F D_l x$$

which gives after integration:

$$x = \frac{x_0}{1. + (A P_1^0 Y_i Dg) / (P F D_l)}$$

where F = wastewater flowrate (liter/hr)

For a biological continuous flow system , once again different biodegradation kinetic models can be assumed, and the material balance equations integrated to yield :

(1) zero-order

$$x = [x_0 - \frac{K_0 V}{F D_l}] / [1. + \frac{A P_1^0 Y_i Dg}{F P D_l}]$$

(2) first-order

$$x = x_0 / [1. + \frac{A P_1^0 Y_i Dg}{F P D_l} + \frac{K_1 V}{F}]$$

(3 a) Monod model without growth

$$x = \frac{[-a + \sqrt{a^2 + 4b}]}{2} \quad (iii)$$

where

$$a = \left[\frac{A P_1^0 Y_i Dg K_2}{P D_1} + F K_2 + V K_1 - F x_0 D_1 \right] /$$

$$\left[\frac{A P_1^0 Y_i Dg}{P} + F D_1 \right]$$

$$b = F x_0 K_2 / \left[\frac{A P_1^0 Y_i Dg}{P} + F D_1 \right]$$

(3 b) Monod model with growth

Using the same formula (iii) but

$$a = \frac{\frac{A P_1^0 Y_i Dg K_2}{P D_1} + F K_2 + K_1 V (B_0 + x_0 Y D_1) - F D_1 x_0}{\frac{A P_1^0 Y_i Dg}{P} + F D_1 - K_1 Y D_1 V}$$

$$b = \frac{F x_0 K_2}{\frac{A P_1^0 Y_i Dg}{P} + F D_1 - K_1 Y D_1 V}$$

After programming (Appendix 5-8), for a nonbiological batch system the theoretical time to strip the solution to 1.0 ppm was compared with the measured time. Results are shown in Table 4.

These results indicate, for example, that benzene and toluene strip out at a very fast rate, while phenol is not subject to stripping.

For a biological batch system, with biological rate constants obtained from Pak (40), the results are shown in Table 5.

The results and examples for continuous systems are also shown in Appendix 7 and 8.

V. CONCLUSIONS

1. A comparison between the VLE based UNIFAC parameters and the LLE based parameters does not reveal many similarities. Thus for the same compound two different activity coefficients were obtained. By comparison with measured values, the LLE predictions were more accurate.
2. Calculation of octanol/water partition coefficients by the fragment method is quite involved, especially for complex molecules(such as naphthalene, or 2,4-D). Compound structures are required, and considerable proficiency is needed in handling the calculations. In this study, the relative error varied from 0 to 170 %.
3. In this study, toluene and naphthalene were found to be highly strippable compounds; nitrobenzene, phenol, 2-chlorophenol and nitrophenol are difficult to strip, or stripped slowly. For a nonbiological system, the theoretical time to strip the solution versus actual time to strip the solution indicated that only 60 to 70 % saturation of the exit air was achieved.
4. Although single compound biodegradation rate constants were not always available, as expected compounds that were not easily stripped were predominantly removed by biodegradation (with the exception of nitrobenzene

which has a very slow rate of biodegradation).

VI. REFERENCES:

- [01]. Duffus, J. H., Environmental Toxicology , John Wiley Sons, N.Y. (1980).
- [02]. Grain, C. F., "Activity Coefficient", Chapt. 11, Handbook of Chemical Property Estimation Methods, Edited by Lyman, W. J., Reehl, W. F., and Rosenblatt, D. H., McGraw-Hill , N.Y. (1982).
- [03]. Burkhard, L. P., "Estimation of Vapor Pressures for Halogenated Aromatic Hydrocarbons by a Group-Contribution Method", I&EC Fundamentals, 24, 119, (1985).
- [04]. Macknick, A. B., and Prausnitz, J. M., "Vapor Pressures of Heavy Liquid Hydrocarbons by a Group-Contribution Method", I&EC Fundamentals, 18, 348, (1979).
- [05]. Edwards, D. R., and Prausnitz, J. M., " Estimation of Vapor Pressure of Heavy Liquid Hydrocarbons Containing N or S by a Group-Contribution Method", I&EC Fundamentals, 20, 280, (1981).
- [06]. Burkhard, L. P., Andren, A. W., and Armstrong, D. E., "Estimation of Vapor Pressure for Polychlorinated Biphenyls: A comparison of Eleven Predictive Methods", Environ. Sci. Technol., 19, 500, (1985).
- [07]. Fredenslund, A., Gmehling, J., and Rasmussen, P., Vapor Liquid Equilibria Using UNIFAC, Elsevier, New York (1977).
- [08]. Gmehling, J., Fredenslund, A., and Rasmussen, P., "Vapor-Liquid Equilibria by UNIFAC Group Contribution: Revision & Extension 2", I&EC Process Design & Dev., 21, 118, (1982).
- [09]. Bell, A. T., " Explanation for Deviations of Fischer-Tropsch Products from A Schalz-Flory Distribution", I&EC Process Design & Dev., 22, 678, (1983).
- [10]. Magnussen, T., Rasmussen, P., and Fredenslund, A., "UNIFAC Parameter Table for Prediction of Liquid-Liquid Equilibria", I&EC Process Design & Dev., 20, 331, (1981).

- [11]. Personal Communication with Dr. F. Anderson (July 29, 1985).
- [12]. Leo, A. J., Hansch, C., and Elkins, D., "Partition Coefficients and Their Uses", Chem. Rev., 71, 525, (1971).
- [13]. Veith, G. D., Austin, N. M., and Morris, R. T., " A Rapid Method for Estimating Log P for Organic Chemicals", Water Res., 13, 43, (1979).
- [14]. McDuffie, B., " Estimation of Octanol-Water Partition Coefficients for Organic Pollutants Using Reverse-Phase HPLC", Chemosphere, 10, 73, (1981).
- [15]. Wasik, S. P., Miller, M. M., May , W. E., and Sonnefeld, W. J, " Determination of the Vapor Pressure, Aqueous Solubility and Octanol/Water Partition Coefficient of Hydrophobic Substances by Coupled Generator Column/Liquid Chromatographic Methods", Residue Rev., 85, 29, (1983).
- [16]. Sarna, L. P., Hodge, P. E., and Webster, G. B., " Octanol/Water Partition Coefficients of Chlorinated Dioxins and Dibenzofurans by Reverse-Phase HPLC Using Several C18 Columns", Chemosphere, 13, 975, (1984).
- [17]. Mackay, D., Russel, P., and Wan, Y. S., " Determination of Air-Water Henry's Law Constant for Hydrophobic Pollutants", Environ. Sci. Technol., 13, 333, (1979).
- [18]. Arbuckle, W. B., " Estimating Activity Coefficients for Use in Calculating Environmental Parameters", Environ. Sci. Technol., 17, 537, (1983).
- [19]. Mackay, D., Wan, Y. S., Bobra, A., and Billington, J., " Volatilization of Organic Pollutants from Water", EPA 600/3-82-019, NTIS PB 82-230939 (April, 1982).
- [20]. Strier, M. P., " Pollutant Treatability : A Molecular Engineering Approach", Environ. Sci. Technol., 14, 28, (1980).
- [21]. Strier, M. P., and Gallup, J. D., "Industrial Effluent Standards for Toxic Pollutants", p. 183, Proceedings 36th Industrial Waste Conference, Purdue University, Ann Arbor Sci. Pub. (1981).
- [22]. Wukasch, R. F., Grady, C. P., and Kirsch, E. J.,

"Prediction of the Fate of Organic Compounds in Biological Wastewater Treatment systems", Water-1980, AICHE Symp. Ser., 77, 137, (1981).

- [23]. Petrasek, A. C., " Behavior of Selected Organic Priority Pollutants in Wastewater Collection and Treatment Systems", WPCF 53rd Annual Conference, Las Vegas, Nevada (September 1980).
- [24]. Hwang, S. T., " Treatability and Pathways of Priority Pollutants in Biological Wastewater Treatment", Water-1980, AICHE Symp. Ser., 77, 316, (1981).
- [25]. Petrasek, A. C., " Removal and Partitioning of the Volatile Priority Pollutants in Conventional Wastewater Treatment Plants", Municipal Environmental Research Lab., U.S. EPA Cincinnati, Ohio (October 1981).
- [26]. Gaudy, A. F., Kincannon, D. F., and Manickam, T. S., " Treatment Compatibility of Municipal Waste and Biologically Hazardous Industrial Compounds", Vol. 1, 2, EPA-600/2-82-075a (June 1982).
- [27]. Stover, E. L., and Kincannon, D. F., " Predicting Treatability of Multiple Organic Priority Pollutant Wastewaters from Single-Pollutant Treatability Studies", p. 641, Proceedings of the 37th Industrial Waste Conference, Purdue University, Ann Arbor Sci. Pub. (1982).
- [28]. Pekin, T. and Moore, A., " Air Stripping of Trace Volatile Organics from Wastewater", p. 765, Proceedings of the 37th Industrial Waste Conference, Purdue University, Ann Arbor Sci. Pub. (1982).
- [29]. Strier, M. P. and Gallup, J. D., " Removal Pathways and Fate of Organic Priority Pollutants in Treatment Systems : Chemical Considerations", p. 813, Proceedings of the 37th Industrial Waste Conference, Purdue University, Ann Arbor Sci. Pub. (1982).
- [30]. Bishop, D. F., " The Role of Municipal Wastewater Treatment in Control of Toxics", Paper presented at the NATO/ CCMS Meeting in Bari, Italy (September 1982).
- [31]. Bishop, D. F., Petrasek, A. C., and Kugelman, I. J., " Control of Specific Organic and Metal Contaminants by Municipal Wastewater Treatment Processes", U.S.

EPA Guide Sheet (October 1981).

