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ABSTRACT

Title of Thesis: Thermal Desorption of Hazardous and Toxic Organic Compounds from Sand Matrices

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Master of Science in Environmental Science.

Thesis directed by: Dr. Joseph W. Bozzelli

Incineration processes are effective and sometimes efficient technologies for the remediation of contaminated solids which result in permanent destruction of most organic hazardous compounds. A less energy intensive , but more efficient process to remove contaminants from the soil is the application of heat and a flow of inert gas where the entire soil mass is not heated to incineration temperatures. This thermal treatment increases volatilization and often affects complete removal of organic compound depending on soil conditions and species volatility.

The goals of this research are to develop an understanding of the mass transport phenomena and adsorption thermodynamics that control the desorption of contaminants from sand specifically determining mass transfer coefficients, film mass transfer

coefficients, and equilibrium constants for a series of target organic pollutants. We also determined particle size effects on each of the above parameters for the pollutant species. We compare these data with soil bed mass transfer parameters and heats of adsorption in view the of absence of intraparticle diffusion effects in sand bed. These parameters will yield a better understanding and allow calculation of required time, temperature, and flow veocity for the desorption process in incineration or thermal desorption processes.

The experiment is based on plug flow deposition of the target contaminant on a well characterized sand column monitoring its travel through the column at varied temperatures, flowrates, and sand particle sizes. Chromatographic response analysis on the results is used to calculate the heats of adsortion of organic materials onto the sand matrices in addition to axial dispersion and film mass transfer coefficients. We study these effects on particle sizes of the sand bed; at sieve #'s 30-35, 35-40, and 40-50.

The amount of contaminant remaining in the sand decreases with the increasing temperatures in the sand bed. We observe that the film mass transfer and dispersion coefficients decrease when the sand particle size increases. The following results have been obtained:

$$\text{Particle Size I} : R_p = 0.027cm$$

$$\text{Particle Size II} : R_p = 0.023cm$$

$$\text{Particle Size III} : R_p = 0.018cm$$

Compound	Molecular Diffusivity ($D_m, cm^2/sec$)	Film Mass Transfer Coefficient ($K_f, cm/sec$)			Dispersion Coefficient ($D_z, cm^2/sec$)		
		I	II	III	I	II	III
Methylene Chloride	0.122	4.41	5.09	6.43	2.47	6.54	9.04
Chloroform	0.117	4.26	5.08	6.51	2.51	2.92	4.12
1,1,1-trichloroethane	0.108	3.95	4.70	6.03	1.63	4.05	5.79
Benzene	0.122	4.45	5.30	6.80	5.40	7.96	9.06
Toluene	0.123	4.47	5.33	6.83	5.14	6.16	8.45
Tetrachloroethylene	0.134	4.89	5.82	7.47	3.25	3.98	4.11
Chlorobenzene	0.132	4.81	5.73	7.36	3.33	6.32	8.77
1,2,4-trichlorobenzene	0.154	5.61	6.68	8.57	4.74	6.53	17.65

These results can be then applied to thermal treatment of contaminated soils and will be utilized to obtain optimum operational conditions for sand decontamination experiments.

Thermal Desorption of Hazardous and Toxic Organic Compounds from Sand Matrices

by

Jaeil Kwon

Thesis submitted to the faculty of the graduate school of the New Jersey Institute of Technology in partial fullfillment of the requirements for the degree of Master of Science in Environmental Science.

1990

APPROVAL OF THESIS

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Korean Chemical Society, June 1985

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Chapter 1

Introduction

Hazardous waste sites frequently contain large quantities of contaminated soils which results from spills, leaking storage tanks, illegal discharges, tanker accidents, and improperly operated landfills. The contaminated soil can be dangerous to the ground water supply and aquifers. In addition, it can be dangerous to inhabitants of the area.

Currently there are several alternatives for the clean-up of soil at sites found to be contaminated with organic pollutants. The first alternative involves excavation of the contaminated soil, transportation to a secure hazardous waste landfill for disposal and backfilling of the excavated areas. The second alternative would be redeposition[1], where the contaminated soil is redistributed in an approved dump site, delaying the problem for future generations. And the third option would entail excavation of contaminated soil, transportation to a thermal treatment facility where the soil would be

rendered non-hazardous and return of treated soil to excavated area.

The cost associated with the transportating and disposing of these contaminated soils in an approved landfill can be prohibitive when large volumes of soil are involved, as in the first and second alternatives. There is also a significant limitation on the number of sites which can accept contaminated wastes with the number decreasing rapidly. Additionally, landfill can not provide a permanent solution to the problem as the soil may have to be handled again at some future date.

Thermal treatment and incineration are viable alternatives which are particularly applicable to solids and can permanently destroy most of the hazardous constituents in the soil, excluding inorganic materials. There has been projected development in this technology[2]. As more nontraditional materials, soils or low energy solids, and sludges, are thermally treated or incinerated additional basic research will be required to effect optimizationd with auxiliary fuel minimized[3]. Even though this strategy is costly due to initial capital investment and, subsequent fuel requirements in the case of soil, it is being accepted[4] as satisfactory because of its high degree of the efficiency and permanent destruction.

In spite of wide acceptance of this technology, there is little understanding about the fundamental mass transfer principles of the organic contaminants through the heated soil matrices and, more importantly, about the limitation of the technology. It would be very valuable to be able to predict efficiency with respect to vapor pressure, heats of adsorption and mass transfer properties of the compounds in the soil.

The goals of this research are to develop an understanding of the mass transport phenomena and adsorption thermodynamics that control the desorption of contaminants from sand, specifically determining axial dispersion coefficients, film mass transfer coefficients, equilibrium constants and particle size effects on each of the above parameters.

The experiment is based on plug flow deposition of the contaminants on a well characterized sand column, monitoring its travel through the column at varied temperatures, flowrates, and sand particle sizes. Chromatographic response analysis on the results is used to estimate the heats of adsortion of organic materials onto the sand matrix in addition to axial dispersion coefficients and film mass transfer coefficients.

In this study we present our determination of equilibrium constants, heats of adsorptions, film mass transfer coefficients and axial dispersion coefficients for each of 8 target compounds:

- Methylene Chloride
- Chloroform
- 1,1,1-Trichloroethane
- Benzene
- Toluene
- Tetrachloroethylene
- Chlorobenzene

- 1,2,4-Trichlorobenzene

With these mass transfer parameters and heats of adsorption we verified the improved mass transfer model[5] for non-porous material, sand.

Chapter 2

Previous Studies

A number of models for simulating sorption rate processes have been developed. One of the simplest models is quantified by a single rate constant, K_F termed the One-Box Model by *Lipadius and Amundson*[6] in which sorption rate is a function of concentration difference between the sorbent and solution. They made the first theoretical contribution by solving the linear chromatographic system where axial dispersion and adsorption/desorption were the significant rate processes.

The One-Box model does not fit experimental data very well, and sorption kinetics data always show a rapid initial uptake followed by a slow approach to equilibrium[7]. Thus many other mass transfer approches were developed. The improved model typically involves subdividing the sorbent into two-compartments.[8]. This concepualization corresponds to physical situations in which there are two classes of sorbing sites, two chemical reactions in series, or a sorbent with an exterior part and an inner part.

Unfortunately, this type of model retains three independent fitting parameters that can not be easily evaluated or estimated for new combinations of chemicals and solids. *Kubin and Kucera*[9][10] extended the development to include axial dispersion, external (gas-to-particle surface) diffusion, intraparticle diffusion and adsortion, in the absence of reaction.

Later *Suzuki and Smith*[11] obtained a solution for the chromatographic curve in the Laplace-domain, which includes the effects of axial dispersion, external and intraparticle diffusion, reversible adsorption and first-order surface reaction. The solution was then used to relate moments of the chromatographic curve properties of the G.C. peak such as width to the transport and surface rate parameters. This allows the use of the results for evaluating surface reaction rates from experimentally determined moments and proves to be valuable.

Because the theory of transient behavior of chromatographic columns is applicable only to catalysts possessing a unimodal pore size distribution, the precise manner in which these two diffusion terms combine was not known. In 1973, *Haynes* and *Sarma*[12] utilized moment analysis to obtain an equation relating quantities extracted from the chromatogram to the model parameters. They finally provide us with some clear and applicable guidance in elucidating mass transfer behavior in these processes.

Jong-In Dong[13] defined a different equilibrium constant for sorption on soil and sand and derived the equations which are identical to those of *Haynes and Sarma*'s. He also developed the applicable equation to estimate the mass transfer parameters

for sand particle utilizing mass balance equations and moment analysis method. We utilize these equations and methods in this study to determine heats of adsorption, dispersion coefficients, and film mass transfer coefficients on silica sand of mesh size 30 - 35, 35 - 40, and 40 - 50.

Chapter 3

Theory

3.1 Mass Transfer of Gas Molecules in a Packed Bed

The transport of gas molecules in a packed bed takes place according to a series of complex and sometimes tortuous steps. Each step may have an influence on the rate of mass transfer of the molecule through the system and therefore contributes to the band-broadening from a spike injection in a chromatographic type experiments. By analyzing the contributions of each step to the shape of a chromatographic response peak, mass transfer parameters in particles can be determined. Mass transfer of organic compounds inside soil beds consists of four major steps:

1. Axial Dispersion along the soil bed

2. Mass Transfer through the film around soil particles

3. Intraparticle Diffusion inside individual soil particle

4. Adsorption/Desorption behaviour between soil surface and fluid phase inside particles.

This mass transfer mechanism can be analyzed through the chromatographic response analysis utilizing mass balance equations and the moment analysis method.

3.2 Mass Transfer on Sand Bed

The sand bed is considered to show very different mass transfer behavior from soil clay or other particle beds which have a complex pore structure. A completely different model[13] has been developed to deal with this sand bed case. Because there is no diffusion inside the sand particles, adsortion/desorption activity is assumed to occur on the outer surface of the particles only. The following equations have, therefore, been developed using mass balance equations and moment analysis method. They are developed and reduced to

$$\mu = \frac{L}{V}(1 + \frac{1-\theta_b}{\theta_b}\frac{3}{R_p}K_b) \tag{3.1}$$

$$\begin{aligned}\sigma^2 &= \frac{2LD_z}{V^3}(1 + \frac{1-\theta_b}{\theta_b}\frac{3}{R_p}K_b)^2 \\ &+ \frac{L}{V}\frac{1-\theta_b}{\theta_b}\frac{6}{R_p}\frac{K_b^2}{K_f}\end{aligned} \tag{3.2}$$

where	μ	average retention time	$min.$
	σ^2	variance	$min.^2$
	L	bed length	cm
	V	superficial gas velocity	cm/sec
	K_b	equilibrium constant defined by a $C_a = K_b' C_z'$ or $C_a = K_b C_z'$	
	a	Surface area of particle per unit volume	cm^{-1}
	C_z'	Concentration of bed fluid	g/cm^3
	θ_b	porosity of bed	
	D_z	dispersion coefficient	cm^2/sec
	K_f	Film mass transfer coefficient	cm/sec
	R_p	Particle Radius	cm

The first term in *Equation(3.1)* is the purge velocity and second term is adsorption equilibria effects combined with velocity. In *Equation(3.2)* the first term is the dispersion effects on variance and the second term is effects on film mass transfer on variance. The absence of the intraparticle diffusion term in sand results in a different chromatographic response from that of soil and we can anticipate from the theory what the different effects of particle size in sand will be.

3.3 Equilibrium Constants, K_b

From the*Equation(3.1)* we obtain by rearrangement the equation:

$$K_b = (\frac{\mu V}{L} - 1)\frac{R_p \theta_b}{3(1-\theta_b)} \tag{3.3}$$

Using *Equation(3.3)* and the average retention time and discharge velocity we can evaluate the equilibium constant. Discharge velocity is the velocity of the gas flow through the particles of the bed, considering the porosity effect. For example at 2.0

scale of flowmeter, the flowrate of carrier gas is $11.70cm^3/min$ at 100 $^\circ C$. Dividing flowrate by cross sectional area of the bed gives us the flow velocity;

$$Velocity = \frac{11.70cm^3/min}{0.1636cm^2} = 71.52cm/min. \tag{3.4}$$

The cross-sectional area is calculated from I.D.(4.546mm) of the bed. In the bed the velocity would increase due to the pore structure. The discharge velocity is obtained by dividing flow velocity by the porosity of the bed. Porosity is defined as the ratio of the void volume in sand bed to the volume of the bed. For example, the porosity of particle size II is 0.4145 and this gives;

$$DischargeV = \frac{71.52cm/min.}{0.4145} = 172.54cm/min. = 2.88cm/sec \tag{3.5}$$

3.4 Mass Transfer Parameters

3.4.1 Axial Dispersion Coefficient, D_z

From the *Equation(3.1)* and *Equation(3.2)* we obtain following equation:

$$\begin{aligned} \frac{\sigma^2}{2\mu^2}\frac{L}{V} &= \frac{1}{V^2}D_z \\ &+ (\frac{1-\theta_b}{\theta_b}\frac{3}{R_p}\frac{K_b^2}{K_f})(1+\frac{1-\theta_b}{\theta_b}\frac{3}{R_p}K_b)^{-2} \end{aligned} \tag{3.6}$$

We can determine axial dispersion coefficient, D_Z by plotting $\frac{\sigma^2}{2\mu^2}\frac{L}{V}$ vs. $1/V^2$ where axial dispersion coefficient, D_Z, is obtained directly from the slope. We measure μ, σ,

we know L, R_p, θ_b and V where K_b from *Equation(3.3)* and K_f from the Y-intercept. Detailed method to evaluate K_f is described in *Section(3.4.2)*.

3.4.2 Film Mass Transfer Coefficient, K_f

Film mass transfer coefficient can be determined experimentally as well as theoretically. The Sherwood Number[13] which characterizes film mass transfer is expressed as follows:

$$Sh \equiv \frac{2R_pK_f}{D_m} \tag{3.7}$$

where R_p Average Particle Radius
K_f Film Mass Transfer Coefficient
D_m Molecular Diffusivity

There is an assumption[14] that at a low Reynolds number the Sherwood Number is 2.0. We calculate the Reynolds Number for each particle size. Since the Renolds Number is smaller than 2 for sand beds, the flow is considered to be laminar[15] and we can assume that the Sherwood Number is 2.0 according to the conclusion[16]. This gives:

$$Sh \equiv \frac{2R_pK_f}{D_m} \simeq 2.0 \tag{3.8}$$

Therefore:

$$K_f = \frac{D_m}{R_p} \tag{3.9}$$

From the *Equation(3.9)* we can estimate the film mass transfer coefficient knowing the molecular diffusivity. The film mass transfer coefficient also can be obtained ex-

perimentally. Using *Equation(3.6)* we can evaluate the film mass transfer coefficient directly from the Y-intercepts.

3.4.3 Molecular Diffusivity, D_m

The Chapman-Enskog fomula for viscosity and thermal conductivity were given in *Bird, Stewart, Lightfoot*[16] and the corresponding formula for cD_m for the gaseous state at low density is:

$$cD_m = 2.2646 \times 10^{-5} \frac{\sqrt{T(\frac{1}{M_A} + \frac{1}{M_B})}}{\sigma_{AB}^2 \Omega_{D,AB}} \tag{3.10}$$

If we approximate c by the ideal-gas law $c = p/RT$, this becomes

$$D_{AB} = 0.0018583 \frac{\sqrt{T^3(\frac{1}{M_A} + \frac{1}{M_B})}}{p\sigma_{AB}^2 \Omega_{D,AB}} \tag{3.11}$$

where	D_{AB}	molecular diffusivity $D_{AB} \equiv D_m$	$cm^2 sec^{-1}$
	c	concentration	$g-mole/cm^{-3}$
	T	temperature	$^\circ K$
	p	pressure	atm
	σ_{AB}	collision diameter $1/2(\sigma_1 + \sigma_2)$	$\mathring{A}$
	$\Omega_{D,AB}$	function of ϵ/kT where $\epsilon = \sqrt{\epsilon_1 \epsilon_2}$	Lennard-Jones parameters
	k	Boltzmann constant	

When ϵ/k is not known *Hirschefelder, Bird & Spotz*[18] recommend

$$\frac{\epsilon}{k} = 1.15 T_b \tag{3.12}$$

$$\sigma = 1.18 V_b^{1/3} \tag{3.13}$$

where	T_b	the normal boiling point	$^\circ K$
	V_b	molar volume of liquid at b.p.	$cc/g-mole$

Our group is also developing a group additivity approach to estimating σ and ϵ/k.

3.5 Heat of Adsorption

There is temperature-dependent term since the temperature dependence of the equilibrium constant should follow a van't Hoff equation[19]:

$$K = K_o exp(\frac{-\Delta H_o}{RT}) \tag{3.14}$$

Since adsorption is exothermic (ΔH is negative), K_b should decrease with increasing temperature. The assumption of identical sites with no interaction between adsorbed molecules implies that the heat of adsorption is independent of coverage. At low sorbate concentration Henry's law[20] is approached. Henry's law states that at low concentration the vapor pressure of the solute obeys the equation:

$$p_B = x_B k_B \tag{3.15}$$

where x_B is the mole fraction of solute and k_B is a constant. Thus at low sorbate concentration we obtain:

$$\frac{dlnK'}{dT} = \frac{\Delta H_o}{RT^2} \tag{3.16}$$

Equation 3.16 may be expressed in logarythmic form as follows.

$$lnK = lnK_o - \frac{\Delta H_o}{R}\frac{1}{T} \tag{3.17}$$

By plotting lnK_b versus $1/T$ we can obtain $-\Delta H_o/R$ from the slope.

Chapter 4

Experimental Method

4.1 Experimental Apparatus

An overall diagram of experimental apparatus is shown in *Figure(4.1)*. A Varian Aerograph Gas Chromatograph Model 1200[21] equipped with Flame Ionization Detector was used for the analysis. A sand bed cartridge column was placed in the oven instead of the column. The bed was prepared with three different particle sizes of sand: mesh#'s 30-35, 35-40, and 40-50. $0.5\mu l$ of target chemical pollutant selected for the study was then injected into the sand bed at varied temperatures and flowrates of carrier gas, N_2. Preheated nitrogen gas passes through injector and carries the target contaminants into the sand bed then to the F.I.D.(Flame Ionization Detector).

The F.I.D. is connected to HP Model 3396A Integrator[22]. Data produced by the integrator are sent to the host computer to be stored and analyzed. The computer

Figure 4.1: Experimental Apparatus

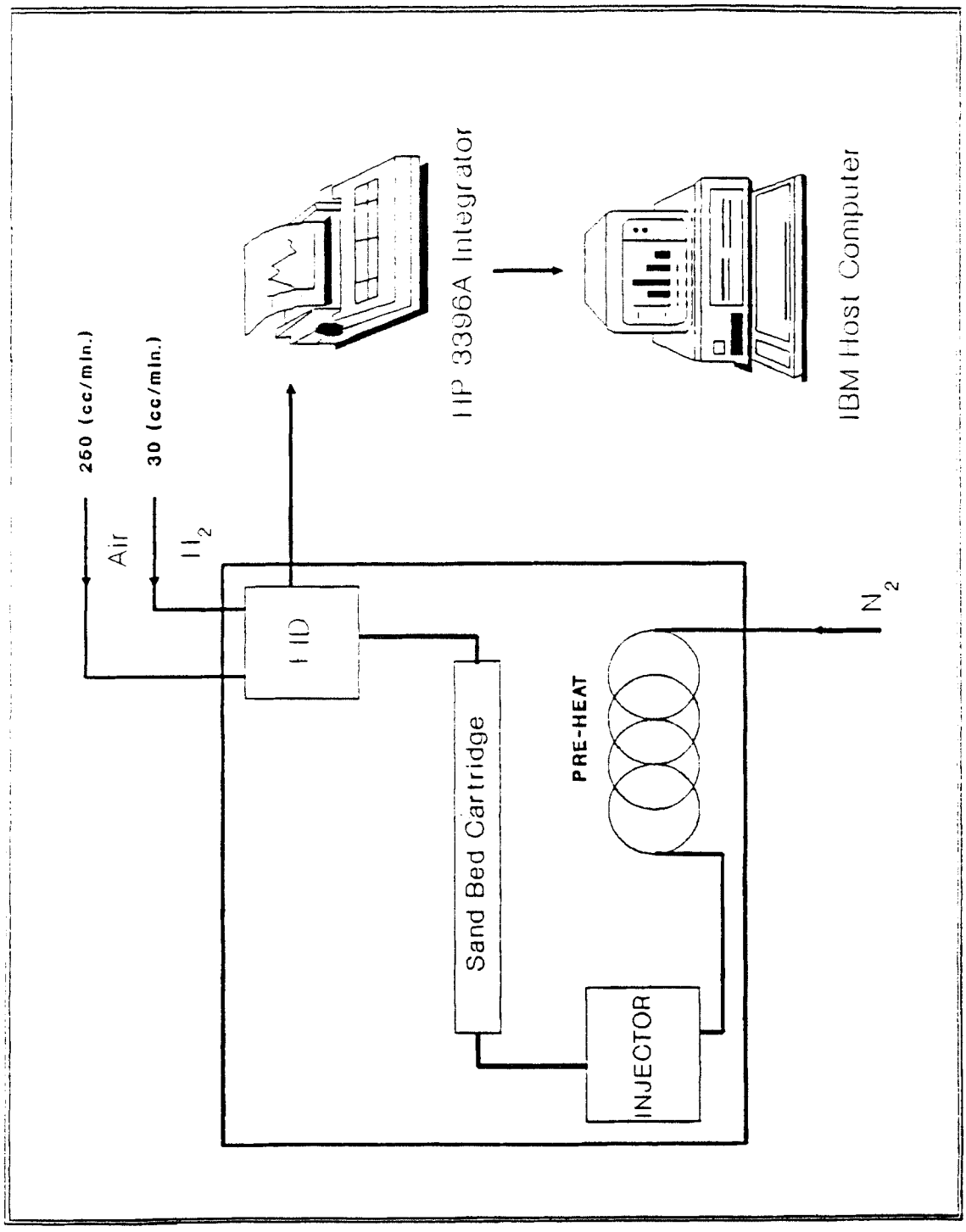


Table 4.1: Target Compounds and Toxicity

Compound	Boiling Point $^{\circ}C$	Molecular Weight	Human Toxicity
Methylene Chloride	39.8	89.9	narcotic in high conc.
Chloroform	61.7	119.4	carcinogen
1,1,1-Trichloroethane	74	133.4	mucous membranes
Benzene	80	78.1	carcinogen
Toluene	111	92.1	mild macrocytic anemia
Tetrachloroethylene	121	165.9	narcotic in high conc.
Chlorobenzene	132	112.6	faint
1,2,4-Trichlorobenzene	214	181.5	narcotic in high conc.

program processes the elution data versus time for mass transfer behavior study. A detailed listing of the program is in *Appendix A*.

4.2 Materials

4.2.1 Target Compounds

We selected 8 substances including 6 chlorocompounds and 4 aromatic compounds for study. Boiling points range from 39.8°C to 214°C. Most of them are known to be toxic and hazardous compounds. Benzene and chloroform, for example, are listed as carcinogens by the U.S. EPA[23]. Compounds studied are listed in *Table(4.1)* along with their physical properties and toxicity.

Table 4.2: Sand Particle Sizes and Porosities

Size	Sieve No.	Average Diameter(cm)	Porosity
I	30 - 35	0.0548	0.4501
II	35 - 40	0.0460	0.4145
III	40 - 50	0.0359	0.4055

4.2.2 Sand Bed Preparation

Sand adsorbent bed cartridge was prepared using stainless steel tubing(ID = $4.564mm$, $Length$ = $29cm$). A 50 lbs-pack of Silica Sand was purchased from Channel, a lumber company. It was also verified not to be carbonate sand by test with acid - Acid + Carbonate yield CO_2 gas. 20 lbs of sand was washed with water and dried in an oven at 200 $°C$ for 24 hours. Dried sand was sieved and separated according to the Mesh No. The stainless steel cartridge was packed with cleaned and screened sand of known mesh size. and installed in the oven. The sand bed column was heated to 400 $°C$ for 4 hours to remove possible remnant organics in the bed. Sand particle sizes and relevant porosities are listed in *Table(4.2)*

4.3 Flowrate Control and Calibrations

After four hours' conditioning in the oven($400°C$) we connect the tubing to flowmeter for carrier gas calibrations and flow verification. Setting the different flow scale of the flowmeter we measured the flowrate with a bubblemeter and stopwatch. At 40, 100, 160, 200, and 260 $°C$ we measure the flowrate varying the flow scale from in 0.5

increments. The calibration of flowmeter is shown in *Figure(4.2)* and flow rate at each temperature is in *Appendix B.*

4.4 Dead Volume Adjustment on Response Peak

We eliminate all other sections except the tubing section including injector volume. FID volume. and all the fittings used to and from bed from the mass transfer consideration so that we can consider the bed section only for the study. We do this by replacing the sand bed with clean G.C. connector tubing($I.D. = 0.8mm$, $Length = 15cm$). The volume of the tubing is less than 1.6% of the total bed volume. We inject the sample through this tubing and analyze the response to estimate the dead volume affected average retention time in the system. Thus we subtract the dead volume effect from packed bed experiment peak response-average rentention time. Dead volume effects in the sand bed were determined at temperatures of 100, 160, and 260 $°C$ with varied flow rate of each temperature. The results are shown in *Figure(4.3)* and listing of all data for each temperature is shown in *Appendix C.*

4.5 Operation

After placing the sand cartridge in the oven, for at least one hour re-conditioning at 400$°C$ was applied, to remove possible organic residuals in the bed prior to the each experiment. 0.5μl of the target compound was injected and integrator started at the same time for complete analysis. An example of a run is shown in *Figure(4.4).* After

Figure 4.2: Calibration of Carrier Gas at various Temperature

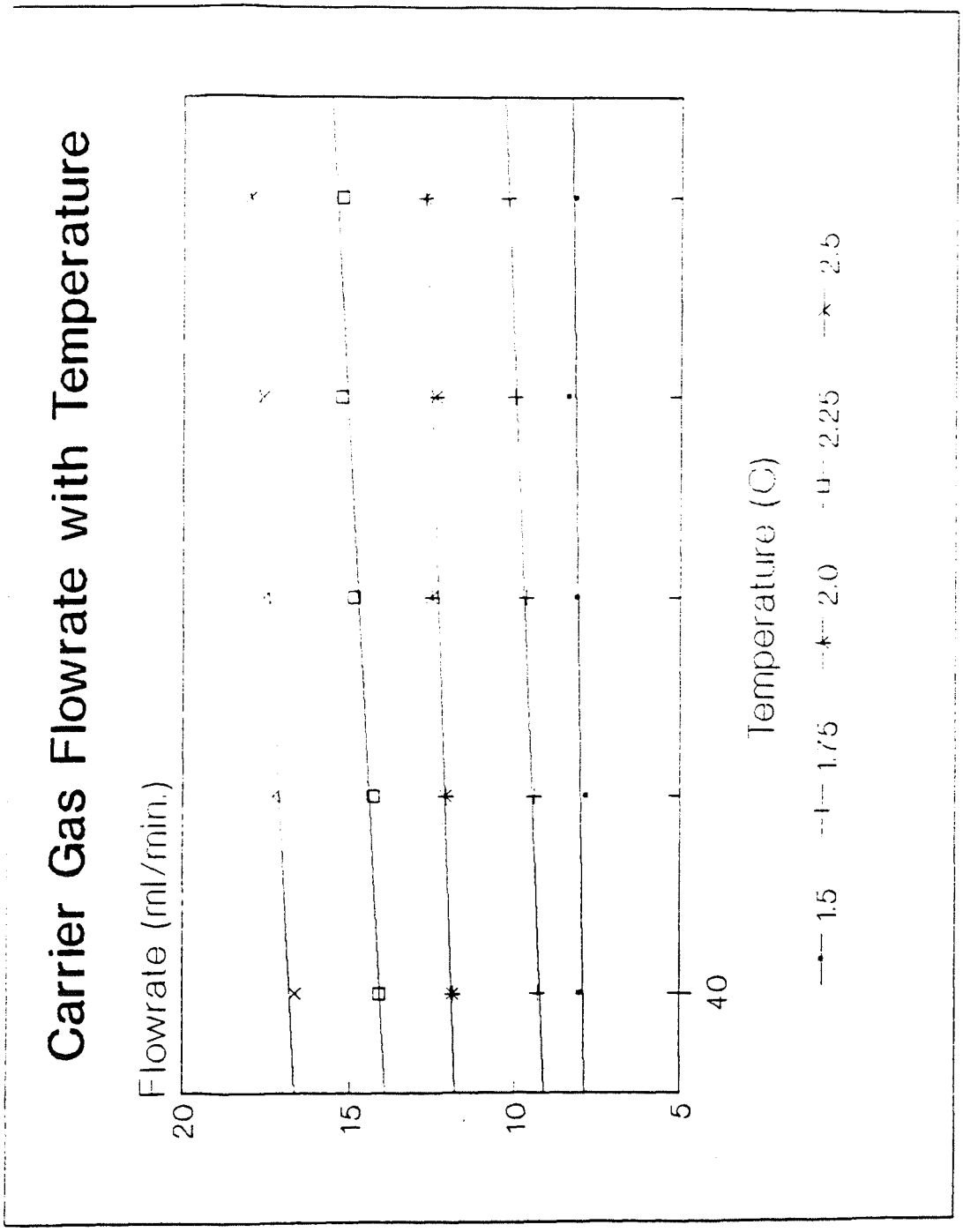
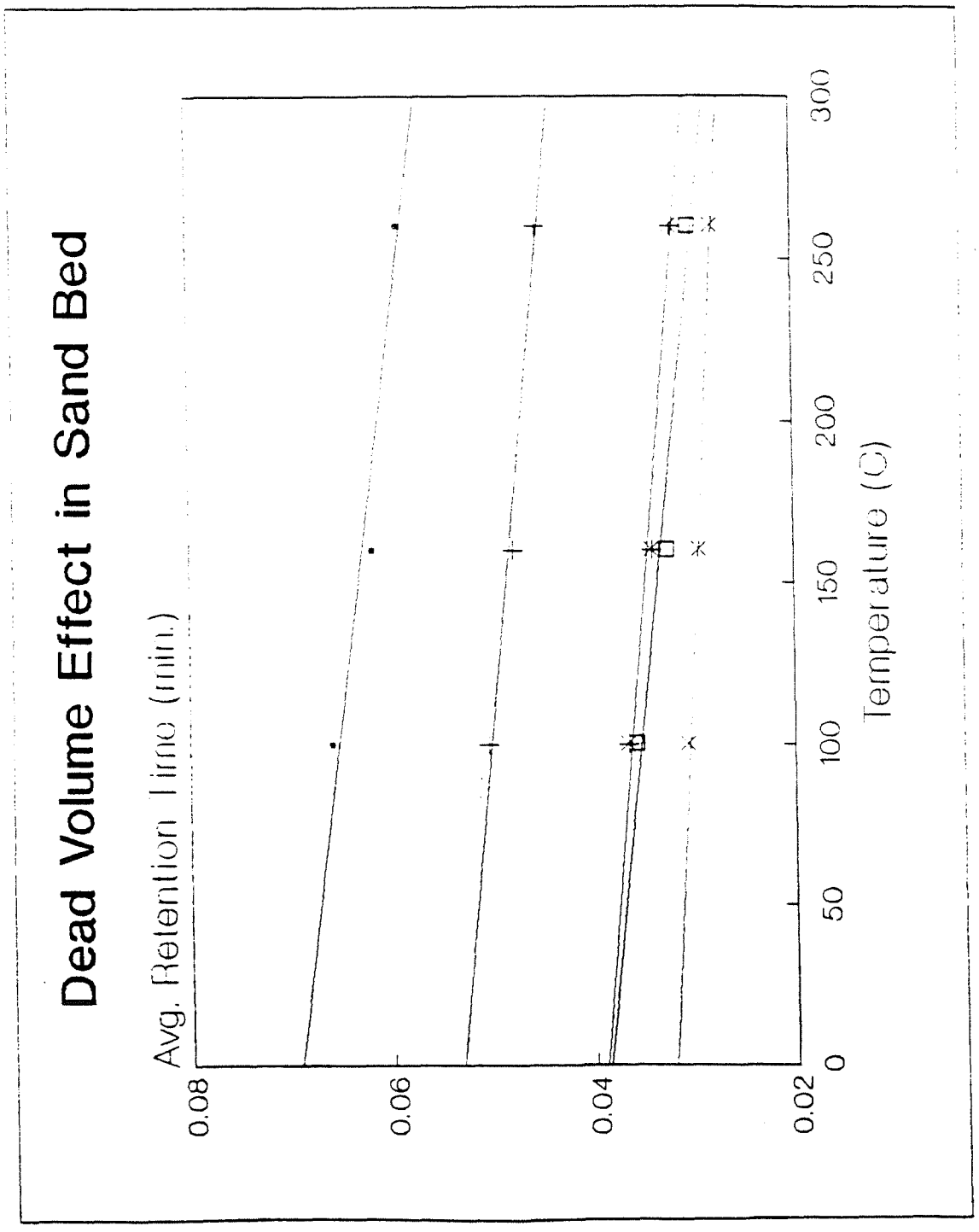


Figure 4.3: Dead Volume Effects at various Temperature



injection and detection we determined the average retention time and variance for each peak using computer program. For each of 8 compounds, the analysis was carried out changing the particle sizes , temperatures, and flow rates.

