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Volatilization of Selected Organic Compounds From a Creosote Waste Land Treatment Facility

by

Eric J Scott

A project report submitted in partial fulfillment
of the requirements for the degree

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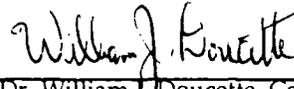
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Volatilization of Selected Organic Compounds From a Creosote Waste Land Treatment Facility

Introduction

The volatilization of hazardous chemicals from hazardous waste treatment, storage, and disposal facilities has received increasing attention in recent years because of the potential for damage to surrounding populations and to the environment in general. A general concern of the public, industry, and regulators in regard to ultimate treatment and disposal of hazardous wastes is that this material should not be treated or disposed of in a manner that allows the migration of hazardous constituents from one compartment of the environment to another in the treatment process. As an example, a hazardous waste should not be applied to the soil for biological treatment if a major fraction of this waste is expected to volatilize into the atmosphere without being transformed into a nonhazardous material.

The need for a model that could predict the mass flux rate of chemicals from land application of waste organic materials has increased due to recent changes in the Resource Conservation and Recovery Act (RCRA) and Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) because of certain preplanning requirements which require engineers to predict the environmental impacts of planned and unplanned releases of these hazardous chemicals to the environment.

Purpose

The purpose of this research was to evaluate the emissions of volatile and semi-volatile compounds which are constituents of a complex creosote waste from laboratory simulations of a land treatment system to assess the potential human exposure to hazardous compounds from this source. In addition, the Thibodeaux-Hwang Air Emission Release Rate (AERR) model was evaluated for its use in predicting emission rates of hazardous constituents of creosote wood preservative waste from land treatment facilities.

A group of hazardous volatile and semi-volatile constituents present in the creosote waste was selected for evaluation in this study and included a variety of polynuclear aromatic hydrocarbons (PNA's), phenol, and chlorinated and substituted phenols. The compounds chosen for study are listed along with several important physical properties of each chemical in the Table 1.

Objectives

The specific objectives of this study were to:

1. Perform air sampling of the creosote waste in a laboratory environment and quantify the amount of each chemical volatilized from samples of waste amended soil obtained from a land treatment facility.
2. Compare the laboratory surface emission flux results to predictions made using the Thibodeaux-Hwang AERR model.

Table 1. Selected volatile and semi-volatile chemicals and their environmental fate properties.

Chemical	Mol Wt	T _B (° C)	T _M (° C)	Vapor Pressure (atm)	Aqueous Solubility (mol/L)	Log (K _{ow})
Toluene	92.10 ¹	111.0 ²	-95.1 ²	2.90E-02 ¹	5.59E-03 ¹	2.69 ³
Phenol	94.11 ⁴	181.7 ⁴	43.0 ⁴	2.63E-04 ⁵	8.71E-01 ⁵	1.46 ⁵
m-Cresol	108.15 ⁴	202.2 ⁴	11.5 ⁴	5.26E-05 ⁵	2.17E-01 ⁵	1.96 ⁵
2,6-Dimethylphenol	122.17 ⁴	212.0 ⁴	49.0 ⁴	3.78E-04 ⁶	1.70E-03 ⁶	2.36 ⁵
Naphthalene	128.19 ⁴	218.0 ⁴	80.6 ⁴	1.03E-04 ⁷	2.34E-04 ⁵	3.01 ⁵
2-Methylnaphthalene	142.20 ⁴	240.0 ⁴	34.6 ⁴	9.21E-05 ⁸	1.83E-04 ⁵	3.86 ⁸
2-Ethyl-naphthalene	156.23 ⁴	258.0 ⁴	-7.4 ⁴	3.36E-05 ⁸	3.55E-04 ⁶	4.21 ⁶
Pentachlorophenol	266.34 ⁴	309.0 ⁴	174 ⁴	1.45E-07 ⁹	5.26E-05 ⁹	5.01 ⁸
Anthracene	178.24 ⁴	354.0 ²	216.2 ⁴	5.04E-05 ¹⁰	7.24E-06 ⁵	4.45 ⁵

T_B is boiling point temperature, T_M is melting point temperature.

¹Sims et al. (1986)

⁶Calculated (see Appendix F)

²Morrison & Boyd (1987)

⁷Sonnefeld (1983)

³Chiou & Schmedding (1982)

⁸Mackay et al. (1982)

⁴CRC

⁹IRP Toxicology Guide (1986)

⁵Verscheuren (1977)

¹⁰Thibodeaux (1979)

Theory

The Thibodeaux-Hwang AERR model (1) was developed to predict the rate of volatilization of individual chemicals within a complex waste mixture applied to soil. The model was developed to describe the chemical mixture applied either on the surface or injected at some depth below the surface.

Figure 1 illustrates a cross-section of such a landfarming operation. An oily waste is injected to a depth h_s or applied to the surface ($h_s = 0$) and penetrates to a depth h_p below the soil surface.

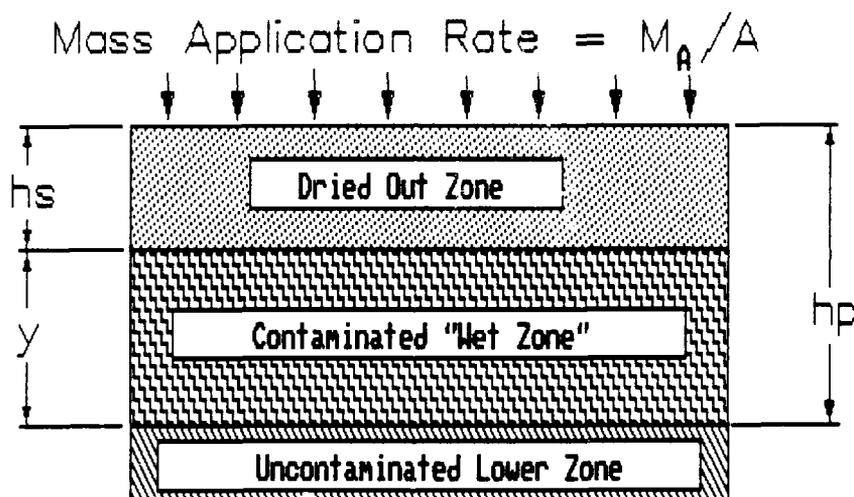


Figure 1. Theoretical soil profile described by the Thibodeaux-Hwang AERR Model.

The individual contaminants within the waste begin a four step volatilization process wherein they are transported (1) through the bulk oil to the liquid-air interface, (2) through the interface to the voids in the soil, (3) through the pores to the atmospheric boundary, and (4) through the atmospheric boundary into the lower atmosphere. The "wet zone" slowly retreats while the "dried out zone"

increases until all the chemical has vaporized. The assumptions that are made in order to simplify the model are:

1. The soil is initially free of chemicals.
2. The soil has uniform structure, particle size distribution and porosity.
3. The chemical is applied and uniformly distributes itself in the soil between h_s and h_p .
4. The chemical does not decompose, react with the soil or adsorb irreversibly onto the soil particles.
5. The temperature in the soil is constant.
6. Chemical contamination is restricted to the original saturated volume. There is no chemical movement either horizontally or vertically in the soil. Any chemical leaving the volume does so through the soil-air interface.
7. In dealing with multiple component wastes it is assumed that no interaction takes place among the individual constituents. Each species is dealt with separately and the total flux rate is equal to the sum of the flux rates for the individual chemicals.

The time it takes for all of a constituent in the oily waste to completely volatilize can be calculated from an equation derived by Thibodeaux and Hwang (1):

$$t_d = \frac{(h_p + h_s) \cdot M_A}{2 \cdot A \cdot D_A' \cdot C_A^*} \quad (1)$$

where t_d = the time (sec) for the initial mass to completely volatilize into the soil vapor phase, M_A = the original mass (μg) applied to the soil, A = the area (cm^2) over which the waste is applied (M_A/A = the mass application rate, $\mu\text{g}/\text{cm}^2$), D_A' is the effective diffusivity (cm^2/sec) of the component in the soil vapor space, and C_A^* is the equilibrium soil vapor phase concentration ($\mu\text{g}/\text{cm}^3$) of the individual component.

The mass flux rate of each component from the soil surface at time t can be calculated using the following equation, which was developed by Thibodeaux and Hwang (1) for use with chemical mixtures:

$$F_A = \frac{D_A' \cdot C_A^*}{\left(h_s^2 + \frac{2 \cdot D_A' \cdot t \cdot A (h_p - h_s) C_A^*}{M_A} \right)^{0.5}} \quad (2)$$

where F_A = the mass flux rate ($\mu\text{g}/\text{cm}^2\text{-sec}$) of the constituent out of the soil and t = the time (sec) at which the flux is measured. This equation only applies as long as t is less than t_d since beyond that point, the soil column is theoretically free of contaminant and the only flux out of the soil is a result of the chemical remaining in the interstices.

The value of C_A^* can be estimated (1) from:

$$C_A^* = \frac{C_{i0} \cdot H_c'}{1 + H_c' \left(\frac{6 \cdot D_A' \cdot Z_o}{D_c \cdot a_s (h_p^2 + h_p \cdot h_s - 2h_s^2)} \right)} \quad (3)$$

In this equation, C_{i0} = the initial concentration ($\mu\text{g}/\text{cm}^3$) of contaminant i in the waste, H_c' = the effective Henry's Law constant ($(\text{g}/\text{cm}^3 \text{ air})/(\text{g}/\text{cm}^3 \text{ oil})$), Z_o = the oil film diffusion length (cm), D_o = the diffusivity (cm^2/sec) of the contaminant in oil, and a_s is the interfacial surface area (cm^2) over which diffusion takes place.

Dupont, et al. (2) carried out a sensitivity analysis on the contaminant diffusion term (the term in brackets in the denominator of Equation 3) and observed that it was much smaller than 1 for virtually all land treatment scenarios. This term can therefore be neglected, simplifying Equation 3 to:

$$C_A^* = H_c' \cdot C_{i0} \quad (4)$$

They also demonstrated that for surface application, soil moisture content, surface penetration depth, soil bulk density, contaminant concentration/waste loading rate and soil particle density significantly affected the predicted flux rates from soil. It was concluded that efforts should be made to improve the measurement and/or prediction of these terms to improve the accuracy of model predictions.

It is known that both the Henry's Law constant and diffusivity vary with ambient temperature, so it would be expected that temperature has a significant effect on the volatilization of chemicals from soil. Farmer et al. (3) investigated the effects of pesticide concentration, temperature, air flow rate, and vapor pressure on the rate of insecticide volatilization from soil and found that each were significant. They also showed that volatilization decreased with time for surface applications. Farmer, Igue, and Spencer (4), in discussing their results concluded that as surface concentrations were depleted, diffusion became the controlling factor in loss rates from their model soil systems.

Farmer et al. (4) studied the effects of bulk density of soils on volatilization rates. They showed that volatilization rates decreased as the bulk density increased. They argued that the apparent total diffusion coefficient is made up of vapor and nonvapor diffusion coefficients. Their data showed that vapor diffusion was dependent on the concentration of dieldrin in the soil and approached zero above 25 $\mu\text{g/g}$. Above 25 $\mu\text{g/g}$ the effect of bulk density was diminished.