- [32]. Robinson, J. A. and Tiedje, J. M., " Nonlinear Estimation of Monod Growth Kinetics Parameters from a Single Substrate Depletion Curve", Appl. Environ. Micro., 45, 1453, (1983).
- [33]. Simkins, S. and Alexander, M., " Models for Mineralization with the Variables of Substrate Concentration and Population Density", Appl. Environ. Micro., 47, 1299, (1984).
- [34]. Alexander, M., " Biodegradation of Organic Chemicals", Environ. Sci. Technol., 18, 106, (1985).
- [35]. Lange's Handbook of Chemistry, 13th Ed., McGraw Hill, N.Y., (1985).
- [36]. Shuzo Ohe, Computer Aided Data Book of Vapor Pressure, Eng. Data Book Publishing Co., Tokyo, Japan.
- [37]. Mackay, D., and Wan, Y. S., " Aqueous Solubility of Polynuclear Aromatic Hydrocarbons", J. Chem. Engr. Data, 22, 399, (1977).
- [38]. Desai, S. S., " Kinetics of Biodegradation of Phenol and 2,6-DCP", Masters Thesis, NJIT (1983).
- [39]. Colish, J. C., " Biodegradation of Phenol and O-Chlorophenol Using Activated Sludge Bacteria", Masters Thesis, NJIT (1984).
- [40]. Pak, D. W., " The Biodegradation of Phenolics Using Mixed Liquor from PVSC Plant", Masters Thesis, NJIT (1985).
- [41]. Kincannon, D. F., " Removal Mechanisms for Toxic Priority Pollutants", JWPCF, 55, 157, (1983).
- [42]. Mueller, J. A., " Secondary, Tertiary and Toxics Treatment", p. 6-49, 6-50, Manhattan College, Bronx, New York (1983).
- [43]. Petrasek, A. C., Kugelman, I. J., Austern, B. M., Pressley, T. A., Winslow, L. A., and Wise, R. H., " Fate of Toxic Organic Compounds in Wastewater Treatment Plants", JWPCF, 55, 1286, (1983).
- [44]. Banerjee, S., " Calculation of Water Solubility of Organic Compounds with UNIFAC Derived Parameters",

Environ. Sci. Technol., 19, 369, (1985).

- [45]. Eugene, R. T., Long, T. C., Wood, D. A., and Eckert, C. A., " Limiting Activity Coefficients of Nonpolar and Polar Solutes in both Volatile and Nonvolatile Solvents by Gas Chromatography", J. Chem. Engr. Data, 27, 399, (1982).
- [46]. Shamat, N. A., and Maier, W. J., " Kinetics of Biodegradation of Chlorinated Organics", JWPCF, 52, 2158, (1980).
- [47]. Beltrame, P., Carniti, P., and Pitea, D., " Kinetics of Phenol Degradation by Activated Sludge in A Continuous Stirred Reactor", JWPCF, 51, 126, (1980).
- [48]. Neufeld, R. D., and Valiknac, T., " Inhibition of Phenol Biodegradation by Thiocyanate", JWPCF, 51, 2283, (1979).
- [49]. Luthy, R. G. , " Treatment of Coal Coking and Coal Gasification Wastewaters", JWPCF, 53, 325, (1981).
- [50]. Lewandowski, G. A., Baltzis, B., and Varuntanya, C., "Kinetics of Biodegradation of Toxic Organic Compounds", paper presented at the summer National Meeting of AIChE, Philadelphia, PA, (Aug. 1984).
- [51]. Pitter, P., " Determination of Biological Degradability of Organic Substances", Water Research, 10, 231, (1976).
- [52]. Vavillin, V. A., " Dependence of Biological Treatment Rate on Species Composition in Activated Sludge or Biofilm- II: From Model to Theory", Biotech. Bioeng, 25, 1539, (1983).
- [53]. Blackburn, J. W., Troxler, W. L., Truong, K. N., Zink, R. P., Meckstroth, S. C., Florance, J. R., Groen, A., and Yagi, O., " Organic Chemical Fate Prediction in Activated Sludge Treatment Processes", IT Contract Nos. 68-03-3027, and 68-03-3074, (1984).
- [54]. Lyman, W. J., " Solubility in Water ", Chapt. 2, Handbook of Chemical Property Estimation Methods, Edited by Lyman, W. J., Reehl, W. F., and Rosenblatt, D. H., McGraw-Hill, N.Y. (1982).
- [55]. Reid, R. C., Prausnitz, J. M., and Sherwood, T. K., The Properties of Gases and Liquids, McGraw-Hill N.Y.

(1977).

- [56]. Gmehling, J., Onken, U., and Arlt, W., Vapor Liquid Equilibrium Data Collection: Aqueous-Organic Systems, 1, part 1a, Pub. by DECHEMA, (1981).

TABLE 1

VAPOR PRESSURE AND HENRY'S LAW CONSTANTS

PRIORITY POLLUTANTS	Ref	Antoine Constants			P	H
		A	B	C	(Atm) (mmHg) (25°C)	(m ³ -atm/mol) (25°C) (Expt.)
1,1,2,2- TETRACHLOROETHANE	35 41	6.6317	1228.1	179.9	.00572 4.3455	4.20*10(-4)
1,1,1,2- TETRACHLOROETHANE	35 25	6.8987	1365.88	209.74	.01582 12.024	3.80*10(-4)
1,1,1- TRICHLOROETHANE	35 41	8.6434	2136.6	302.8	.17563 133.48	4.90*10(-3)
1,1,2- TRICHLOROETHANE	35 25	6.9518	1314.4	209.2	.02875 21.853	7.40*10(-4)
1,1- DICHLOROETHANE	35 42	6.9770	1174.02	229.06	.29864 226.97	4.71*10(-3) (20°C)
TRICHLOROETHYLENE	35 25	6.5183	1018.6	192.7	.09090 69.085	1.17*10(-2)
DICHLOROMETHANE	35 2	7.4092	1325.9	252.6	.56505 429.44	2.60*10(-3)
2-NITROPHENOL	36 42	7.7410	2163.44	230.29	.00024 .18481	7.17*10(-5) (20°C)

PHENOL	35 41	7.133	1516.79	174.95	.00046 .35250	1.30*10(-6)

TOLUENE	35 19	6.9546	1344.8	219.48	.03743 28.444	6.70*10(-3)

CHLOROBENZENE	35 19	6.9781	1431.05	217.55	.01575 11.969	3.70*10(-3)

NITROBENZENE	35 41	7.1156	1746.60	201.8	.00034 .25974	2.40*10(-5)

1,2- DICHLOROBENZENE	35 41	7.14378	1704.49	219.42	.00195 1.4797	1.90*10(-3)

1,3- DICHLOROBENZENE	35 41	7.0401	1607.05	213.38	.00262 1.9886	2.60*10(-3)

2-CHLOROTOLUENE	35 2	7.3680	1735.8	230.0	.00479 3.6384	2.60*10(-3)

CHLOROANILINE	35 2	7.56265	1998.6	220.0	.00033 .25416	9.70*10(-6)

2,6- DICHLOROPHENOL	36	8.20323	2431.8	236.759	.00011 .08185	

2-CHLOROPHENOL	36	7.23217	1774.35	233.312	.00304 2.3075	

BENZO(A) PYRENE						

PHENANTHRENE	35 42	7.26082	2379.04	203.76	.000001 .000726	1.21*10 ⁽⁻⁴⁾ (20°C)

DIPHENYLAMINE	36 43	7.97321	2729.39	233.943	.000004 .002708	1.70*10 ⁽⁻⁵⁾

DIETHYLPHTHALATE	36	8.325	2916.98	241.744	.000003 .002452	

NAPHTHALENE	35 42	6.8181	1585.86	184.82	.000239 .181931	3.36*10 ⁽⁻⁴⁾ (20°C)

1,4-DIOXANE	35	7.43155	1554.68	240.34	.049152 37.3551	

BENZENE	35	6.90565	1211.03	220.79	.125237 95.1800	5.55*10 ⁽⁻³⁾

TABLE 2

INFINITE-DILUTION ACTIVITY COEFFICIENTS
(CALCULATED USING UNIFAC METHOD)

PRIORITY POLLUTANTS	ACTIVITY COEFFICIENT (LLE)		ACTIVITY COEFFICIENT (VLE)	
	Cal. (a)	Lit. (b)	Cal. (a)	Lit. (c)
1,1,2,2- TETRACHLOROETHANE	11438		11046	11100
1,1,1,2- TETRACHLOROETHANE	7102		6830	
1,1,1- TRICHLOROETHANE	2875		2374	2370
1,1,2- TRICHLOROETHANE	2278		2688	
1,1- DICHLOROETHANE	1842		795	
TRICHLOROETHYLENE	6.5×10^7			
DICHLOROMETHANE	254		249	
2-NITROPHENOL	113		51	
PHENOL	54.5		6.4	57 (44°C)
TOLUENE	7265		12096	12100

CHLOROBENZENE	10149		19158	19200

NITROBENZENE	3576		3338	3340

1,2-DICHLOROBENZENE	28371		172939	173000

1,3-DICHLOROBENZENE	28371		172939	173000

2-CHLOROTOLUENE	29020		94676	

CHLOROANILINE	1638		748	

2,6-DICHLOROPHENOL	7400			

2-CHLOROPHENOL	350			

BENZO(A) PYRENE	3.3×10^8	1.2×10^8	1.3×10^9	2.8×10^9

PHENANTHRENE	1.1×10^6	1.8×10^6	4.2×10^6	7.4×10^6

DIPHENYLAMINE				

DIETHYLPHTHALATE				

NAPHTHALENE	55855	68300	138891	139000

1,4-DIOXANE

35.5

26.4

4.4
(20°C)

BENZENE

2582

2417

(a). Detailed calculation see Appendix

(b). See References: 35, 45.

(c). See References: 44, 56.