4.6 Data Processing

A Fortran program has developed and utilized to calculate the mass transfer parameters and heats of adsorption for each particle sizes from the input data.

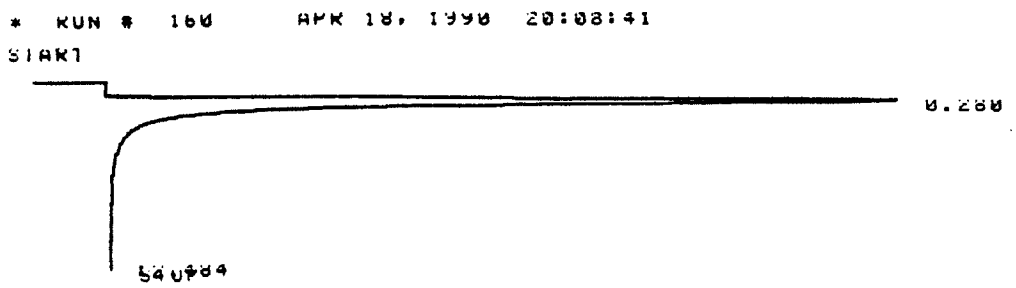
- Average retention time
- Variance
- Flowrate
- Experiment Temperature
- Dead volume effects
- Cross-sectional Area
- Temperature conversion factor

A sample input data and output data is shown in *Figure(4.5)*. For convenience, each set of data was named according to experiment temperatures. The list of filenames is in *Appendix D*.

The first row of input consists of filename, experiment temperature, temperature conversion factor (from $°C$ to $°K$) and cross-sectional area of the bed. The next

Figure 4.4: Sample Chromatogram and Peak Analysis

Particle Size : 0.0274*cm*
Injector Temp. : 150°*C*
Detector Temp. : 200°*C*
Bed Temp. : 140°*C*
Carrier Gas : $11.70 ml/cm^3$
Scale : 2.0




```
Closing signal file M:SIGNAL  .BNC

RUN#   160          APR 18, 1990  20:08:41

SIGNAL FILE: M:SIGNAL.BNC
AREA%
      RT      AREA TYPE  WIDTH      AREA%


 *   1              -114.008
  6              -114.05
  11             -114.067
  16             -114.117
  21             -114.167
  26             -114.183
  31             -114.2

*  FILELENGTH (MIN.)
71.5
XBASE 7
7114
TOTAL AREA=      23821.1
AVG. RETENTION TIME =          0.372485      MIN.
VARIANCE            =          0.0288098     MIN.
```

Figure 4.5: Sample Input and Output Data for Caculation

(A) Input Data

3081	80.0	1.2047	.1636
7.8794	.5132	.06925	.0288
9.0351	.3712	.05310	.0155
11.7010	.3058	.0390	.0124
13.8316	.2718	.0386	.0104
16.5015	.2202	.0324	.0079

(B) Output Data

FILENAME: 3081 80.0 (353.15)			
1.5	.0072703	.216642	.986198
2.0	.0046411	.164764	.901579
2.5	.0056851	.098239	.791698
3.0	.0061220	.070305	.735252
3.5	.0055888	.049395	.721847

five rows consist of flowrate at experiment temperature, average retention time, dead volume effect, and variance at different flowrate. The output comes with flowmeter scale and equilibrium constant, data of X and Y for plot $\frac{\sigma^2}{2\mu^2}\frac{L}{V}$ vs $1/V^2$ to estimate mass transfer parameters.

4.7 Quality Assurance

Each set of experiments was duplicated or verified by repeated experiments a minimum two times. Toluene was analyzed six times in order to determine the best experimental conditions. All results were consistent.

Chapter 5

Results and Discussion

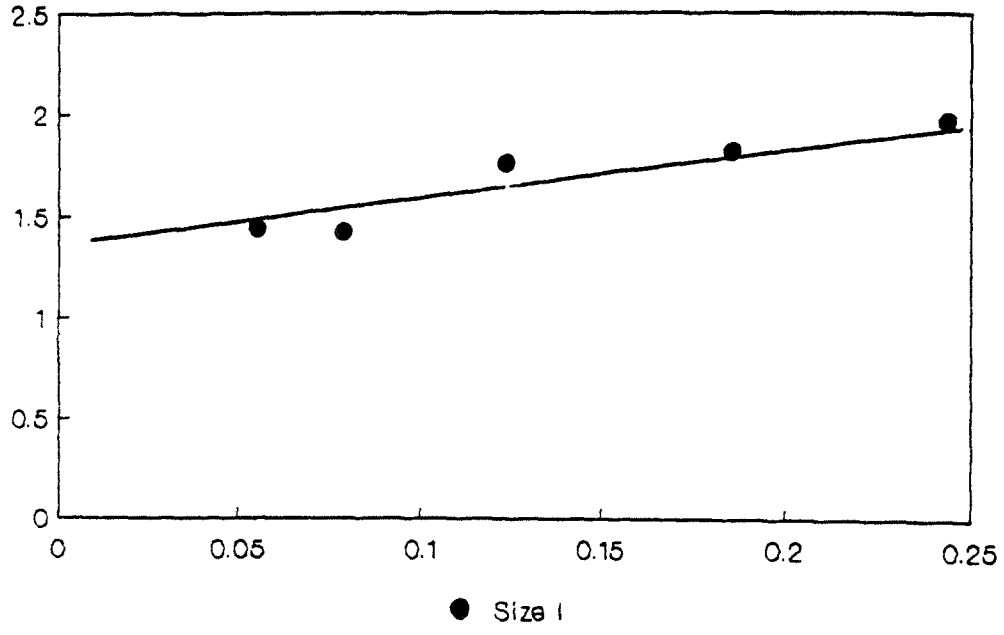
Chromatographic response analysis described in Chapter 3 has been utilized to study the mass transfer phenomena and heats of adsorption. Using *Equation(3.3)* and *Equation(3.17)* we obtain equilibrium constants, as well as, heats of adsorption from plot $1/T$ vs $ln(K_b/T)$. From *Equation(3.6)* we also obtain mass transfer coefficients and film mass transfer coefficients. The following sections detail the data obtained for each of the target compounds.

5.1 Methylene Chloride

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.1)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle size are shown in *Figure(5.1)*, *Figure(5.2)* and *Figure(5.3)* respectively.

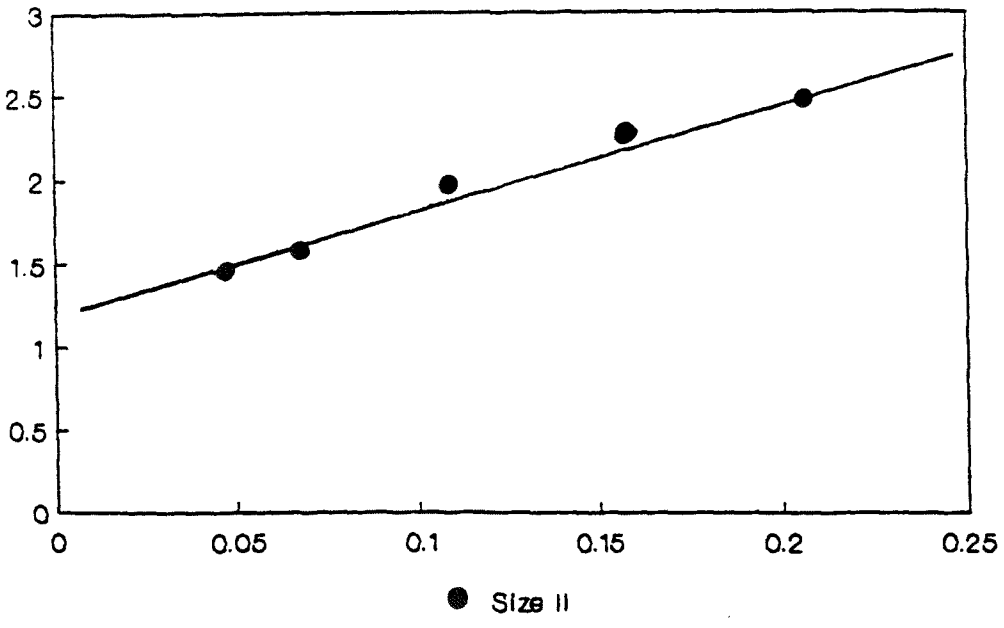
The heats of adsorption are plotted versus particle size in *Figure(5.4)* which shows

Figure 5.1: Heats of Adsorption of CH_2Cl_2 : Size I



Methylene Chloride at 60 C

Figure 5.2: Heats of Adsorption of CH_2Cl_2 : Size II

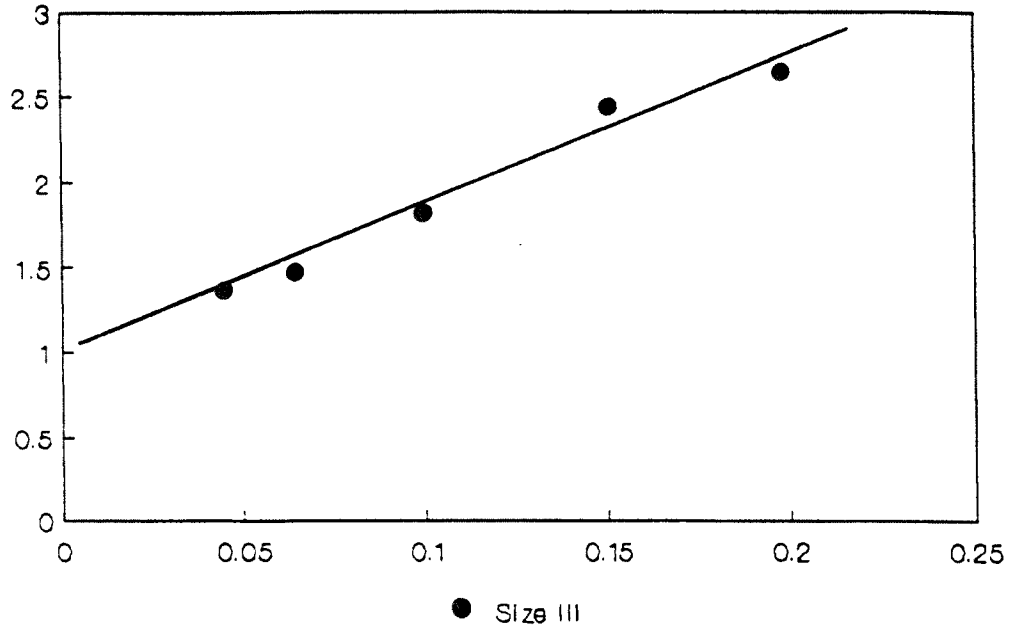


Methylene Chloride at 60 C

Table 5.1: Equilibrium Constants and Heats of Adsortion of CH_2Cl_2

Size	Temperature $°C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $°K$
I	50	12.651	2.577
	60	8.753	
	80	6.725	
	100	4.914	
	120	3.422	
II	50	11.518	2.265
	60	10.314	
	80	6.707	
	100	5.491	
	120	4.076	
III	50	9.782	2.158
	60	9.408	
	80	5.882	
	100	4.913	
	120	3.793	

Figure 5.3: Heats of Adsorption of CH_2Cl_2 : Size III



a slight increse in $-\Delta H/R$ with particle size.

Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.5)*,*Figure(5.6)*, and *Figure(5.7)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.8)*. Both coefficients show a decrease with increasing particle size.

Mass transfer parameters of Methylene Chloride at each temperature are listed in *Table(5.2)*.

Figure 5.4: Particle Size Dependence of $-\Delta H/R$

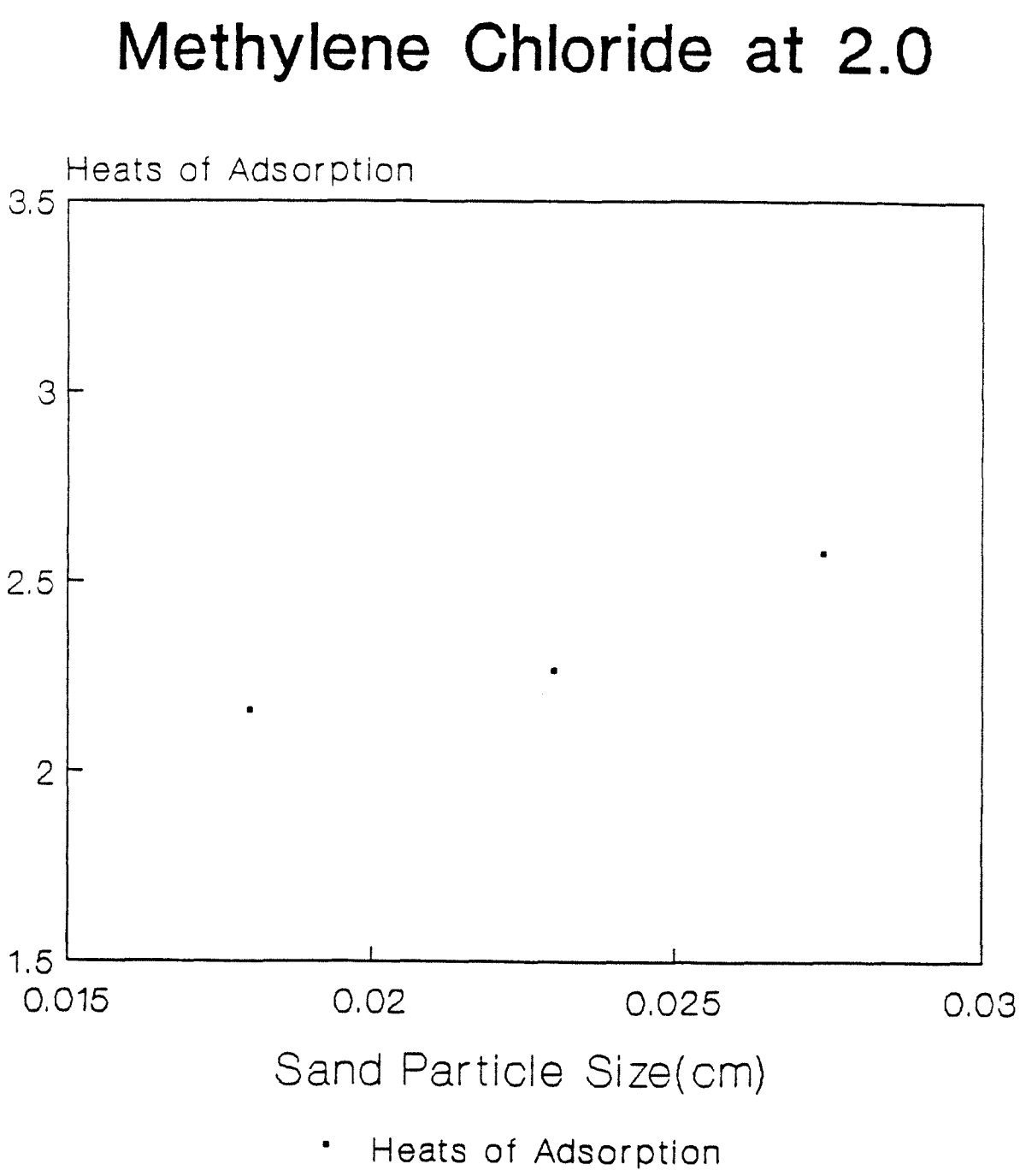
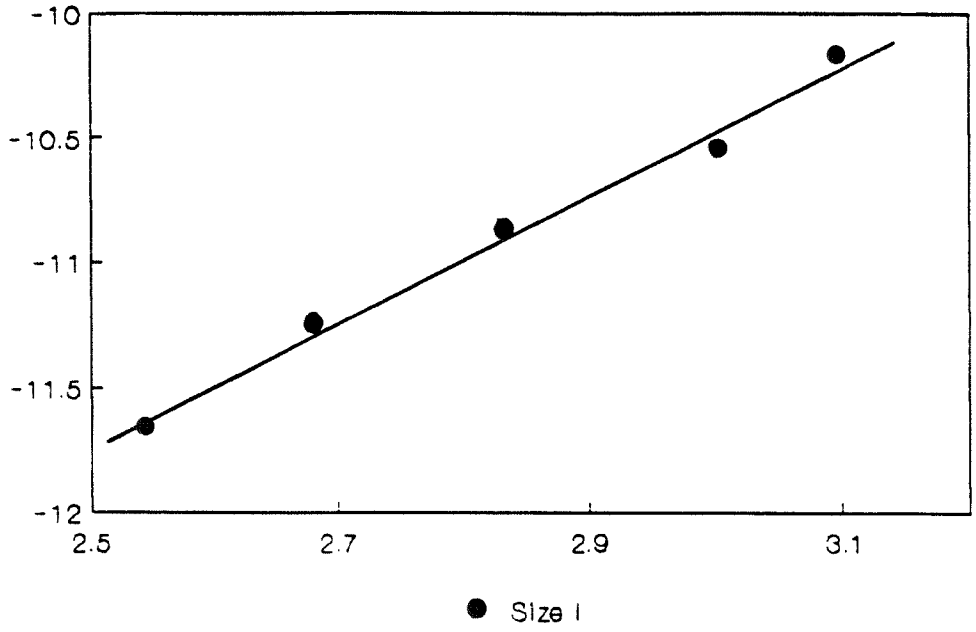
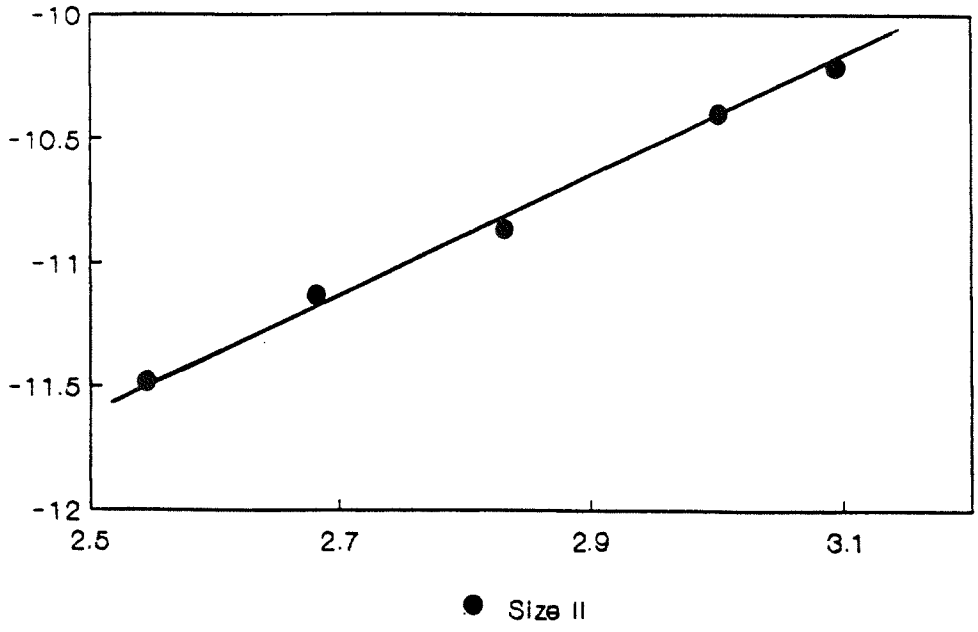


Figure 5.5: Dispersion Coefficient of CH_2Cl_2 : Size I



Methylene Chloride at 2.0

Figure 5.6: Dispersion Coefficient of CH_2Cl_2 : Size II



Methylene Chloride at 2.0

Figure 5.7: Dispersion Coefficient of CH_2Cl_2 Size III

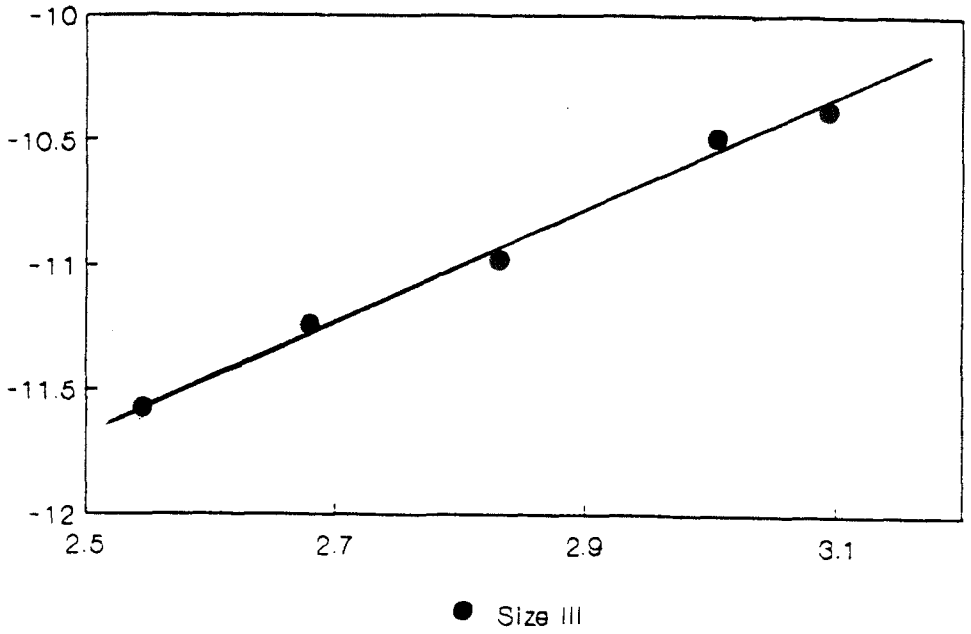


Table 5.2: Evaluated Mass Trasfer Parameters of Methylene Chloride

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	2.471	4.41	
II	6.542	5.09	0.1218
III	9.042	6.43	

Figure 5.8: Particle Size Dependence of D_z on Methylene Chloride

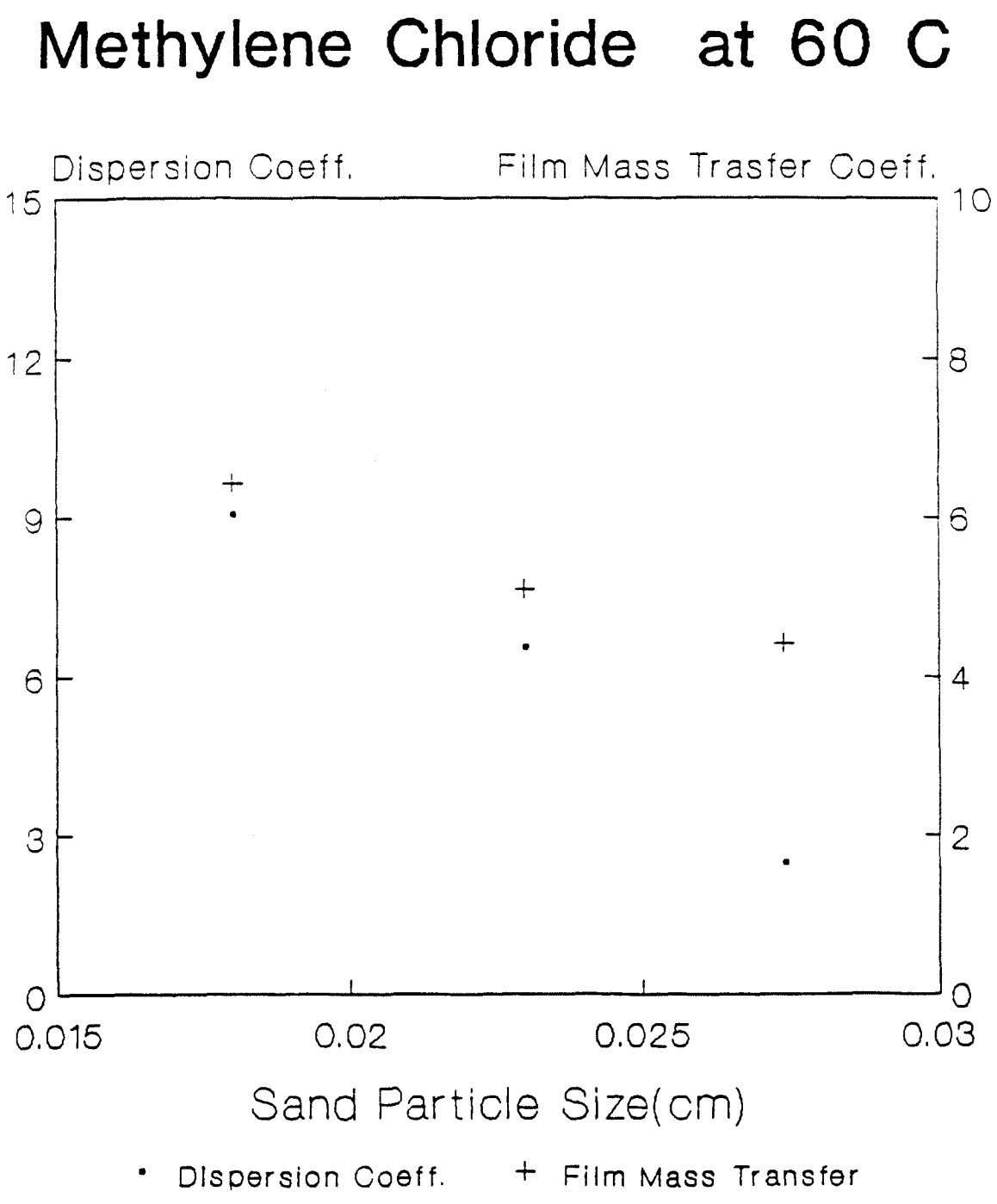
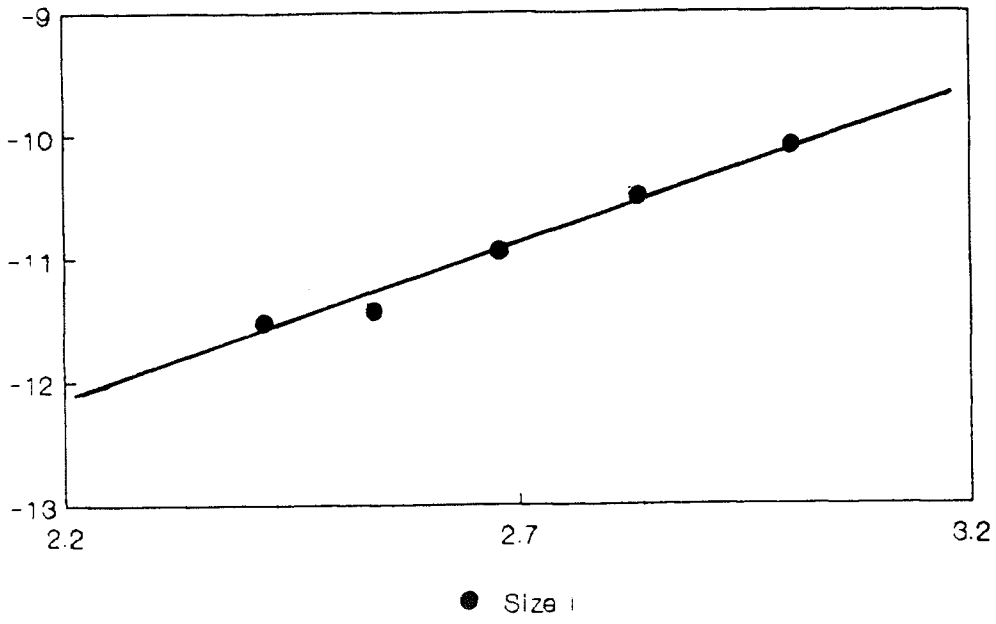