Parameter Estimation

One difficulty with the Thibodeaux-Hwang AERR model is that a number of the chemical properties it requires for input have not been measured for many chemicals of interest. Because of this a method of estimation for these properties must be used.

In Equation 1, D_A' , the effective soil diffusion coefficient, has been correlated to the properties of the soil. Its value is found using a relationship that was suggested by Lyman et al. (5)

$$D_A' = D_A \cdot S_a^{10/3} / S_t^2 \quad (5)$$

where D_A is the species air diffusivity ($\mu\text{g}/\text{cm}^2\text{-sec}$), S_a is the soil air filled porosity and S_t is the soil total porosity. D_A must also be estimated for some chemicals.

According to Thibodeaux (6), if the diffusivity for a chemical can be found at a temperature other than the desired temperature its value can be corrected by using the ratios of the dynamic viscosities of air at the two temperatures involved

$$D_A@T_2 = D_A@T_1 \left(\frac{T_2 \cdot \mu_1}{T_1 \cdot \mu_2} \right) \quad (6)$$

where μ_1 and μ_2 are the viscosities of air ($\text{N}\cdot\text{sec}/\text{m}^2$) at temperatures T_1 and T_2 , (K) respectively.

Where a value for D_A cannot be found for a chemical Lyman et al. (5) recommend either the Fuller, Schettler and Giddings (FSG) method or the Wilke-Lee (WL) method for its estimation. The FSG method gives best results for chlorinated aliphatics while aromatics, alkanes, and ketones were shown to deviate by 5% from measured values. This method uses the following relationship:

$$D_A = \frac{10^{-3} \cdot T^{1.75} \cdot M_r^{0.5}}{P(V_A^{1/3} + V_B^{1/3})^2} \quad (7)$$

where T is the temperature (K) of interest, M_r can be considered an average molecular weight as defined in the reference, V_A and V_B are the molar volumes (cm^3/mol) for air and the gas in question, and P is the atmospheric pressure (atm).

Using the WL method

$$D_A = \frac{B' \cdot T^{3/2} \cdot M_r^{1/2}}{P \cdot \sigma_{AB}^2 \cdot \Omega} \quad (8)$$

where T , M_r , and P are as previously defined, $B' = 0.00217 - 0.00050(1/M_A + 1/M_B)^2$, σ_{AB} is the characteristic length, (Angstroms) and Ω is the collision integral (dimensionless) as defined in Lyman, et al (5). The WL method is said to be useable for a wider range of chemicals than the FSG method.

In calculating C_A^* , a value for H_c' , the effective Henry's Law constant is needed. Measured values for this property are rarely available. It can be estimated using chemical properties that are more commonly found, i.e., H_c , the aqueous phase Henry's Law constant ($(\text{g}/\text{cm}^3 \text{ air})/(\text{g}/\text{cm}^3 \text{ water})$), and K_{sw} , the partition coefficient for the chemical between solvent and water. In the case of an oily waste, hexane has been used to approximate the oil's characteristics, and thus the K_{sw} for hexane can be used (7). If H_c is known, H_c' can be calculated from

$$H_c' = H_c / K_{sw} \quad (9)$$

H_c can be converted from H_A , the Henry's Law constant in $\text{atm} \cdot \text{L}/\text{mole}$ by

$$H_c = H_A (1000 \text{ g water}/\text{L water}) (1 \text{ mole water}/18 \text{ g water}) (1/1 \text{ atm}) \quad (10)$$

When a value for H_c or H_A cannot be found, H_A can be approximated according to Neely et al. (8) from

$$H_A = P/S \quad (11)$$

where P is the vapor pressure (atm) and S is the aqueous solubility (mole/L) of the constituent of interest.

If the vapor pressure of a chemical has not been measured, its value can be estimated according to an equation presented by Neely et al (7)

$$\ln(P) = -(4.4 + \ln(T_b)[1.803(\frac{T_b}{T} - 1) - 0.803 \cdot \ln(T_b/T)] - 6.8(\frac{T_b}{T} - 1)) \quad (12)$$

In this equation T_b is the chemical's boiling point (K), T_m is the melting point (K) and T is the ambient temperature (K). Vapor pressure, P is given in atmospheres. The last term of Equation 12 is omitted for chemicals which are liquids at room temperature.

It may also be necessary in some cases to approximate the solubility of a chemical in water. For this, Neely et al. (7) recommend a correlation equation based on the octanol/water partition coefficient, K_{ow} , for neutral organics.

$$\log(S) = -\log(K_{ow}) + 0.76 - 0.01 \cdot T_m \quad (13)$$

In this equation T_m is in °C and 25°C is used for liquids. Solubility, S , is in mole/L.

The solvent/water partition coefficient, K_{sw} is difficult to find for most organic chemicals and must be estimated. Correlation equations are available which are of the form

$$\log(K_{ow}) = a \cdot \log(K_{sw}) + b \quad (14)$$

where a and b are the slope and intercept of the solvent regression equation (5), respectively.

Experimental values for K_{ow} are not available for some organic chemicals. In this case, Lyman et al. (5) recommend Leo's fragment constant method for calculating $\log(K_{ow})$.

Materials and Methods

Laboratory Air and Soil Sampling.

A preliminary study was performed to determine optimum flow rate and sampling volumes for air sampling. A creosote mixture was made by adding 15 mL of creosote waste to 18.3 mL of Penreco™ Oil 2257 to simulate actual waste application practices at a wood preserving waste land treatment facility (creosote mixed with a light oil at a weight ratio of 45:55). The creosote waste was obtained from a land treatment facility and had been stored for an extended period in a metal drum. The properties of the Penreco™ oil were felt to be approximately the same as that used by the land treatment facility. Each of four 500 mL erlenmeyer flasks received 8.3 mL of the mixture, and were capped with an impinger dispersion tube (Figure 2).

Breathing air was used as purge gas and was fed at a flow rate of 200 mL/min to each flask. The effluent gas was exhausted through the exit port of the dispersion tube which was connected, using Teflon™ tubing, to a glass "T". One end of the "T" was used for venting exhaust air to the atmosphere. A piece of Teflon™ tubing was connected to the other end of the "T" followed by a straight piece of glass tubing and a brass Swagelock™ fitting. Figure 2 is a representation of one of the flasks.

Two Tenax™ tubes were connected in series at the Swagelock™ fitting. The second tube in series was used to detect break-through from the first tube. The sampling tubes were then connected to a constant volume air sampling pump operated in constant pressure mode at 20 inches of water suction. A flow rate controller was connected below each sample train and adjusted to flow rates of 10, 20, 30, 60, and 100 mL/min in successive tests.

Air samples were for 10, 20, and 60 minutes following initial waste application. Sorbent tubes were desorbed and analyzed on an HP 5880 GC for

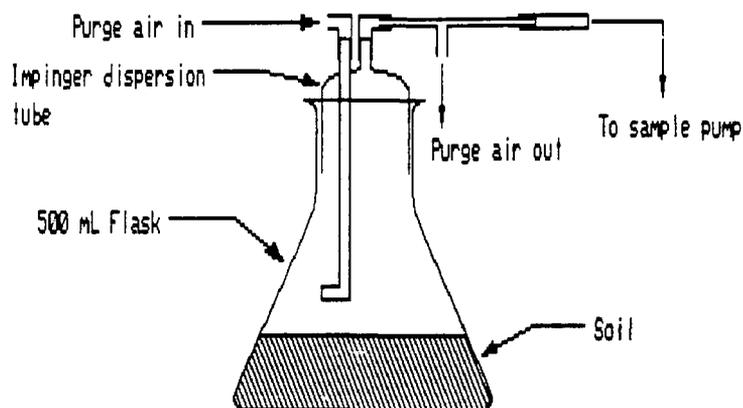


Figure 2. Air sampling apparatus used in laboratory study.

compound separation/quantification. These data were used to evaluate and adjust flow rates and sample volumes that were used in subsequent tests.

Laboratory soil emission measurement procedures.

Four erlenmeyer flasks were prepared for emission sampling using the apparatus described above. A mass application rate of 0.12 mL/cm^2 was used to simulate comparable rates used in the industry. An 8.3 mL volume of the creosote mixture described above was added to 280 g of a previously uncontaminated soil obtained from a land treatment facility in Wiggins, Mississippi, in each of three 500 mL erlenmeyer flasks. Before using the soil it was sieved through a No. 40 seive and the particle density and water content were determined using a method described by the American Society of Agronomy and Soil Sciences Society of America (9). The creosote waste mixture was stirred into the soil until the soil appeared to be uniformly coated with the waste. A fourth flask was prepared as a control by adding 280 g of soil without waste.

Air samples were taken at 0, 1, 5, 10, 50, and 100 hours using a purge flow rate of 200 mL/min in each flask and sample flow rates of approximately 30 mL/min at 0, 1, 5, and 10 hours, and 50 to 60 mL/min at 100 hours. All air

samples were taken for 20 minutes. Total sample volumes varied from 600 to 1260 mL using this sampling approach.

Soil samples were taken at 0, 10, 50, and 100 hours. They were used to provide a means of conducting a mass balance for the compounds of interest. Soil samples of approximately 20 grams and were placed into 120 mL amber glass bottles with Teflon™ lined lids. One hundred mL of dichloromethane were added to each bottle. The mixture was frozen until analyzed. Each time soil samples were taken, the soil was stirred, the soil samples were taken, and air samples were collected for that time period.

Creosote waste analysis.

Acid-Base/Neutral Extraction and Cleanup. Standard methods outlined in SW-846, Method 3650 (10), for the extraction of semi-volatiles from soil and waste produced a mixture in which the creosote waste was distributed between both the aqueous and organic phases and the phase boundary could not be distinguished. A modified method used at the Utah Water Research Laboratory was followed which consists of dilution of 1 mL of waste in 25 mL of methylene chloride and 15 mL of water for acid-base cleanup. When this modification was incorporated prior to the standard method positive results were achieved.

The final acid-base/neutral procedure utilized in this study was begun by adding 1 mL of creosote waste to 25 mL of methylene chloride. This was then extracted by adding 15 mL of distilled water, adjusting the pH to 12 or more, shaking for 2 minutes and allowing the mixture to settle for 10 minutes. The extraction was repeated three times after which the base/neutral fraction was collected into a 120 mL amber glass bottle with Teflon™ lined lids.

The aqueous fraction was put into a clean separatory funnel where 20 mL of methylene chloride were added. The pH was adjusted to 2 or less with concentrated sulfuric acid. The separatory funnel was shaken for 2 minutes and allowed to settle for 10 minutes. This step was repeated two more times and the organic fraction was collected in a 120 mL amber glass bottle. The base/neutral

and acid fractions were refrigerated at 4° C until they could be analyzed by GC analysis. This mixture was used to determine the concentration of naphthalene, 2-methylnaphthalene, 2-ethylnaphthalene, pentachlorophenol, and anthracene in the waste mixture.

Methanol extract for Purge and Trap separation. A methanol extract was made by filling a test tube 75% full with methanol, adding approximately 2 grams of creosote waste, filling the tube to the top with methanol, and sealing the tube so that no air bubbles remained. This mixture was mixed with a vortex mixer for 5 minutes and centrifuged for 15 minutes.