TABLE 3

OCTANOL/WATER PARTITION COEFFICIENTS (Kow)

PRIORITY POLLUTANTS	Log Kow Cal.	Log Kow Lit.
1,1,2,2- TETRACHLOROETHANE	2.78	2.56
1,1,1,2- TETRACHLOROETHANE	3.17	2.56
1,1,1- TRICHLOROETHANE	2.62	2.49
1,1,2- TRICHLOROETHANE	2.19	2.17
1,1- DICHLOROETHANE	1.92	1.79
TRICHLOROETHYLENE	2.28	2.29 2.42
DICHLOROMETHANE	1.26	1.25
2-NITROPHENOL	1.20	2.00
PHENOL	1.46	1.46

TOLUENE	2.79	2.69 2.21
---------	------	--------------

CHLOROBENZENE	2.84	2.84 2.98
---------------	------	--------------

NITROBENZENE	1.87	1.85 1.83
--------------	------	--------------

1,2- DICHLOROBENZENE	3.55	3.55 3.40
-------------------------	------	--------------

1,3- DICHLOROBENZENE	3.38	3.38 3.44
-------------------------	------	--------------

2-CHLOROTOLUENE	3.50	3.42
-----------------	------	------

CHLOROANILINE	1.61	1.88
---------------	------	------

2,6- DICHLOROPHENOL	2.88	
------------------------	------	--

2-CHLOROPHENOL	2.17	2.19 2.16
----------------	------	--------------

BENZO(A) PYRENE		6.5 7.77
-----------------	--	-------------

PHENANTHRENE	4.54	4.46
--------------	------	------

DIPHENYLAMINE	3.51	3.50
---------------	------	------

DIETHYLPHTHALATE3.41

NAPHTHALENE

3.37

3.37

3.35

1,4-DIOXANE

0.01

-0.42

BENZENE

2.13

2.13

1. Log Kow Lit. see References: 12, 13, 15, 16.

2. Log Kow Cal. see Appendix 2.

TABLE 3A

MEASURED VS. PREDICTED HENRY'S LAW CONSTANTS (H)

PRIORITY POLLUTANTS	H Lit. @ 25°C	H ^a Cal.	E ^b %
1,1,2,2- TETRACHLOROETHANE	.42*10(-3)	.12*10(-2)	186
1,1,1,2- TETRACHLOROETHANE	.38*10(-3)	.20*10(-2)	430
1,1,1- TRICHLOROETHANE	.49*10(-2)	.91*10(-2)	86
1,1,2- TRICHLOROETHANE	.74*10(-3)	.12*10(-2)	62
1,1- DICHLOROETHANE	.47*10(-2) (20°C)	.10*10(-1)	110
TRICHLOROETHYLENE	.117*10(-1)		
DICHLOROMETHANE	.26*10(-2)	.26*10(-2)	0
2-NITROPHENOL	.717*10(-4)	.50*10(-6)	99
PHENOL	.13*10(-5)	.45*10(-6)	65

TOLUENE	.67*10(-2)	.49*10(-2)	27
---------	------------	------------	----

CHLOROBENZENE	.37*10(-2)	.29*10(-2)	22
---------------	------------	------------	----

NITROBENZENE	.24*10(-4)	.22*10(-4)	8
--------------	------------	------------	---

1,2-DICHLOROBENZENE	.19*10(-2)	.10*10(-2)	47
---------------------	------------	------------	----

1,3-DICHLOROBENZENE	.26*10(-2)	.13*10(-2)	50
---------------------	------------	------------	----

2-CHLOROTOLUENE	.26*10(-2)	.25*10(-2)	4
-----------------	------------	------------	---

CHLOROANILINE	.97*10(-5)	.97*10(-5)	0
---------------	------------	------------	---

2,6-DICHLOROPHENOL		.15*10(-4)	
--------------------	--	------------	--

2-CHLOROPHENOL		.20*10(-4)	
----------------	--	------------	--

BENZO (A) PYRENE			
------------------	--	--	--

PHENANTHRENE	.121*10(-3) (20°C)	.20*10(-4)	67
--------------	-----------------------	------------	----

DIPHENYLAMINE	.170*10(-4)		
---------------	-------------	--	--

DIETHYLPHTHALATE			
------------------	--	--	--

NAPHTHALENE	.336*10(-3) (20°C)	.24*10(-3)	30
-------------	-----------------------	------------	----

1,4-DIOXANE		.31*10(-4)	
-------------	--	------------	--

BENZENE	.555*10(-2)	.58*10(-2)	4
---------	-------------	------------	---

$$a. H = 18 \times 10^{-6} \times P^0 \times \gamma$$

$$b. \text{Error \%} = \frac{|H_{\text{Cal.}} - H_{\text{Lit.}}|}{H_{\text{Lit.}}} \times 100$$

TABLE 4
Nonbiological Batch Systems
Air Flowrate : 30 liters/hr
Reaction Volume : 2.0 liters

Compound	Initial Aqueous Conc. (ppm)	Vapor Press. @ 25°C (mmHg)	Theoretical Time to Strip the Solution to 1 ppm (hr)	Actual Time to Strip the Solution to 1 ppm (hr) *
phenol	100	0.3525	-----	-----
2-chloro- phenol	20	2.3075	252	350
2,6-dichloro- phenol	20	0.0800	340	450
toluene	100	28.444	1.55	2.5
nitrobenzene	20	0.2597	220	330
benzene	20	95.180	1.25	

* See References: 38, 39, 40.

TABLE 5
Biological Batch System

Air Flowrate : 30 liters/hr

Reaction Volume : 2.0 liters

Compound	Initial Aqueous Conc. (ppm)	Vapor Press. @ 25°C (mmHg)	Theoretical Time to Treat the Solution to 1 ppm (hr) [Zero-Order]	Theoretical Time to Treat the Solution to 1 ppm (hr) [First-Order]
phenol	100	0.3525	24.75(1.24)	41.9(---)
2-chloro- phenol	20	2.3075	63.3(1.73)	20(230)
2,6-dichloro- phenol	20	0.0800	271.4(211.)	75(24.4)

** Shown in parenthesis are the values using phenol-acclimated organisms.

TABLE 6
KINETIC MODEL SURVEY

The following models have been tried by most of the workers to obtain the kinetic rate constants.

Zero order model: $-dS / dt = K_0$
 First order model: $-dS / dt = K_1 S$
 Monod model: $U = U_m S / [K_m + S]$

where

S_0 : Initial Substrate Conc., ppm.

S : Substrate Conc., ppm.

t : Time, hour.

K_0 : Zero Order Rate Constant.

K_1 : First Order Rate Constant.

U_m : Max. Specific Growth Rate Constant, hr^{-1} .

K_m : Michaelis-Menten Constant, mg/liter or ppm.

Y : Yield Coefficient

K_d : Endogenous Respiration Coefficient, hr^{-1} .

Ref	Compd	Conc. (ppm)	Model	Reactor type	Comments (Temp., PH, Organisms)
46	2,4-D	111	Monod, $U_m = 0.096$ $K_m = 5.4$ $Y = 0.14$	Batch	20°C, PH=7.0 Pseudomonas putida
46	2,4-D	111	Monod, $U_m = 0.092$ $K_m = 2.7$ $Y = 0.14$	Chemostat	"
47	PHE	360	Monod, $U_m = 0.17$ $K_m = 245$ $K_d = 0.008$ $Y = 0.45$	CSTR	20°C, PH=7.2 Mixed Culture
48	PHE	<100	Monod, $U_m = 0.287$ $K_m = 2.11$ $K_d = 0.01$ $Y = 1.20$	"	22°C, PH=7.0 Mixed Culture
49	PHE	400	1st order $K_o = 0.004$ 1-mg/ day $K_d = 8.33 \times 10^{-4}$ $Y = 0.13$	Continuous	Mixed Culture
40	PHE	100	zero order $K_o = 4. (80)$	Batch	20°C, PH=7.2 Mixed Culture
51	PHE	84	zero order $K_o = 3.36$ mg/l-hr	"	"

50	OCP	10	zero order $K_o = 0.17664$	"	25°C, PH=7.4 PVSC Mixed Culture
40	OCP	20	zero order $K_o = 0.3(11)$	"	"
51	OCP	120	zero order $K_o = 1.5$ mg/l-hr	"	20°C, PH=7.2 Mixed Culture
40	2,6-DCP	20	zero order $K_o = 0.07$ (0.09)	"	"
51	NB	123	zero order $K_o = 0.861$ mg/l-hr	"	"
51	2-NP	151	zero order $K_o = 1.06$ mg/l-hr	"	"

* Shown in parenthesis are the degradation rates after prior acclimation to phenol.

APPENDIX 1

```

C
C
C *****
C *
C *   REGRESSION EQUATION FOR THE ESTIMATION  OF AQUEOUS   *
C *   SOLUBILITY FOR ALKYL HALIDES           *
C *
C *****
C
C
C Data input :  log Kow, M.W.
C               where  Kow  = Octanol/Water Partition Coefficient
C                   M.W. = Molecular Weight
C                   let   A  = log Kow
C                       B  = M.W.
C
C   IMPLICIT REAL*4 (A-K,O-Z)
C   5 READ(14,10)A,B
C  10 FORMAT(F4.2)
C     IF(P.EQ.0.0)GO TO 40
C     S=(10**(-1.221*A+.832))*1000.*B
C     WRITE(15,20)S
C  20 FORMAT('S=',5X,E9.3,5X,'ppm',/)
C     GO TO 5
C  40 STOP
C     END

```

APPENDIX 1 (Continue)

```

C
C
C *****
C *
C * REGRESSION EQUATION FOR THE ESTIMATION OF AQUEOUS *
C * SOLUBILITY FOR AROMATICS AND CHLORINATED HYDROCARBONS *
C * LAW CONSTANTS *
C *
C *****
C
C
C Data input : log Kow, M.W.
C      where   Kow  = Octanol/Water Partition Coefficient
C              M.W. = Molecular Weight
C      let     A   = log Kow
C              B   = M.W.
C
C      IMPLICIT REAL*4 (A-K,O-Z)
C      5 READ(24,10)A,B
C      10 FORMAT(F4.2)
C      IF(P.EQ.0.0)GO TO 40
C      S=(10**(-1.37*A+7.26))/1000.*B
C      WRITE(15,20)S
C      20 FORMAT('S=',5X,E9.3,5X,'ppm',/)
C      GO TO 5
C      40 STOP
C      END

```

APPENDIX 1 (Continue)

C
C
C
C
C
C
C
C
C
C
C
C
C
C
C

```
*****
*
*   REGRESSION EQUATION FOR THE ESTIMATION OF AQUEOUS
*   SOLUBILITY FOR BENZENE AND ITS DERIVATIVES
*
*****
```

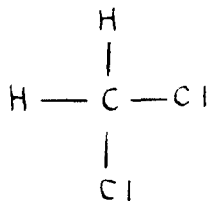
```
Data input : log Kow, M.W.
      where   Kow  = Octanol/Water Partition Coefficient
              M.W. = Molecular Weight
      let     A   = log Kow
              B   = M.W.
```

```
IMPLICIT REAL*4 (A-K,O-Z)
5 READ(34,10)A,B
10 FORMAT(F4.2)
   IF(P.EQ.0.0)GO TO 40
   S=(10**(-0.996*A+0.339))*1000.*B
   WRITE(15,20)S
20 FORMAT('S=',5X,E9.3,5X,'ppm',/)
   GO TO 5
40 STOP
END
```