Figure 5.9: Heats of Adsorption of $CHCl_3$: Size I



Chloroform at 2.0

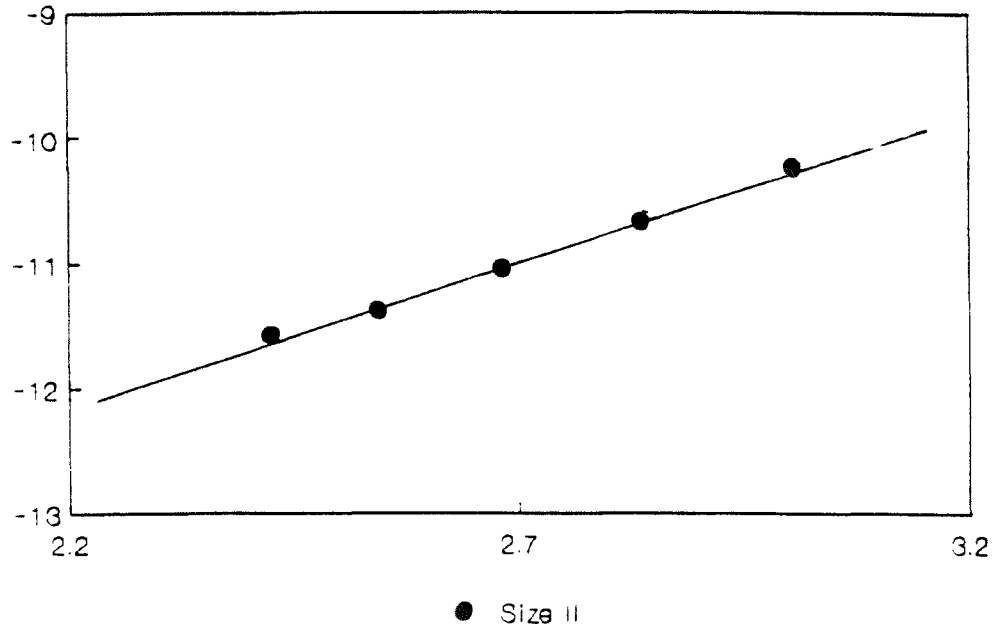
5.2 Chloroform

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.3)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.9)*, *Figure(5.10)* and *Figure(5.11)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.12)* which shows slight increase in $-\Delta H/R$ with particle size.

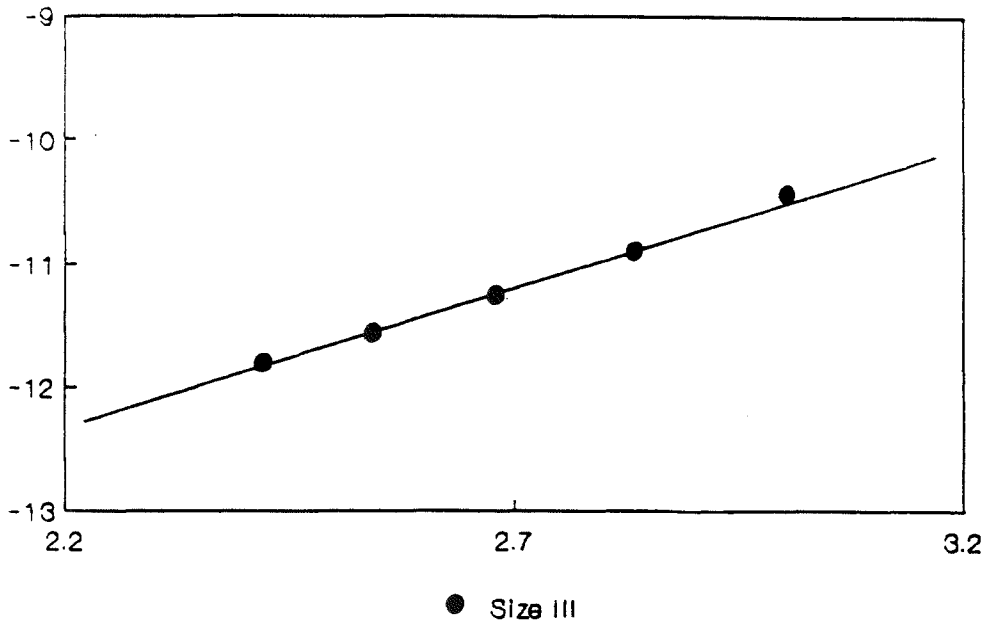
Mass transfer parameters of Chloroform at each temperature are listed in *Table(5.4)*. Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.13)*, *Figure(5.14)* and *Figure(5.15)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.16)*. Both coefficients show a decrease

Figure 5.10: Heats of Adsorption of $CHCl_3$: Size II



Chloroform at 2.0

Figure 5.11: Heats of Adsorption of $CHCl_3$: Size III



Chloroform at 2.0

Table 5.3: Equilibrium Constants and Heats of Adsortion of $CHCl_3$

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
I	60	14.121	2.648
	80	9.594	
	100	6.306	
	120	4.052	
	140	4.223	
II	60	12.597	2.448
	80	8.330	
	100	5.747	
	120	4.227	
	140	3.972	
III	60	10.143	2.374
	80	6.590	
	100	4.835	
	120	3.620	
	140	3.236	

Figure 5.12: Particle Size Dependence of $-\Delta H/R$

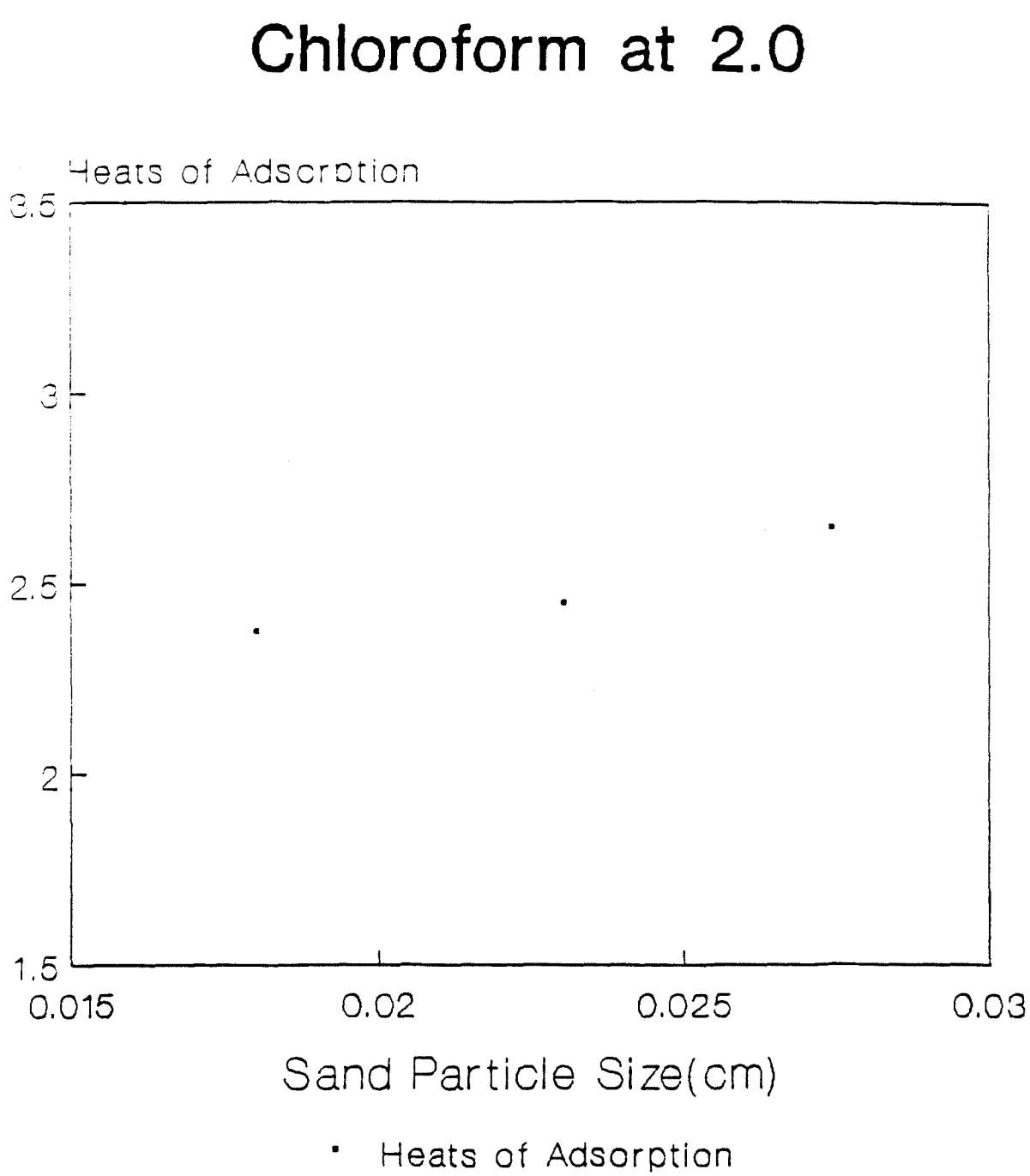
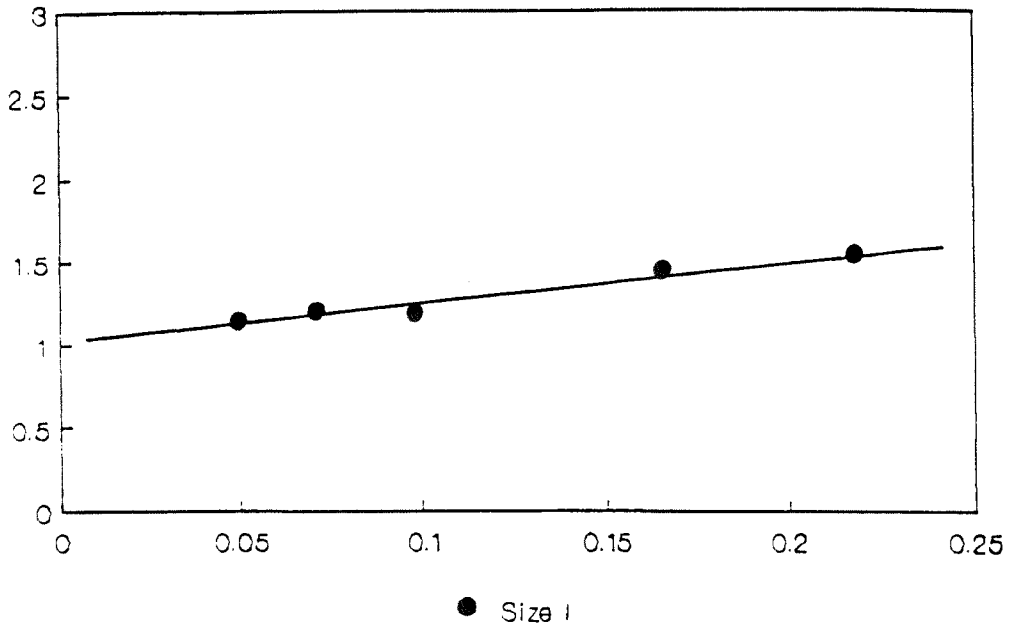
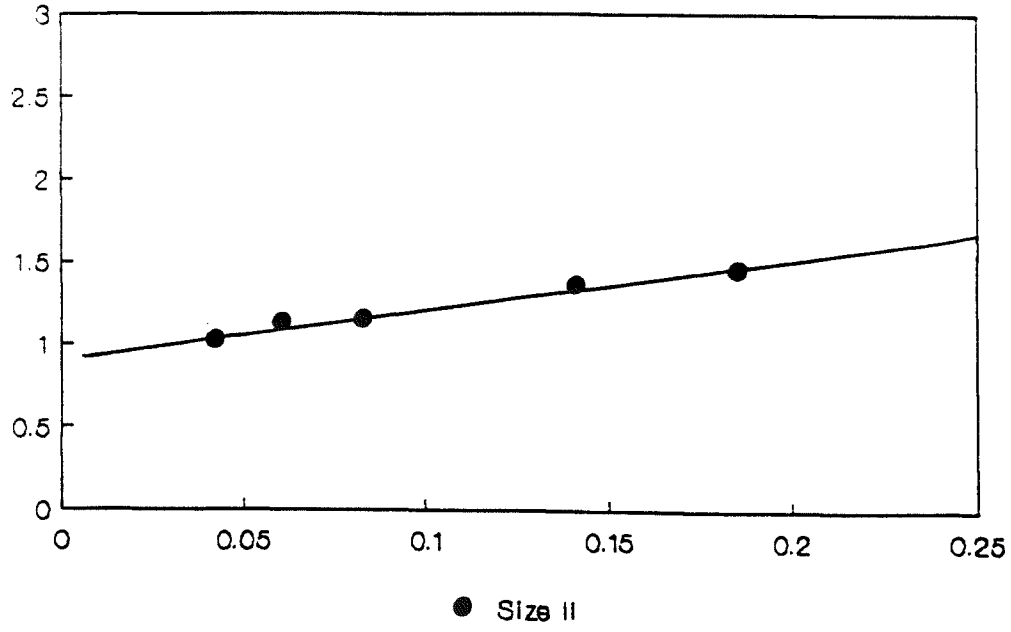


Figure 5.13: Dispersion Coefficient of $CHCl_3$: Size I



Chloroform at 80 C

Figure 5.14: Dispersion Coefficient of $CHCl_3$: Size II



Chloroform at 80 C

Figure 5.15: Dispersion Coefficient of $CHCl_3$: Size III

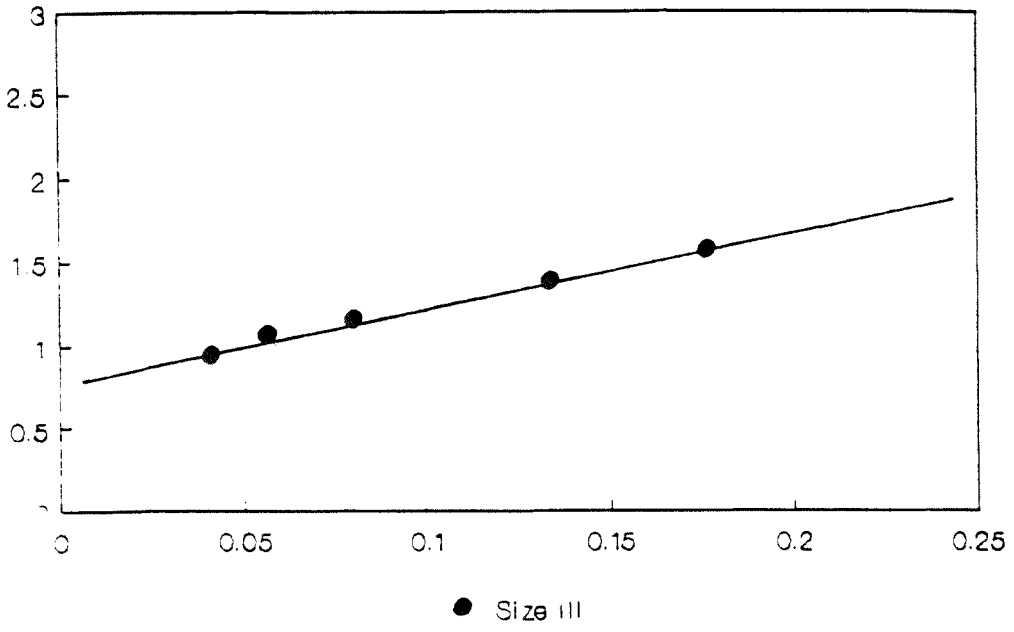


Table 5.4: Evaluated Mass Trasfer Parameters of Chloroform

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	2.506	4.26	
II	2.915	5.08	0.1168
III	4.131	6.51	

Figure 5.16: Particle Size Dependence of D_z

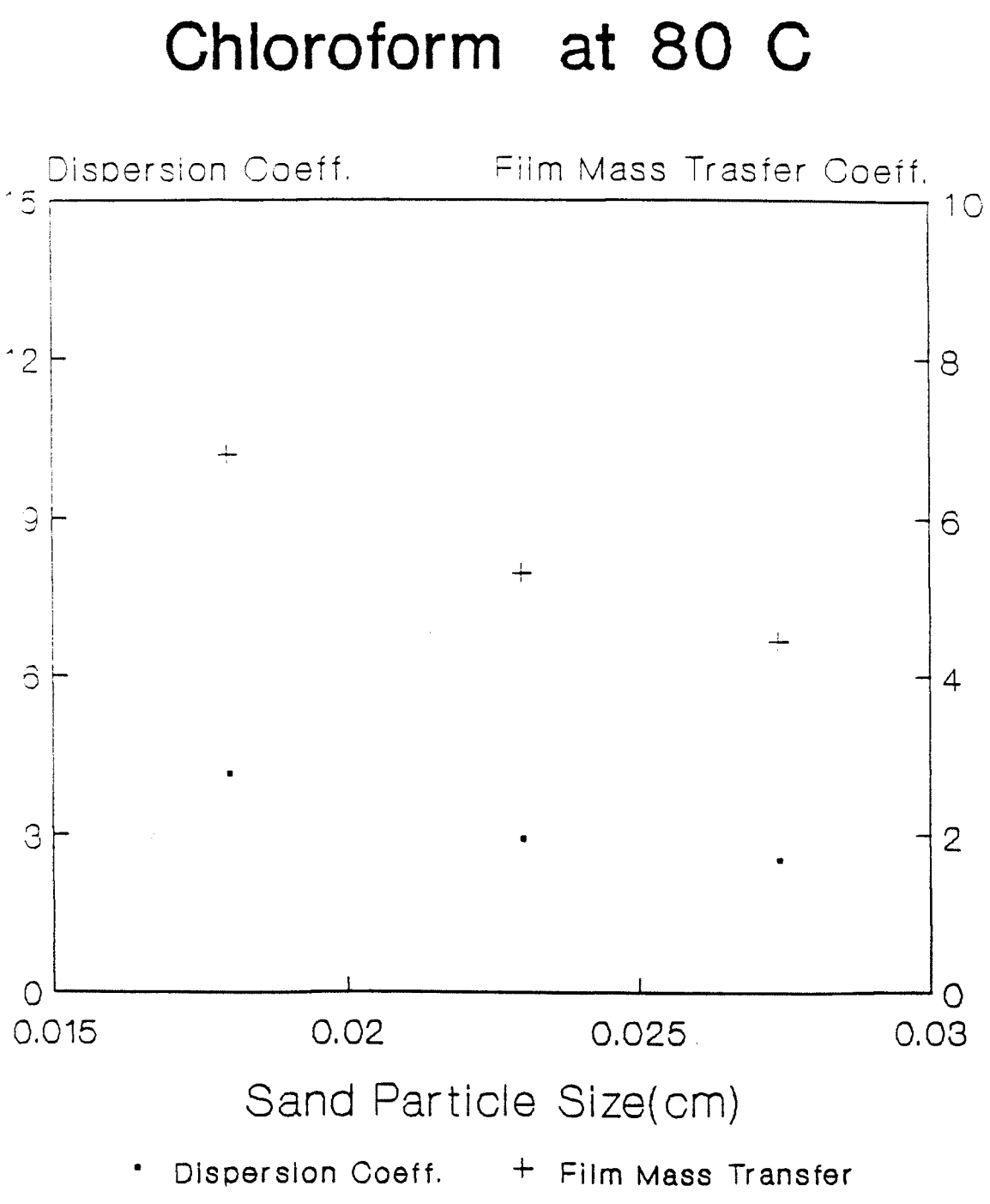


Table 5.4: Evaluated Mass Trasfer Parameters of Chloroform

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	2.506	4.26	
II	2.915	5.08	0.1168
III	4.131	6.51	

5.3 1,1,1-Trichloroethane

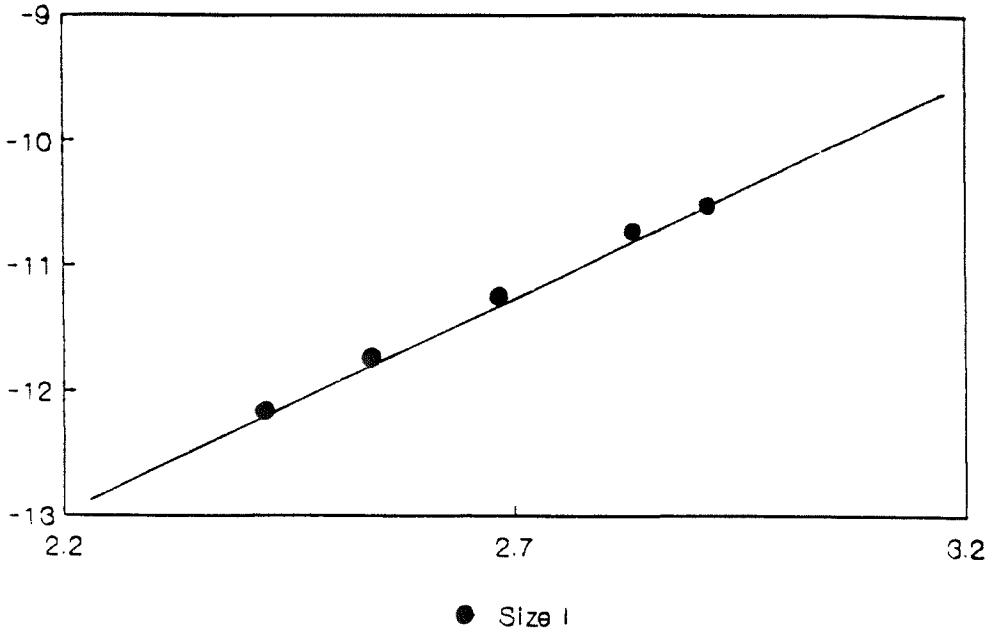
Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.5)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.17)*, *Figure(5.18)* and *Figure(5.19)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.20)* which shows slight increase in $-\Delta H/R$ with particle size.

Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.21)*,*Figure(5.22)*, and *Figure(5.23)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.24)*. Both coefficients show a decrease with increasing particle size.

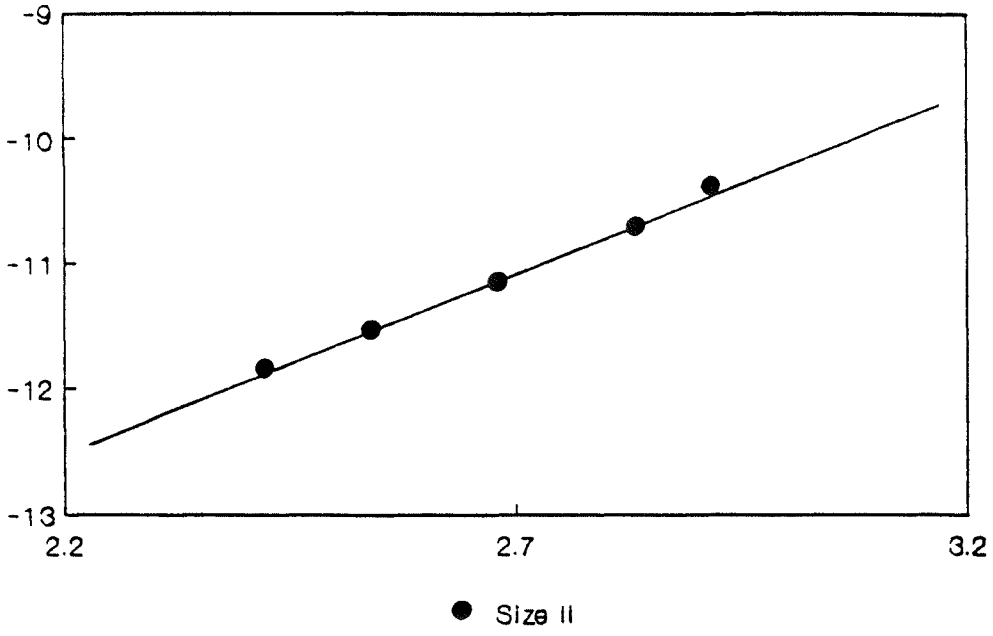
Mass transfer parameters of 1,1,1-Trichloroethane at each temperature are listed in *Table(5.6)*.