The methanol extract was then subjected to "purge-and-trap" separation by adding 5 mL of distilled water to a "purge-and-trap" vessel, and adjusting the flow of nitrogen gas through the column to 30 mL/min to an accuracy of +/- 0.1mL/min. Two hundred fifty µL of the methanol extract were added and purged for 12 minutes. The volatile organics were collected on Tenax™ traps and were thermally desorbed into an HP 5880 GC for separation/quantification. The concentration of toluene, phenol, cresol, and 2,6-dimethylphenol were found using this method.

Soil Extraction.

Soil samples were extracted by using a tissuemizer for 1 1/2 minutes. Methylene chloride had been added when the samples were taken. The liquid in the sample was poured through a drying column containing 4 to 6 inches of sodium sulfate into clean Kaderna Danish flasks with concentrator tubes attached. The liquid was concentrated to 10 mL, placed in 15 mL clear glass bottles, and frozen until GC analysis could be accomplished.

To determine the loss of chemicals through the tissuemizer extraction process a mixed standard solution of the nine chemicals being studied was added to three clean soil samples in amber glass bottles. The samples were then prepared in the same manner as above and analyzed. Four additional bottles were prepared and a similar amount of mixed standard was added to three of the bottles. All were

extracted and analyzed. The three with standard solution added served to quantify the losses due to volatilization and were compared with the three soil samples to see how much was adsorbed by the soil. The sample without standard solution added was tissued last and was used to see how much cross contamination occurred throughout the extraction process.

The moisture contents of soils from each flask were determined from the soil that remained after the volatilization experiment. A method prescribed by the American Society of Agronomy and Soil Sciences Society of America (9) was used.

Chromatography Procedures.

A Hewlett-Packard (HP) 5880 Gas Chromatograph (GC) with a flame ionization detector and SPB-5 capillary column were used for separation and quantification of specific waste constituents. An Envirochem model 850 thermal tube desorber was used for Tenax™ trap desorption.

The temperature program used on the GC was as follows:

<u>Temperature</u>	<u>Slope</u>	<u>Time</u>
40 °C		4 minutes
	6°/min	
230 °C		0 minutes

A standard dilution of 30,000 µg/mL in methylene chloride was made for each of the test chemicals (except anthracene which was made to 10,000 µg/mL because of its lower solubility in methylene chloride) from which dilutions of 120, 600, 1,000 and 3,000 µg/mL (40, 200, 333, and 1,000 µg/mL for anthracene) were made for standard curve preparation.

Spike Recovery.

Known amounts of standard dilutions of the test compounds were injected directly onto Tenax™ traps and into clean glass tubes while in the loading chamber of the thermal desorber to determine recovery efficiencies from the Tenax™. The Tenax™ traps were prepared using methods developed for the Environmental Protection Agency at the Environmental Monitoring Systems Laboratory (11). The Tenax™ traps were then thermally desorbed into the GC to quantitate compound recovery from the sorbent material. The masses injected onto the Tenax™ tubes were 0.24, 1.2, 2 and 6 µg/tube (0.08, 0.4, 0.67 and 2 µg/tube for anthracene). Calibration curves were developed from the data of the Tenax™ traps and the empty glass tubes for determining spike recovery efficiencies.

Model Calculations

Measured values for parameters required by the Thibodeaux-Hwang AERR model are hard to find for many organic chemicals which have been disposed of in the environment. Appendix F contains a listing of those values found in recent literature for the chemicals studied in this project and their isomers. Where a measured value could not be found, estimates were made using the methods described previously.

The expected emission rates were calculated using the Thibodeaux-Hwang AERR model. Table 2 gives the values for each input value that was calculated using parameter estimation methods. The theoretical evaporation times (t_d) were also calculated to see if any were shorter than the sampling period so that the model was not extended beyond the period for which it is considered valid.

Since the soil was remixed at 10, 50, and 100 hours, a modification to the standard model was necessary since it assumes that the soil remains undisturbed after application of the material to be treated. It was assumed that after being mixed, the creosote became redistributed uniformly in the soil and that the mass remaining in the soil was proportional to the depth of the wet zone remaining at

the mixing time calculated using an equation derived by Thibodeaux (12). The mass is equal to

$$M_A = M_{A0} \cdot y / h_p \quad (15)$$

where M_{A0} is the mass of constituent A at time = 0, and y is the depth of the remaining wet zone.

The soil moisture content was measured at the beginning of the experiments and after the 100 hour sample was taken. A straight line interpolation between the beginning and ending values was included in the model equations for adjusting the value of S_s .

Table 2. Input values for Thibodeaux-Hwang AERR model which were calculated using parameter estimation techniques.

Chemical	Da (FSG) (cm ² /sec)	Da(WL) (cm ² /sec)	D'a (cm ² /sec)	Ksw	HA (atm ³ L/mol)	Hc (g/cm ³)/(g/cm ³)	Hc (g/cm ³)/(g/cm ³)	Ca* (g/cm ³)
Toluene	0.0804	0.0860	2.26E-02	5.61E+02	5.19E+00	2.12E-01	3.78E-04	1.67E-03
Phenol	0.0852	0.0874	2.30E-02	2.99E+00	3.02E-04	1.23E-05	4.13E-06	4.96E-05
m-Cresol	0.0773	0.0789	2.08E-02	2.51E+01	2.42E-04	9.91E-06	3.95E-07	2.20E-05
2,6-Dimethylphenol	0.0717	0.0750	1.98E-02	1.38E+02	2.22E-01	9.09E-03	6.60E-05	1.91E-03
Naphthalene	0.0702	0.0722	1.90E-02	2.19E+03	4.27E-01	1.75E-02	7.98E-06	2.65E-01
2-Methylnaphthalene	0.0655	0.0668	1.76E-02	8.15E+04	5.03E-01	2.06E-02	2.52E-07	8.35E-03
2-Ethylnaphthalene	0.0616	0.0625	1.65E-02	3.62E+05	9.46E-02	3.87E-03	1.07E-08	5.39E-05
Pentachlorophenol	0.0592	0.0573	1.51E-02	1.09E+07	2.76E-03	1.13E-04	1.03E-11	2.29E-07
Anthracene	0.0597	0.0591	1.56E-02	1.00E+06	6.96E+00	2.85E-01	2.83E-07	3.68E-03

Results and Discussion

Chromatography.

Calibration curves for each constituent of interest were plotted for direct injection and spike procedures. Appendix A contains these plots along with the accompanying statistical data from linear regression analyses. It had been hoped that the direct injection data could be used to represent the actual peak areas for the concentrations injected and that spike recovery efficiencies could be evaluated from the direct injection data.

In every case the regression line for the spike data fell above that for direct injection data. The direct injection data are compared graphically with the spike data in Appendix A. The slopes of the two lines for each chemical were compared to see if the data sets represented distinct populations. Table A-1 and Table A-2 in Appendix A were derived using a method for comparing the slopes of two lines outlined by Kleinbaum and Kupper (13), where a weighted average of the variances of the slopes was derived and divided into the difference of the two slopes. This value was compared against the value from the t-distribution for the a 95% confidence interval. The analysis showed that the two slopes of the calibration lines were not equal, with the exception of toluene.

In the range of concentrations used to generate the calibration curves, the recovery efficiencies for the spikes was higher than for the direct injection data, so it was decided to assume 100% recovery from Tenax™ for the purposes of the experiment. It was expected that the recovery efficiency was high for Tenax™ and would not affect the results of the experiment.

Creosote waste analysis.

Purge and trap separation of a methanol extract was chosen for quantification of toluene, phenol, m-cresol, and 2,6-dimethylphenol in the creosote waste because these chemicals were not detected in the acid/base-neutral extractions. Acid/base-neutral extraction was used for naphthalene, 2-

methylnaphthalene, 2-ethylnaphthalene, pentachlorophenol, and anthracene. Table 3 gives the average values for each constituent and the 95% confidence intervals for the data collected. Waste analysis data are in Appendix B.

Table 3. Concentrations of individual chemicals in creosote waste.

Chemical	Average Concentration ($\mu\text{g/g}$)	Standard Deviation ($\mu\text{g/g}$)	Method
Toluene	5.56	0.25	Purge & Trap
Phenol	15.1	0.34	Purge & Trap
Cresol	70.1	6.02	Purge & Trap
2,6-Dimethylphenol	36.5	3.82	Purge & Trap
Naphthalene	41,800	2,980	Acid-Base/Neutral extraction
2-Methylnaphthalene	41,800	4,650	Acid-Base/Neutral extraction
2-Ethylnaphthalene	6,360	1,710	Acid-Base/Neutral extraction
Pentachlorophenol	27,900	4,540	Acid-Base/Neutral extraction
Anthracene	16,400	7,090	Acid-Base/Neutral extraction

As mentioned above, the creosote waste had been stored in a metal drum for an extended period of time. A GC/MS analysis of the waste at the time it was obtained showed similar concentrations for the semi-volatile constituents but the volatile constituents had much higher values. It would appear that the volatile chemicals had partitioned into the drum's headspace and disappeared.

Laboratory air sampling.

Three of the nine chemicals studied (2-ethylnaphthalene, anthracene, and pentachlorophenol) were not detected at levels sufficient for quantification at any time during the 100 hour sampling period. Plots for the other six chemicals showing their flux rates over time are given in Appendix C. From Equation 2 it can be seen that the flux rate at a given time should be linearly proportional to the inverse square root of time. A linear regression analysis was performed on the data from each flask for each of the six chemicals. Only the data collected at 0, 1, and 5 hours were included since the 10, 50, and 100 hour samples were taken after mixing the soil.

Table 4 summarizes the results of the linear regression analyses. A positive slope indicates that the flux rate declined over time. Only four of the 18 slopes were positive indicating that in general, the flux rates tended to increase within the first 5 hours of the experiment.

Table 4. Comparison of Regression outputs for Flux vs 1/SQRT(t) using only the data for 0, 1, and 5 hours.

Compound	Slope	y-intrept	r ²	W/in 95% Conf. Int?
Toluene				
Flask 1	3.359E-05	9.637E-06	0.92340	Yes
Flask 2	1.776E-06	2.976E-05	0.26734	No
Flask 3	1.909E-05	8.622E-06	0.55584	No
Phenol				
Flask 1	-2.666E-06	4.861E-05	0.02617	No
Flask 2	-1.728E-05	7.207E-05	0.32271	No
Flask 3	-1.805E-06	5.030E-05	0.01013	No
m-Cresol				
Flask 1	5.298E-06	1.845E-05	0.16585	No
Flask 2	-1.742E-05	5.295E-05	0.60756	No
Flask 3	-2.020E-06	3.930E-05	0.00617	No
2,6-Dimethylphenol				
Flask 1	-1.723E-05	8.120E-05	0.32463	No
Flask 2	-2.410E-05	8.569E-05	0.23833	No
Flask 3	-3.841E-05	1.330E-04	0.33785	No
Naphthalene				
Flask 1	-8.968E-05	2.344E-04	0.52697	No
Flask 2	-1.527E-04	3.772E-04	0.81480	Yes
Flask 3	-3.584E-04	8.039E-04	0.45117	No
2-Methylnaphthalene				
Flask 1	-1.293E-04	4.124E-05	0.22488	No
Flask 2	-3.903E-05	9.517E-05	0.63055	No
Flask 3	-1.133E-04	2.616E-04	0.50048	No

The data from each flask were analyzed separately giving three sets of data for each of the constituents. A correlation coefficient for a 95% confidence interval at the 5% level of significance (14) was compared against the data generated correlation coefficients to judge whether the data fit a straight line.