APPENDIX 2

Leo's Fragment Method For Calculating
Octanol/Water Partition Coefficients

Examples:



$$f_{\text{C}} = 0.2$$

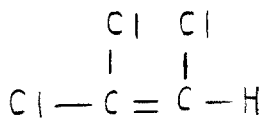
$$2f_{\text{H}} = 2 \times 0.23$$

$$2f_{\text{Cl}} = 2 \times 0.06$$

$$2F_{\text{mhG2}} = 2 \times 0.3$$

$$(2-1)F_{\text{b}} = 1 \times -0.12$$

$$\log K_{\text{ow}} = 1.26$$



$$2F_{\text{mhG2}} = 2 \times 0.3$$

$$2f_{\text{C}} = 2 \times 0.2$$

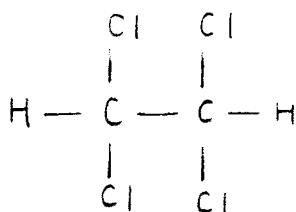
$$3f_{\text{Cl}} = 3 \times 0.5$$

$$3f_{\text{H}} = 3 \times 0.23$$

$$F = -0.55$$

$$(4-1)F_{\text{b}} = 3 \times -0.12$$

$$\log K_{\text{ow}} = 2.28$$



$$2f_{\text{C}} = 2 \times 0.2$$

$$4f_{\text{Cl}} = 4 \times 0.06$$

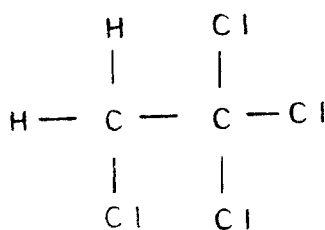
$$2f_{\text{H}} = 2 \times 0.23$$

$$4F_{\text{mhG2}} = 4 \times 0.3$$

$$(4-1)F_{\text{b}} = 3 \times -0.12$$

$$\frac{(4-1)F_{mhV4} = 3*0.28}{}$$

$$\log Kow = 2.78$$



$$2f_C = 2*0.2$$

$$4f_{Cl} = 4*0.06$$

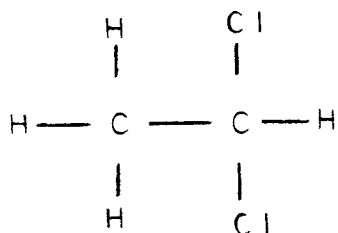
$$2f_H = 2*0.23$$

$$(4-1)F_b = 3*-0.12$$

$$3F_{mhG3} = 3*0.53$$

$$\frac{(4-1)F_{mhV} = 3*0.28}{}$$

$$\log Kow = 3.17$$



$$2f_C = 2*0.2$$

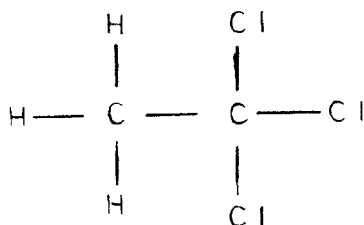
$$2f_{Cl} = 2*0.06$$

$$4f_H = 4*0.23$$

$$(2-1)F_b = -0.12$$

$$\frac{2F_{mhG2} = 2*0.3}{}$$

$$\log Kow = 1.92$$



$$2f_C = 2*0.2$$

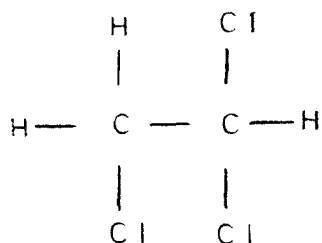
$$3f_{Cl} = 3*0.06$$

$$3f_H = 3*0.23$$

$$(3-1)F_b = 2*-0.12$$

$$\frac{3F_{mhG3} = 3*0.53}{}$$

$$\log Kow = 2.62$$



$$2f_{\text{C}} = 2 \times 0.2$$

$$3f_{\text{Cl}} = 3 \times 0.06$$

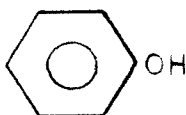
$$3f_{\text{H}} = 3 \times 0.23$$

$$(3-1)F_{\text{b}} = 2 \times -0.12$$

$$2F_{\text{mhG2}} = 2 \times 0.3$$

$$\underline{(3-1)F_{\text{mhV}} = 2 \times 0.28}$$

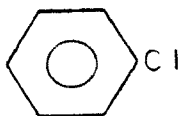
$$\log K_{\text{ow}} = 2.19$$



$$f_{\text{C6H5}} = 1.9$$

$$\underline{f_{\text{OH}} = -0.44}$$

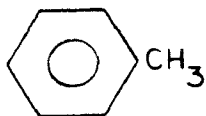
$$\log K_{\text{ow}} = 1.46$$



$$f_{\text{C6H5}} = 1.9$$

$$\underline{f_{\text{Cl}} = 0.94}$$

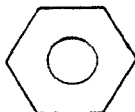
$$\log K_{\text{ow}} = 2.84$$



$$f_{\text{C6H5}} = 1.9$$

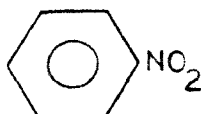
$$\underline{f_{\text{CH3}} = 0.89}$$

$$\log K_{\text{ow}} = 2.79$$



$$\underline{6f_{\text{CH}} = 6 \times 0.355}$$

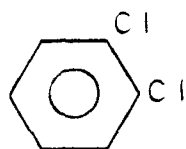
$$\log K_{\text{ow}} = 2.13$$



$$f_{\text{C6H5}} = 1.9$$

$$\underline{f_{\text{NO2}} = -0.03}$$

$$\log K_{ow} = 1.87$$

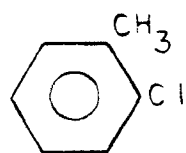


$$-f_H = -0.23$$

$$f_{C_6H_5} = 1.9$$

$$\underline{2f_{Cl} = 2 \times 0.94}$$

$$\log K_{ow} = 3.55$$



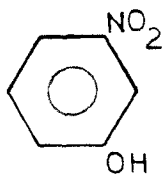
$$-f_H = -0.23$$

$$f_{C_6H_5} = 1.9$$

$$f_{CH_3} = 0.89$$

$$\underline{f_{Cl} = 0.94}$$

$$\log K_{ow} = 3.50$$



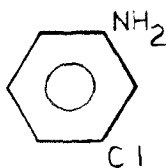
$$-f_H = -0.23$$

$$f_{C_6H_5} = 1.9$$

$$f_{OH} = -0.44$$

$$\underline{f_{NO_2} = -0.03}$$

$$\log K_{ow} = 1.20$$



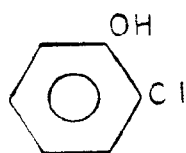
$$f_{C_6H_5} = 1.9$$

$$f_{NH_2} = -1.0$$

$$f_{Cl} = 0.94$$

$$\underline{-f_H = -0.23}$$

$$\log K_{ow} = 1.61$$



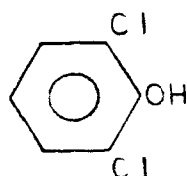
$$-f_H = -0.23$$

$$f_{C_6H_5} = 1.9$$

$$f_{OH} = -0.44$$

$$\underline{f_{Cl} = 0.94}$$

$$\log Kow = 2.17$$



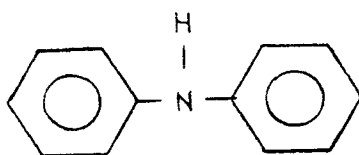
$$f_{C_6H_5} = 1.9$$

$$-2f_H = -2 \times 0.23$$

$$2f_{Cl} = 2 \times 0.94$$

$$\underline{f_{OH} = -0.44}$$

$$\log Kow = 2.88$$

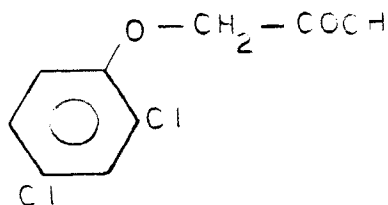


$$2f_{C_6H_5} = 2 \times 1.9$$

$$f_{NH} = -0.09$$

$$\underline{(2-1)F_{bYN} = -0.2}$$

$$\log Kow = 3.51$$



$$f_{C_6H_5} = 1.9$$

$$f_{-O-} = -0.61$$

$$f_C = 0.2$$

$$2f_H = 2 \times 0.23$$

$$f_{COOH} = -1.11$$

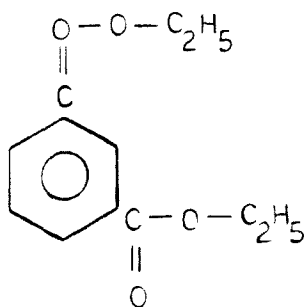
$$(3-1)F_b = 2 \times -0.12$$

$$F_{P1} = -0.42 \times (-0.61 - 1.11)$$

$$-2f_H = -2 \times 0.23$$

$$\underline{2f_{Cl} = 2 \times 0.94}$$

$$\log Kow = 2.74$$



$$fC6H5 = 1.9$$

$$2fCOO = 2 * -0.56$$

$$2fC2H5 = 2 * (5 * 0.23 + 2 * 0.2)$$

$$-fH = -0.23$$

$$\underline{2(2-1)Fb = 2 * -0.12}$$

$$\log Kow = 3.41$$

```
*****
*
*  CALCULATE THE VAPOR PRESSURE BY USING ANTOINE'S EQUATION  *
*
*****
```

```

IMPLICIT REAL*4 (A-H,O-Z)
100 READ(4,10)A,B,C
  10 FORMAT(F7.5,1X,F8.3,1X,F7.3)
    IF(A.EQ.0.0) GO TO 200
    P=(10**(A-B/(25.0+C)))/760.0
    WRITE(6,12)
      12 FORMAT(' ')
    WRITE(6,15)A,B,C
      15 FORMAT('A=',F7.5,5X,'B=',F8.3,5X,'C=',F7.3)
    WRITE(6,20)P
      20 FORMAT('THE VAPOR PRESSURE IS : ',F15.9,' Atm ')
    GO TO 100
200 STOP
    END