Figure 5.17: Heats of Adsorption of $C_2H_3Cl_3$: Size I



1,1,1-trichloroethane at 2.0

Figure 5.18: Heats of Adsorption of $C_2H_3Cl_3$: Size II



1,1,1-trichloroethane at 2.0

Table 5.5: Equilibrium Constants and Heats of Adsortion of $C_2H_3Cl_3$

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
	70	9.230	
	80	7.741	
I	100	4.971	3.423
	120	3.109	
	140	2.101	
	70	10.707	
	80	8.131	
II	100	5.191	2.965
	120	3.816	
	140	2.980	
	70	8.835	
	80	6.901	
III	100	4.377	2.522
	120	3.700	
	140	3.048	

Figure 5.19: Heats of Adsorption of $C_2H_3Cl_3$: Size III

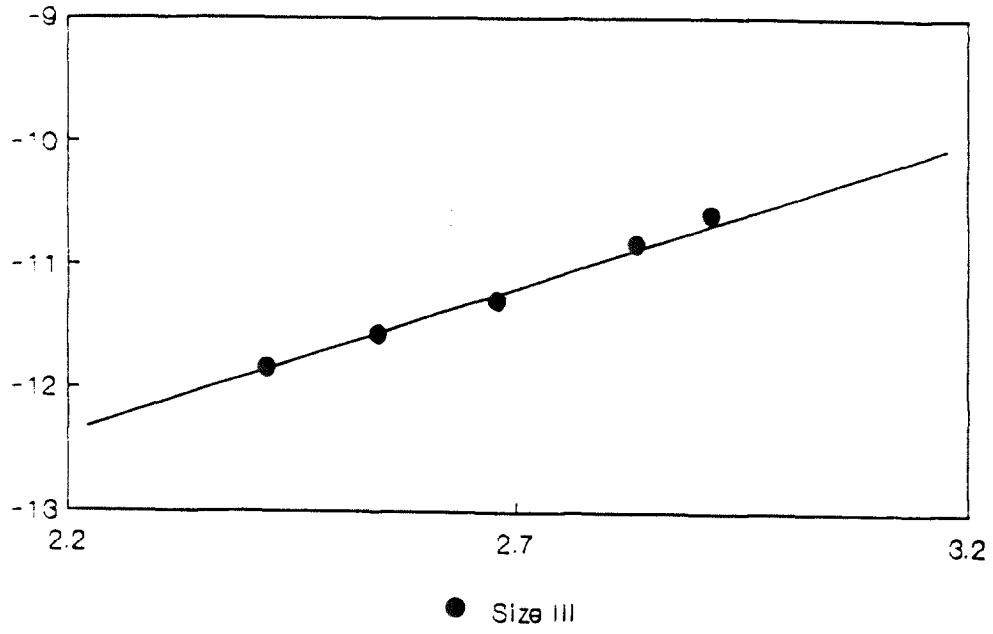


Table 5.6: Evaluated Mass Trasfer Parameters of 1,1,1-Trichloroethane

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	1.634	3.95	
II	4.049	4.70	0.1082
III	5.787	6.03	

Figure 5.20: Particle Size Dependence of $-\Delta H/R$

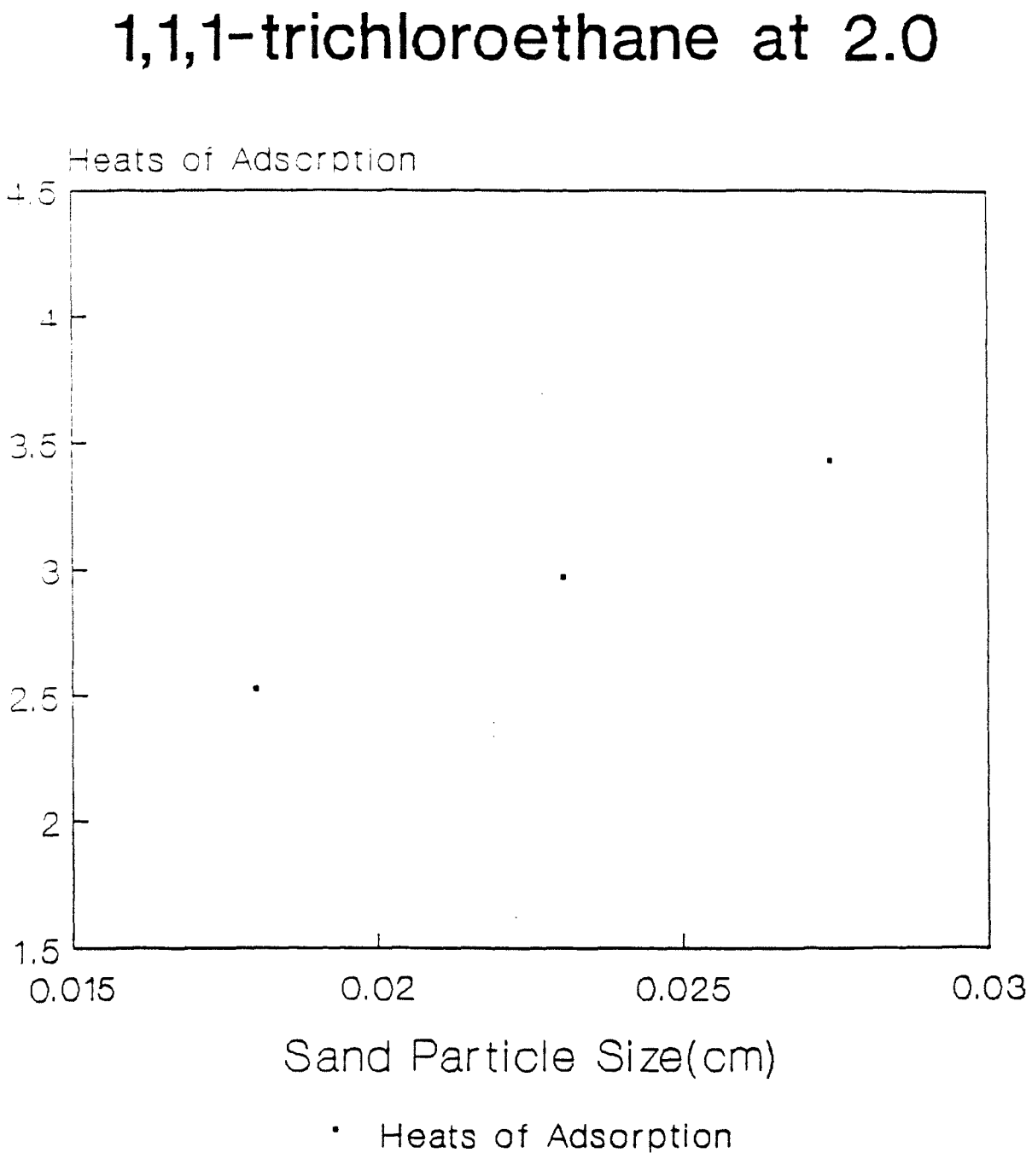
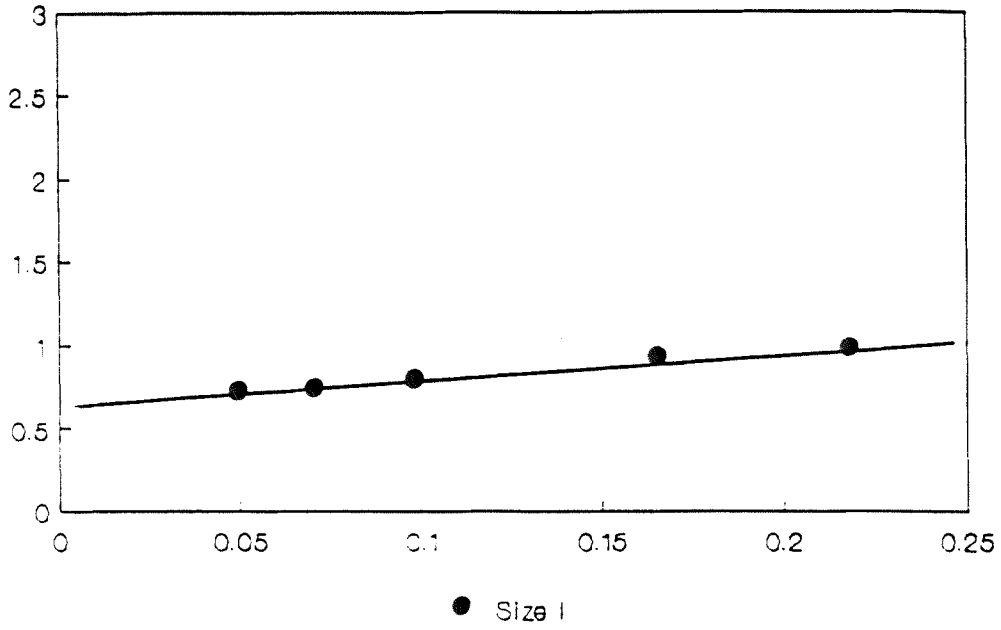
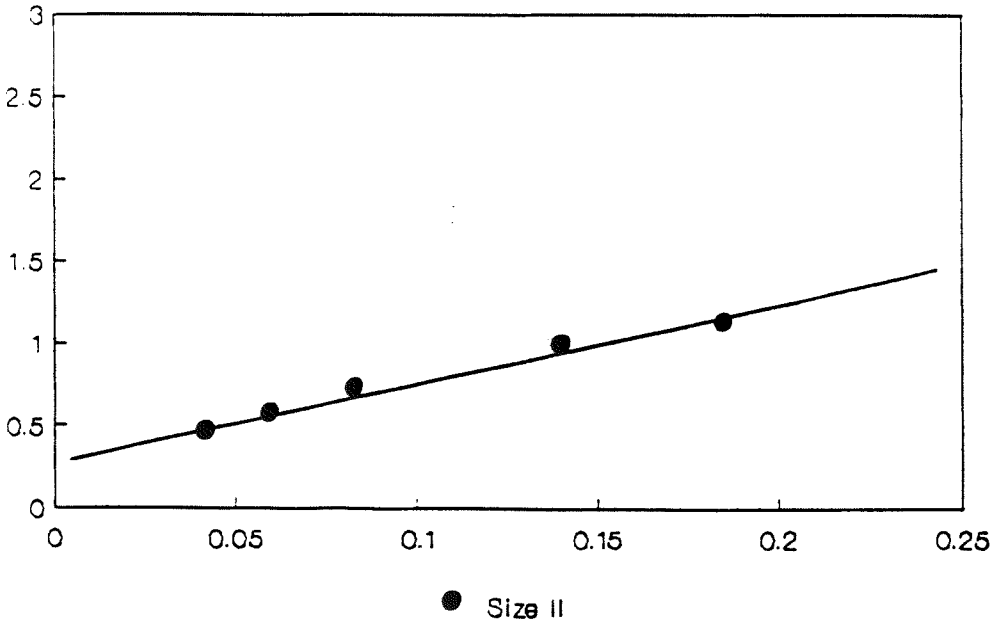


Figure 5.21: Dispersion Coefficient of $C_2H_3Cl_3$: Size I



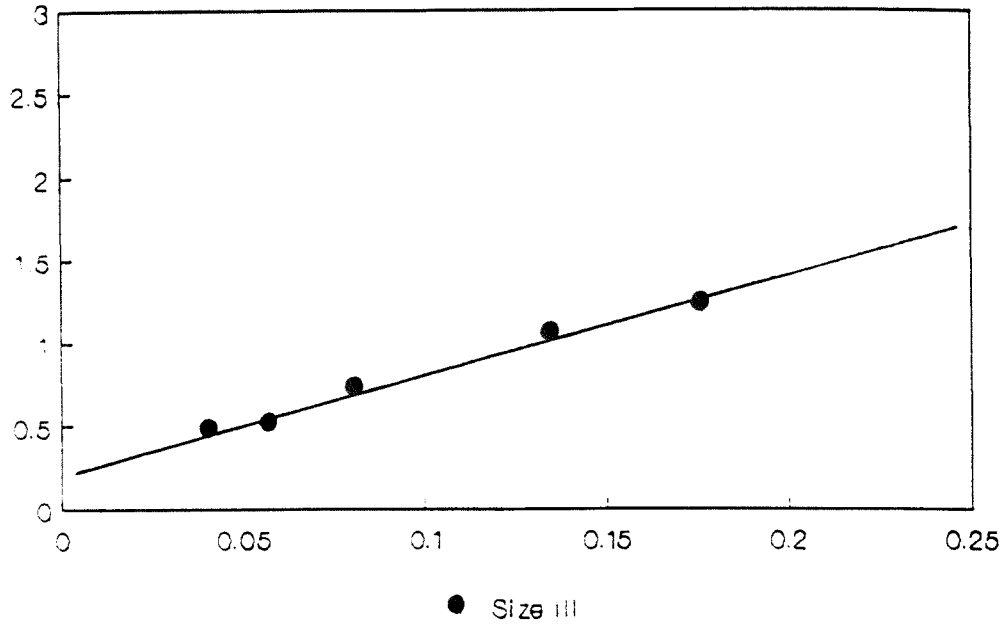
1,1,1-trichloroethane at 80 C

Figure 5.22: Dispersion Coefficient of $C_2H_3Cl_3$: Size II



1,1,1-trichloroethane at 80 C

Figure 5.23: Dispersion Coefficient of $C_2H_3Cl_3$: Size III



1,1,1-trichloroethane at 80 C

5.4 Benzene

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.7)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.25)*, *Figure(5.26)* and *Figure(5.27)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.28)* which shows slight increase in $-\Delta H/R$ with particle size.

Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.29)*,*Figure(5.30)*, and *Figure(5.31)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.32)*. Both coefficients show a decrease with increasingparticle size.

Figure 5.24: Particle Size Dependence of D_z

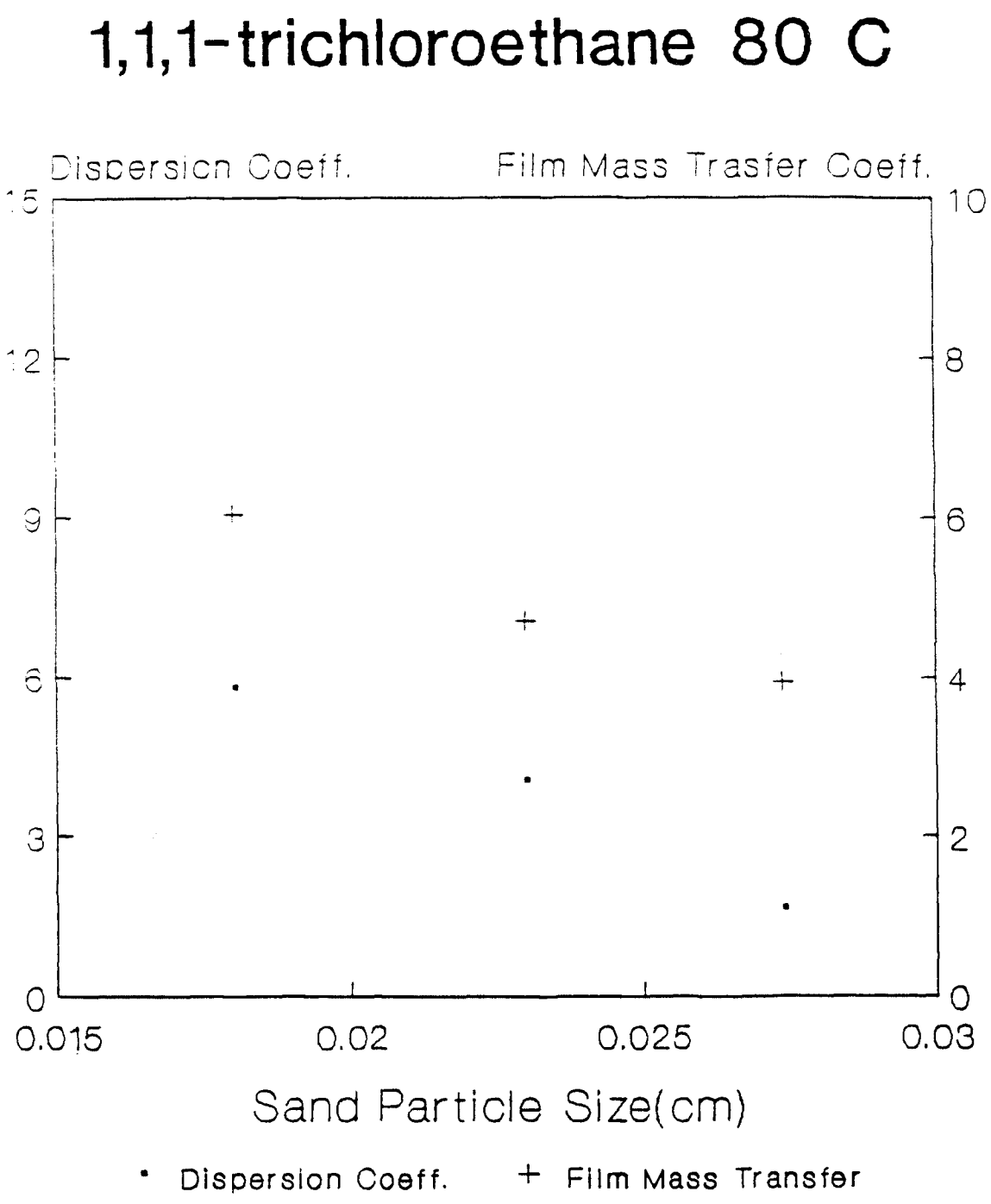
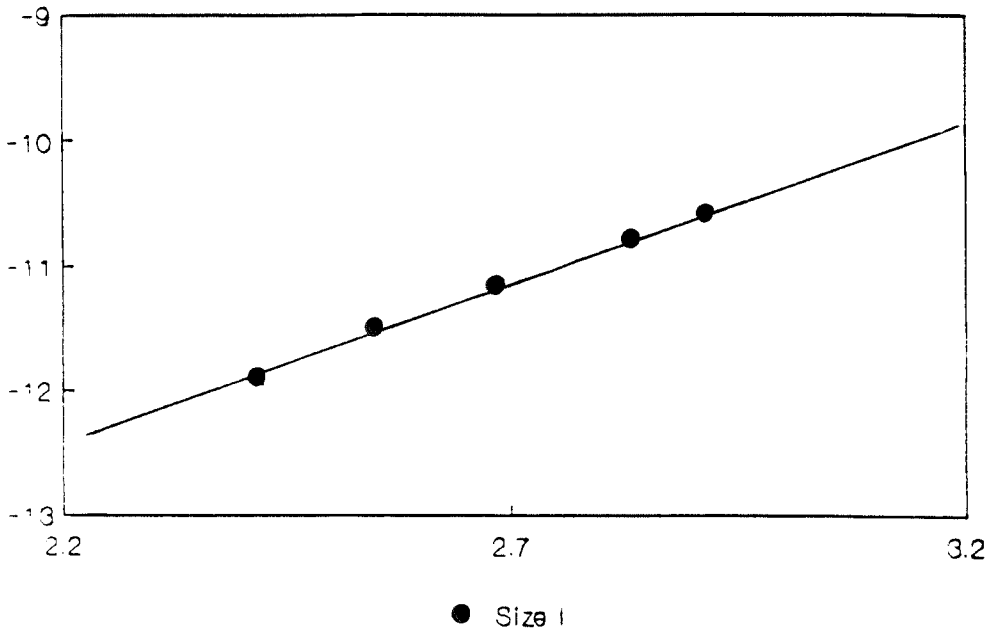
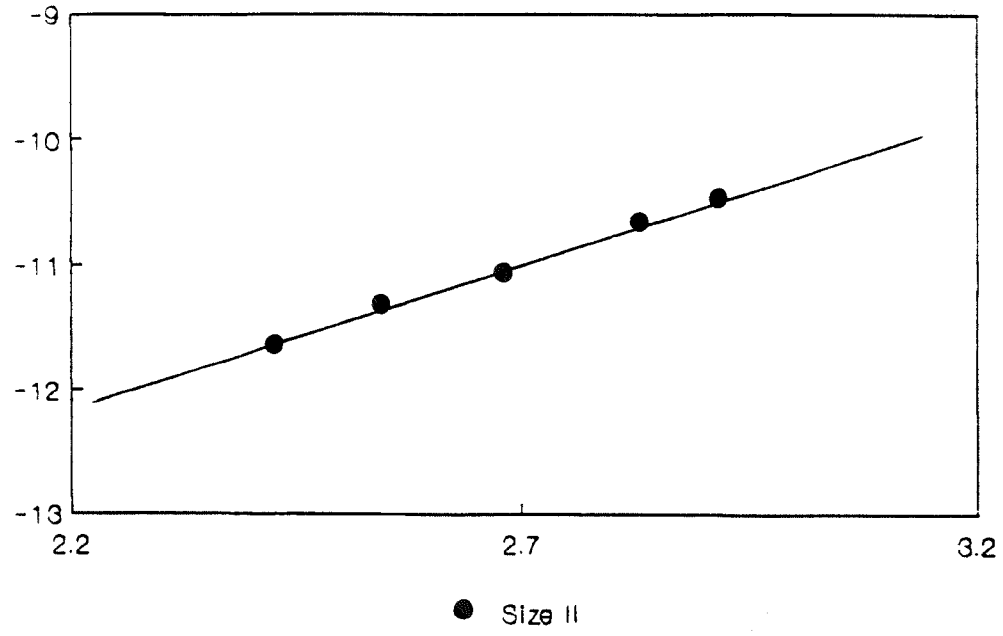


Figure 5.25: Heats of Adsortion of C_6H_6 : Size I



Benzene at 2.0

Figure 5.26: Heats of Adsortion of C_6H_6 : Size II

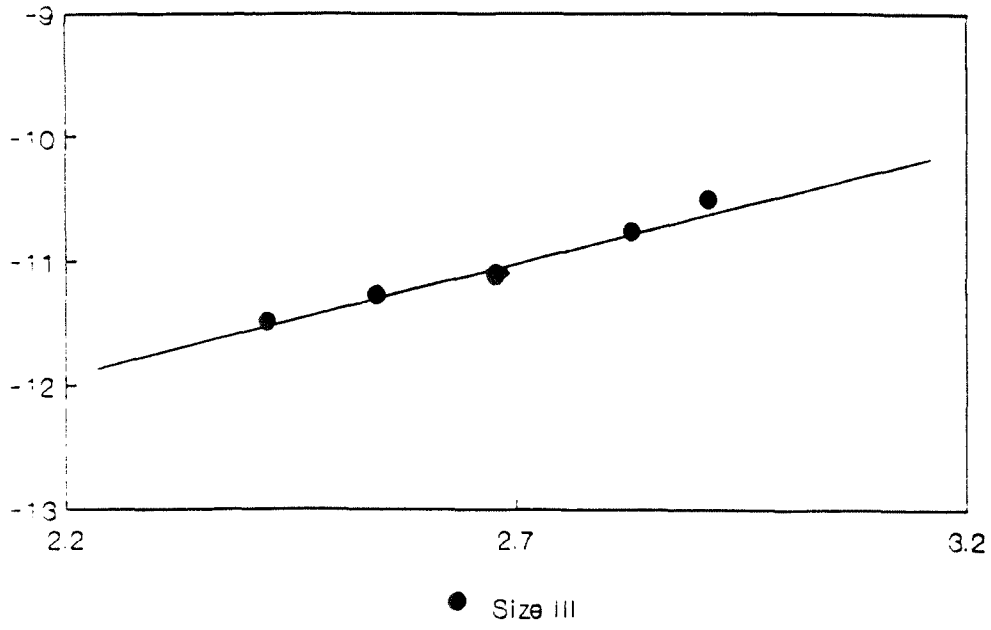


Benzene at 2.0

Table 5.7: Equilibrium Constants and Heats of Adsortion of C_6H_6

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
I	70	8.752	2.682
	80	7.346	
	100	5.555	
	120	4.140	
	140	2.678	
II	70	9.985	2.338
	80	8.524	
	100	5.750	
	120	5.033	
	140	3.713	
III	70	9.465	1.914
	80	7.523	
	100	5.169	
	120	4.924	
	140	4.344	

Figure 5.27: Heats of Adsorption of C_6H_6 : Size III



Benzene at 2.0

Mass transfer parameters of Benzene at each temperature are listed in *Table(5.8)*.

Figure 5.28: Particle Size Dependence of $-\Delta H/R$

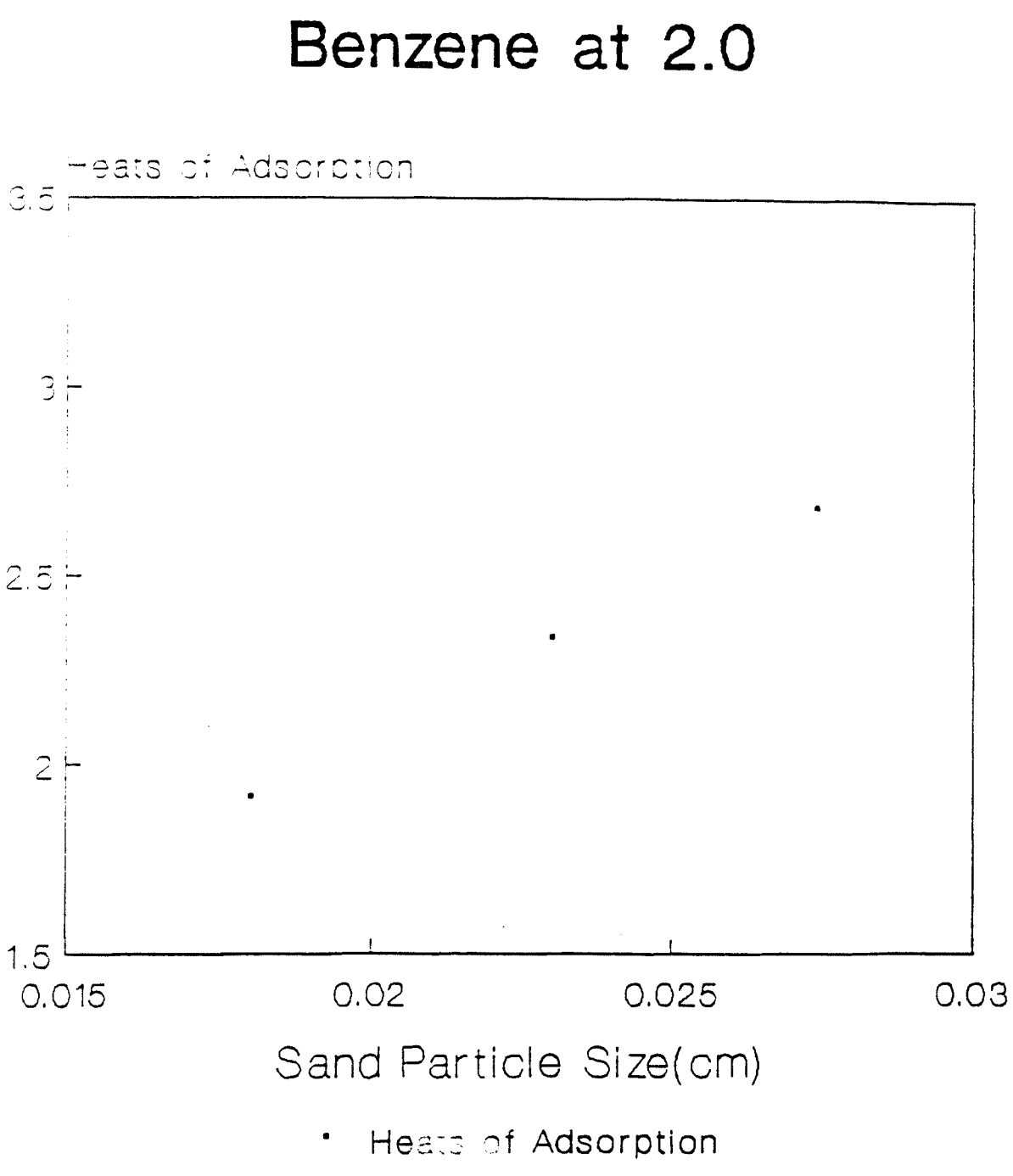
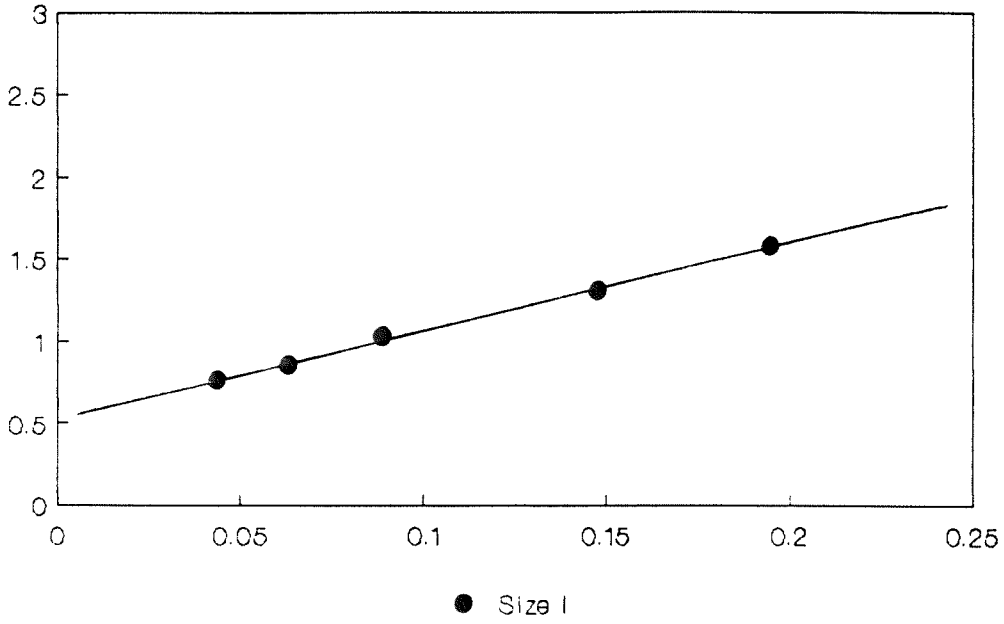
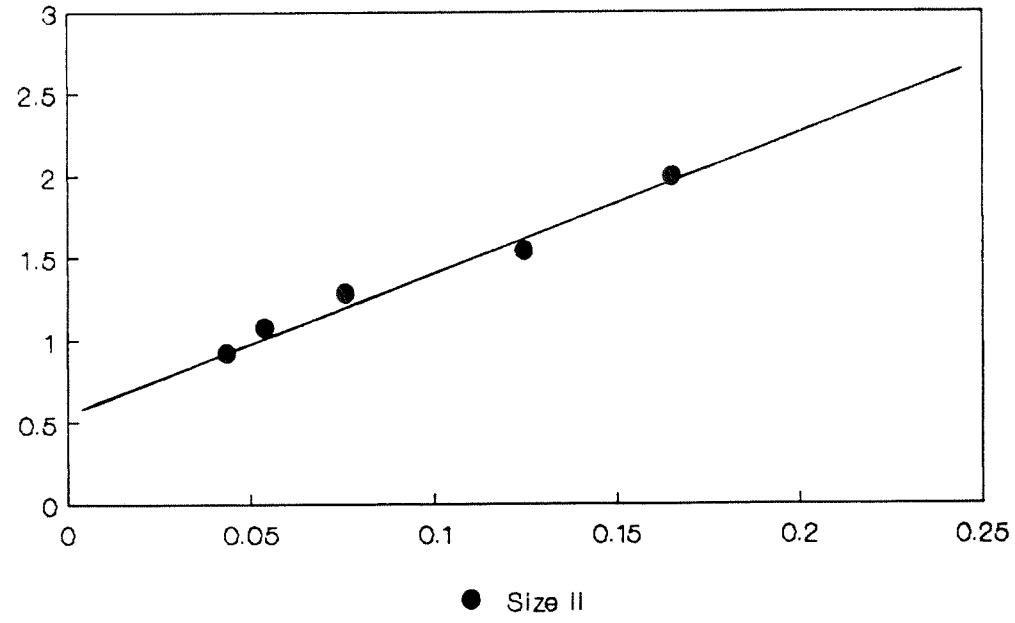