Toluene. The mass flux rate for toluene declined during the air sampling period in all three flasks as shown in Figure 3. Only the data for flask 1 met the criteria established for fitting a straight line, while the correlation coefficients for the other two flasks were fairly low. A plot of the regression line for flask 1 is given in Figure 4. The slopes of the regression lines were all positive, which combined with the high correlation between the flux rate and $1/t^2$ data for Flask 1, favor a conclusion that it volatilized according to the proposed model.

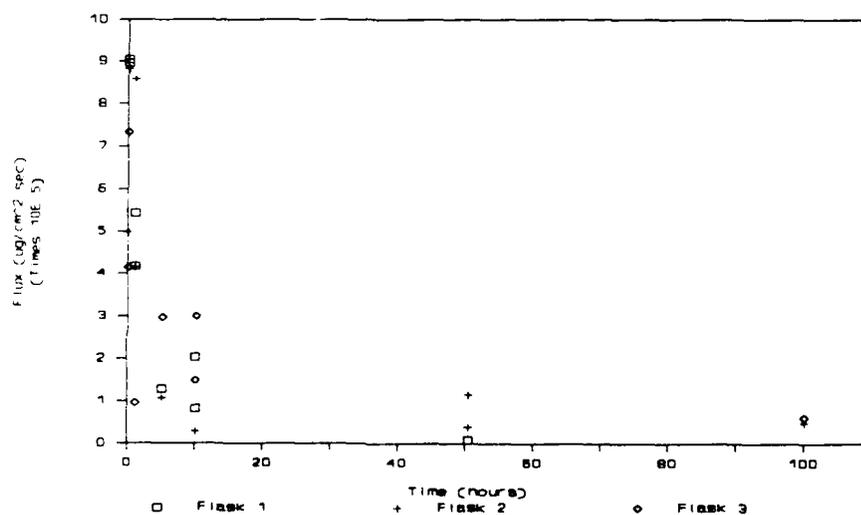


Figure 3. Flux rate vs. time for Toluene.

m-Cresol. Cresol data for flask 1 gave a positive slope for the regression line but the correlation coefficient was very low. The other two data sets gave negative slopes and low correlation coefficients leaving a very low probability that cresol emissions followed the model.

Naphthalene. The volatilization data for Flask 2 yielded a correlation coefficient that falls above the correlation coefficient for a 95% confidence interval but the slope of the regression line is negative indicating that the flux rate increased over time. Figure 5 is typical of the naphthalene data.

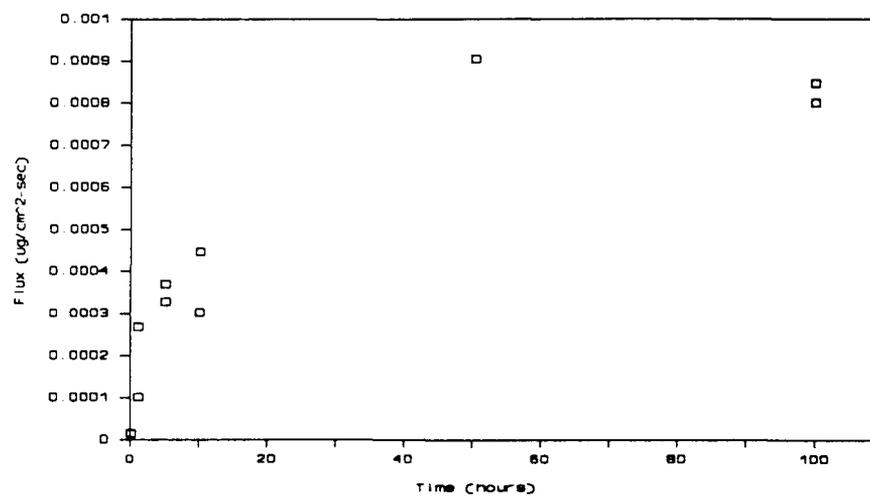


Figure 4. Comparison of mass flux rate for naphthalene over time.

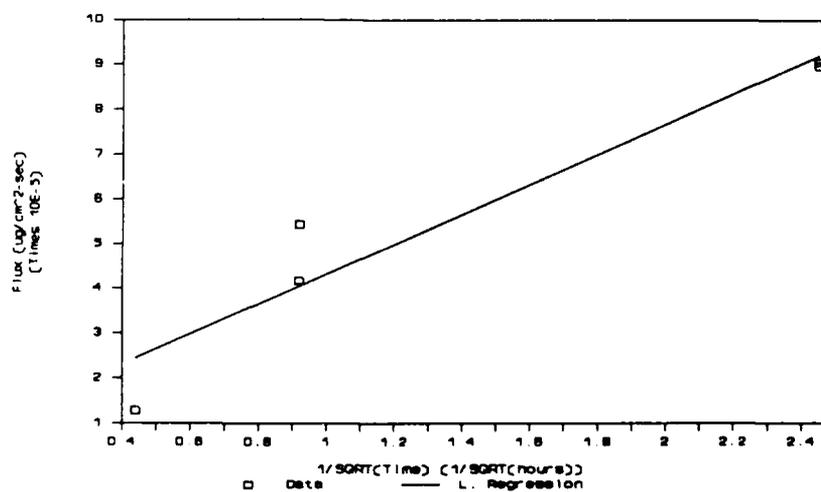


Figure 5. Mass flux rate for Toluene in flask 1 plotted against the inverse square of time.

All other chemicals. All other data sets yielded negative slopes and small correlation coefficients leaving doubt concerning the adequacy of the Thibodeaux-Hwang AERR model the characterization of the volatilization of these chemicals.

Laboratory Soil Samples.

Average compound losses through the tissuemizer extraction process are summarized in Table 5. When the mixed standard was incorporated into soil samples the average loss of constituents varied between 22.3% and 31.1%. Tissuemizing the standard mixed only in methylene chloride gave losses from 21.3% to 37%. Pentachlorophenol was the only chemical for which the loss of chemical was greater from the standard extracted without soil than from the standard mixed with soil. Analysis of variance results (Appendix D) showed that no significant difference existed between the two sets of data.

On the average, 2.5% greater loss occurred when the standard was mixed with soil, suggesting that some of the chemical was adsorbed by the soil or lost in some other way associated with its contact with soil. The percentages obtained from the standard mixed with soil (Table 5) were used as correction factors in calculating the concentrations of each chemical in the soil for mass balance calculations.

Table 5. Tissuemizer soil extraction losses.

Chemical	W/Soil percent	W/o Soil percent
Toluene	30.1	29.4
Phenol	24.6	21.3
m-Cresol	25.5	22.0
2,6-dimethylphenol	24.7	21.7
Naphthalene	25.2	22.1
2-Methylnaphthalene	23.4	20.6
2-Ethylnephthalene	24.3	21.3
Pentachlorophenol	31.1	37.2
Anthracene	22.3	21.7

Percent refers to percentage of original mass loss through the extraction procedure.

Analysis of soil extracts yielded results that were below the detection limit for toluene, phenol, m-cresol, and 2,6-dimethylphenol. It is most probable that the concentrations of these chemicals were so low that any quantifiable amounts were lost in the extraction process. All other chemicals were detected at sufficient levels for quantification.

Data for naphthalene show 46.7%, 44.5%, and 16.2% average losses for Flasks 1, 2, and 3, respectively, over the 100 hour study period. The values for Flask 3 do not show the same trend as those for Flasks 1 and 2 in that the 0-hour value is lower than the 10-hour value. The discrepancy is most likely due to sampling and analytical error. This conclusion is supported by the fact that the data show a net gain of naphthalene over the first ten hour period. Figure 6 shows the decline in naphthalene concentration over time and is typical of plots for the other chemicals which appear in Appendix D.

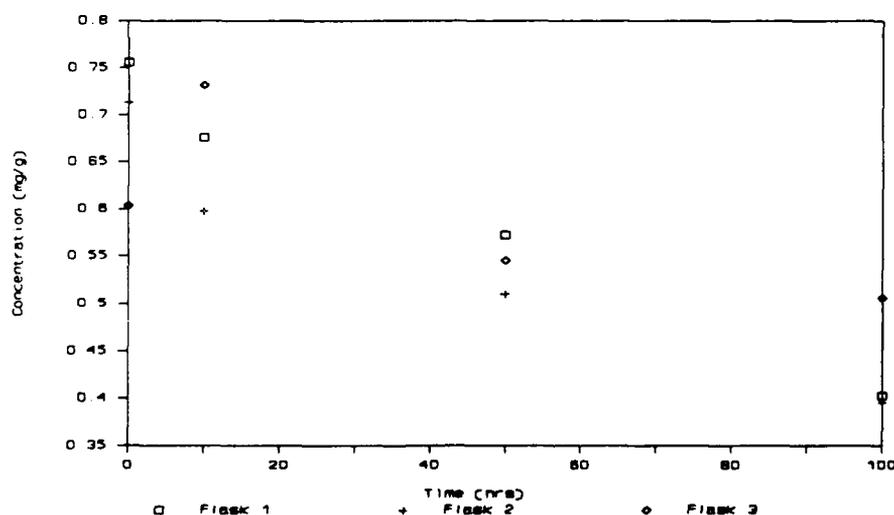


Figure 6. Variation of soil concentration of naphthalene with time.

Analysis of pentachlorophenol data showed losses of 13.0%, 47.1% and 17.8% for the three flasks. In this case, Flask 2 data are atypical and sampling and analytical error is thought to cause the discrepancy. Data for 2-ethylnaphthalene

in Flask 3 and anthracene in Flask 2 also show net gains of these chemicals and are thought to be in error.

Overall comparison of the concentrations in the three flasks shows good agreement between them except for those cases already noted. Table 6 lists the losses for each chemical. The chemicals are listed in the general order of decreasing volatility as can be seen by comparing the relative amounts of each chemical which was lost.

Table 6. Loss of parent chemicals based on soil concentration data measured at 100 hours after the start of experiments.

Chemical	Flask 1 percent	Flask 2 percent	Flask 3 percent	Average	95% CI
Toluene	NV	NV	NV	NV	NV
Phenol	NV	NV	NV	NV	NV
m-Cresol	NV	NV	NV	NV	NV
2,6-dimethylphenol	NV	NV	NV	NV	NV
Naphthalene	46.7	44.5	16.2	35.8	+/-23.5
2-Methylnaphthalene	16.3	21.6	-8.6	9.7	+/-22.2
2-Ethyl-naphthalene	9.6	12.8	-13.4	3.0	+/-19.7
Pentachlorophenol	12.9	47.1	17.8	26.0	+/-25.4
Anthracene	4.8	-1.2	8.9	4.2	+/-7.0

NV indicates that no value was measured.

A negative value means that a gain was found.

Percent refers to percentage of original mass lost over the course of the experiments.