```

```

*****
*
*      UNIFAC METHOD FOR CALCULATING INFINITE-DILUTION
*      ACTIVITY COEFFICIENTS
*
*****

```

Data input : AMN = Group Interaction Parameters,
NC = Number of Components,
NG = Number of Groups,
NU = Number of Groups in Component i,
R = Volume Parameters,
Q = Surface Area Parameters,
T = Temperature.

```

IMPPLICIT REAL*8 (A-H,O-Z)
REAL*8 NT(10),NU(10,10)
DIMENSION THETA(10),THXX(10,10),XXX(10,10)
DIMENSION PLN(10,10),AMN(10,10),PHI(10,10)
DIMENSION R(10),Q(10),RQ(20),RI(20),QI(20)
DIMENSION X(10),XQ(10),XY(10),GAMA1(10),GAMA2(10)
DATA R(1),R(2),R(3),R(4)/.5313D0,1.1562D0,1.2663D0,.92D0/
DATA Q(1),Q(2),Q(3),Q(4)/.4D0,.844D0,.968D0,1.4D0/
DATA NC,NG,Z/2,4,1.0D1/
DATA T/2.980D2/
DATA NU(1,1),NU(1,2),NU(1,3),NU(1,4)/4.0D0,1.0D0,1.0D0,0.0D0/
DATA NU(2,1),NU(2,2),NU(2,3),NU(2,4)/0.0D0,0.0D0,0.0D0,1.0D0/
DATA AMN(1,1),AMN(1,2),AMN(1,3),AMN(1,4)/0.0D0,-8.781D2,1.670D2
,C8.594D2/
DATA AMN(2,1),AMN(2,2),AMN(2,3),AMN(2,4)/7.778D2,0.0D0,-4.713D1
,C3.907D2/
DATA AMN(3,1),AMN(3,2),AMN(3,3),AMN(3,4)/-1.468D2,-1.073D2,0.0D
OC,5.695D3/
DATA AMN(4,1),AMN(4,2),AMN(4,3),AMN(4,4)/3.728D2,-9.727D1,2.037
DC2,0.0D0/
WRITE(20,21) T
21 FORMAT(' By Using UNIFAC-LLE Parameters ,Temp= ',F5.1,'K',/)
WRITE(20,23)
23 FORMAT(' COMP 1 : 2-CHLOROTOLUENE COMP 2 : WATER ',/)
WRITE(20,16)
16 FORMAT(' The Structure of COMP 1 : ',//////////)
WRITE(20,11)
11 FORMAT(' Group No R Q ',/)
WRITE(20,12)NU(1,1),R(1),Q(1)
12 FORMAT(' ACH ',F3.0,4X,2F10.5,/)
WRITE(20,13)NU(1,2),R(2),Q(2)
13 FORMAT(' ACCl ',F3.0,4X,2F10.5,/)

```

```

        WRITE(20,14) NU(1,3),R(3),Q(3)
14  FORMAT('      ACCH      ',F3.0,4X,2F10.5,/)
        WRITE(20,15) NU(2,4),R(4),Q(4)
15  FORMAT('      Water      ',F3.0,4X,2F10.5,/)
        WRITE(20,26)
26  FORMAT(' The Group-Interaction Parameters Array Amn is : ',/)
        WRITE(20,24)((AMN(I,J),J=1,4),I=1,4)
24  FORMAT(5X,4F13.5,/)
1000 READ(22,10)X(1),X(2)
10  FORMAT(D13.8,1X,D13.8)
        IF(X(1).EQ.9.00000000D0)GO TO 400
        WRITE(20,25)X(1),X(2)
25  FORMAT('// ' X(1)= 'D13.8,5X,' X(2)= 'D13.8,/)
        DO 30 M=1,NG
        DO 30 N=1,NG
        PHI(M,N)=DEXP(-1.0D0*AMN(M,N)/T)
30  CONTINUE
        SUMN=0.0D0
        SUMR=0.0D0
        SUMQ=0.0D0
        DO 70 I=1,NC
        RI(I)=0.0D0
        QI(I)=0.0D0
        NT(I)=0.0D0
        DO 40      J=1,NG
        RI(I)=RI(I)+NU(I,J)*R(J)
        QI(I)=QI(I)+NU(I,J)*Q(J)
        NT(I)=NT(I)+NU(I,J)
40  CONTINUE
        SUMN=SUMN+X(I)*NT(I)
70  CONTINUE
        RR=RI(1)/RI(2)
        QQ=QI(1)/QI(2)
        DO 50 I=1,NC
        RQ(I)=RI(I)-QI(I)
50  CONTINUE
        DO 60 I=1,NC
        XY(I)=Z/2.0D0*RQ(I)-(RI(I)-1.0D0)
60  CONTINUE
        C=DLOG(RR)
        E=DLOG(QQ/RR)
        G=DLOG(1.0D0/RR)
        A=DLOG(RR/QQ)
        GAMAC1=C+(Z*QI(1)/2.0D0)*E+XY(1)-RR*XY(2)
        GAMAC2=G+(Z*QI(2)/2.0D0)*A+XY(2)-XY(1)/RR
        GAMA1(1)=GAMAC1
        GAMA1(2)=0.0D0
        GAMA2(1)=0.0D0
        GAMA2(2)=GAMAC2
        SUMQQ=0.0D0
        DO 80 J=1,NG

```



```

SUMJ=0.0D0
DO 75 I=1,NC
SUMJ=SUMJ+X(I)*NU(I,J)
75 CONTINUE
XQ(J)=SUMJ/SUMN
SUMQQ=SUMQQ+XQ(J)*Q(J)
80 CONTINUE
DO 90 J=1,NG
THETA(J)=XQ(J)*Q(J)/SUMQQ
90 CONTINUE
DO 150 I=1,NC
SUMXXX=0.0D0
DO 100 J=1,NG
XXX(I,J)=NU(I,J)/NT(I)
SUMXXX=SUMXXX+XXX(I,J)*Q(J)
100 CONTINUE
DO 110 J=1,NG
THXX(I,J)=XXX(I,J)*Q(J)/SUMXXX
110 CONTINUE
DO 140 K=1,NG
SUM1=0.0D0
SUM2=0.0D0
DO 130 M=1,NG
SUM1=SUM1+THXX(I,M)*PHI(M,K)
SUM3=0.0D0
DO 120 N=1,NG
SUM3=SUM3+THXX(I,N)*PHI(N,M)
120 CONTINUE
SUM2=SUM2+THXX(I,M)*PHI(K,M)/SUM3
130 CONTINUE
PLN(I,K)=Q(K)*(1.0D0-DLOG(SUM1)-SUM2)
140 CONTINUE
150 CONTINUE
IF(X(1).EQ.1.00000000D0)GO TO 300
DO 200 I=1,NC
ANS=GAM1(I)
DO 180 K=1,NG
SUM1=0.0D0
SUM2=0.0D0
DO 170 M=1,NG
SUM1=SUM1+THETA(M)*PHI(M,K)
SUM3=0.0D0
DO 160 N=1,NG
SUM3=SUM3+THETA(N)*PHI(N,M)
160 CONTINUE
SUM2=SUM2+THETA(M)*PHI(K,M)/SUM3
170 CONTINUE
PPLN=Q(K)*(1.0D0-DLOG(SUM1)-SUM2)
ANS=ANS+NU(I,K)*(PPLN-PLN(I,K))
180 CONTINUE
GAMMA=DEXP(ANS)

```

```
      WRITE(20,190)I,GAMMA
190  FORMAT(' THE AC OF COMP #',I2,' IS : ',F18.5)
200  CONTINUE
      GO TO 1000
300  DO 350 I=1,NC
      ANS=GAMA2(I)
      DO 330 K=1,NG
      SUM1=0.0D0
      SUM2=0.0D0
      DO 320 M=1,NG
      SUM1=SUM1+THETA(M)*PHI(M,K)
      SUM3=0.0D0
      DO 310 N=1,NG
      SUM3=SUM3+THETA(N)*PHI(N,M)
310  CONTINUE
      SUM2=SUM2+THETA(M)*PHI(K,M)/SUM3
320  CONTINUE
      PPLN=Q(K)*(1.0D0-DLOG(SUM1)-SUM2)
      ANS=ANS+NU(I,K)*(PPLN-PLN(I,K))
330  CONTINUE
      GAMMA=DEXP(ANS)
      WRITE(20,340)I,GAMMA
340  FORMAT(' THE AC OF COMP #',I2,' IS : ',F18.5)
350  CONTINUE
      GO TO 1000
400  STOP
      END
```

APPENDIX 5

```

*****
*
*          MASS BALANCE FOR
*          NONBIOLOGICAL BATCH SYSTEM
*
*****

```

```

Data input : CONIN = INFLUENT CONCENTRATION (ppm)
              DG = DENSITY OF GAS PHASE (mole/l)
              DL = DENSITY OF LIQUID PHASE (mole/l)
              PW = VAPOR PRESSURE OF PURE WATER (mmHg)
              PC = VAPOR PRESSURE OF POLLUTANT (mmHg)
              GC = ACTIVITY COEFFICIENT OF POLLUTANT
              V = REACTION VOLUME (l)
              P = SYSTEM PRESSURE (mmHg)

```

```

IMPLICIT REAL*4 (A-H,O-Z)
CHARACTER*1 COL(71)
DIMENSION TIME(100),Y(100)
CHARACTER*1 STAR
CHARACTER*1 BLANK
CHARACTER*1 S
DATA STAR/'*'/
DATA BLANK/' '/
DATA S/'-'/
DATA TI,TF,MM/0.,7.,71/
DATA CONIN,A,P,V,DG,DL,PW/20.,30.,760.,3.,0.0408,55.5,
%25.209/
DATA PC,GC/95.18,2582./
CONC(T)=CONIN*EXP(-A*PC*GC*DG*T/P/V/DL)

```

```

      FIND CONC. & CONMAX.