Figure 5.29: Dispersion Coefficient of C_6H_6 : Size I



Benzene at 100 C

Figure 5.30: Dispersion Coefficient of C_6H_6 : Size II



Benzene at 100 C

Figure 5.31: Dispersion Coefficient of C_6H_6 : Size III

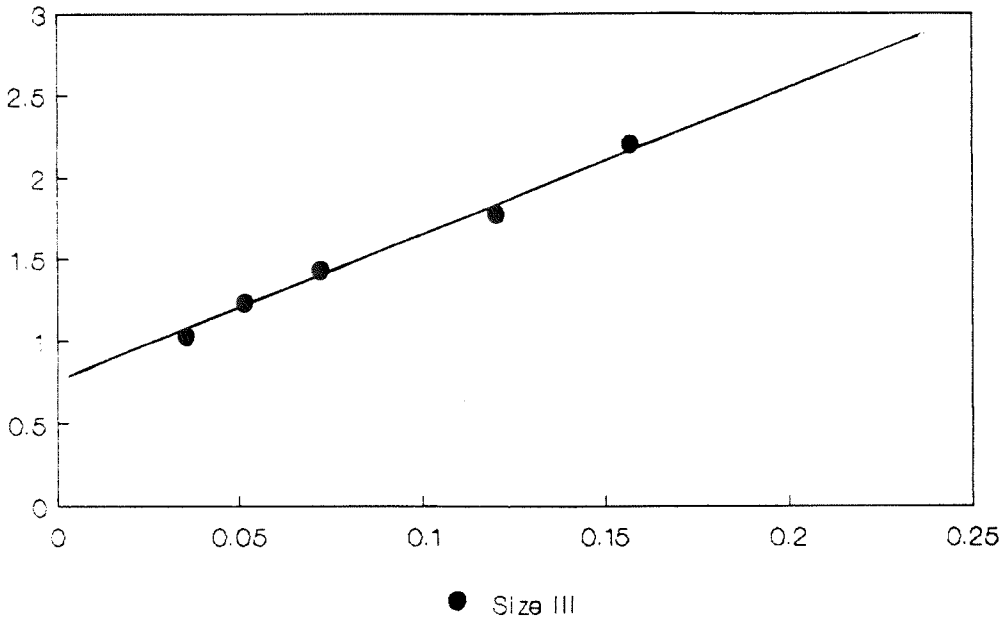


Table 5.8: Evaluated Mass Trasfer Parameters of Benzene

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	5.401	4.45	
II	7.958	5.30	0.1219
III	9.058	6.80	

Figure 5.32: Particle Size Dependence of D_z

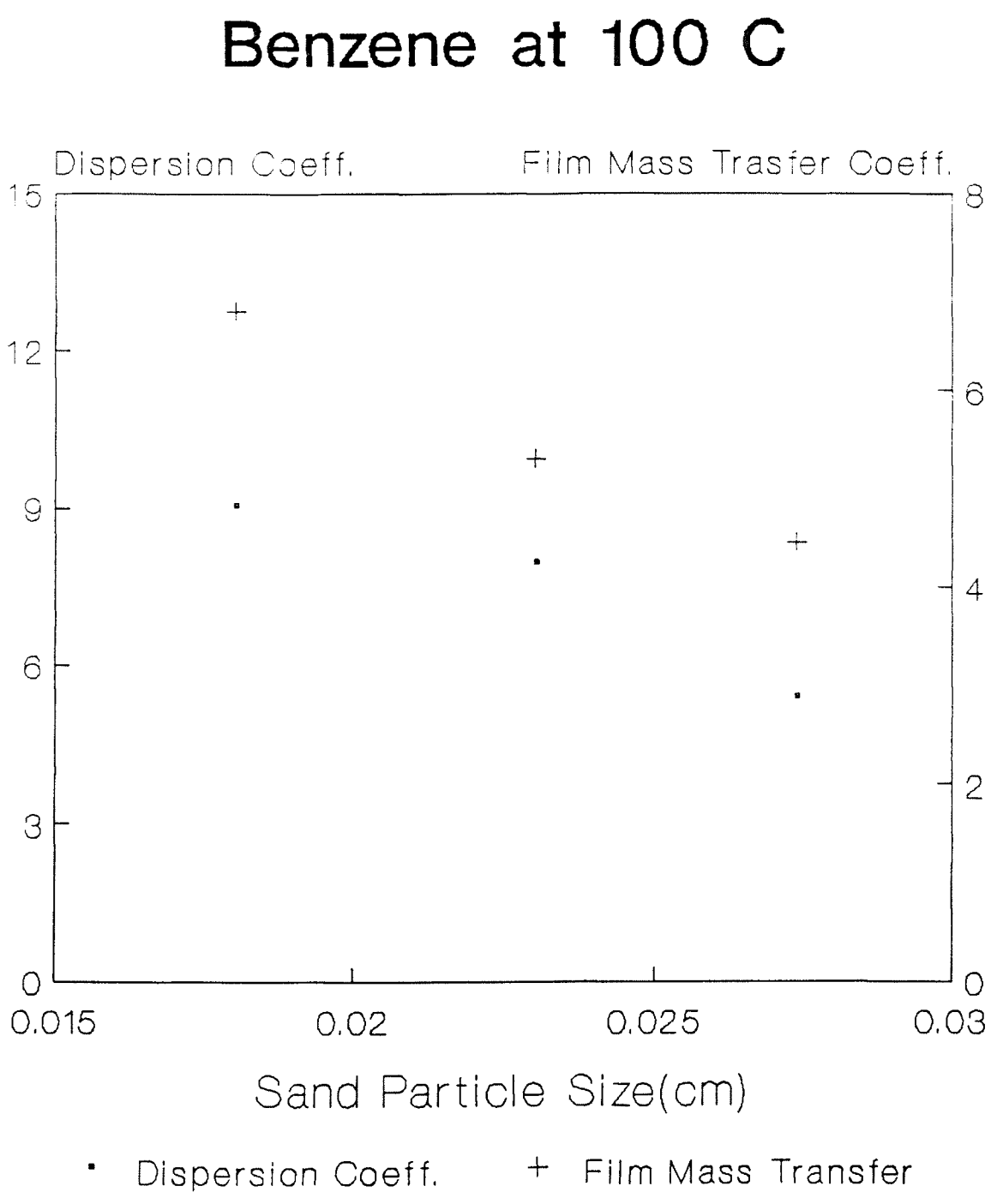
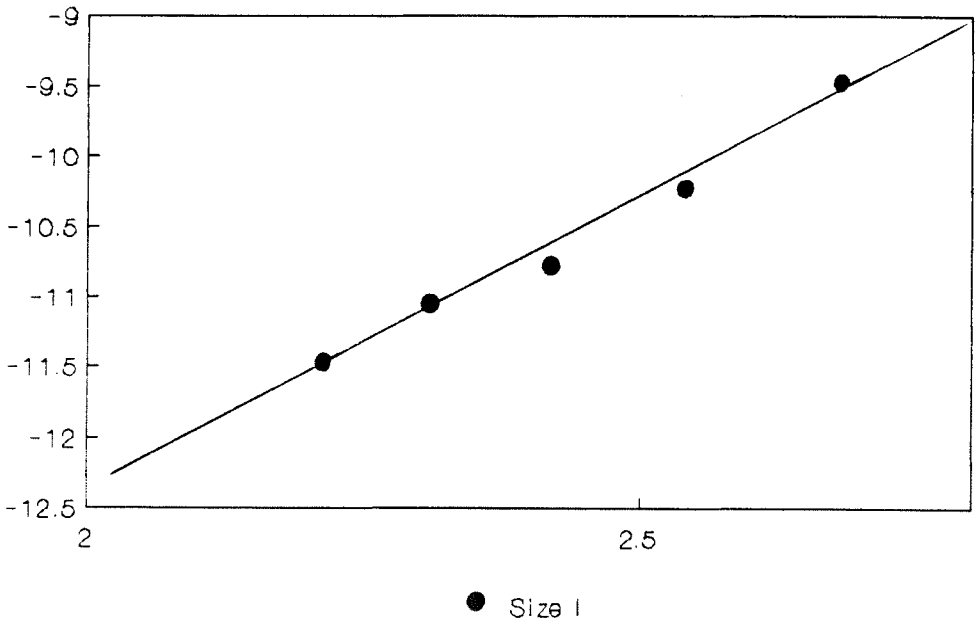


Figure 5.33: Heats of Adsorption of C_7H_8 : Size I



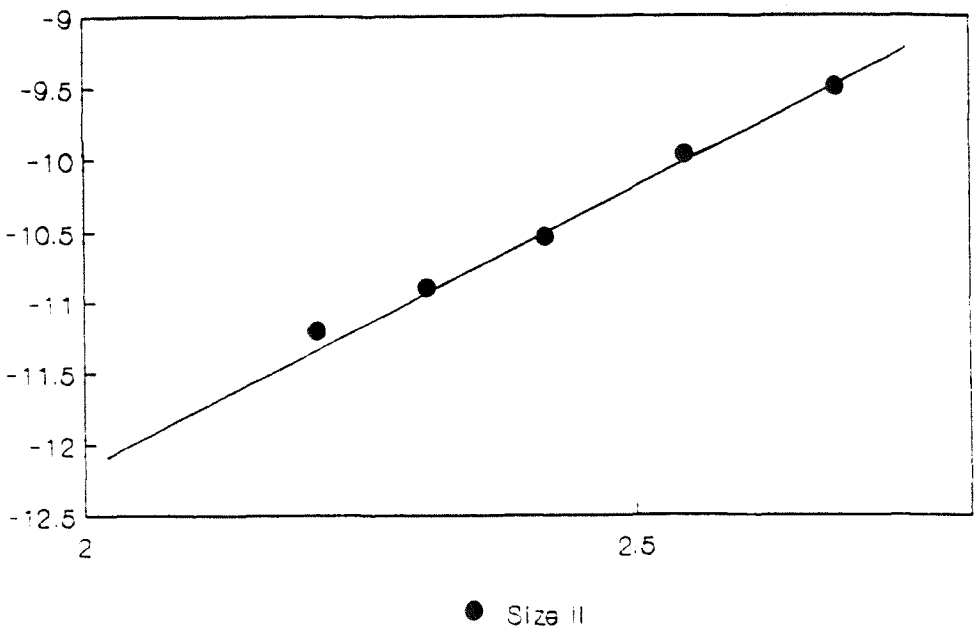
5.5 Toluene

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.9)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.33)*, *Figure(5.34)* and *Figure(5.35)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.36)* which shows slight increase in $-\Delta H/R$ with particle size.

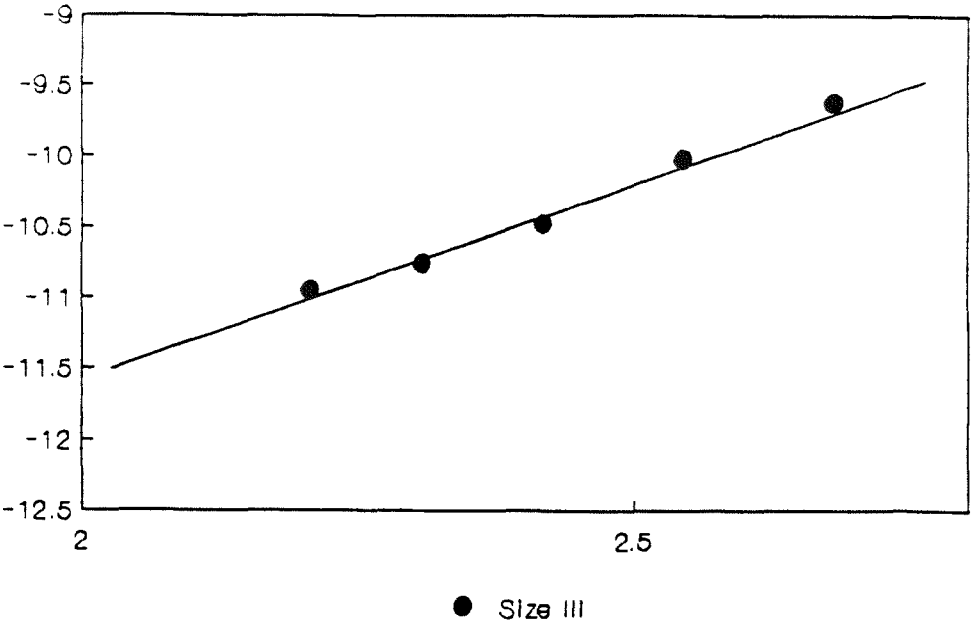
Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.37)*,*Figure(5.38)*, and *Figure(5.39)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.40)*. Both coefficients show a decrease with increasing particle size.

Figure 5.34: Heats of Adsorption of C_7H_8 : Size II



Toluene at 2.0

Figure 5.35: Heats of Adsorption of C_7H_8 : Size III



Toluene at 2.0

Table 5.9: Equilibrium Constants and Heats of Adsortion of C_7H_8

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
I	100	29.221	4.074
	120	13.527	
	140	8.371	
	160	7.015	
	180	4.754	
II	100	28.332	3.653
	120	18.457	
	140	10.705	
	160	8.193	
	180	6.320	
III	100	24.889	2.921
	120	17.545	
	140	11.093	
	160	8.791	
	180	8.090	

Figure 5.36: Particle Size Dependence of $-\Delta H/R$

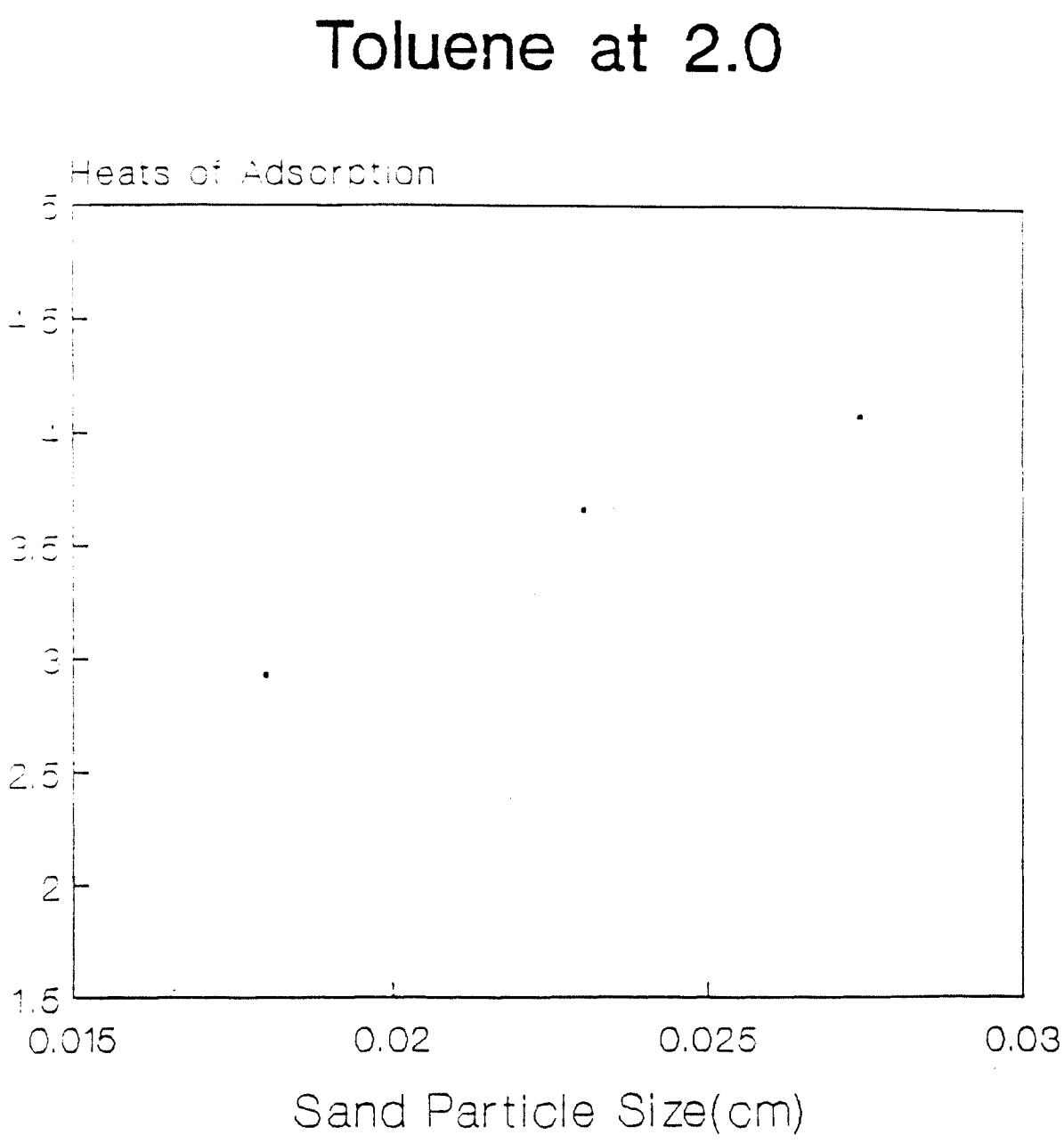


Figure 5.37: Dispersion Coefficient of C_7H_8 : Size I

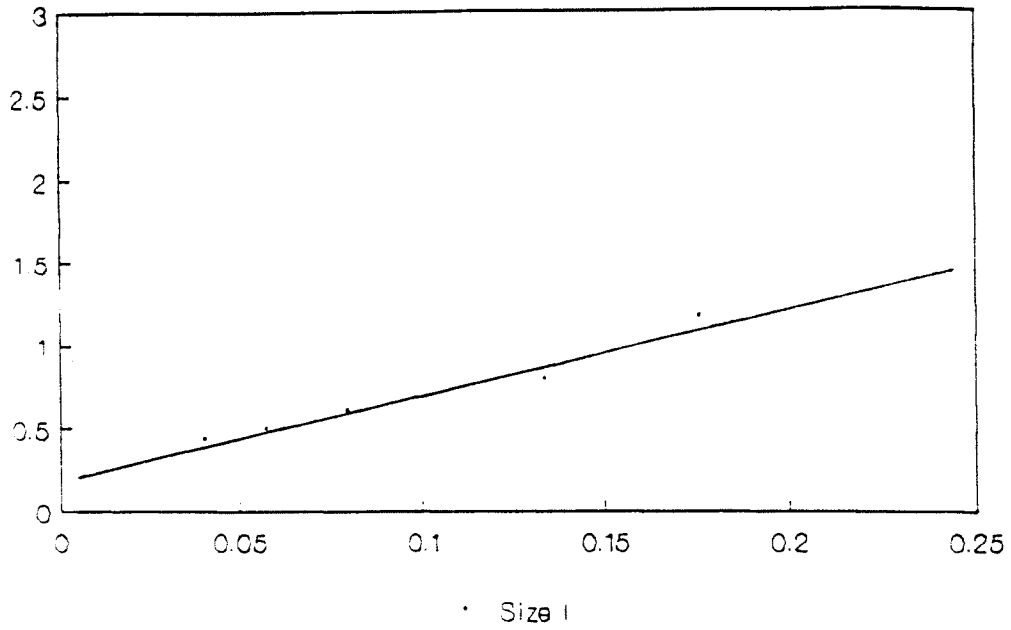


Figure 5.38: Dispersion Coefficient of C_7H_8 : Size II

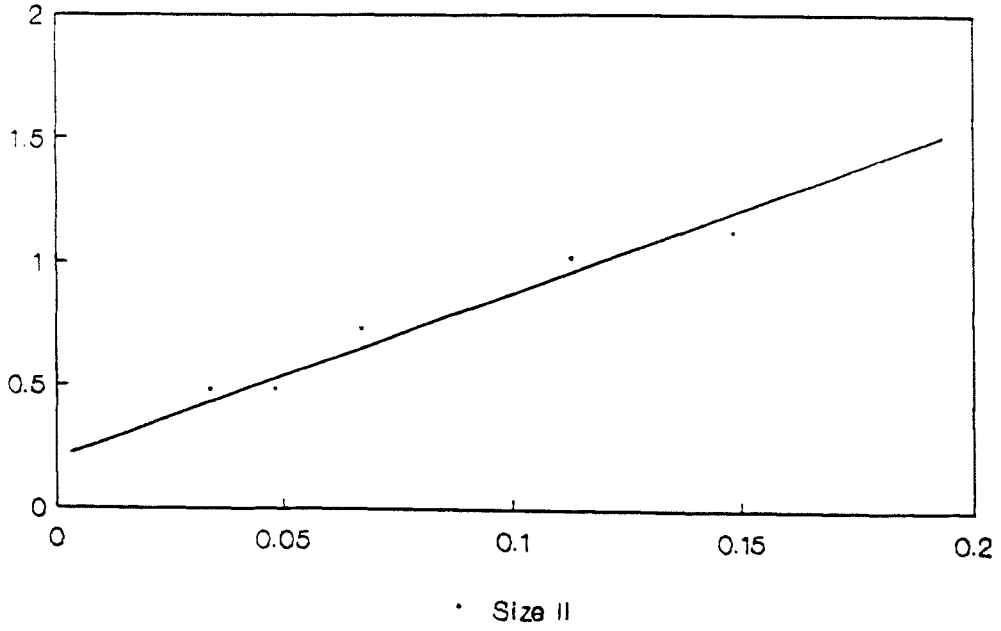
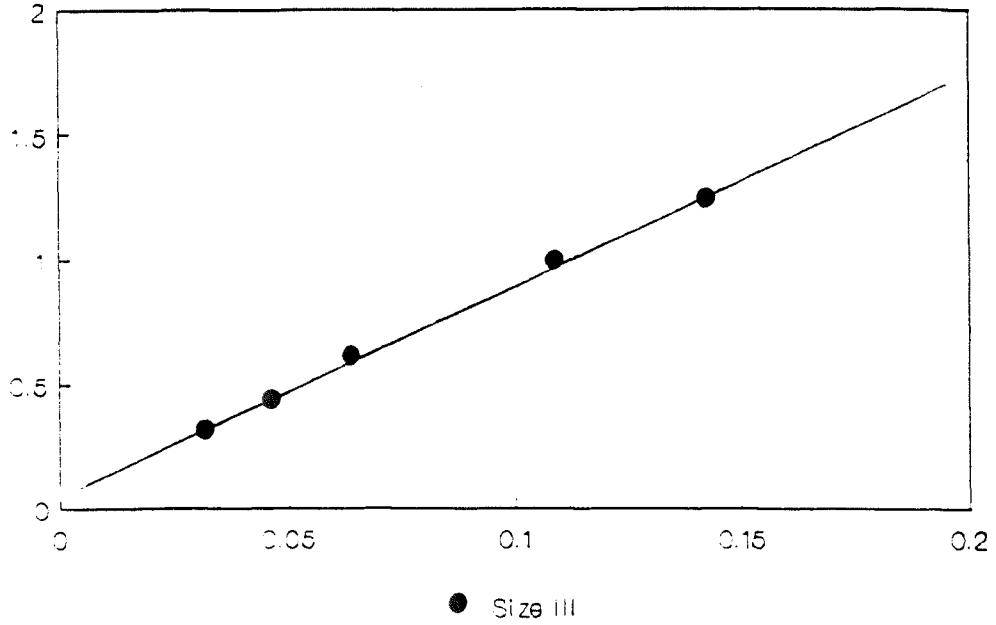


Figure 5.39: Dispersion Coefficient of C_7H_8 : Size III



Toluene at 120 C

Mass transfer parameters of Toluene at each temperature are listed in *Table(5.10)*.

Figure 5.40: Particle Size Dependence of D_z

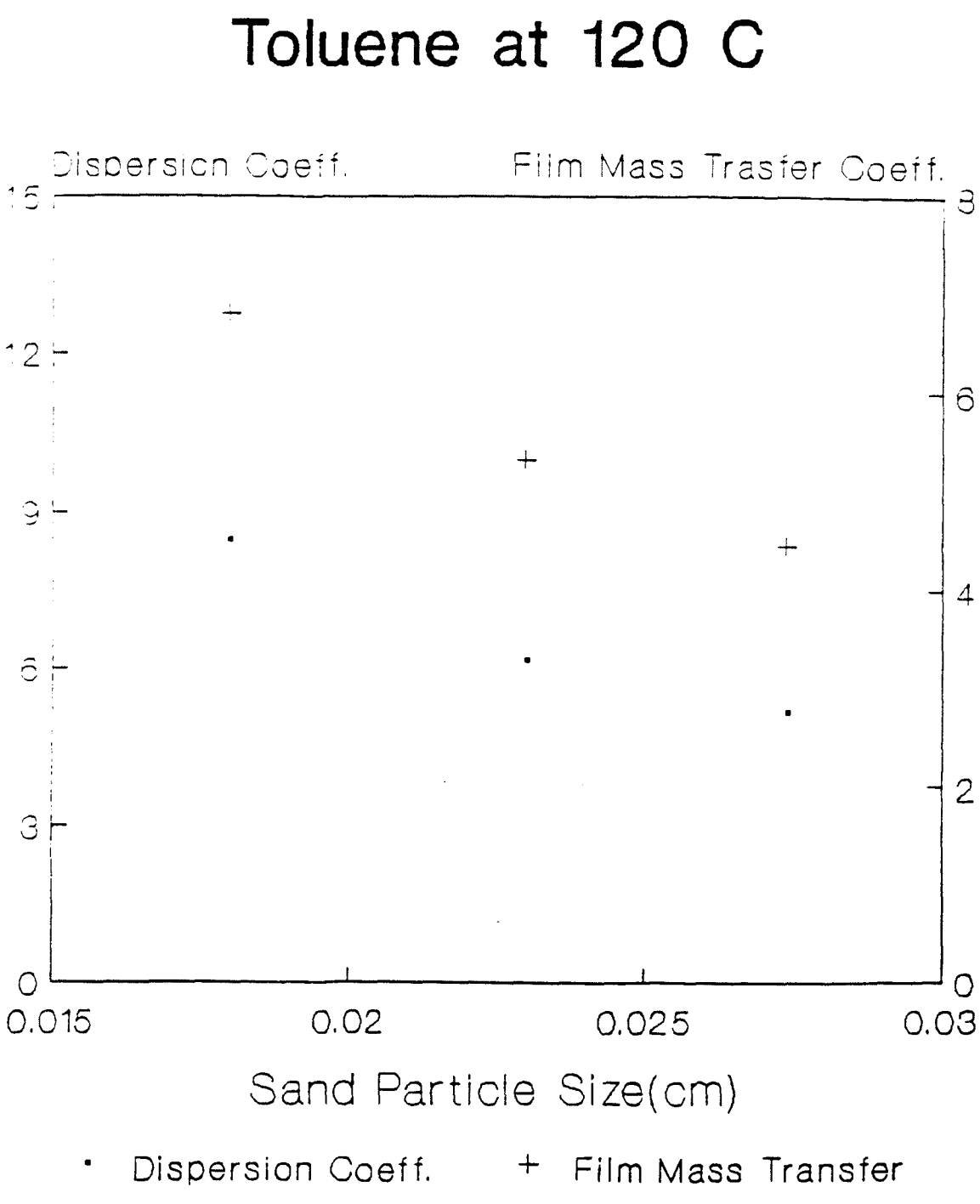


Table 5.10: Evaluated Mass Trasfer Parameters of Toluene

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	5.144	4.47	
II	6.156	5.33	0.1225
III	8.450	6.83	

5.6 Tetrachloroethylene

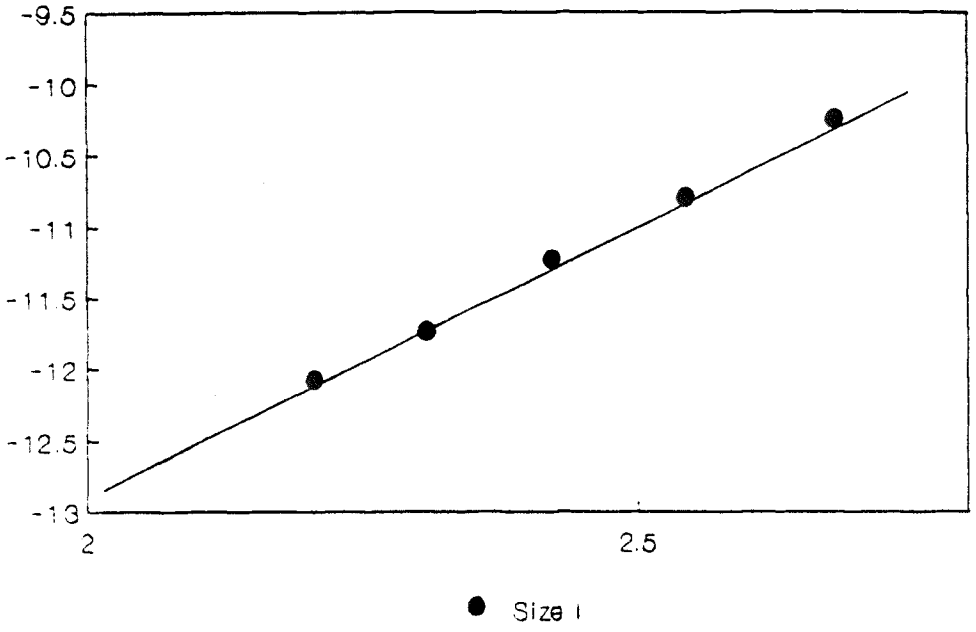
Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.11)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.41)*, *Figure(5.42)* and *Figure(5.43)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.44)* which shows slight increase in $-\Delta H/R$ with particle size.

Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.45)*,*Figure(5.46)*, and *Figure(5.47)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.48)*. Both coefficients show a decrease with increasing particle size.

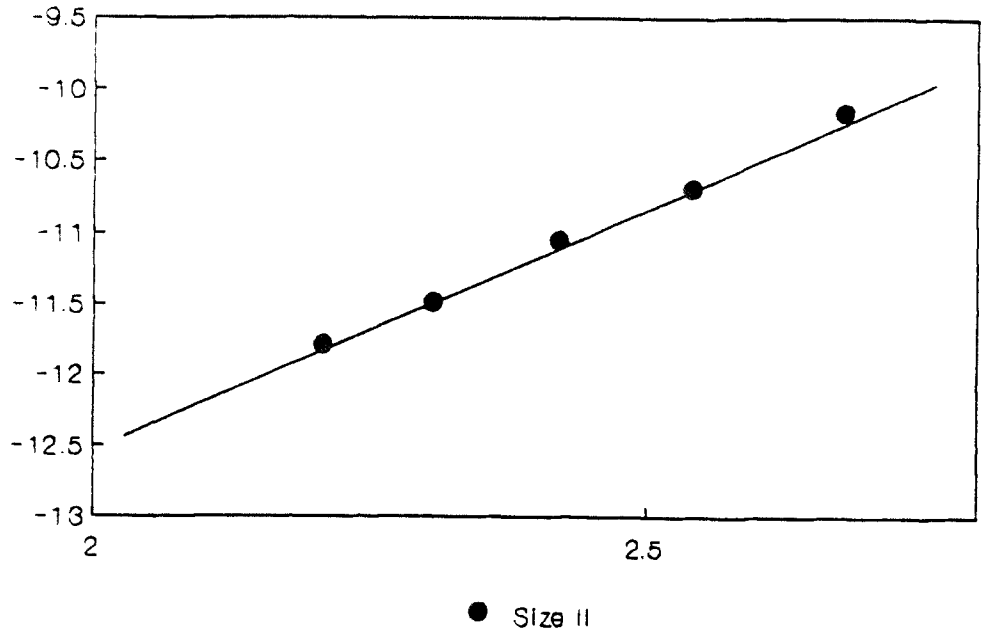
Mass transfer parameters of Tetrachloroethylene at each temperature are listed in *Table(5.12)*.

Figure 5.41: Heats of Adsorption of C_2Cl_4 : Size I



Tetrachloroethylene at 2.0

Figure 5.42: Heats of Adsorption of C_2Cl_4 : Size II



Tetrachloroethylene at 2.0

Table 5.11: Equilibrium Constants and Heats of Adsortion of C_2Cl_4

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
I	100	13.561	3.924
	120	8.148	
	140	5.637	
	160	3.556	
	180	2.578	
II	100	14.519	3.381
	120	8.780	
	140	6.640	
	160	4.523	
	180	3.514	
III	100	13.803	3.224
	120	8.274	
	140	6.510	
	160	4.524	
	180	3.561	

Figure 5.43: Heats of Adsorption of C_2Cl_4 : Size III

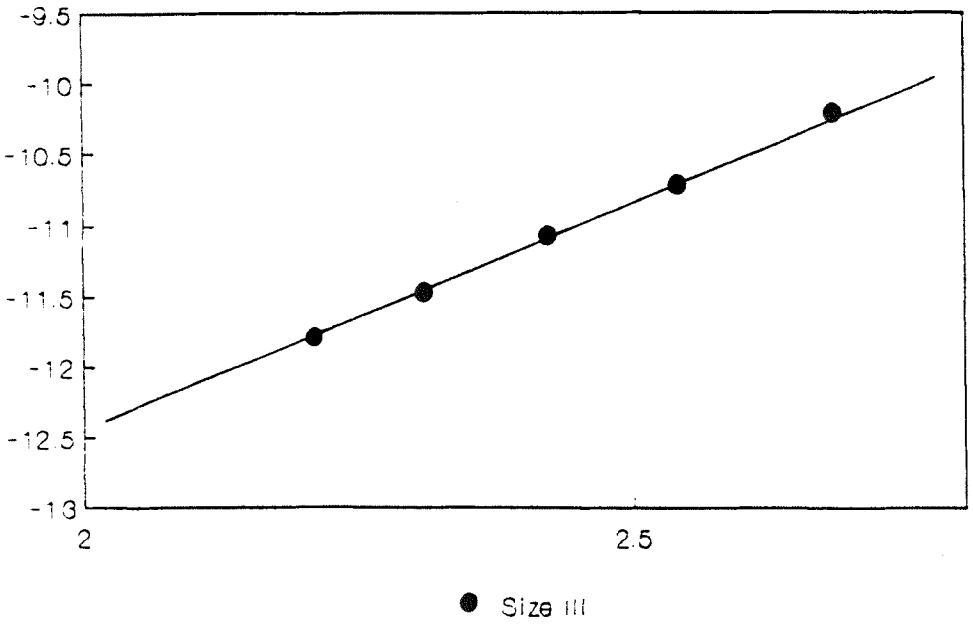


Table 5.12: Evaluated Mass Trasfer Parameters of Tetrachloroethylene

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	3.247	4.89	
II	3.975	5.82	0.1339
III	4.110	7.47	

Figure 5.44: Particle Size Dependence of $-\Delta H/R$

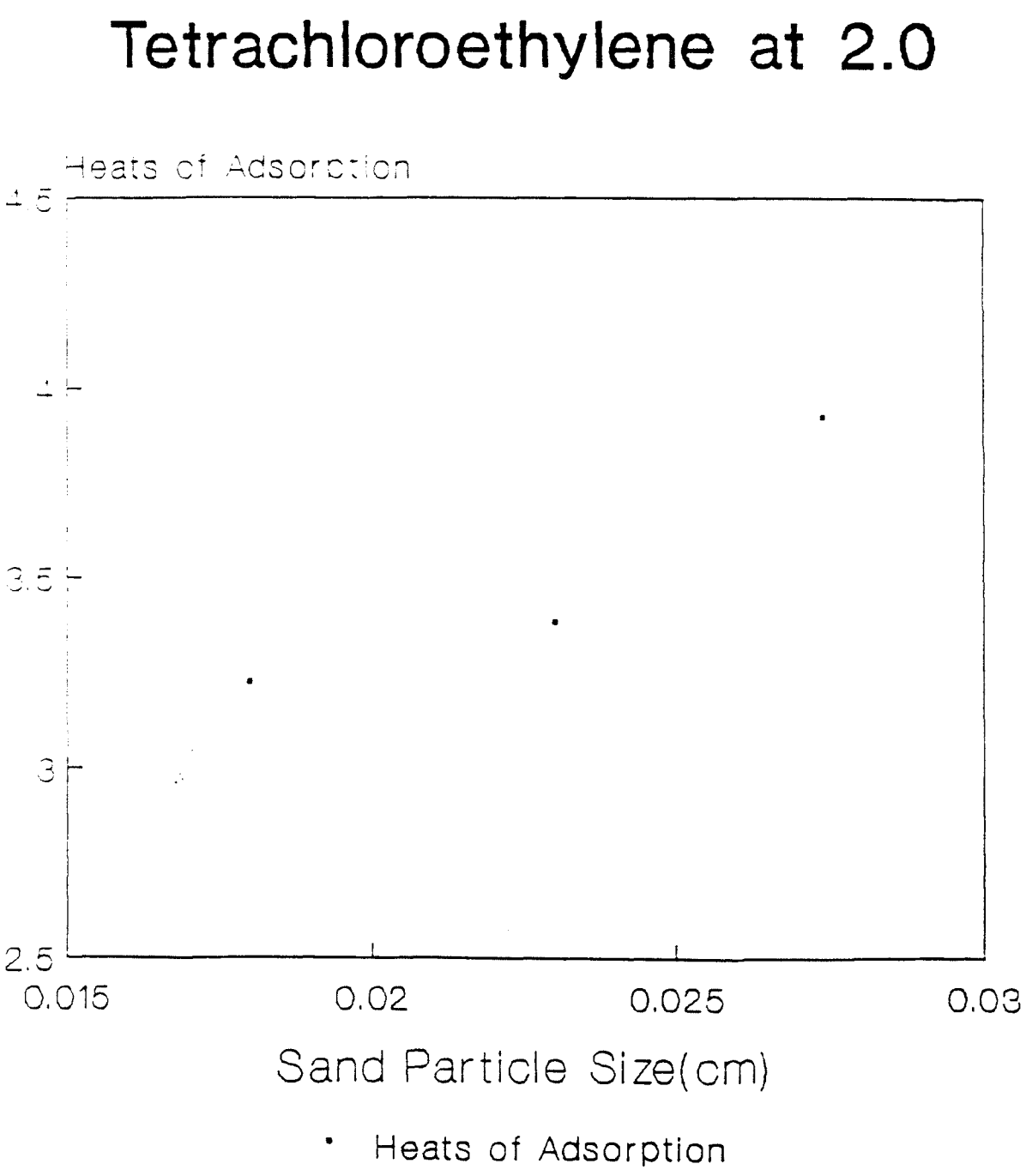
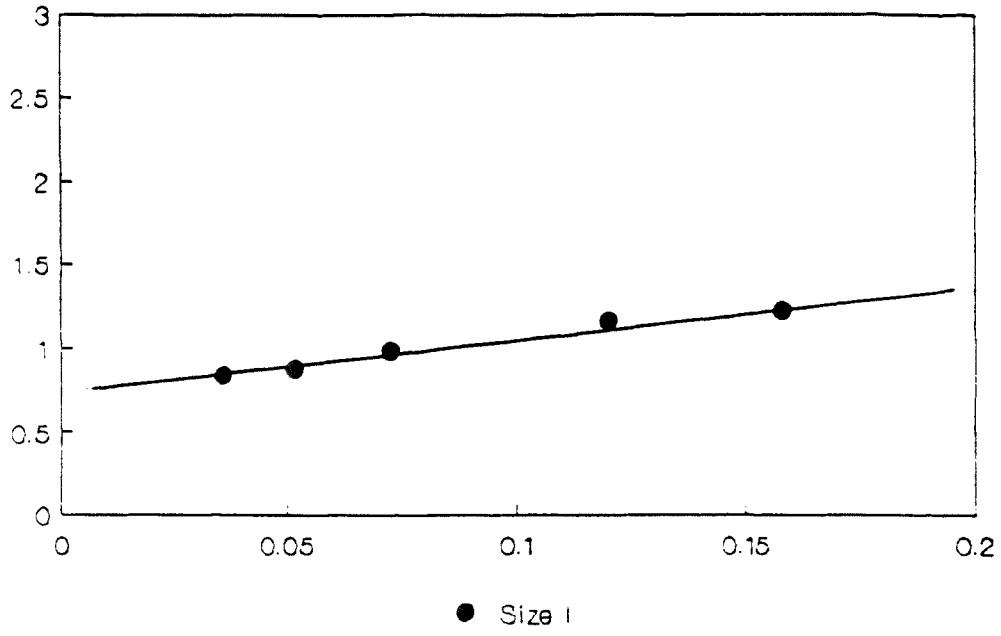
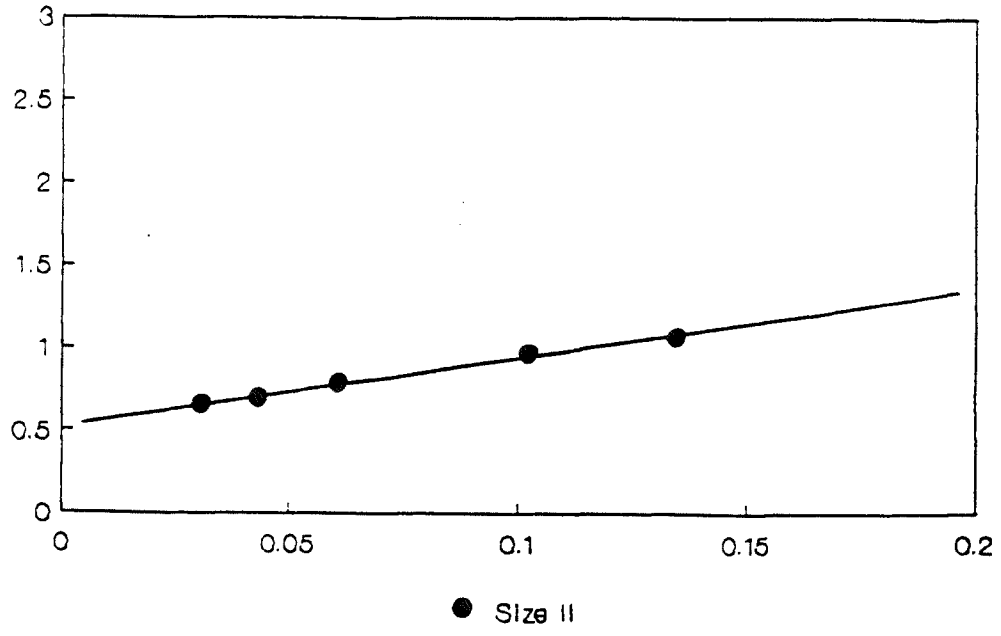


Figure 5.45: Dispersion Coefficient of C_2Cl_4 : Size I



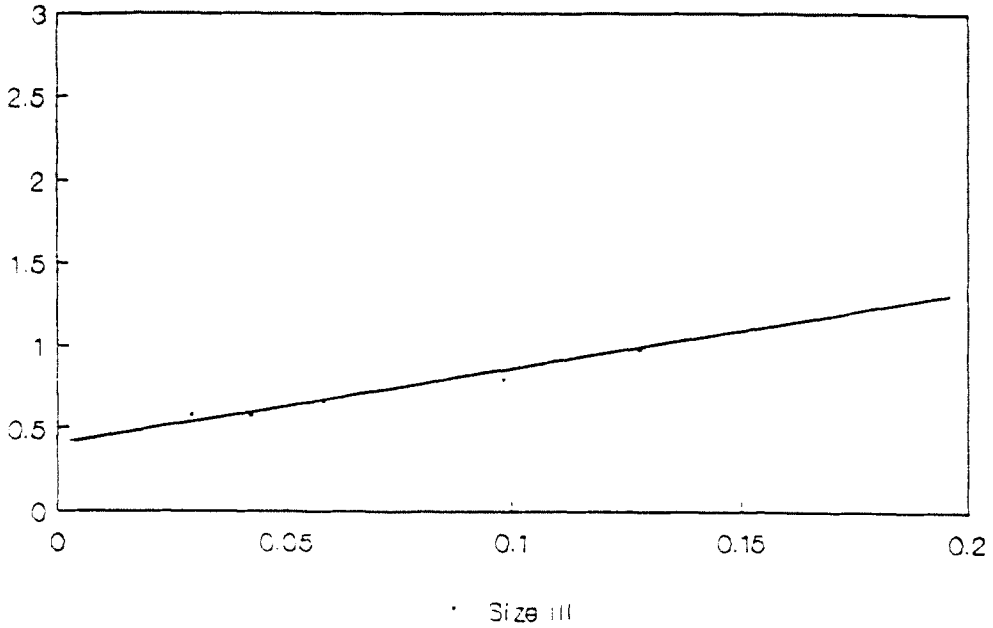
Tetrachloroethylene at 140

Figure 5.46: Dispersion Coefficient of C_2Cl_4 : Size II



Tetrachloroethylene at 140

Figure 5.47: Dispersion Coefficient of C_2Cl_4 : Size III



Tetrachloroethylene at 140

5.7 Chlorobenzene

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.13)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.49)*, *Figure(5.50)*, and *Figure(5.51)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.52)* which shows slight increase in $-\Delta H/R$ with particle size.

Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.53)*,*Figure(5.54)*, and *Figure(5.55)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.56)*. Both coefficients show a decrease with increasing particle size.

Figure 5.48: Particle Size Dependence of D_z

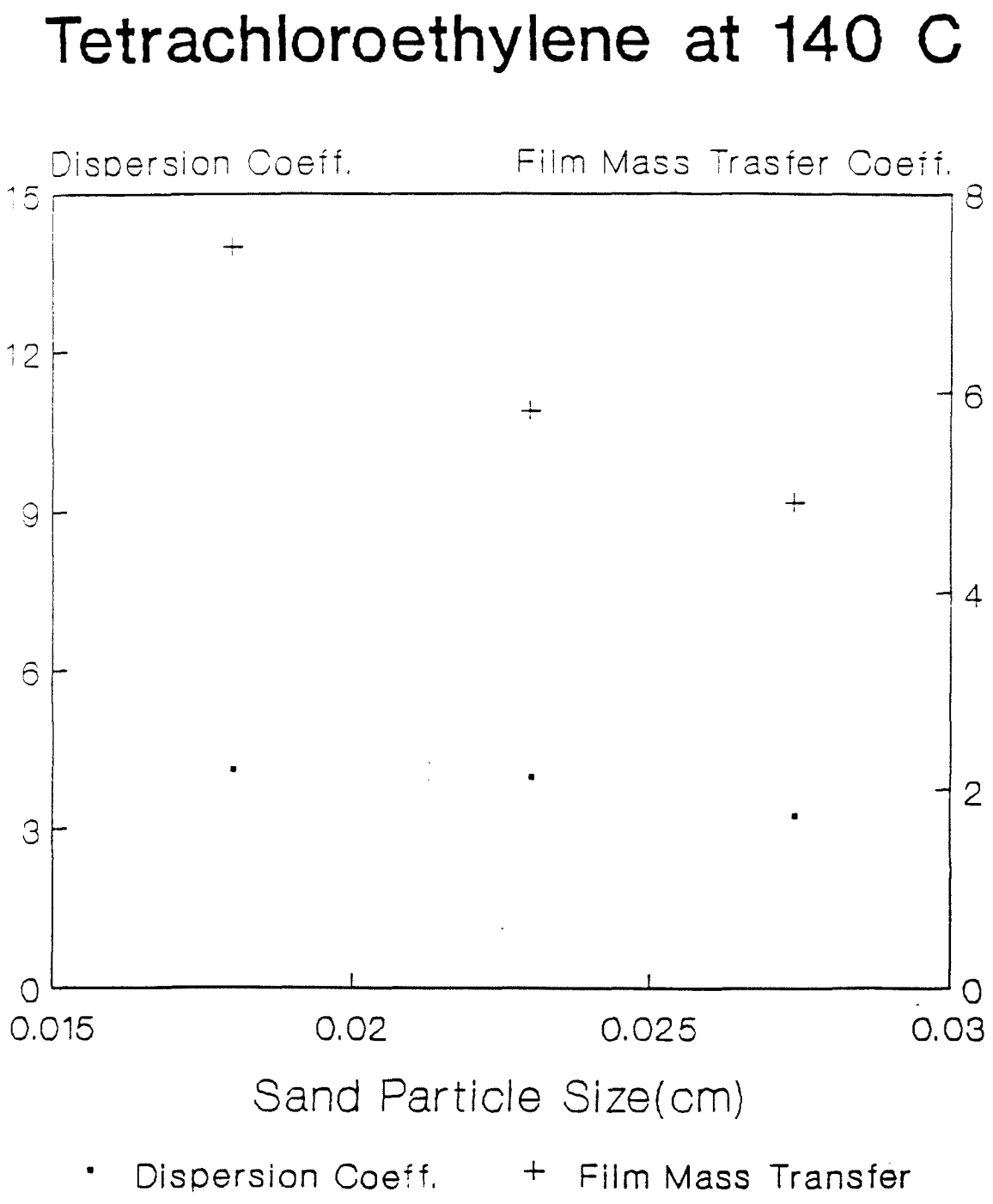
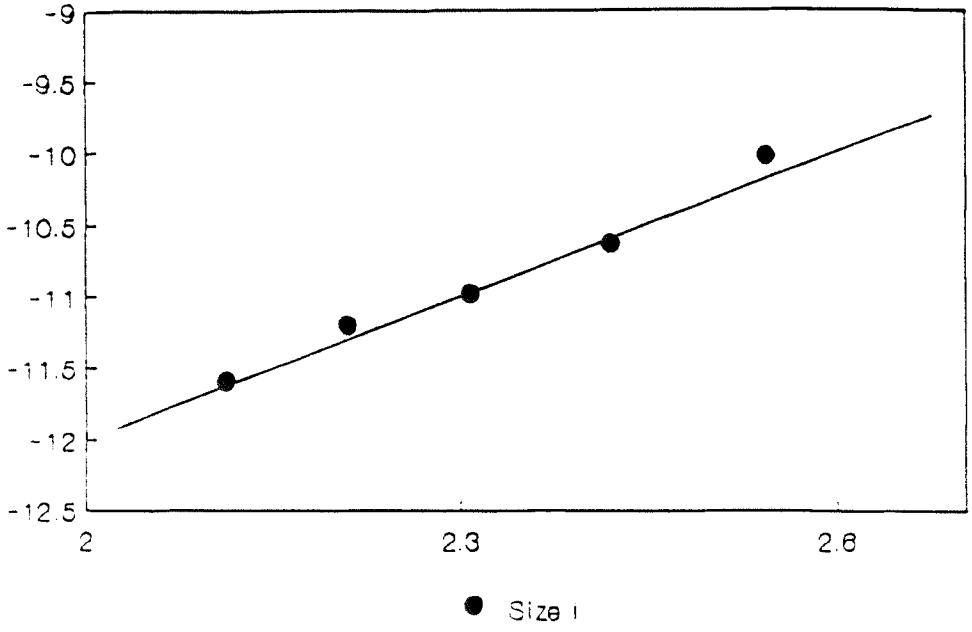
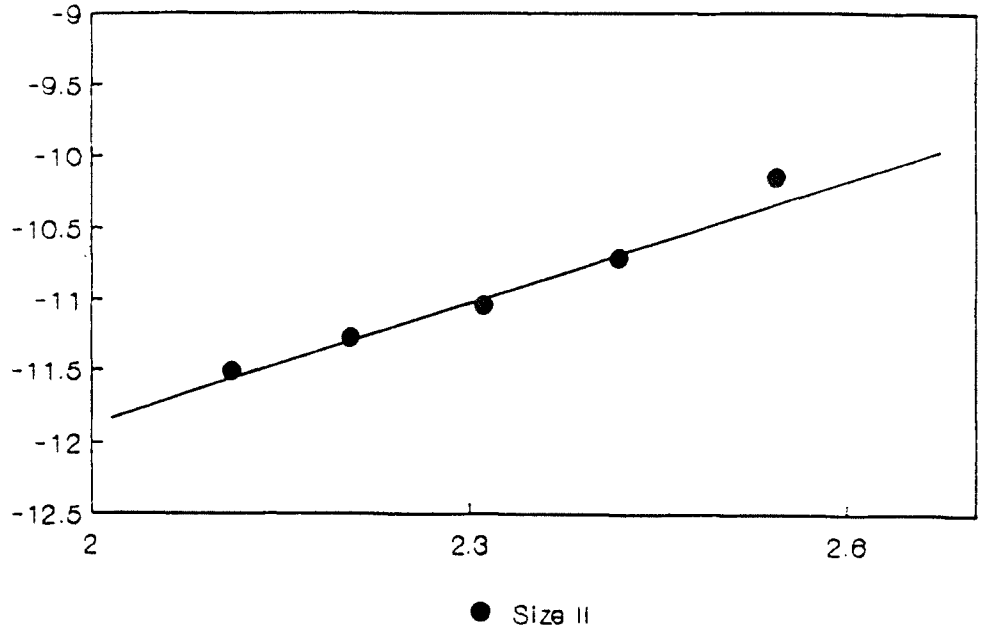


Figure 5.49: Heats of Adsortion of C_6H_5Cl : Size I



Chlorobenzene at 2.0

Figure 5.50: Heats of Adsortion of C_6H_5Cl : Size II

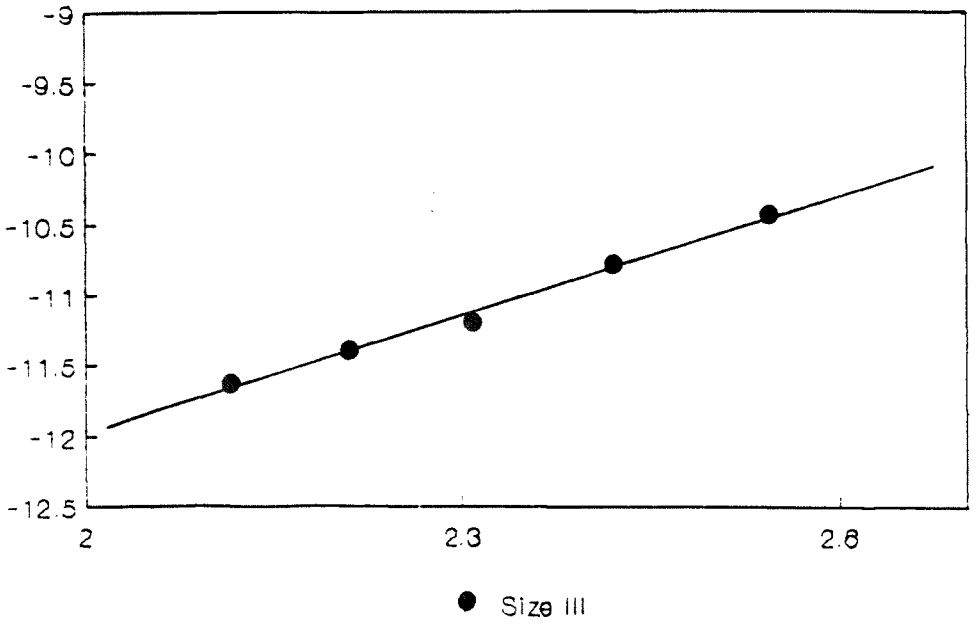


Chlorobenzene at 2.0

Table 5.13: Equilibrium Constants and Heats of Adsortion of C_6H_5Cl

Size	Temperature $^\circ C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $^\circ K$
I	120	17.731	3.357
	140	9.501	
	160	7.208	
	180	6.311	
	200	4.581	
II	120	14.910	2.951
	140	8.857	
	160	6.713	
	180	6.001	
	200	4.744	
III	120	11.874	2.862
	140	8.553	
	160	5.671	
	180	5.121	
	200	4.235	

Figure 5.51: Heats of Adsorption of C_6H_5Cl : Size III



Chlorobenzene at 2.0

Mass transfer parameters of Chlorobenzene at each temperature are listed in *Table(5.14)*.