Soil moisture content was measured at the beginning and end of the experiment. A loss of moisture from 10.78% at the beginning to 3.3% was seen. This loss of moisture from the soil is believed to have a pronounced impact on the flux rate of the individual chemicals as can be seen by looking at Equation 5. The air filled porosity, S_a , increases as moisture content decreases, which would increase the effective diffusion coefficient.

Comparison of volatilization data with soil extract data.

Losses due to volatilization were calculated using flux data for naphthalene and 2-methylnaphthalene since these two chemicals were the only ones with both flux and soil extract data. The mass lost during each time period was found by using the average of the flux rates at the beginning and end of each period, and multiplying this value by the time increment and soil surface area. This mass was subtracted from the original mass found at time 0 and was divided by the mass of soil to calculate the concentration that would result if volatilization were the only loss. It can be seen from Table 7 that the measured flux rates accounted for only a small portion of the losses from the soil as measured in the soil extracts. Refer to Appendix E for complete data analysis.

Table 7. Loss of chemicals from soil accounted for by flux data.

Chemical	Flask 1 percent	Flask 2 percent	Flask 3 percent	Avg	95% CI
Naphthalene	2.9	5.8	18.6	9.1	+/-11.5
2-Methylnaphthalene	2.5	2.3	-18.5	9.8	+/-16.6

A negative value means that a gain was found.

Percent refers to percentage of original mass lost over the course of the experiments.

The validity of the data for Flask 3 is questionable as was mentioned above. Data for Flasks 1 and 2 show that less than 6% of the total loss of these two constituents can be accounted for by volatilization data. If the data are accurate, other mechanisms remove far more of these chemicals than does volatilization. This conclusion invalidates assumption 4 of the model which states that the chemicals do not decompose, react, etc., but does not explain why volatilization of some of the chemicals would tend to increase over time.

Parameter estimation and model calculations.

The model predicts that soil mixing creates a spike in the flux rate curve. Equation 2 illustrates that the flux rate approaches infinity as the time approaches zero in the case of this experiment because h_0 is equal to zero making the

denominator increasingly smaller with each time increment in the negative direction. The spikes last only a few minutes however, and the flux rate soon returns to near what it would have been if mixing had not occurred. According to the model, replicate measured flux rates can vary widely over a short sampling period in this region of the flux curve.

A better time to take air samples would have been just before mixing the soil or at some time after mixing when the flux rate curve would be expected to be more stable. However, for the purposes of this experiment, air sampling was performed right after mixing to evaluate the potentially high loss of hazardous chemicals from this process. This aspect may explain some of the variation in measured flux rates.

Plots of the predicted flux rates and measured values (see Appendix F) show that in some cases, the data are relatively close to the predicted rates while in other cases little agreement exists between the two sets of numbers. The flux data for the three flasks were combined and compared to predicted values by calculating 95% confidence intervals for the data and observing whether the predicted value fell within that range. The ratios of the average measured concentrations to the predicted values were also calculated. The results are summarized in Table 8.

A careful examination of Table 8 reveals that the model overpredicted the mass flux rates for only one chemical, naphthalene. A few of the flux rates were over predicted but not consistently nor to the degree as the predictions for naphthalene. All other flux rates were underpredicted by as little as 6% and as much as 1300%. For all chemicals except naphthalene the predictions were within 2 orders of magnitude.

The effects of soil moisture content on the effective soil diffusion, D_A' , coefficient can be seen by examining Equation 5. As mentioned above, soil moisture content declined from 10.78% to 3.3% which correspond to correction factors due to soil air filled porosities, $S_A^{10/3}$ of 9.814E-02 and 1.592E-01, respectively, which would cause a 62% increase in D_A' . This would explain, in

part at least the increase in flux rates of some of the chemicals with longer evaporation times (t_d).

Table 8. Comparison of measured flux rates to predicted rates.

Time	Average Flux Rate	W/in 95% CI?	Average/Predicted
Toluene			
0.17	7.22E-05	Yes	1.05
1.18	4.66E-05	Yes	1.80
5.17	1.77E-05	Yes	1.41
Phenol			
0.17	3.82E-05	No	1.93
1.18	5.45E-05	No	7.31
5.17	4.75E-05	No	13.13
10.17	4.84E-05	No	2.73
50.50	3.98E-06	No	4.73
100.17	1.65E-05	No	1.41
m-Cresol			
0.17	2.43E-05	No	0.90
1.18	3.69E-05	No	3.64
5.17	2.64E-05	No	5.38
10.17	2.82E-05	Yes	1.06
50.50	4.52E-05	No	2.88
100.17	3.71E-05	No	1.36
2,6-Dimethylphenol			
0.17	3.20E-05	No	0.18
1.18	8.75E-05	Yes	1.32
5.17	7.17E-05	No	2.23
10.17	8.02E-05	Yes	0.84
50.50	9.08E-05	No	4.65
Naphthalene			
0.17	2.06E-05	No	2.97E-04
1.18	1.37E-04	No	5.24E-03
5.17	4.69E-04	No	3.73E-02
10.17	4.03E-04	No	6.78E-03
50.50	8.52E-04	No	3.31E-02
100.17	9.59E-04	No	2.81E-02
2-Methylnaphthalene			
0.17	9.44E-06	No	0.18
1.18	3.96E-05	Yes	2.06
5.17	1.27E-04	No	13.63
10.17	4.09E-05	Yes	0.78
50.50	2.79E-04	Yes	8.35
100.17	6.42E-04	No	9.89

Conclusions

A creosote waste was examined in laboratory studies and a modeling exercise to estimate the potential for volatilization of hazardous constituents during landfarming operations. Nine constituents, toluene, phenol, m-cresol, 2,6-dimethylphenol, naphthalene, 2-methylnaphthalene, 2-ethylnaphthalene, pentachlorophenol, and anthracene were included in the study. Based on data and information collected during the study, the following conclusions were drawn:

1. Analysis of the creosote waste showed that the more volatile constituents were found to have lower concentrations in general than multiple ringed aromatics. Concentrations varied from 5.6 $\mu\text{g/g}$ for toluene to 41,800 $\mu\text{g/g}$ for 2-methylnaphthalene.
2. Of the nine chemicals studied, consisting of 27 sets of mass flux rate data, only 2 sets of flux data yielded a straight line from linear regression analysis of mass flux rate against the inverse square of time by established criteria. A set for toluene met this criteria and appeared to follow the model. Another set of data for naphthalene met the criteria for a straight line but the slope of the regressed line had a negative slope showing that the flux rate increased, contrary to that suggested by the model. A third set of data for m-cresol had a positive slope but did not qualify as a straight line.
3. Soil concentrations of the nine test chemicals were found to show a decrease in concentrations over time. The total losses of two chemicals (naphthalene and 2-methylnaphthalene) in soil were compared to mass flux data for the entire study period. The amount of each chemical that volatilized represented less than 6% of the total loss as determined by soil concentrations at the beginning and end of the study period. The fourth assumption of the Thibodeaux-Hwang AERR model, which states that the chemicals do not decompose, react with the soil or adsorb irreversibly, is invalid for these chemicals.

Engineering Significance

The need of the practicing engineer to predict the volatilization rates for organic materials which have been applied to or spilled on soil has increased in recent years by requirements of federal regulations governing the use, shipping and disposal of hazardous chemicals in the United States. Both the Resource Conservation and Recovery Act (RCRA) and the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) have specific requirements for assessing the impact of these actions upon the environment.

The Thibodeaux-Hwang AERR model was developed to predict the rate at which chemicals volatilize from soil surfaces (reference 1). Several experimenters have looked at the validity of the assumptions made to simplify the model and the impact each parameter has on the accuracy of the model (references 2, 3, 4, and 7).

This study has shown that in laboratory experiments, several important parameters need close attention. Soil moisture content is inversely related to flux rates and should be controlled or measured in order to assess its impacts. Bulk density affects the rate of chemical movement from the soil interstices to the atmosphere and should receive attention in experiments that involve mass flux measurements. Temperature may also affect certain parameters of the model and should be controlled or measured to assess its impact.

Analysis of the data in this experiment can be interpreted to show that an actual increase in volatilization rates can occur as soil moisture content decreases because the effective diffusion coefficient increases as the air filled porosity increases. Decreasing moisture content, therefore, will have a much greater effect on the flux rates of less volatile chemicals such as naphthalene than on volatile chemicals such as toluene because they remain in the soil for much greater time spans.

The relative amounts of two of the test chemicals lost from a soil column due to volatilization were found to be very small (3% to 6%) compared to the total

loss observed over the experimental period. The relative importance of volatilization as a loss mechanism should be expected to increase as the volatility of the chemical in question increases. For nonvolatile constituents such as naphthalene and 2-methylnaphthalene, the Thibodeaux-Hwang model would not be very useful in predicting the total loss of chemicals because of the importance of other mechanisms (leaching, biodegradation, etc) to their fate in soil systems.

Soil mixing is known to have a short term impact on the rate of volatilization, which coincides with predictions of the Thibodeaux-Hwang AERR model.

The need for accurate values for parameters needed for input to the Thibodeaux-Hwang AERR model is emphasized by the difficulty in using estimation techniques, especially when one considers that many techniques exist and choosing the most appropriate equation or relationship can become tedious and time consuming. Estimation techniques, in general were useful in calculating the needed model parameters.

Estimation methods are used in many aspects of engineering design and evaluation and most engineers are accustomed to these procedures. Other estimation techniques, such as structural design, water distribution system designs, etc. use correction factors. Since correction factors have not been included in the estimation techniques included in this paper, the results should be viewed with caution and not relied on beyond their perceived accuracy.

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Appendix A - Chromatography

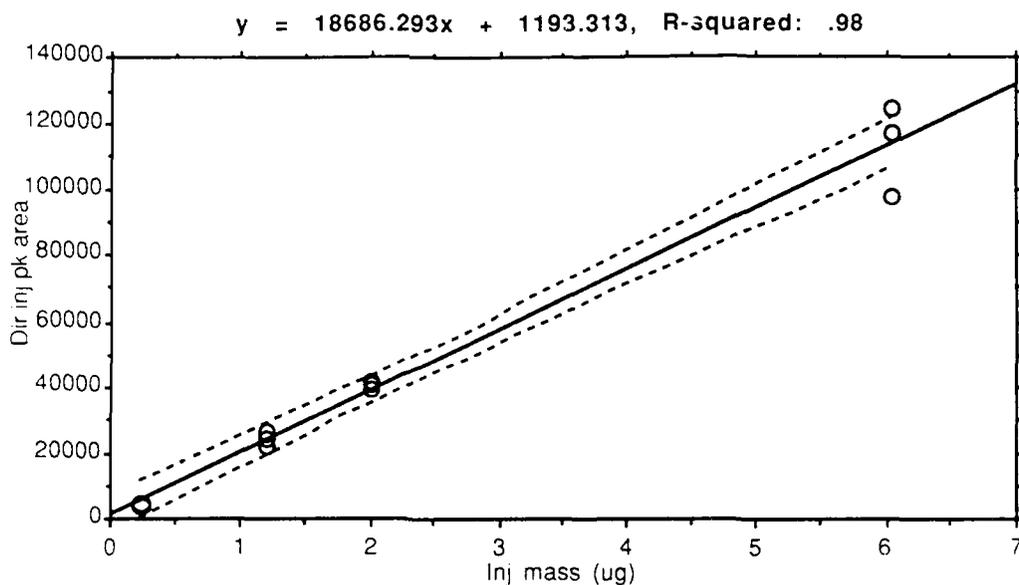


Figure A-1. Toluene standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter	Value	Std. Err.	Std. Value	t-Value	Probability
INTERCEPT	1193.313				
SLOPE	18686.293	833.449	.99	22.42	1.0000E-4

Confidence Intervals Table

Parameter	95% Lower	95% Upper	90% Lower	90% Upper
MEAN (X Y)	41446.266	49634.851	42210.135	48870.981
SLOPE	16829.034	20543.552	17175.542	20197.045

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF	R	R-squared	Adj. R-squared	Std. Error
11	.99	.98	.979	6364.671

Analysis of Variance Table

Source	DF	Sum Squares	Mean Square	F-test
REGRESSION	1	2.036E10	2.036E10	502.676
RESIDUAL	10	405090333.292	40509033.329	p = 1.0000E-4
TOTAL	11	2.077E10		

No Residual Statistics Computed

Figure A-2. Statistical Data - toluene standard curve.