```

```

      ZTIME=TI+0.0
      DELTA=(TF-TI)/(MM-1)
      CONMAX=0.0
      DO 10 J=1,MM
      TIME(J)=ZTIME
      Y(J)=CONC(TIME(J))
      IF(CONMAX.LT.Y(J)) CONMAX=Y(J)
      ZTIME=ZTIME+DELTA
10  CONTINUE
      WRITE(6,20) (TIME(J),Y(J),J=1,20)
20  FORMAT(10X,'TIME=',F6.2,2X,'Hour',5X,'Conc. IS :',F8.3,2X,
%'ppm')
      WRITE(6,30)

```

```

30 FORMAT(' ',//)
   WRITE(6,40)
40 FORMAT(' ',15X,'HORIZONTAL-AXIS IS Conc.-AXIS',/)
   WRITE(6,50)
50 FORMAT(' ',15X,'VERTICAL-AXIS IS TIME-AXIS',///)
C
C      PRINT Conc.-AXIS
C
      DO 60 L=1,MM
      COL(L)=S
60 CONTINUE
      WRITE(6,70) (COL(LL),LL=1,MM)
70 FORMAT(1X,71A1)
C
C      PRINT TIME-AXIS & Y(M)
C
      DO 100 M=1,20
      DO 80 N=1,MM
      COL(N)=BLANK
80 CONTINUE
      MXA=(MM-1)*Y(M)/CONMAX+1.5
      COL(MXA)=STAR
      WRITE(6,90) COL
90 FORMAT('| ',71A1)
100 CONTINUE
      STOP
      END

```

APPENDIX 6

```

C
C
C
C *****
C *
C *
C *      MASS BALANCE FOR
C *      BIOLOGICAL BATCH SYSTEM WITH ZERO-ORDER
C *      AND FIRST-ORDER BIODEGRADATION
C *
C *****
C
C      Data input : CONIN = INFLUENT CONCENTRATION (ppm)
C                    CK0 = ZERO-ORDER CONSTANT
C                    CK1 = FIRST-ORDER CONSTANT
C                    DG = DENSITY OF GAS PHASE (mole/l)
C                    DL = DENSITY OF LIQUID PHASE (mole/l)
C                    PW = VAPOR PRESSURE OF PURE WATER (mmHg)
C                    PC = VAPOR PRESSURE OF POLLUTANT (mmHg)
C                    GC = ACTIVITY COEFFICIENT OF POLLUTANT
C                    A = AIR FLOWRATE (l/hr)
C                    V = REACTION VOLUME (l)
C                    P = SYSTEM PRESSURE (mmHg)
C
C      SUBROUTINE ZERO(Z0,T)
C      DATA A,P,V,DG,DL,PW/30.,760.,3.,0.0408,55.5,25.209/
C      DATA CONIN,PC,GC/100.,0.3525,54.5/
C      DATA CK0/3.939/
C      AA=A*PC*GC*DG/(P*V*DL)
C      Z0=(CONIN+CK0/(AA*DL*94000))*EXP(-AA*T)-CK0/(AA*DL*94000)
C      RETURN
C      END
C
C      SUBROUTINE FIRST(Z1,T)
C      DATA A,P,V,DG,DL,PW/30.,760.,3.,0.0408,55.5,25.209/
C      DATA CONIN,PC,GC/100.,0.3525,54.5/
C      DATA CK1/.11/
C      AA=A*PC*GC*DG/(P*V*DL)
C      Z1=CONIN*EXP(-(AA+CK1)*T)
C      RETURN
C      END
C
C      IMPLICIT REAL*4 (A-H,O-Z)
C      CHARACTER*1 COL(71)
C      DIMENSION TIME(100),Y(100,100),CONMAX(2)
C      CHARACTER*1 STAR
C      CHARACTER*1 BLANK
C      CHARACTER*1 S
C      DATA STAR/'*'/
C      DATA BLANK/' '/
C      DATA S/'-'/

```

```
DATA TI,TF,MM/0.,14000.,71/
DATA A,V/30.,3./
```

```
C
C      FIND CONC. & CONMAX.
C
```

```
      ZTIME=TI+0.0
      DELTA=(TF-TI)/(MM-1)
      DO 10 J=1,MM
      TIME(J)=ZTIME
      CONMAX(I)=0.0
      CALL ZERO(Z0,ZTIME)
      CALL FIRST(Z1,ZTIME)
      Y(1,J)=Z0
      Y(2,J)=Z1
      IF(CONMAX(1).LT.Y(1,J)) CONMAX(1)=Y(1,J)
      IF(CONMAX(2).LT.Y(2,J)) CONMAX(2)=Y(2,J)
      ZTIME=ZTIME+DELTA
10  CONTINUE
      DO 100 I=1,2
      WRITE(6,11)
11  FORMAT(14X, ' BIOLOGICAL BATCH SYSTEM FOR PHENOL ')
      WRITE(6,12)
12  FORMAT(' ',/)
      WRITE(6,13) A
13  FORMAT(15X, ' AIR FLOWRATE= ',F5.1,1X,'l/hr',/)
      WRITE(6,14) V
14  FORMAT(15X, ' REACTION VOLUME= ',F5.1,1X,'l',/)
      WRITE(6,20) (TIME(J),Y(I,J),J=1,44)
20  FORMAT(10X, 'TIME=',F7.2,2X, 'Hour',4X, 'Conc. IS :',F8.3,2X,
      &'ppm')
      WRITE(6,30)
30  FORMAT(' ',/////////)
      WRITE(6,40)
40  FORMAT(' ',15X, 'HORIZONTAL-AXIS IS Conc.-AXIS',/)
      WRITE(6,50)
50  FORMAT(' ',15X, 'VERTICAL-AXIS IS TIME-AXIS',//)
```

```
C
C      PRINT Conc.-AXIS
C
```

```
      DO 60 L=1,MM
      COL(L)=S
60  CONTINUE
      WRITE(6,70) (COL(LL),LL=1,MM)
70  FORMAT(1X,71A1)
```

```
C
C      PRINT TIME-AXIS & Y(I,M)
C
```

```
      DO 100 M=1,44
      DO 80 N=1,MM
      COL(N)=BLANK
80  CONTINUE
```

```
      MXA=(MM-1)*Y(I,M)/CONMAX(I)+1.5  
      COL(MXA)=STAR  
      WRITE(6,90) COL  
90    FORMAT('|',71A1)  
100   CONTINUE  
      STOP  
      END
```

APPENDIX 7

```

*****
*
*           MASS BALANCE FOR
*   BIOLOGICAL CONTINUOUS FLOW SYSTEM WITH ZERO-ORDER
*           AND FIRST-ORDER BIODEGRADATION
*
*****

```

```

Data input : CONIN = INFLUENT CONCENTRATION (ppm)
              CK0 = ZERO-ORDER CONSTANT
              CK1 = FIRST-ORDER CONSTANT
              DG = DENSITY OF GAS PHASE (mole/l)
              DL = DENSITY OF LIQUID PHASE (mole/l)
              PW = VAPOR PRESSURE OF PURE WATER (mmHg)
              PC = VAPOR PRESSURE OF POLLUTANT (mmHg)
              GC = ACTIVITY COEFFICIENT OF POLLUTANT
              V = REACTION VOLUME (l)
              P = SYSTEM PRESSURE (mmHg)
              A = AIR FLOWRATE (l/hr)
              F = WASTEWATER FLOWRATE (l/hr)

```

```

IMPLICIT REAL*4 (A-H,O-Z)
DATA A,F,P,V,DG,DL,PW/30.,.36,760.,2.,.0408,55.5,25.209/
DATA CONIN,PC,GC/100.,0.3525,54.45/
DATA CK0,CK1/3.94,0.11/
CONC0=(CONIN-CK0*V/F/DL)/(1.+A*PC*GC*DG/(F*P*DL))
CONC1=CONIN/(1.+A*PC*GC*DG/(F*P*DL)+CK1*V/F)
WRITE(6,10)
10 FORMAT(9X, ' BIOLOGICAL CONTINUOUS SYSTEM FOR PHENOL ')
WRITE(6,20)
20 FORMAT(' ',//)
WRITE(6,30) A
30 FORMAT(15X, ' AIR FLOWRATE= ',F5.1,1X,'l/hr',/)
WRITE(6,40) F
40 FORMAT(15X, ' WASTEWATER FLOWRATE= ',F5.2,1X,'l/hr',/)
WRITE(6,50) V
50 FORMAT(15X, ' REACTION VOLUME= ',F5.1,1X,'l',/)
WRITE(6,55)
55 FORMAT(15X, ' ZERO-ORDER REACTION ',//)
WRITE(6,60) CONIN
60 FORMAT(15X, 'INFLUENT CONC. IS : ',F8.3,2X,'ppm')
WRITE(6,70) CONC0
70 FORMAT(15X, 'EFFLUENT CONC. IS : ',F8.3,2X,'ppm',///)
WRITE(6,75)
75 FORMAT(15X, ' FIRST-ORDER REACTION ',//)
WRITE(6,80) CONIN
80 FORMAT(15X, 'INFLUENT CONC. IS : ',F8.3,2X,'ppm')

```



```
WRITE(6,90) CONC1  
90 FORMAT(15X, 'EFFLUENT CONC. IS : ',F8.3,2X,'ppm')  
STOP  
END
```

APPENDIX 8

```

C
C
C
C *****
C *
C *
C *      MASS BALANCE FOR
C *      BIOLOGICAL CONTINUOUS SYSTEM FOR MONOD MODEL
C *      [W/O GROWTH]
C *
C *****
C
C
C      Data input : CONIN = INFLUENT CONCENTRATION   (ppm)
C                   CK1  = MONOD MODEL CONSTANT
C                   CK2  = MONOD MODEL CONSTANT
C                   DG   = DENSITY OF GAS PHASE      (mole/l)
C                   DL   = DENSITY OF LIQUID PHASE   (mole/l)
C                   PW   = VAPOR PRESSURE OF PURE WATER (mmHg)
C                   PC   = VAPOR PRESSURE OF POLLUTANT (mmHg)
C                   GC   = ACTIVITY COEFFICIENT OF POLLUTANT
C                   B0   = INITIAL BIOMASS CONCENTRATION
C                   Y    = YIELD COEFFICIENT
C                   A    = AIR FLOWRATE (l/hr)
C                   F    = WASTEWATER FLOWRATE (l/hr)
C                   V    = REACTION VOLUME (l)
C                   P    = SYSTEM PRESSURE (mmHg)
C
C
C      SUBROUTINE QUAD(A,B,C,X1,X2)
C      IMPLICIT REAL*4 (A-H,O-Z)
C      XX=-B/(2.*A)
C      D=XX*XX-C/A
C      IF(D) 1,2,2
C 1 GO TO 3
C 2 XY=SQRT(D)
C   X1=XX+XY
C   X2=XX-XY
C 3 RETURN
C   END
C
C
C      IMPLICIT REAL*4 (A-H,O-Z)
C      DATA A,F,P,V,DG,DL,PW/120.,0.36,760.,3.,0.0408,55.5,
C      %25.209/
C      DATA CONIN,PC,GC/100.,0.3525,54.5/
C      DATA CK1,CK2,B0,Y/0.2,25.0,2000.,0.011/
C      A0=1.0
C      A1=A*PC*GC*DG*CK2/(P*DL)
C      A2=(A*PC*GC*DG/P)+F*DL
C      A3=(A*PC*GC*DG/P)+F*DL-CK1*DL*Y*V

```

```
AA=(A1+F*CK2+V*CK1-CONIN*F*DL)/A2
BB=CONIN*F*CK2/A2
CC=(A1+F*CK2+CK1*(B0+Y*CONIN*DL)*V-F*DL*CONIN)/A3
DD=CONIN*F*CK2/A3
WRITE(*,*)A0,AA,BB,CC,DD
CALL QUAD(A0,AA,BB,X1,X2)
WRITE(6,10) X1,X2
10 FORMAT(2F10.3)
CALL QUAD(A0,CC,DD,X1,X2)
WRITE(6,10) X1,X2
STOP
END
```