Figure 5.52: Particle Size Dependence of $-\Delta H/R$

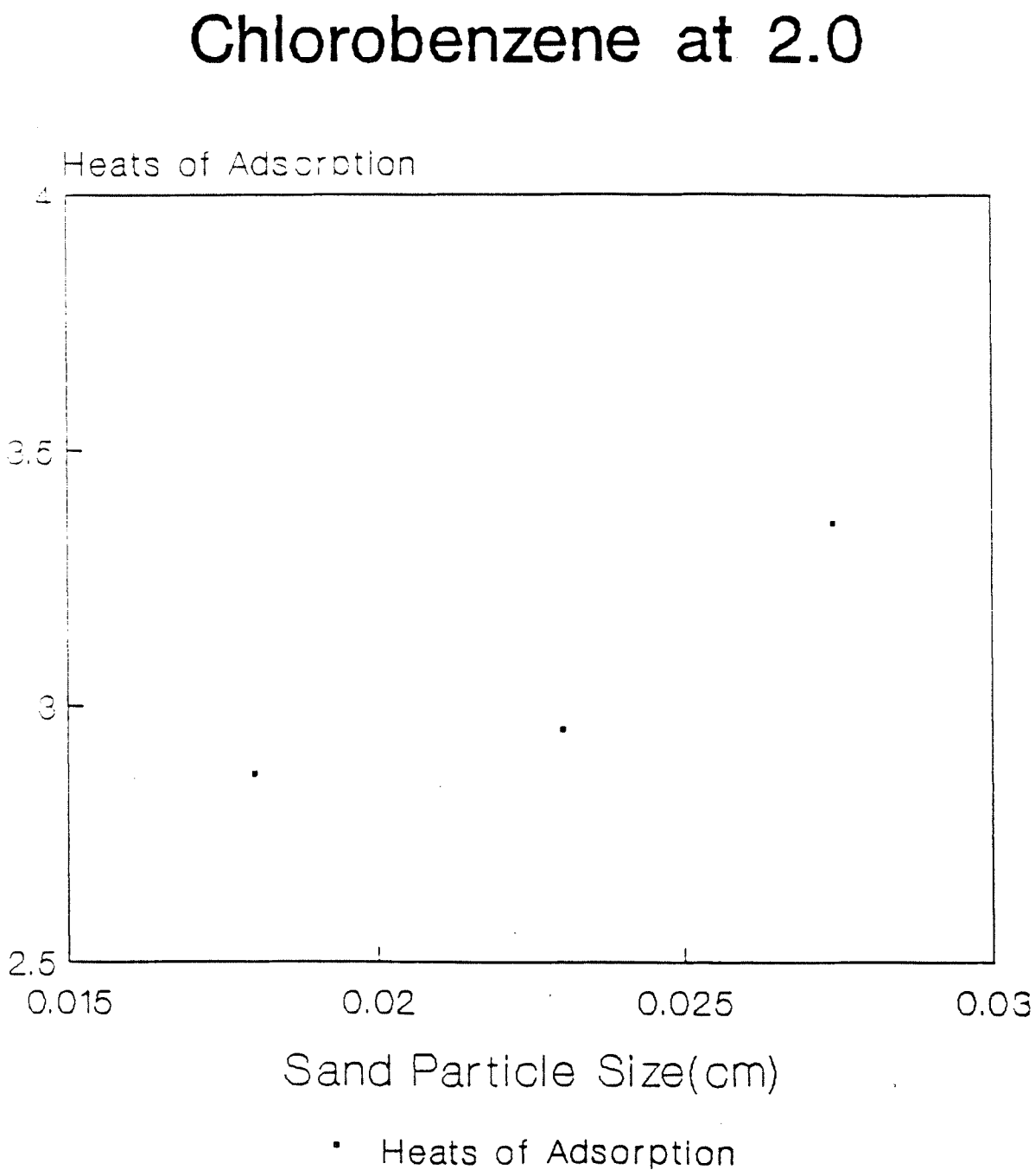


Figure 5.53: Dispersion Coefficient of of C_6H_5Cl : Size I

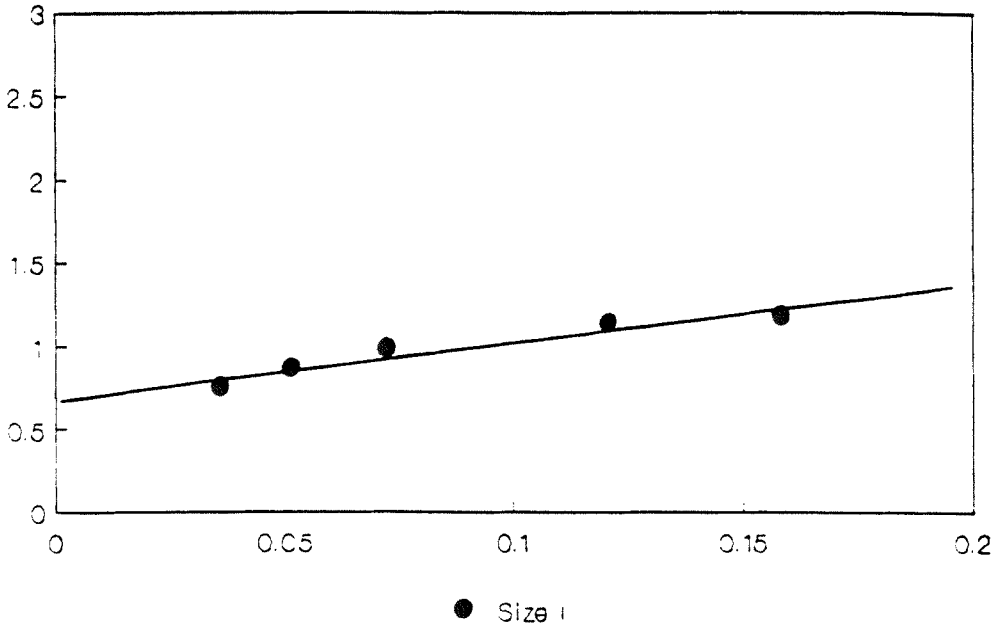


Figure 5.54: Dispersion Coefficient of C_6H_5Cl : Size II

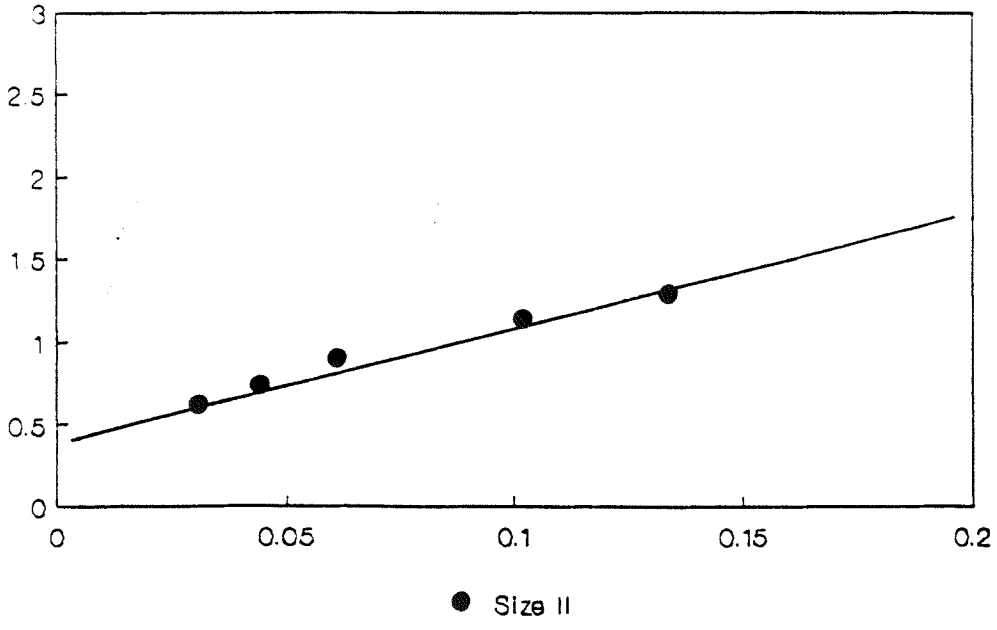


Figure 5.55: Dispersion Coefficient of C_6H_5Cl : Size III

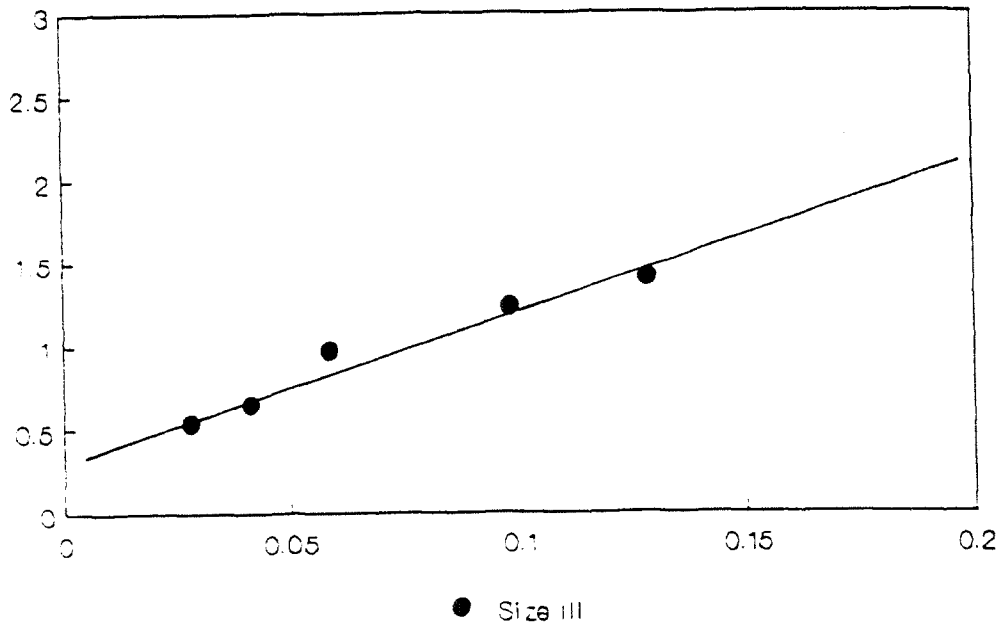


Table 5.14: Evaluated Mass Trasfer Parameters of Chlorobenzene

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	3.328	4.81	
II	6.320	5.73	0.1319
III	8.768	7.36	

Figure 5.56: Particle Size Dependence of D_z

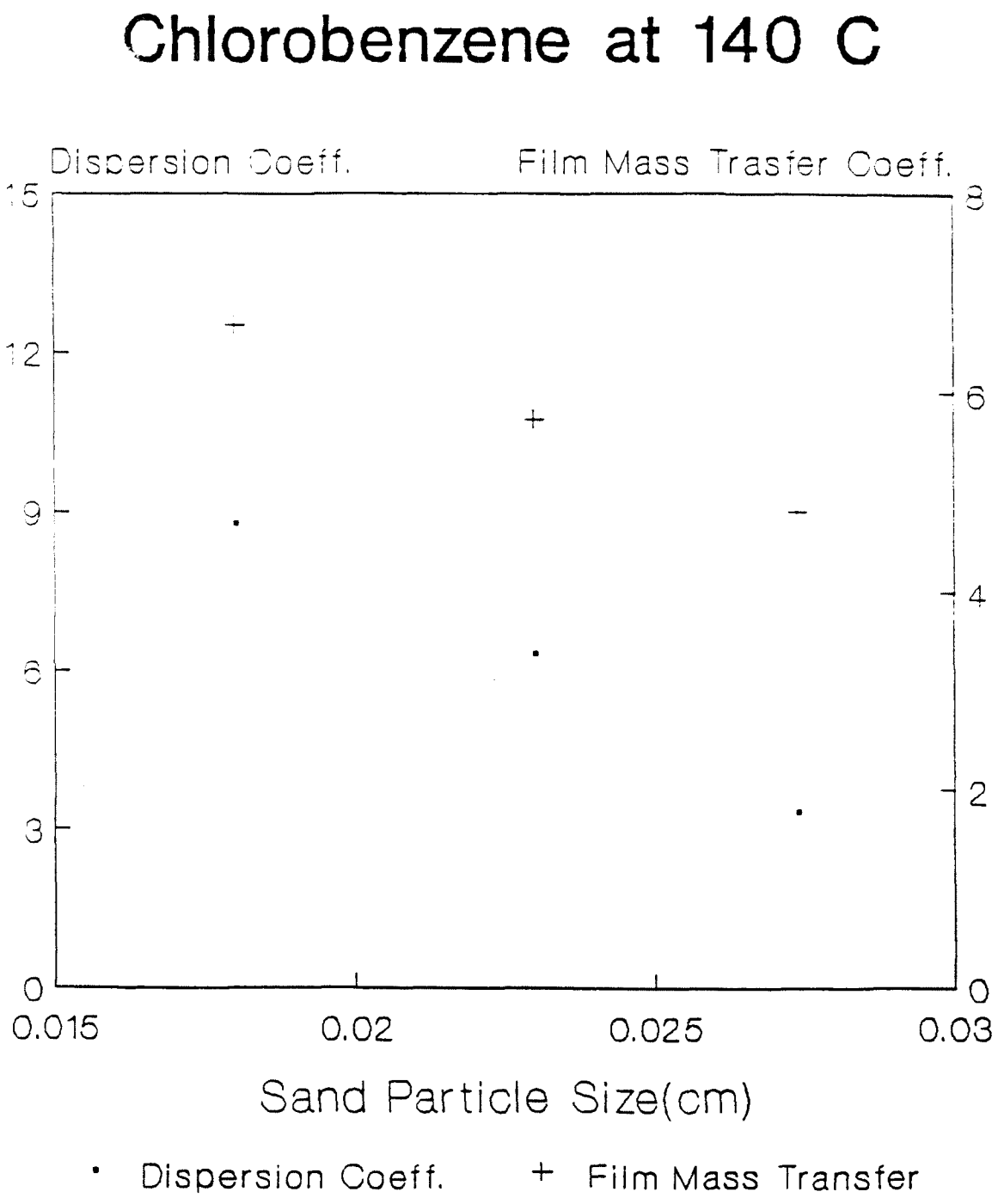
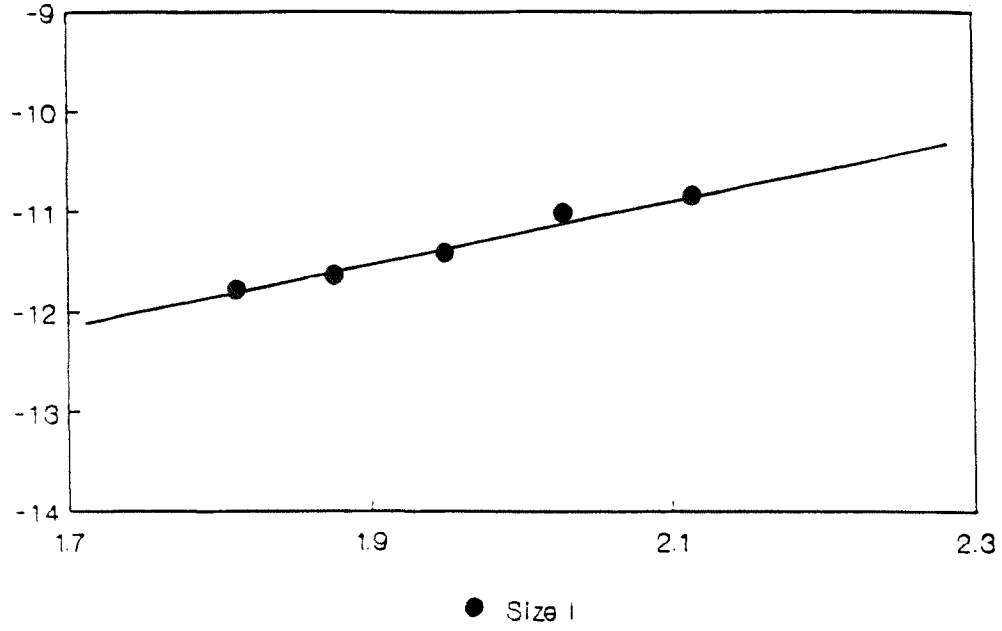


Figure 5.57: Heats of Adsorption of $C_6H_3Cl_3$: Size I



'.2,4-trichlorobenzene at 2.0

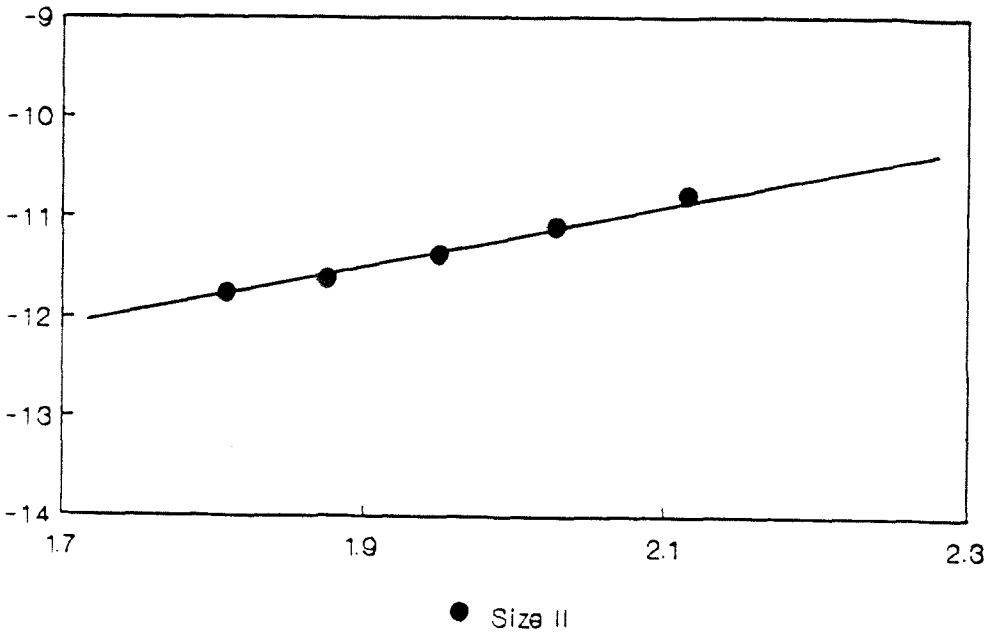
5.8 1,2,4-Trichlorobenzene

Equilibrium constants at various temperature and heats of adsorption are shown in *Table(5.15)* for each particle sizes. The graphs $1/T$ vs $ln(K_b/T)$ for each particle sizes are shown in *Figure(5.57)*, *Figure(5.58)* and *Figure(5.59)* respectively.

The heats of adsorption are plotted versus particle size in *Figure(5.60)* which shows slight increase in $-\Delta H/R$ with particle size.

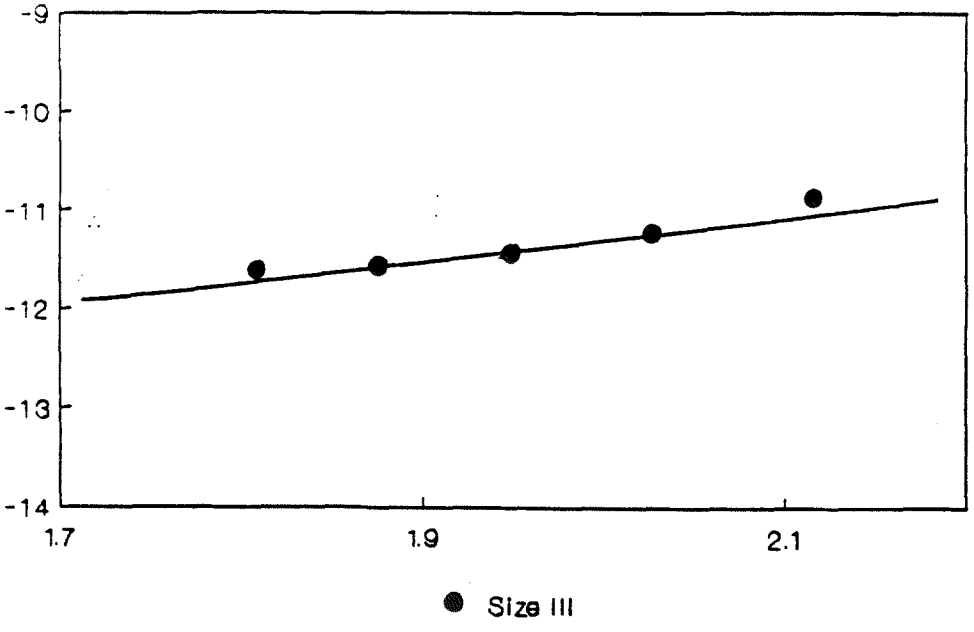
Plots $1/V^2$ vs. $\frac{\sigma^2 L}{2\mu^2 V}$ for each size are displayed in *Figure(5.61)*,*Figure(5.62)*, and *Figure(5.63)* respectively. The particle size effect on dispersion and film mass transfer coefficients are illustrated in *Figure(5.64)*. Both coefficients show a decrease with increasing particle size.

Figure 5.58: Heats of Adsorption of $C_6H_3Cl_3$: Size II



1,2,4-trichlorobenzene at 2.0

Figure 5.59: Heats of Adsorption of $C_6H_3Cl_3$: Size III



1,2,4-trichlorobenzene at 2.0

Table 5.15: Equilibrium Constants and Heats of Adsortion of $C_6H_3Cl_3$

Size	Temperature $°C$	Equilibrium Const. $K_b \times 1000$	Heats of Adsorption $-\Delta H/R \times 1000$ $°K$
I	200	9.444	3.340
	220	8.491	
	240	5.328	
	260	4.546	
	280	4.372	
II	200	9.728	3.226
	220	7.596	
	240	5.836	
	260	4.618	
	280	4.453	
III	200	8.820	2.405
	220	6.245	
	240	5.467	
	260	4.969	
	280	4.855	

Figure 5.60: Particle Size Dependence of $-\Delta H/R$

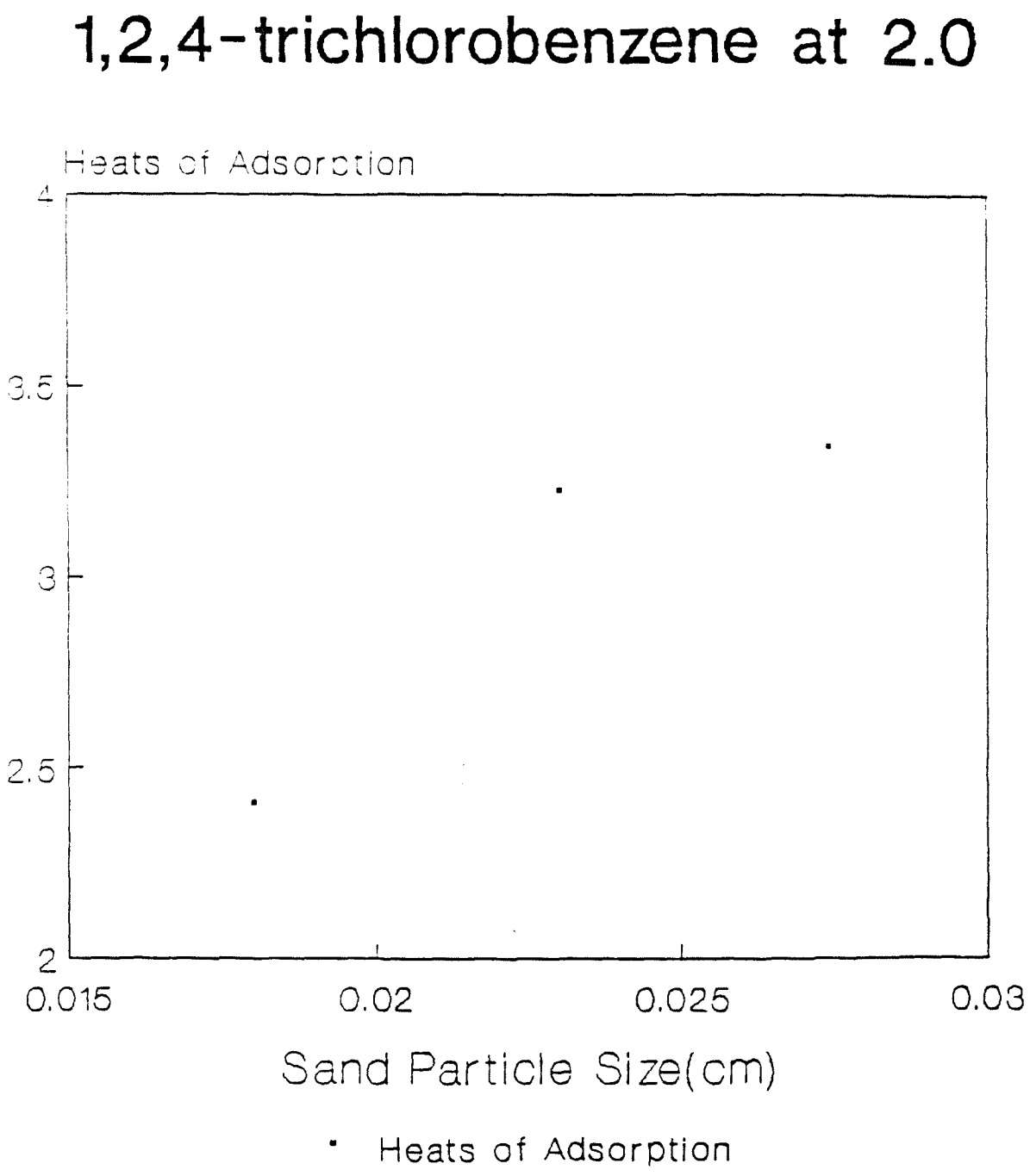
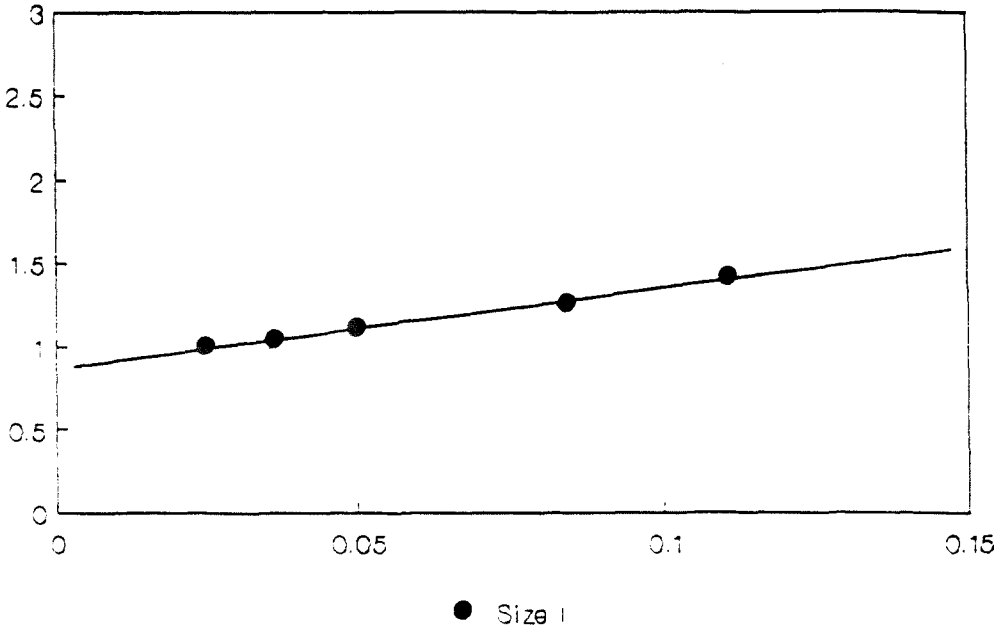
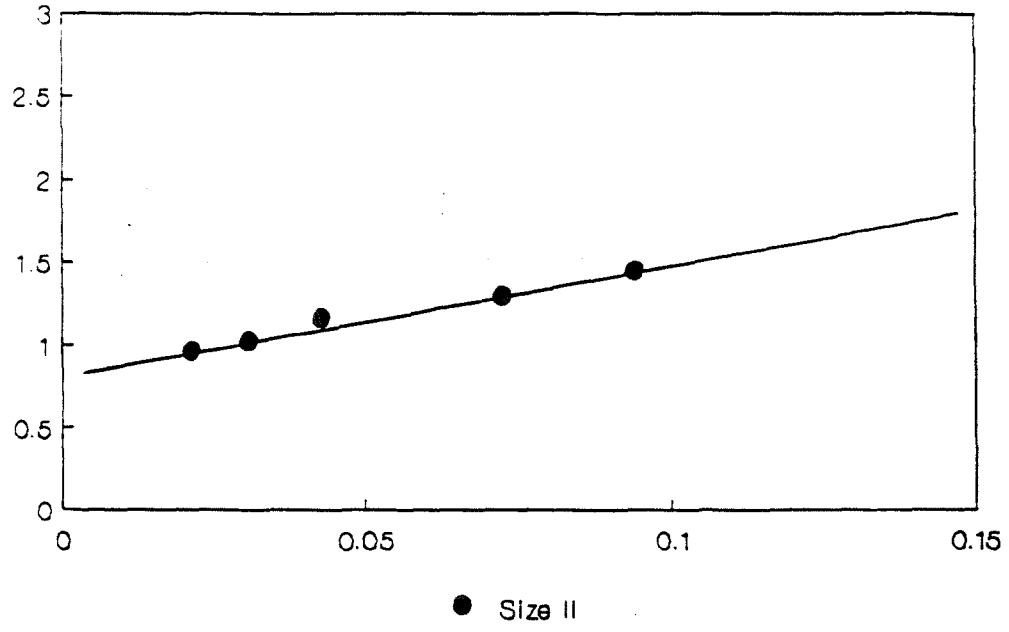


Figure 5.61: Dispersion Coefficient of $C_6H_3Cl_3$: Size I



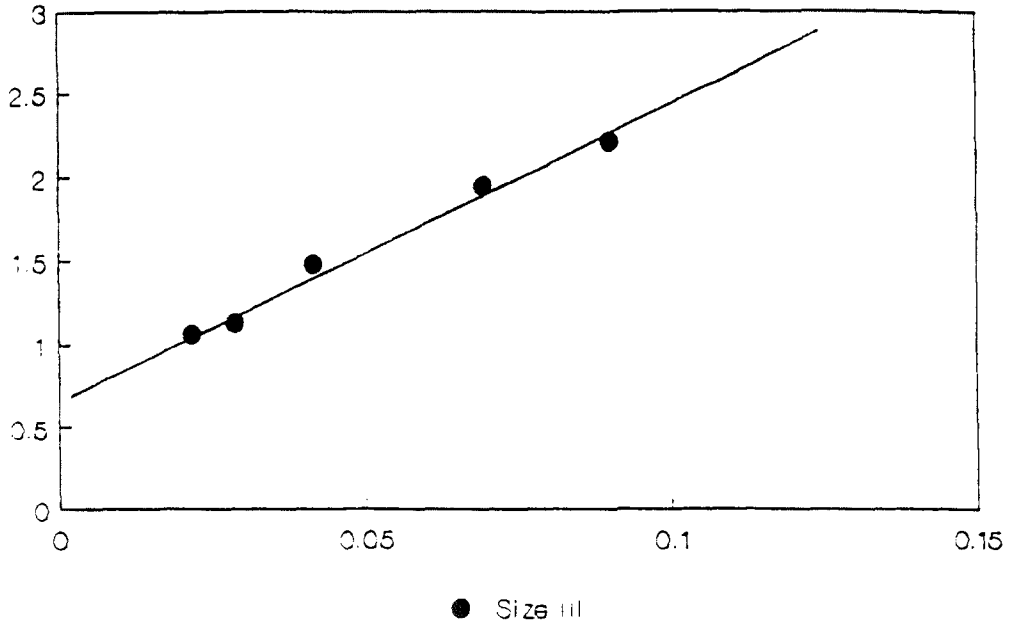
1,2,4-trichlorobenzene at 220 C

Figure 5.62: Dispersion Coefficient of $C_6H_3Cl_3$: Size II



1,2,4-trichlorobenzene at 220 C

Figure 5.63: Dispersion Coefficient of $C_6H_3Cl_3$: Size III



1,2,4-trichlorobenzene at 220 C

Mass transfer parameters of 1,2,4-Trichlorobenzene at each temperature are listed in *Table(5.16)*.