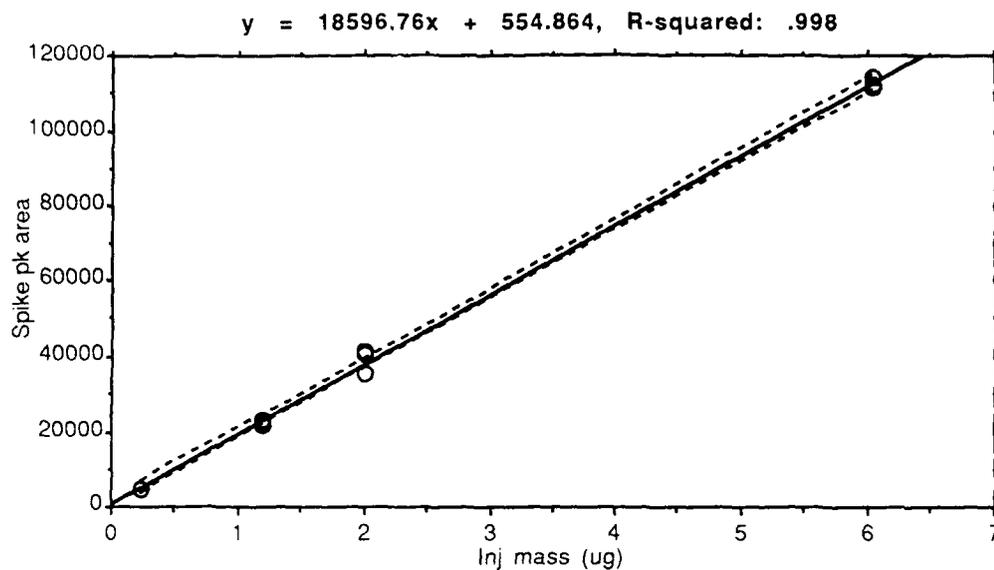


Figure A-3. Toluene spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	554.864				
SLOPE	18596.76	236.454	999	78.648	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	43528.051	45851.199	43744.765	45634.485
SLOPE	18069.845	19123.675	18168.151	19025.369

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R	R-squared:	Adj. R-squared:	Std. Error:
11	.999	.998	.998	1805.693

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	2.017E10	2.017E10	6185.584
RESIDUAL	10	32605269.114	3260526.911	p = 1.0000E-4
TOTAL	11	2.020E10		

No Residual Statistics Computed

Figure A-4. Statistical Data - toluene spike curve.

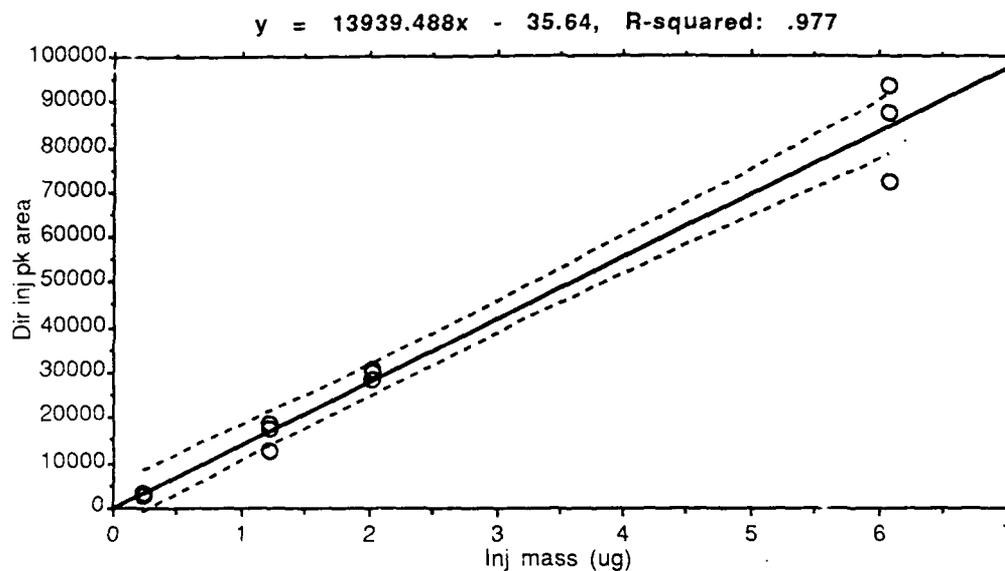


Figure A-5. Phenol standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter	Value	Std. Err.	Std. Value	t-Value	Probability
INTERCEPT	-35.64				
SLOPE	13939.488	682.687	.988	20.419	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	29880.618	36630.065	30510.238	36000.445
SLOPE	12418.186	15460.789	12702.015	15176.961

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF	R	R-squared	Adj. R-squared	Std. Error
11	.988	.977	.974	5246.084

Analysis of Variance Table

Source	DF	Sum Squares	Mean Square	F-test
REGRESSION	1	1.147E10	1.147E10	416.918
RESIDUAL	10	275213949.748	27521394.975	$p = 1.0000E-4$
TOTAL	11	1.175E10		

No Residual Statistics Computed

Figure A-6. Statistical Data - phenol standard curve.

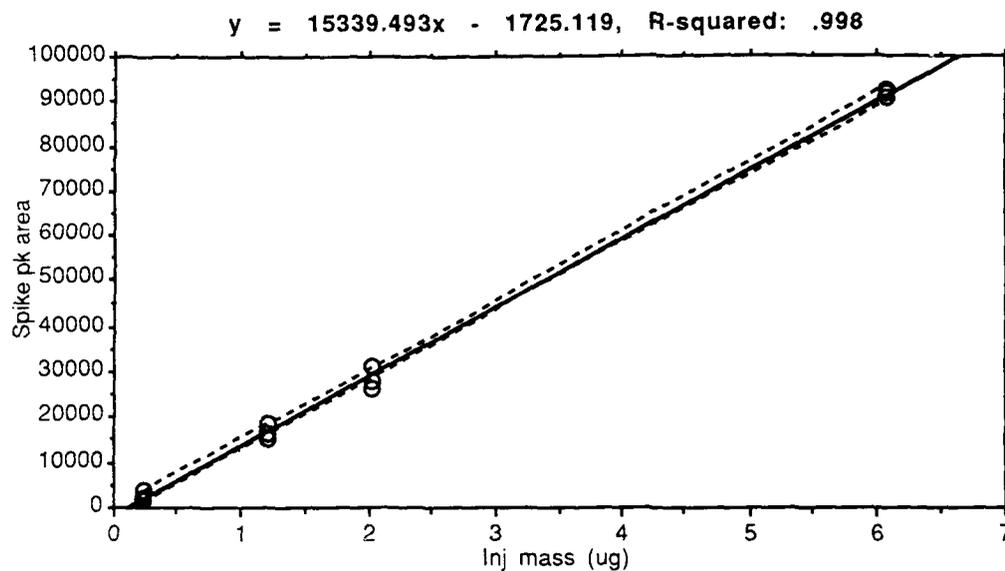


Figure A-7. Phenol spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-1725.119				
SLOPE	15339.493	197.947	.999	77.493	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	33930.913	35887.937	34113.473	35705.377
SLOPE	14898.387	15780.6	14980.684	15698.303

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.999	.998	.998	1521.12

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	1.389E10	1.389E10	6005.128
RESIDUAL	10	23138045.946	2313804.595	$p = 1.0000E-4$
TOTAL	11	1.392E10		

No Residual Statistics Computed

Figure A-8. Statistical Data - phenol spike curve.

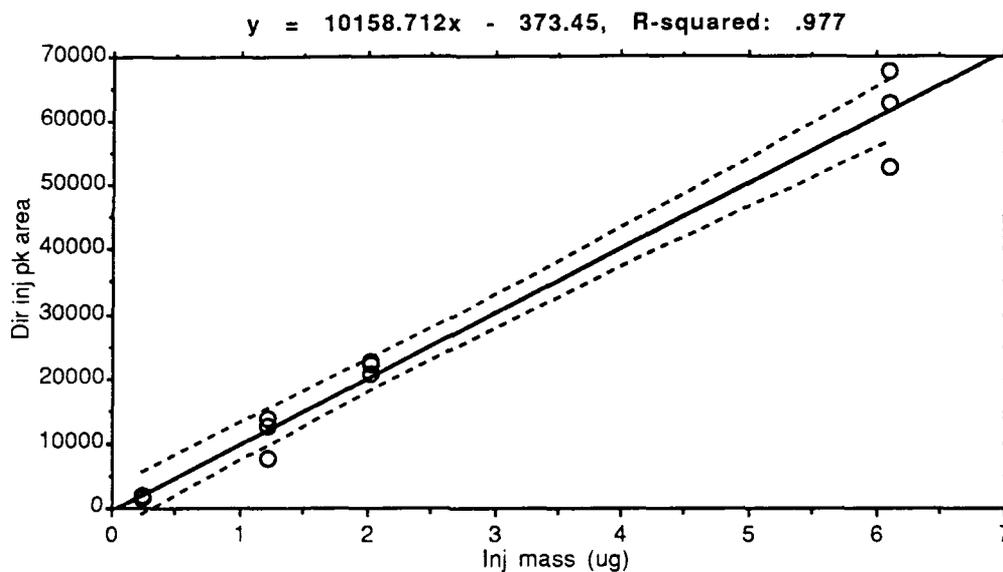


Figure A-9. m-Cresol standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-373.45				
SLOPE	10158.712	497.437	.988	20.422	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	21495.609	26427.879	21955.715	25967.774
SLOPE	9050.221	11267.202	9257.032	11060.392

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.988	.977	.974	3833.662

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	6.13E9	6.13E9	417.062
RESIDUAL	10	146969669.454	14696966.945	p = 1.0000E-4
TOTAL	11	6.277E9		

No Residual Statistics Computed

Figure A-10. Statistical Data - m-cresol standard curve.