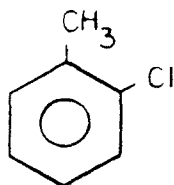
APPENDIX 9

SAMPLE OUTPUT OF APPENDIX 6

By Using UNIFAC-LLE Parameters ,Temp= 298.0 K

COMP 1 : 2-CHLOROTOLUENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACCl	1.	1.15620	.84400
ACCH ₃	1.	1.26630	.96800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-878.10000	167.00000	859.40000
777.80000	.00000	-47.13000	390.70000
-146.80000	-107.30000	.00000	5695.00000
372.80000	-97.27000	203.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 29020.37865
THE AC OF COMP # 2 IS : 1.00000

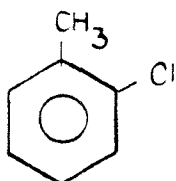
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 126.73131

By Using UNIFAC-VLE Parameters ,Temp= 298.0 K

COMP 1 : 2-CHLOROTOLUENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACCl	1.	1.15620	.84400
ACCH ₃	1.	1.26630	.96800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	538.20000	167.00000	903.80000
-237.70000	.00000	375.50000	920.40000
-146.80000	-126.90000	.00000	5695.00000
362.30000	678.20000	377.60000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 94676.38542
THE AC OF COMP # 2 IS : 1.00000

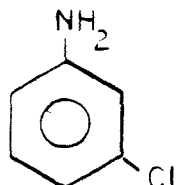
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 591.49319

By Using UNIFAC-LLE Parameters ,Temp= 298.0 K

COMP 1 : CHLOROANILINE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACCl	1.	1.15620	.84400
ACNH ₂	1.	1.06000	.81600
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-878.10000	1.64000	859.40000
777.80000	.00000	323.30000	390.70000
-218.90000	699.10000	.00000	-239.80000
372.80000	-97.27000	-109.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 1637.71612
THE AC OF COMP # 2 IS : 1.00000

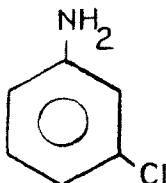
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 5.85387

By Using UNIFAC-VLE Parameters ,Temp= 298.0 K

COMP 1 : CHLOROANILINE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACCl	1.	1.15620	.84400
ACNH ₂	1.	1.06000	.81600
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	538.20000	668.20000	903.80000
-237.70000	.00000	323.30000	920.40000
650.40000	699.10000	.00000	-339.50000
362.30000	678.20000	213.00000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 747.77186
THE AC OF COMP # 2 IS : 1.00000

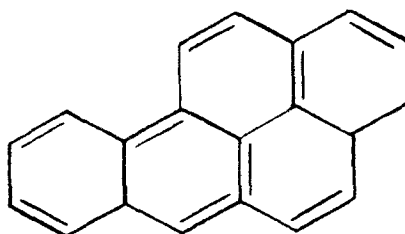
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 4.89710

By Using UNIFAC-LLE Parameters ,Temp= 298.0 K

COMP 1 : BENZOAPYRENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	12.	.53130	.40000
C=C	2.	.66050	.48500
AC	4.	.36520	.12000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	.00000	859.40000
340.70000	.00000	340.70000	896.00000
.00000	-94.78000	.00000	859.40000
372.80000	220.60000	372.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 331635173.10828
THE AC OF COMP # 2 IS : 1.00000

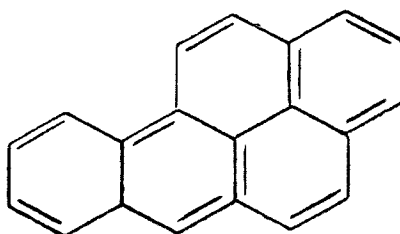
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 212.61697

By Using UNIFAC-VLE Parameters ,Temp= 298.0 K

COMP 1 : BENZOAPYRENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	12.	.53130	.40000
C=C	2.	.66050	.48500
AC	4.	.36520	.12000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	.00000	903.80000
340.70000	.00000	340.70000	896.00000
.00000	-94.78000	.00000	903.80000
362.30000	692.70000	362.30000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 1333503804.73548
THE AC OF COMP # 2 IS : 1.00000

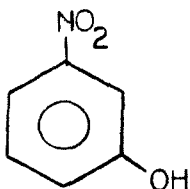
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 266.66718

By Using UNIFAC-LLE Parameters ,Temp= 298.0 K

COMP 1 : NITROPHENOL COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACOH	1.	.89520	.68000
ACNO ₂	1.	1.41990	1.10400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	1649.00000	-11.19000	859.40000
-473.20000	.00000	-16.13000	-595.90000
7.18000	-230.40000	.00000	439.90000
372.80000	344.50000	32.92000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 112.88467
THE AC OF COMP # 2 IS : 1.00000

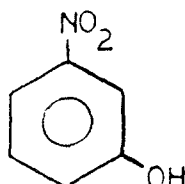
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 2.05141

By Using UNIFAC-VLE Parameters ,Temp= 298.0 K

COMP 1 : NITROPHENOL COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	4.	.53130	.40000
ACOH	1.	.89520	.68000
ACNO2	1.	1.41990	1.10400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	1329.00000	194.90000	903.80000
25.34000	.00000	-16.13000	-601.80000
1824.00000	-230.40000	.00000	360.70000
362.30000	324.50000	399.50000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 51.05171
THE AC OF COMP # 2 IS : 1.00000

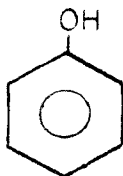
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 2.06118

COMP 1 : PHENOL

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACOH	1.	.89520	.68000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	1649.00000	859.40000
-473.20000	.00000	-595.90000
372.80000	344.50000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 54.45103
 THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

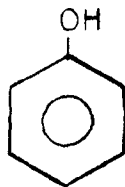
THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 1.96432

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : PHENOL

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACOH	1.	.89520	.68000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	1329.00000	903.80000
3000.00000	.00000	-601.80000
362.30000	324.50000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 6.37026
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 1.44395

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : TOLUENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACCH ₃	1.	1.26630	.96800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	167.00000	859.40000
-146.80000	.00000	5695.00000
372.80000	203.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 7264.61049
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 459.12018

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : TOLUENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACCH ₃	1.	1.26630	.96800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	167.00000	903.80000
-146.80000	.00000	5695.00000
362.30000	377.60000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 12096.40919
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

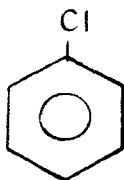
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 647.56965

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : CHLOROBENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACCl	1.	1.15620	.84400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-878.10000	859.40000
777.80000	.00000	390.70000
372.80000	-97.27000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 10148.67827
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 110.48083

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : CHLOROBENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACCl	1.	1.15620	.84400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	538.20000	903.80000
-237.70000	.00000	920.40000
362.30000	678.20000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 19158.03528
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

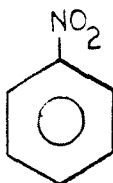
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 450.36428

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : NITROBENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACNO ₂	1.	1.41990	1.10400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-11.19000	859.40000
7.18000	.00000	439.90000
372.80000	32.92000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 3575.55655
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

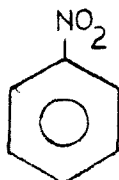
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 76.68600

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : NITROBENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	5.	.53130	.40000
ACNO ₂	1.	1.41990	1.10400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	194.90000	903.80000
1824.00000	.00000	360.70000
362.30000	399.50000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 3337.74713
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

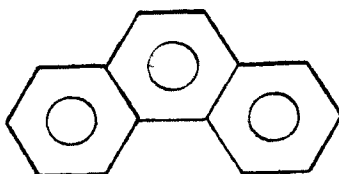
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 67.63355

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : PHENANTHRENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	10.	.53130	.40000
C=C	2.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	859.40000
340.70000	.00000	896.00000
372.80000	220.60000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 1073412.79325
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

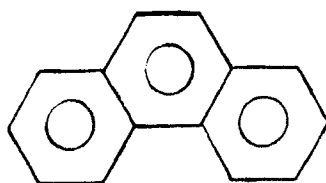
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 198.28430

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : PHENANTHRENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	10.	.53130	.40000
C=C	2.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	903.80000
340.70000	.00000	634.20000
362.30000	692.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 4178929.47931
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

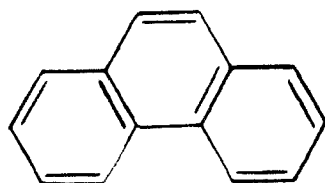
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 177.54709

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : PHENANTHRENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH=CH	5.	1.11670	.86700
C=C	2.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	896.00000
.00000	.00000	896.00000
220.60000	220.60000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 234002.36230
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

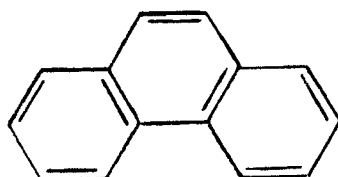
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 165.80595

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : PHENANTHRENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH=CH	5.	1.11670	.86700
C=C	2.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	634.00000
.00000	.00000	634.00000
692.70000	692.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 722170232.43666
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

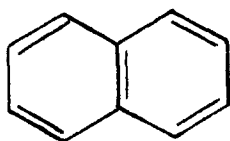
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 82.33202

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	8.	.53130	.40000
C=C	1.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	859.40000
340.70000	.00000	896.00000
372.80000	220.60000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 55854.53570
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

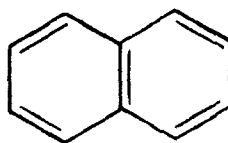
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 257.02312

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	8.	.53130	.40000
C=C	1.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-94.78000	903.80000
340.70000	.00000	634.20000
362.30000	692.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 106629.81743
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

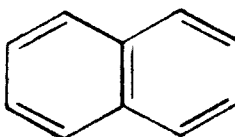
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 251.51702

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH=CH	4.	1.11670	.86700
C=C	1.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	896.00000
.00000	.00000	896.00000
220.60000	220.60000	.00000

X(1)= .000000000D+00 X(2)= .100000000D+01

THE AC OF COMP # 1 IS : 15310.40732
THE AC OF COMP # 2 IS : 1.00000

X(1)= .100000000D+01 X(2)= .000000000D+00

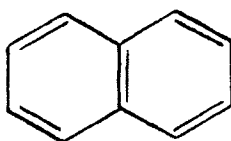
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 210.69216