5.9 Data Summaries and Comparison

5.9.1 Heats of Adsorption

We obtained heats of adsorption at each particle size for eight compounds. They are summarized in *Table(5.17)*. Since the mass transfer parameters and heats of adsorption in the soil particle at particle size ($R_p = 0.023cm$) are identical to Size II of this study it might be meaningful to compare these data with those of soil experiments. The heats of adsorption of sand particle II are compared with the results from soil study of

Figure 5.64: Particle Size Dependence of D_z

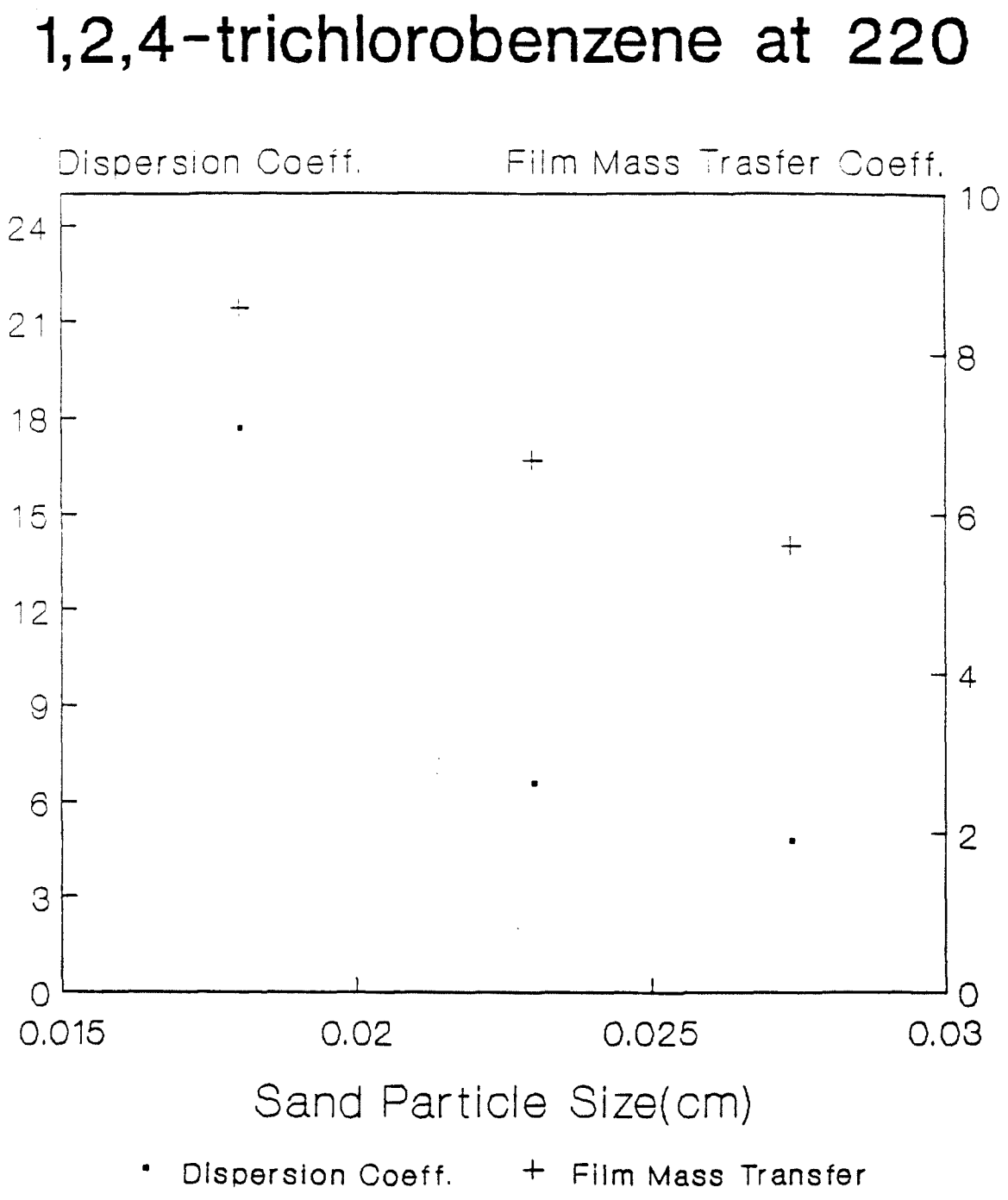


Table 5.16: Evaluated Mass Trasfer Parameters of 1,2,4-Trichlorobenzene

Size	Dispersion Coefficinet ($D_z, cm^2/sec$)	Film Mass Coefficient ($K_f, cm/sec$)	Molecular Diffusivity ($D_m, cm^2/sec$)
I	4.739	5.61	
II	6.534	6.68	0.1536
III	17.65	8.57	

Table(5.18).

The $-\Delta H/R \times 1000$ of sand range from 2.27 $^\circ K$ to 3.65 $^\circ K$ while those of soil vary from 4 $^\circ K$ to 7 $^\circ K$. We observe that heats of adsorption of respective compounds of sand particle are smaller, approximately one half, that of corresponding data for soil. At this time we credit this difference for a given compound in soil vs sand to the intraparticle pores which exist in soil but not in sand.

5.9.2 Mass transfer Parameters

We also obtained mass transfer parameters at each particle size for target compounds. They are summarized in *Table(5.19).* The mass transfer parameters of sand particle II are compared with the results of soil studies in *Table(5.20).*

We observe that the sand bed shows very different mass transfer behavior contrast to that of soil bed. The turbulence terms - Axial dispersion, Film mass transfer -

Table 5.17: Summary of Heats of Adsorption

Particle Size I : $R_p = 0.027cm$
Particle Size II : $R_p = 0.023cm$
Particle Size III : $R_p = 0.018cm$

Compounds	B_p	M_w	$-\Delta H/R \times 1000$ °K at particle size		
	°C		I	II	III
Methylene Chloride	39.8	92.13	2.577	2.265	2.158
Chloroform	61.7	119.4	2.648	2.448	2.374
1,1,1-trichloroethane	74	133.4	3.423	2.965	2.522
Benzene	80	78.1	2.682	2.338	1.914
Toluene	111	92.13	4.074	3.653	2.921
Tetrachloroethylene	121	165.85	3.924	3.381	3.224
Chlorobenzene	132	112.6	3.357	2.951	2.862
1,2,4-trichlorobenzene	214	181.5	3.340	3.226	2.405

Table 5.18: Comparison of $-\Delta H/R$ with Soil Data

Particle Size : II, Sieve No. 35 - 40 : R_p= 0.023cm

Compound	Sand	Soil
Methylene Chloride	2.27	*
Chloroform	2.45	*
1,1,1-trichloroethane	2.97	*
Carbon Tetrachloride	-	*
Benzene	2.34	*
Toluene	3.65	*
Tetrachloroethylene	3.38	-
Chlorobenzene	2.95	*
1,2,4-trichlorobenzene	3.25	*

* indicates the preliminary data of J.I.Dong[24]
approximately two times that of our values for sand

Table 5.19: Summary of Mass Transfer Parameters

Compound	Molecular Diffusivity ($D_m, cm^2/sec$)	Film Mass Transfer Coefficient ($K_f, cm/sec$)			Dispersion Coefficient ($D_z, cm^2/sec$)		
		I	II	III	I	II	III
Methylene Chloride	0.122	4.41	5.09	6.43	2.47	6.54	9.04
Chloroform	0.117	4.26	5.08	6.51	2.51	2.92	4.12
1.1.1-trichloroethane	0.108	3.95	4.70	6.03	1.63	4.05	5.79
Benzene	0.122	4.45	5.30	6.80	5.40	7.96	9.06
Toluene	0.123	4.47	5.33	6.83	5.14	6.16	8.45
Tetrachloroethylene	0.134	4.89	5.82	7.47	3.25	3.98	4.11
Chlorobenzene	0.132	4.81	5.73	7.36	3.33	6.32	8.77
1.2.4-trichlorobenzene	0.154	5.61	6.68	8.57	4.74	6.53	17.65

Table 5.20: Comparison of Mass transfer Parameters with Soil Data

Particle Size : Sieve No. 35 - 40 : $R_p = 0.023cm$

Compound	Molecular Diffusivity ($D_m, cm^2/sec$)		Film Mass Transfer Coefficient ($K_f, cm/sec$)		Dispersion Coefficient ($D_z, cm^2/sec$)	
	Temp. $^\circ C$		Sand	Soil	Sand	Soil
Methylene Chloride	60	0.122	5.09	*	6.54	*
Chloroform	80	0.117	5.08	*	2.92	*
1,1,1-trichloroethane	80	0.108	4.70	*	4.05	*
Carbon Tetrachloride	-	-	-	*	-	*
Benzene	100	0.122	5.30	*	7.96	*
Toluene	120	0.123	5.33	*	6.16	*
Tetrachloroethylene	140	0.134	5.82	*	3.98	*
Chlorobenzene	140	0.132	5.73	*	6.32	*
1,2,4-trichlorobenzene	220	0.154	6.68	*	6.53	*

* Preliminary data[25] - higher values than we obtained for sand.

are predominant over molecular diffusivity. The film mass transfer coefficient of sand matrices vary from 4.70 cm/sec to 6.68cm/sec while those of soil vary from 4.8 cm/sec to 8 cm/sec. Sand's value of K_f are slightly smaller than soil's for all compounds. The dispersion coefficients of sand vary from 3 cm^2/sec to 8 cm^2/sec. The D_z of soil vary from 2.6 cm^2/sec to 6.7 cm^2/sec. The absence of the intraparticle diffusion effect could be believed to result in this difference.

Chapter 6

Conclusion

The plug flow deposition of the hazardous toxic compounds on a well characterized sand column was carried out at varied sand particle sizes; Sieve No. 30 - 35, 35 - 40, and 40 - 50. Temperatures ranged from 50 to 280 $^{\circ}C$. The carrier gas, N_2, flow rate varied from 7.9 to 16.5 cm^3/min. Eight toxic compounds were studied:

- Methylene Chloride
- Chloroform
- 1,1,1-Trichloroethane
- Benzene
- Toluene
- Tetrachloroethylene

- Chlorobenzene
- 1.2.4-Trichlorobenzene

A gas chromatograph was utilized and chromatographic response analysis on the results is employed to study the mass transfer mechanism of organic contaminants in sand matrices. Axial dispersion coefficients, film mass transfer coefficients, and molecular diffusivities were evaluated.

Equilibrium constants were strongly dependent on temperature and showed linearity for van't Hoff plots and heats of adsorption for each compound were determined for varied particle size of sand adsorbent beds.

The amount of contaminant remaining in the sand bed decreased, with the increasing temperature in sand bed. The particle size dependence of each of above parameters was observed. The mass transfer parameters decreased when the particle size of sand increased.

The mass transfer parameters and heats of adsorption of sand bed in which no diffusion was considered were compared with those data of soil bed. The heats of adsorption of sand bed were approximately half of those for corresponding pollutant on soil. While different mass transfer behaviors were observed and following results have been obtained:

$$\text{Particle Size I} : R_p = 0.027cm$$

$$\text{Particle Size II} : R_p = 0.023cm$$

$$\text{Particle Size III} : R_p = 0.018cm$$

Compound	Molecular Diffusivity ($D_m, cm^2/sec$)	Film Mass Transfer Coefficient ($K_f, cm/sec$)			Dispersion Coefficient ($D_z, cm^2/sec$)		
		I	II	III	I	II	III
Methylene Chloride	0.122	4.41	5.09	6.43	2.47	6.54	9.04
Chloroform	0.117	4.26	5.08	6.51	2.51	2.92	4.12
1,1,1-Trichloroethane	0.108	3.95	4.70	6.03	1.63	4.05	5.79
Benzene	0.122	4.45	5.30	6.80	5.40	7.96	9.06
Toluene	0.123	4.47	5.33	6.83	5.14	6.16	8.45
Tetrachloroethylene	0.134	4.89	5.82	7.47	3.25	3.98	4.11
Chlorobenzene	0.132	4.81	5.73	7.36	3.33	6.32	8.77
1,2,4-Trichlorobenzene	0.154	5.61	6.68	8.57	4.74	6.53	17.65

These results can be then applied to thermal treatment of contaminated soils and will be of use in obtaining optimum operational conditions for sand decontamination processes.

Chapter 7

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Appendix A

FORTRAN PROGRAMS for CALCULATION

A.1 Fortran Program I for Mass Transfer Parameter Calculation

MASS TRANSFER CALCULATION PROGRAM FOR PARTICLE SIZE I

WRITTEN BY JAEIL KWON

```
DIMENSION FD(5,10)

DATA READING

READ(1,1000) IFILE,TEMP,TEMPF,XAREA
TEP=TEMP+273.15
WRITE(2,1500)
WRITE(2,2000) IFILE,TEMP,TEP
WRITE(2,1800)
SCALE=1.0
DO 500 i=1,5
READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
FR=FD(i,1)
FART=FD(i,2)
GDEAD=FD(i,3)
VAR=FD(i,4)

CALCULATION

VEL=FR/XAREA
AVEL=VEL*TEMPF
RRT=FART-GDEAD
RVEL=AVEL/.4501
B=((RVEL*RRT)/29-1)*0.007469
DVEL=RVEL/60
DISPX=1/DVEL**2
DISPY=(VAR*14.5)/RRT**2/DVEL
SCALE=SCALE+0.5
WRITE(2,2100) SCALE,B,DISPX,DISPY
CONTINUE

FORMATTING

FORMAT(I4,5X,3F9.4)
FORMAT(4F9.4)
FORMAT(1X,'----------------------------------------')
FORMAT(1X,'----------------------------------------')
FORMAT(3X,'FILENAME:',2X,I4,3X,F5.1,3X,'(',F6.2,')')
FORMAT(1X,F5.1,3X,F10.7,2X,F9.6,1X,F9.6)
STOP
END
```

A.2 Fortran Program II for Mass Transfer Parameter Calculation

MASS TRANSFER CALCULATION PROGRAM FOR PARTICLE SIZE II

WRITTEN BY JAEIL KWON

```
DIMENSION FD(5,10)

DATA READING

READ(1,1000) IFILE,TEMP,TEMPF,XAREA
TEP=TEMP+273.15
WRITE(2,1500)
WRITE(2,2000) IFILE,TEMP,TEP
WRITE(2,1800)
SCALE=1.0
DO 500 i=1,5
READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
FR=FD(i,1)
FART=FD(i,2)
GDEAD=FD(i,3)
VAR=FD(i,4)

CALCULATION

VEL=FR/XAREA
AVEL=VEL*TEMPF
RRT=FART-GDEAD
RVEL=AVEL/.4055
B=((RVEL*RRT)/29-1)*0.004075
DVEL=RVEL/60
DISPX=1/DVEL**2
DISPY=(VAR*14.5)/RRT**2/DVEL
SCALE=SCALE+0.5
WRITE(2,2100) SCALE,B,DISPX,DISPY
CONTINUE

FORMATTING

FORMAT(I4,5X,3F9.4)
FORMAT(4F9.4)
FORMAT(1X,'-----------------------------------------')
FORMAT(1X,'-----------------------------------------')
FORMAT(3X,'FILENAME:',2X,I4,3X,F5.1,3X,'(',F6.2,')')
FORMAT(1X,F5.1,3X,F10.7,2X,F9.6,1X,F9.6)
STOP
END
```

A.3 Fortran Program III for Mass Transfer Parameter Calculation

MASS TRANSFER CALCULATION PROGRAM FOR PARTICLE SIZE III

WRITTEN BY JAEIL KWON

```
DIMENSION FD(5,10)

DATA READING

READ(1,1000) IFILE,TEMP,TEMPF,XAREA
TEP=TEMP+273.15
WRITE(2,1500)
WRITE(2,2000) IFILE,TEMP,TEP
WRITE(2,1800)
SCALE=1.0
DO 500 i=1,5
READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
FR=FD(i,1)
FART=FD(i,2)
GDEAD=FD(i,3)
VAR=FD(i,4)

CALCULATION

VEL=FR/XAREA
AVEL=VEL*TEMPF
RRT=FART-GDEAD
RVEL=AVEL/.4145
B=((RVEL*RRT)/29-1)*0.005428
DVEL=RVEL/60
DISPX=1/DVEL**2
DISPY=(VAR*14.5)/RRT**2/DVEL
SCALE=SCALE+0.5
WRITE(2,2100) SCALE,B,DISPX,DISPY
CONTINUE

FORMATTING

FORMAT(I4,5X,3F9.4)
FORMAT(4F9.4)
FORMAT(1X,'----------------------------------------')
FORMAT(1X,'----------------------------------------')
FORMAT(3X,'FILENAME:',2X,I4,3X,F5.1,3X,'(',F6.2,')')
FORMAT(1X,F5.1,3X,F10.7,2X,F9.6,1X,F9.6)
STOP
END
```

A.4 Fortran Program IV for H_{ads} Calculation

HEAT OF ADSORPTION CALCULATION PROGRAM FOR PARTICLE SIZE I

WRITTEN BY JAEIL KWON

```
      DIMENSION FD(5,10)

      DATA READING

      READ(1,1000) IFILE
      WRITE(2,1500)
      WRITE(2,2000) IFILE
      WRITE(2,1800)
      SCALE=1.25
      DO 500 i=1,5
      READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
      TEMP=FD(i,1)
      FR=FD(i,2)
      FART=FD(i,3)
      GDEAD=FD(i,4)

      CALCULATION

      VEL=FR/0.1636
      TEP=TEMP+273.15
      XRT=(1/TEP)*1000
      TEMPF=TEP/293.15
      AVEL=VEL*TEMPF
      RRT=FART-GDEAD
      RVEL=AVEL/.4501
      B=((RVEL*RRT)/29-1)*0.007469
      YLN=ALOG(B/TEP)
      WRITE(2,2100) TEMP,B,XRT,YLN
      CONTINUE

      FORMATTING

      FORMAT(I4)
      FORMAT(4F9.4)
      FORMAT(1X,'-----------------------------------------------')
      FORMAT(1X,'-----------------------------------------------')
      FORMAT(3X,'FILENAME:',2X,I4,3X,'  at 2.0 SCALE  ')
      FORMAT(3X,F5.1,3X,F9.7,2X,F6.4,2X,F8.4)
      STOP
      END
```

A.5 Fortran Program V for H_{ads} Calculation

HEAT OF ADSORPTION CALCULATION PROGRAM FOR PARTICLE SIZE II

WRITTEN BY JAEIL KWON

```
DIMENSION FD(5,10)

DATA READING

READ(1,1000) IFILE
WRITE(2,1500)
WRITE(2,2000) IFILE
WRITE(2,1800)
SCALE=1.25
DO 500 i=1,5
READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
TEMP=FD(i,1)
FR=FD(i,2)
FART=FD(i,3)
GDEAD=FD(i,4)

CALCULATION

VEL=FR/0.1636
TEP=TEMP+273.15
XRT=(1/TEP)*1000
TEMPF=TEP/293.15
AVEL=VEL*TEMPF
RRT=FART-GDEAD
RVEL=AVEL/.4055
B=((RVEL*RRT)/29-1)*0.004075
YLN=ALOG(B/TEP)
WRITE(2,2100) TEMP,B,XRT,YLN
CONTINUE

FORMATTING

FORMAT(I4)
FORMAT(4F9.4)
FORMAT(1X,'-----------------------------------------------')
FORMAT(1X,'-----------------------------------------------')
FORMAT(3X,'FILENAME:',2X,I4,3X,'  at 2.0 SCALE  ')
FORMAT(3X,F5.1,3X,F9.7,2X,F6.4,2X,F8.4)
STOP
END
```

A.6 Fortran Program VI for H_{ads} Calculation

HEAT OF ADSORPTION CALCULATION PROGRAM FOR PARTICLE SIZE III

WRITTEN BY JAEIL KWON

```
DIMENSION FD(5,10)

DATA READING

READ(1,1000) IFILE
WRITE(2,1500)
WRITE(2,2000) IFILE
WRITE(2,1800)
SCALE=1.25
DO 500 i=1,5
READ(1,1100) FD(i,1),FD(i,2),FD(i,3),FD(i,4)
TEMP=FD(i,1)
FR=FD(i,2)
FART=FD(i,3)
GDEAD=FD(i,4)

CALCULATION

VEL=FR/0.1636
TEP=TEMP+273.15
XRT=(1/TEP)*1000
TEMPF=TEP/293.15
AVEL=VEL*TEMPF
RRT=FART-GDEAD
RVEL=AVEL/.4055
B=((RVEL*RRT)/29-1)*0.004075
YLN=ALOG(B/TEP)
WRITE(2,2100) TEMP,B,XRT,YLN
CONTINUE

FORMATTING

FORMAT(I4)
FORMAT(4F9.4)
FORMAT(1X,'-------------------------------------------------')
FORMAT(1X,'-------------------------------------------------')
FORMAT(3X,'FILENAME:',2X,I4,3X,'  at 2.0 SCALE  ')
FORMAT(3X,F5.1,3X,F9.7,2X,F6.4,2X,F8.4)
STOP
END
```

A.7 HP 3396A Integrator Program for Peak Analysis

GAS CHROMATOGRAM RESPONSE ANALYSIS FOR

AVERAGE RETENTION TIME AND VARIANCE

```
 10   OPEN #11: NAME "M:SIGNAL.ENC"
 20   INIT_ACCESS #11
 25   SUM=0
 26   VSUM=0
 30   TAREA=0
 40   NN=1
 45   NX=1
 50   PRINT "FILELENGTH (MIN.) "
 60   INPUT T
 65   PRINT "XBASE ?":INPUT XBASE
 67
 68
 69
 70   NT=T*300
 80   XAREA=SLICE_AREA+XBASE
 82   IF XAREA<0 THEN XAREA=0
 90   TAREA=TAREA+XAREA
 93   SUM=SUM+SLICE_NUM/300*XAREA
 95   INC_SLICE_NUM (1)
100   NN=NN+1
110   IF NN>NT THEN GOTO 130
120   GOTO 80
130   PRINT "TOTAL AREA=";TAREA
135   AVGT=SUM/TAREA
137   PRINT "AVG. RETENTION TIME =";AVGT;"MIN."
140   CLOSE #11
150   OPEN #11: NAME "M:SIGNAL.ENC"
155   INIT_ACCESS #11
157   XAREA=SLICE_AREA+XBASE
158   IF XAREA<0 THEN XAREA=0
160   VSUM=VSUM+(SLICE_NUM/300-AVGT)^2*XAREA
170   INC_SLICE_NUM (1)
180   NX=NX+1
190   IF NX>NT THEN GOTO 210
200   GOTO 157
210   VAR=VSUM/TAREA
220   PRINT "VARIANCE                    =";VAR;"MIN."
230   CLOSE #11
240   END
```

A.8 HP 3396A Integrator Program for GC BASE LINE

GAS CHROMATOGRAM BASE LINE CALCULATION

```
10    OPEN #11: NAME "M:SIGNAL.BNC"
20    INIT_ACCESS #11
30    N=1
40    PRINT N,SLICE_AREA
50    N=N+5
60    INC_SLICE_NUM (5)
70    IF N>50 THEN GOTO 90
80    GOTO 40
85
90    N=N+50
100   INC_SLICE_NUM (50)
110   PRINT N,SLICE_AREA
120   GOTO 90
```

Appendix B

FLOW RATE CALIBRATIONS

Flow Rate of Carrier Gas at varied Temperature

1.5(Scale)	1.75	2.0	2.25	2.5
50 (Temp.)				
7.879236	9.034741	11.70064	13.83099	16.50096
60				(ml/min.)
7.879283	9.034888	11.70077	13.83119	16.50115
70				
7.87933	9.035036	11.7009	13.83139	16.50134
80				
7.879377	9.035184	11.70103	13.83159	16.50153
90				
7.879424	9.035332	11.70116	13.83178	16.50172
100				
7.879471	9.035479	11.70128	13.83198	16.50191
110				
7.879518	9.035628	11.70141	13.83218	16.5021
120				
7.879565	9.035775	11.70154	13.83238	16.5023
130				
7.879612	9.035924	11.70167	13.83258	16.50249
140				
7.879659	9.036072	11.7018	13.83277	16.50268
150				
7.879707	9.036219	11.70192	13.83297	16.50287
160				
7.879753	9.036368	11.7[illegible]205	13.83317	16.50306

Flowrate of Carrier Gas at various Temperature

1.5(Scale)	1.75	2.0	2.25	2.25
170 (Temp.)				
7.879801	9.036515	11.70218	13.83337	16.50325
180				(ml/min.)
7.879848	9.036663	11.70231	13.83357	16.50344
190				
7.879895	9.036811	11.70244	13.83376	16.50363
200				
7.879942	9.036959	11.70257	13.83396	16.50382
210				
7.879989	9.037108	11.70269	13.83416	16.50402
220				
7.880036	9.037255	11.70282	13.83436	16.50421
230				
7.880083	9.037403	11.70295	13.83456	16.5044
240				
7.88013	9.037551	11.70308	13.83475	16.50459
250				
7.880177	9.037699	11.70321	13.83495	16.50478
260				
7.880224	9.037847	11.70334	13.83515	16.50497
270				
7.880271	9.037994	11.70346	13.83535	16.50516
280				
7.880318	9.038142	11.70359	13.83555	16.50535

Appendix C

DEAD VOLUME EFFECTS

Dead Volume Effects on Sand Bed at Varied Temperature

1.5(Scale)	1.75	2.0	2.25	2.25
50 (Temp.)				
6.925318E-02	.0531049	3.898534E-02	3.860437E-02	3.213724E-02
				(min.)
60				
6.925182E-02	5.310388E-02	.0389844	3.860325E-02	3.213669E-02
70				
6.925045E-02	5.310286E-02	3.898347E-02	3.860212E-02	3.213614E-02
80				
6.924909E-02	5.310184E-02	3.898254E-02	.038601	3.213558E-02
90				
6.924773E-02	5.310082E-02	3.898161E-02	3.859987E-02	3.213503E-02
100				
6.924636E-02	.0530998	3.898067E-02	3.859874E-02	3.213447E-02
110				
.069245	5.309878E-02	3.897974E-02	3.859762E-02	3.213392E-02
120				
6.924363E-02	5.309776E-02	3.897881E-02	3.859649E-02	3.213337E-02
130				
6.924227E-02	5.309674E-02	3.897787E-02	3.859537E-02	3.213282E-02
140				
6.924091E-02	5.309572E-02	3.897694E-02	3.859424E-02	3.213227E-02
150				
6.923955E-02	.0530947	3.897601E-02	3.859311E-02	3.213171E-02
160				
6.923818E-02	5.309367E-02	3.897508E-02	3.[illegible]39E-02	3.213116E-02

Dead Volume Effects on Sand Bed at Varied Temperature

1.5(Scale)	1.75	2.0	2.25	2.25
170 (Temp.)				
6.923681E-02	5.309266E-02	3.897414E-02	3.859086E-02	3.213061E-02
180				(min.)
6.923545E-02	5.309164E-02	3.897321E-02	3.858974E-02	3.213006E-02
190				
6.923409E-02	5.309062E-02	3.897228E-02	3.858861E-02	.0321295
200				
6.923272E-02	.0530896	3.897135E-02	3.858749E-02	3.212895E-02
210				
6.923136E-02	5.308857E-02	3.897041E-02	3.858636E-02	3.212839E-02
220				
6.922999E-02	5.308755E-02	3.896948E-02	3.858524E-02	3.212784E-02
230				
6.922863E-02	5.308653E-02	3.896855E-02	3.858411E-02	3.212729E-02
240				
6.922726E-02	5.308552E-02	3.896761E-02	3.858299E-02	3.212674E-02
250				
.0692259	.0530845	3.896668E-02	3.858186E-02	3.212619E-02
260				
6.922454E-02	5.308347E-02	3.896575E-02	3.858073E-02	3.212563E-02
270				
6.922318E-02	5.308245E-02	3.896482E-02	3.857961E-02	3.212508E-02
280				
6.922181E-02	5.308143E-02	3.896389E-02	3.857848E-02	3.212453E-02

Appendix D

DATA FILENAMES

Compound	Heats of Adsorption Particle Size			Mass Transfer Parameters Particle Size		
	I	II	III	I	II	III
Methylene Chloride	1011	1022	1033	1061	1062	1063
Chloroform	2011	2022	2033	2081	2082	2083
1,1,1-trichloroethane	3011	3022	3033	3081	3082	3083
Benzene	4111	4122	4133	4101	4102	4103
Toluene	5111	5122	5133	5121	51222	5123
Tetrachloroethylene	6111	6122	6133	6141	6142	6143
Chlorobenzene	7111	7122	7133	7141	7142	7143
1,2,4-trichlorobenzene	8211	8222	8233	8221	82222	8223