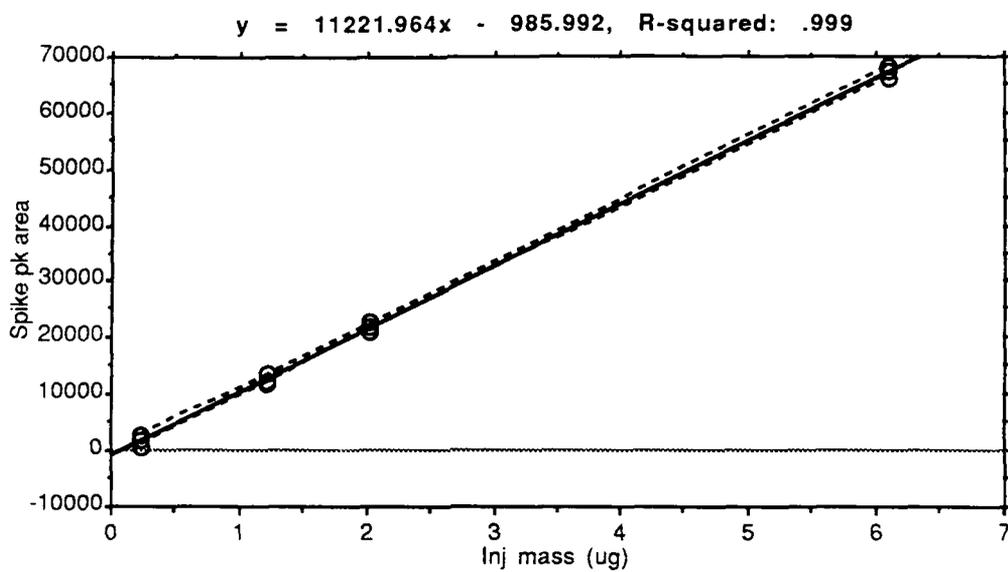


Figure A-11. m-Cresol spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-985.992				
SLOPE	11221.964	112.563	.999	99.695	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	25338.171	26454.273	25442.286	26350.158
SLOPE	10971.128	11472.799	11017.926	11426.001

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.999	.999	.999	867.503

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	7.48E9	7.48E9	9939.088
RESIDUAL	10	7525616.303	752561.63	$p = 1.0000E-4$
TOTAL	11	7.487E9		

No Residual Statistics Computed

Figure A-12. Statistical Data - m-cresol spike curve.

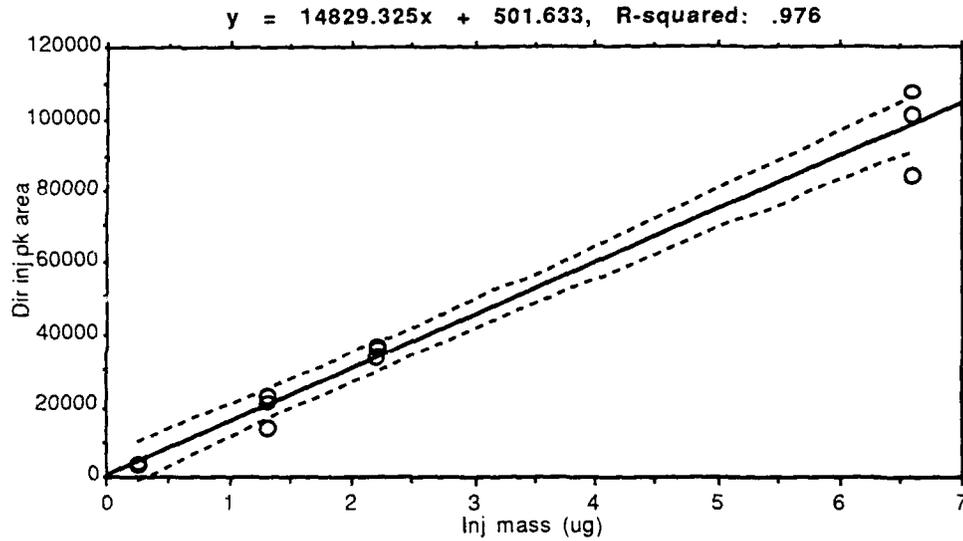


Figure A-13. 2,6-Dimethylphenol standard curve.

Simple Regression X1: Inj mass (ug) Y1: Dir inj pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	501.633				
SLOPE	14829.325	734.186	.988	20.198	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	34946.934	42812.916	35680.71	42079.14
SLOPE	13193.264	16465.386	13498.503	16160.147

Simple Regression X1: Inj mass (ug) Y1: Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.988	.976	.974	6113.924

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	1.525E10	1.525E10	407.973
RESIDUAL	10	373800620.343	37380062.034	p = 1.0000E-4
TOTAL	11	1.562E10		

No Residual Statistics Computed

Figure A-14. Statistical Data - 2,6-dimethylphenol standard curve.

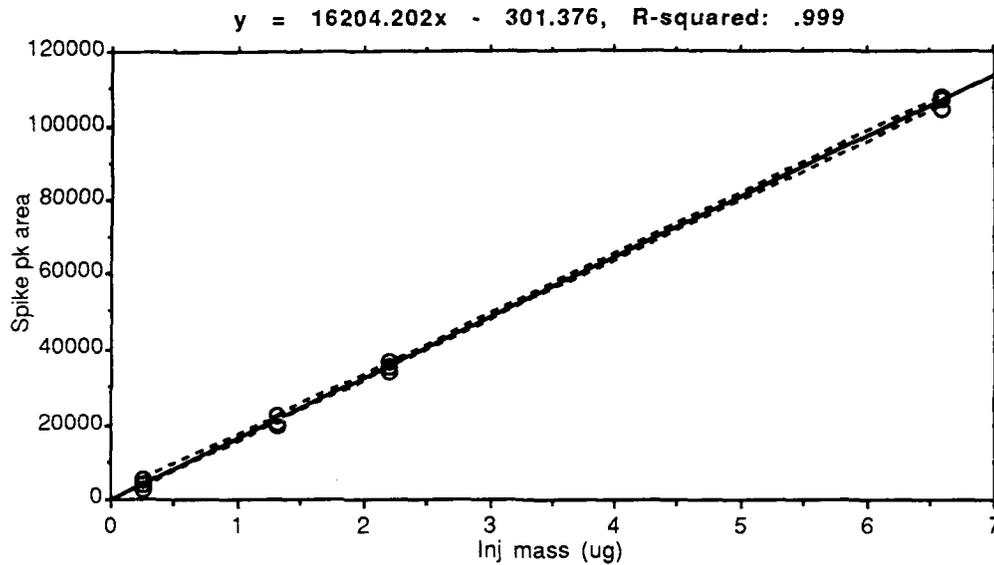


Figure A-15. 2,6-dimethylphenol spike curve.

Simple Regression X₁: Inj mass (ug) Y₁: Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-301.376				
SLOPE	16204.202	145.478	1	111.386	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	40855.783	42414.417	41001.179	42269.021
SLOPE	15880.019	16528.386	15940.502	16467.903

Simple Regression X₁: Inj mass (ug) Y₁: Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	1	.999	.999	1211.466

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	1.821E10	1.821E10	12406.831
RESIDUAL	10	14676507.28	1467650.728	p = 1.0000E-4
TOTAL	11	1.822E10		

No Residual Statistics Computed

Figure A-16. Statistical Data - 2,6-dimethylphenol spike curve.

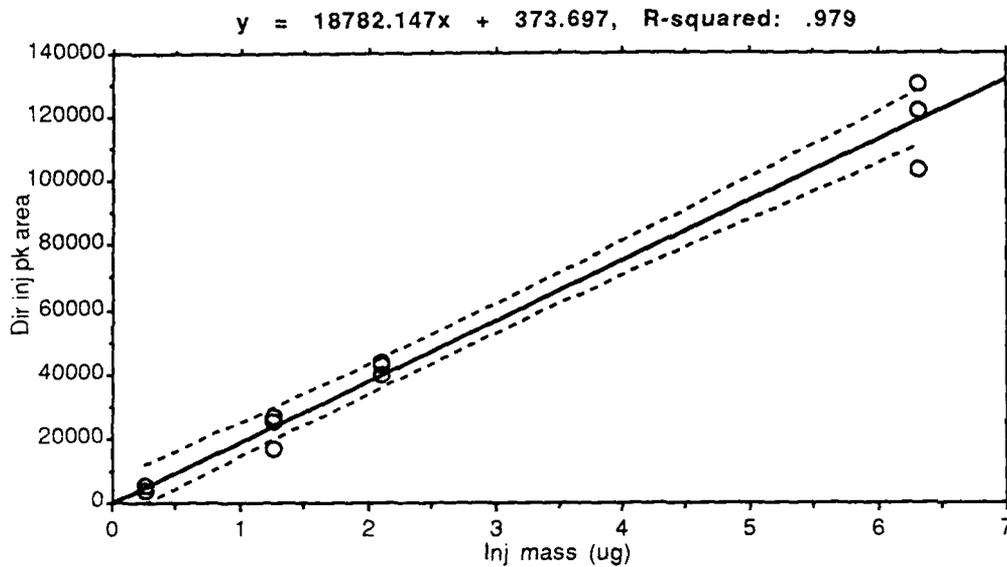


Figure A-17. Naphthalene standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err:	Std. Value:	t-Value:	Probability:
INTERCEPT	373.697				
SLOPE	18782.147	869.623	.989	21.598	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	42493.531	51422.702	43326.486	50589.747
SLOPE	16844.276	20720.017	17205.823	20358.47

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.989	.979	.977	6940.299

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	2.247E10	2.247E10	466.475
RESIDUAL	10	481677446.103	48167744.61	p = 1.0000E-4
TOTAL	11	2.295E10		

No Residual Statistics Computed

Figure A-18. Statistical Data - naphthalene standard curve.

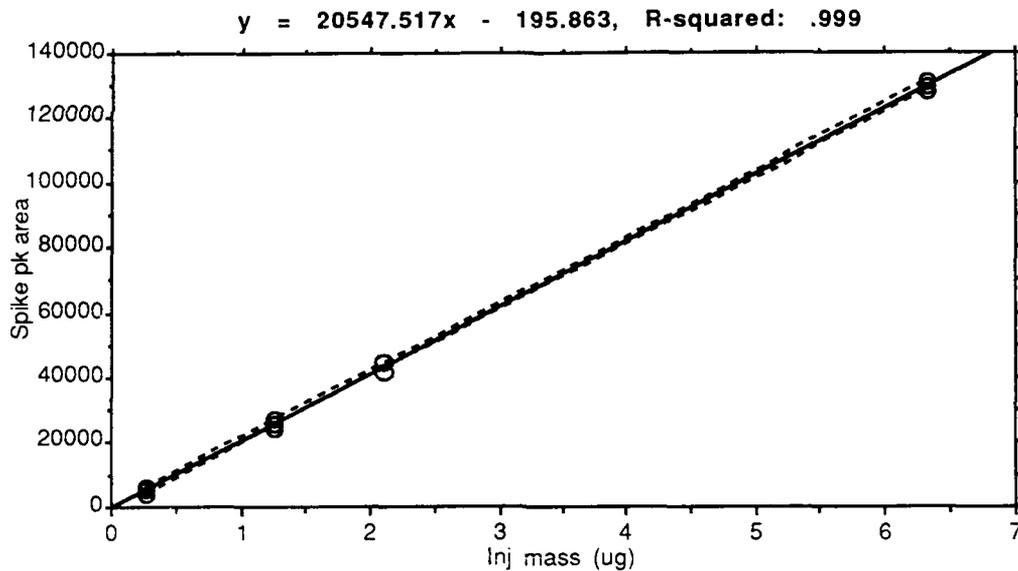


Figure A-19. Naphthalene spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-195.863				
SLOPE	20547.517	164.745	1	124.723	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	49921.33	51612.904	50079.128	51455.106
SLOPE	20180.4	20914.634	20248.893	20846.141

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	1	.999	.999	1314.795

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	2.689E10	2.689E10	15555.948
RESIDUAL	10	17286858.243	1728685.824	$p = 1.0000E-4$
TOTAL	11	2.691E10		

No Residual Statistics Computed

Figure A-20. Statistical Data - naphthalene spike curve.