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH=CH	4.	1.11670	.86700
C=C	1.	.66050	.48500
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	634.20000
.00000	.00000	634.20000
692.70000	692.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 6098894.71677
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

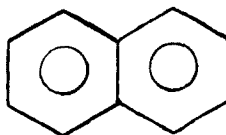
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 104.71891

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	8.	.53130	.40000
AC	2.	.36520	.12000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	859.40000
.00000	.00000	859.40000
372.80000	372.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 152668.82608
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

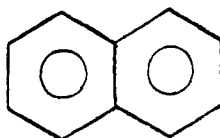
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 354.20473

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : NAPHTHALENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	8.	.53130	.40000
AC	2.	.36520	.12000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	.00000	903.80000
.00000	.00000	903.80000
362.30000	362.30000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 138891.00945
THE AC OF COMP # 2 IS : 1.00000

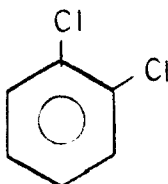
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 430.13334

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : 1,2-DICHLOROBENZENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACCl	2.	1.15620	.84400
ACH	4.	.53130	.40000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	777.80000	390.70000
-878.10000	.00000	859.40000
-97.27000	372.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 28370.96594
THE AC OF COMP # 2 IS : 1.00000

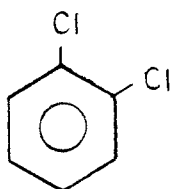
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 60.89894

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : 1,2-DICHLOROBENZENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACCl	2.	1.15620	.84400
ACH	4.	.53130	.40000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-237.70000	920.40000
538.20000	.00000	903.80000
678.20000	362.30000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 172939.26946
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

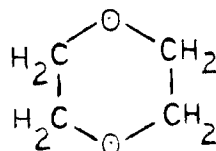
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 446.86822

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : 1,4-DIOXANE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH ₂	2.	.67440	.54000
CH ₂ O	2.	.91830	.78000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	662.10000	1300.00000
1571.00000	.00000	212.80000
342.40000	64.42000	.00000

X(1)= .000000000D+00 X(2)= .100000000D+01

THE AC OF COMP # 1 IS : 35.54103
THE AC OF COMP # 2 IS : 1.00000

X(1)= .100000000D+01 X(2)= .000000000D+00

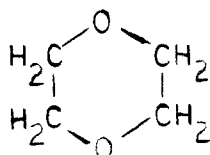
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 8.64408

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : 1,4-DIOXANE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH ₂	2.	.67440	.54000
CH ₂ O	2.	.91830	.78000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	251.50000	1318.00000
83.36000	.00000	-314.70000
300.00000	540.50000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 26.35740
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

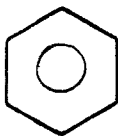
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 2.15713

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : BENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	6.	.53130	.40000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	859.40000
372.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2582.04018
THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

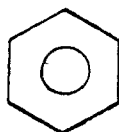
THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 363.08974

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : BENZENE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
ACH	6.	.53130	.40000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	903.80000
362.30000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2417.15867
THE AC OF COMP # 2 IS : 1.00000

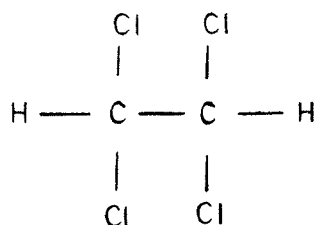
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 440.92297

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 :1,1,2,2-TETRACHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl ₂	2.	2.06060	1.68400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	740.40000
370.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 11438.43167
 THE AC OF COMP # 2 IS : 1.00000

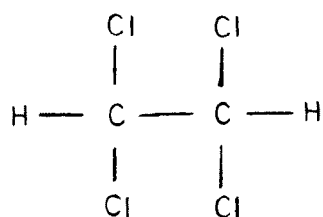
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 129.42969

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 :1,1,2,2-TETRACHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl ₂	2.	2.06060	1.68400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	708.70000
370.40000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 11046.07875
 THE AC OF COMP # 2 IS : 1.00000

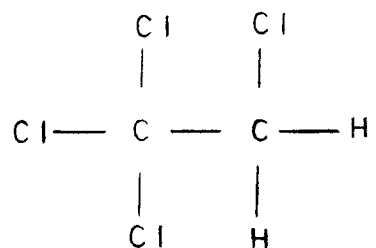
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 111.47554

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 :1,1,1,2-TETRACHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CCl ₃	1.	2.64010	2.18400
CH ₂ Cl	1.	1.46540	1.26400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-157.10000	770.00000
249.20000	.00000	740.40000
356.80000	315.90000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 7102.42980
 THE AC OF COMP # 2 IS : 1.00000

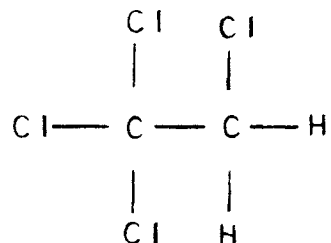
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 122.43041

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 :1,1,1,2-TETRACHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CCl ₃	1.	2.64010	2.18400
CH ₂ Cl	1.	1.46540	1.26400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-157.10000	698.20000
249.20000	.00000	708.70000
353.70000	325.40000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 6829.65667
 THE AC OF COMP # 2 IS : 1.00000

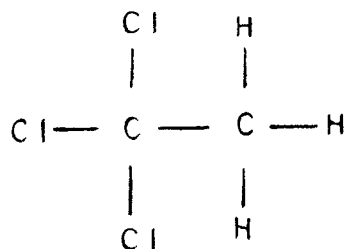
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 93.78877

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : 1,1,1-TRICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH ₃	1.	.90110	.84800
CCl ₃	1.	2.64010	2.18400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	7.50000	1300.00000
21.23000	.00000	793.20000
342.40000	356.80000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2875.03138
 THE AC OF COMP # 2 IS : 1.00000

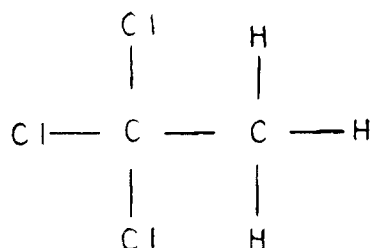
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 223.44827

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : 1,1,1-TRICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH ₃	1.	.90110	.84800
CCl ₃	1.	2.64010	2.18400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	24.90000	1318.00000
36.70000	.00000	826.70000
300.00000	353.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2373.63092
 THE AC OF COMP # 2 IS : 1.00000

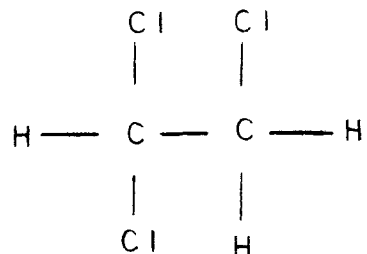
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 251.63373

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : 1,1,2-TRICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl ₂	1.	2.06060	1.68400
CH ₂ Cl	1.	1.46540	1.26400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-21.35000	740.40000
110.50000	.00000	770.00000
370.70000	315.90000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2277.89538
 THE AC OF COMP # 2 IS : 1.00000

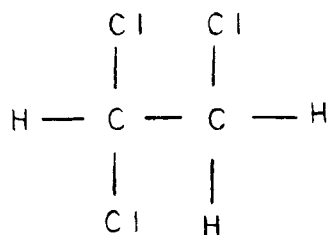
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 134.92654

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : 1,1,2-TRICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl ₂	1.	2.06060	1.68400
CH ₂ Cl	1.	1.46540	1.26400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-84.53000	708.70000
108.30000	.00000	698.20000
370.40000	325.40000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 2688.26401
 THE AC OF COMP # 2 IS : 1.00000

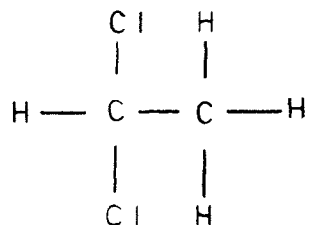
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 110.69151

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : 1,1-DICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH3	1.	.90110	.84800
CHCl2	1.	2.06060	1.68400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	-243.90000	1300.00000
27.90000	.00000	740.40000
342.40000	370.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 1841.58078
 THE AC OF COMP # 2 IS : 1.00000

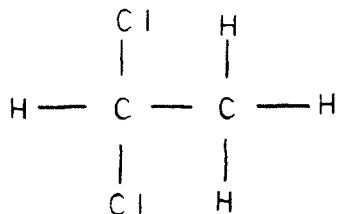
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 241.81020

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : 1,1-DICHLOROETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CH ₃	1.	.90110	.84800
CHCl ₂	1.	2.06060	1.68400
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	53.76000	1318.00000
34.01000	.00000	708.70000
300.00000	370.40000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 795.00223
 THE AC OF COMP # 2 IS : 1.00000

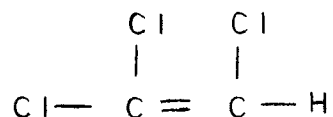
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 187.19823

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : TRICHLOROETHYLENE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CCl=CHCl	1.	3.30920	2.86000
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	1153.00000
1429.00000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 64787335.68779
THE AC OF COMP # 2 IS : 1.00000

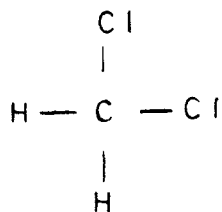
X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
THE AC OF COMP # 2 IS : 1316.66299

By Using UNIFAC-LLE Parameters ,Temp= 298.0K

COMP 1 : DICHLOROMETHANE COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl	1.	2.25640	1.98800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	740.40000
370.70000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 253.63824
 THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

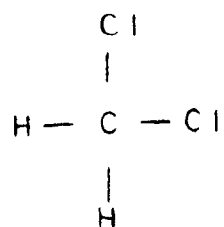
THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 155.75217

By Using UNIFAC-VLE Parameters ,Temp= 298.0K

COMP 1 : DICHLOROMETHANE

COMP 2 : WATER

The Structure of COMP 1 :



Group	No	R	Q
CHCl	1.	2.25640	1.98800
Water	1.	.92000	1.40000

The Group-Interaction Parameters Array Amn is :

.00000	708.70000
370.40000	.00000

X(1)= .00000000D+00 X(2)= .10000000D+01

THE AC OF COMP # 1 IS : 248.46621
 THE AC OF COMP # 2 IS : 1.00000

X(1)= .10000000D+01 X(2)= .00000000D+00

THE AC OF COMP # 1 IS : 1.00000
 THE AC OF COMP # 2 IS : 134.14663