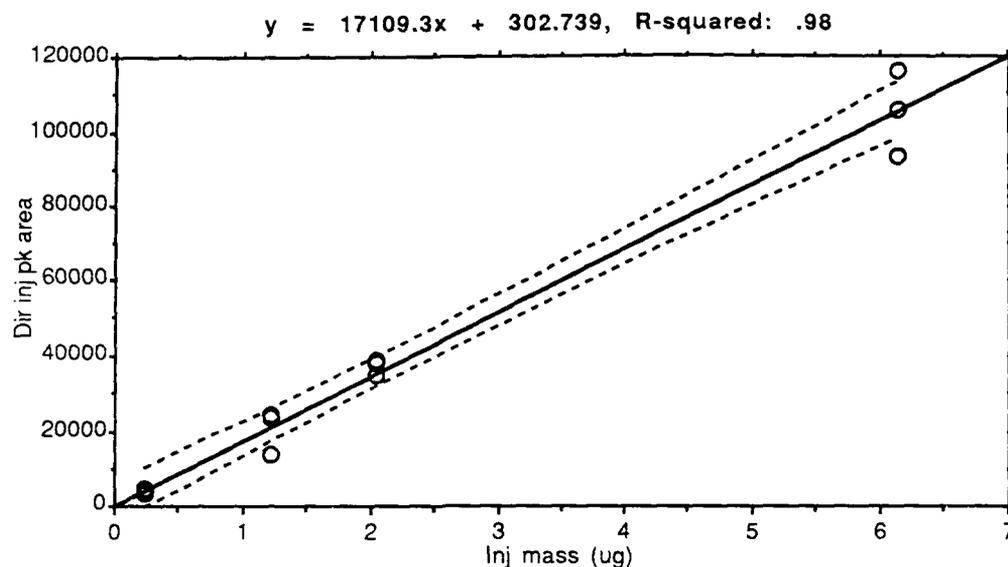


Figure A-21. 2-Methylnaphthalene standard curve.

Simple Regression X1: Inj mass (ug) Y1: Dir inj pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	302.739				
SLOPE	17109.3	782.112	.99	21.876	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	37684.583	45498.934	38413.542	44769.974
SLOPE	15366.439	18852.161	15691.604	18526.997

Simple Regression X1: Inj mass (ug) Y1: Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.99	.98	.977	6073.792

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	1.765E10	1.765E10	478.549
RESIDUAL	10	368909515.501	36890951.55	p = 1.0000E-4
TOTAL	11	1.802E10		

No Residual Statistics Computed

Figure A-22. Statistical Data - 2-methylnaphthalene standard curve.

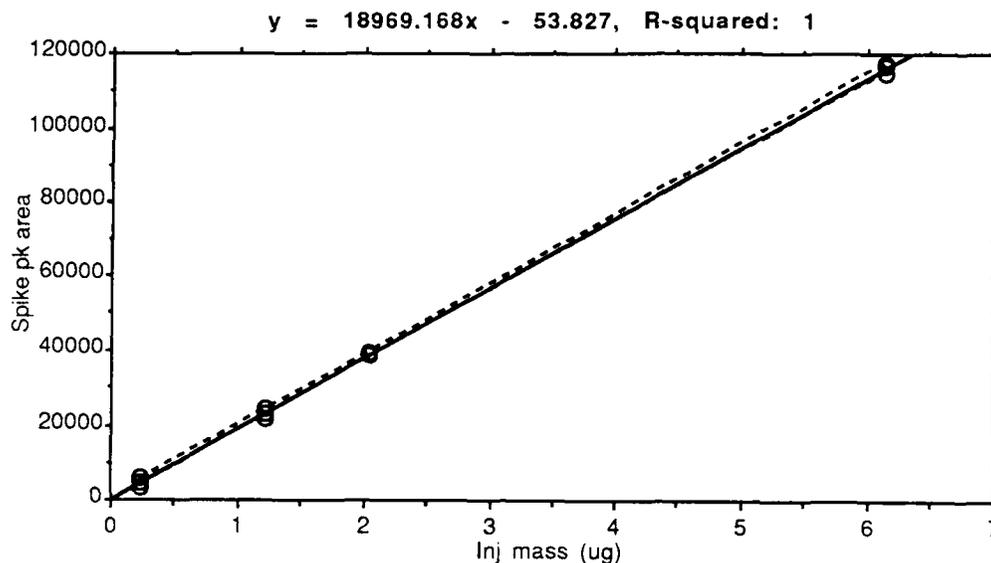


Figure A-23. 2-Methylnaphthalene spike curve.

Simple Regression X₁: Inj mass (ug) Y₁: Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-.53.827				
SLOPE	18969.168	131.423	1	144.337	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	45066.972	46380.061	45189.463	46257.57
SLOPE	18676.305	19262.03	18730.944	19207.391

Simple Regression X₁: Inj mass (ug) Y₁: Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	1	1	.999	1020.613

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	2.170E10	2.170E10	20833.193
RESIDUAL	10	10416510.509	1041651.051	p = 1.0000E-4
TOTAL	11	2.171E10		

No Residual Statistics Computed

Figure A-24. Statistical Data - 2-methylnaphthalene spike curve.

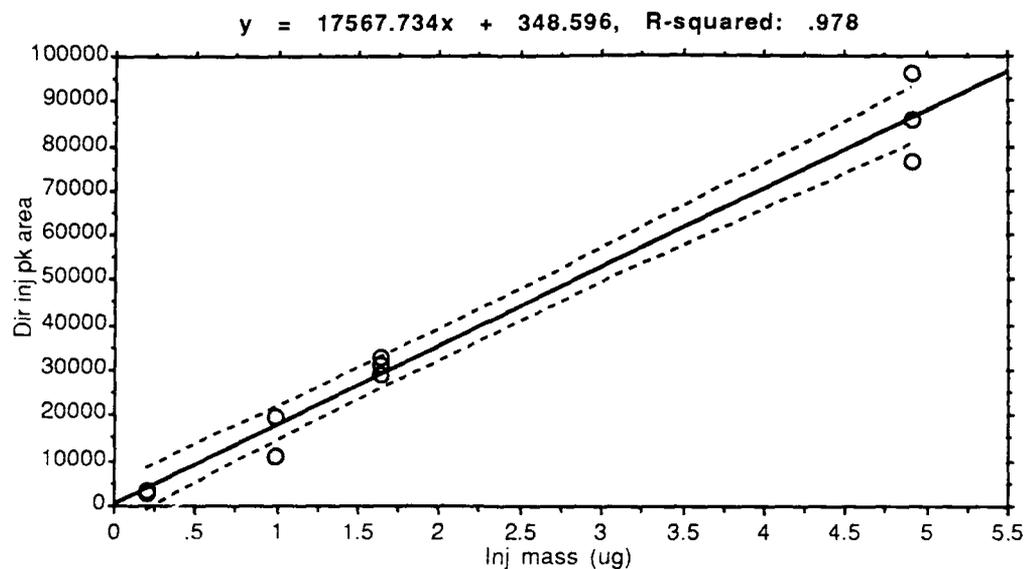


Figure A-25. 2-Ethyl-naphthalene standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	348.596				
SLOPE	17567.734	833.327	.989	21.081	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	30952.355	37617.779	31574.137	36995.997
SLOPE	15710.747	19424.721	16057.204	19078.264

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.989	.978	.976	5180.776

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	1.193E10	1.193E10	444.428
RESIDUAL	10	268404414.214	26840441.421	p = 1.0000E-4
TOTAL	11	1.220E10		

No Residual Statistics Computed

Figure A-26. Statistical Data - 2-ethyl-naphthalene standard curve.

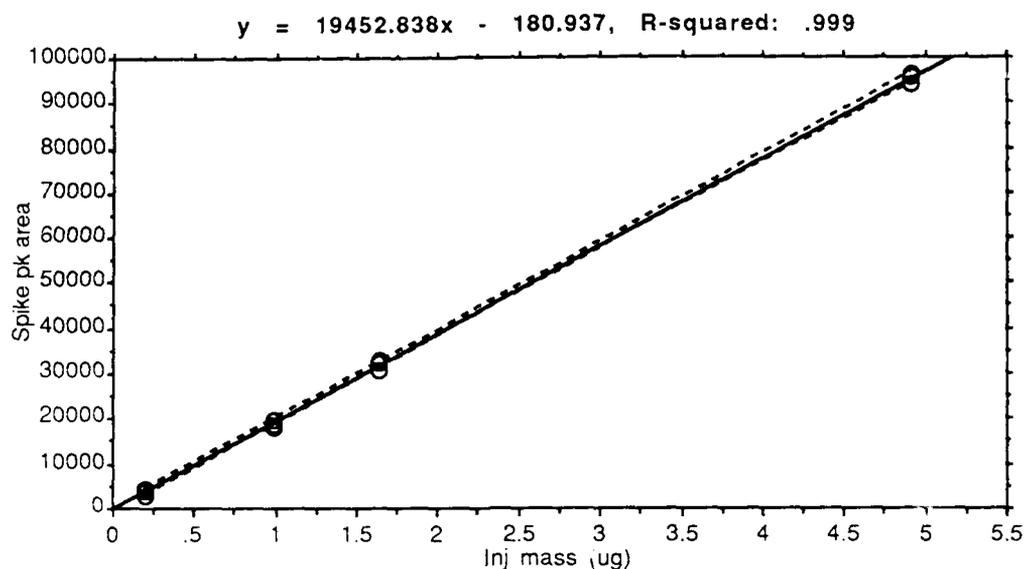


Figure A-27. 2-Ethynaphthalene spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter	Value	Std. Err.	Std. Value:	t-Value	Probability:
INTERCEPT	-180.937				
SLOPE	19452.838	161.263	1	120.628	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	36752.146	38042.021	36872.471	37921.695
SLOPE	19093.479	19812.197	19160.524	19745.152

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF	R	R-squared	Adj. R-squared	Std. Error
11	1	.999	.999	1002.57

Analysis of Variance Table

Source	DF	Sum Squares	Mean Square	F-test:
REGRESSION	1	1.463E10	1.463E10	14551.095
RESIDUAL	10	10051467	1005146.7	p = 1.0000E-4
TOTAL	11	1.464E10		

No Residual Statistics Computed

Figure A-28. Statistical Data - 2-ethynaphthalene spike curve.

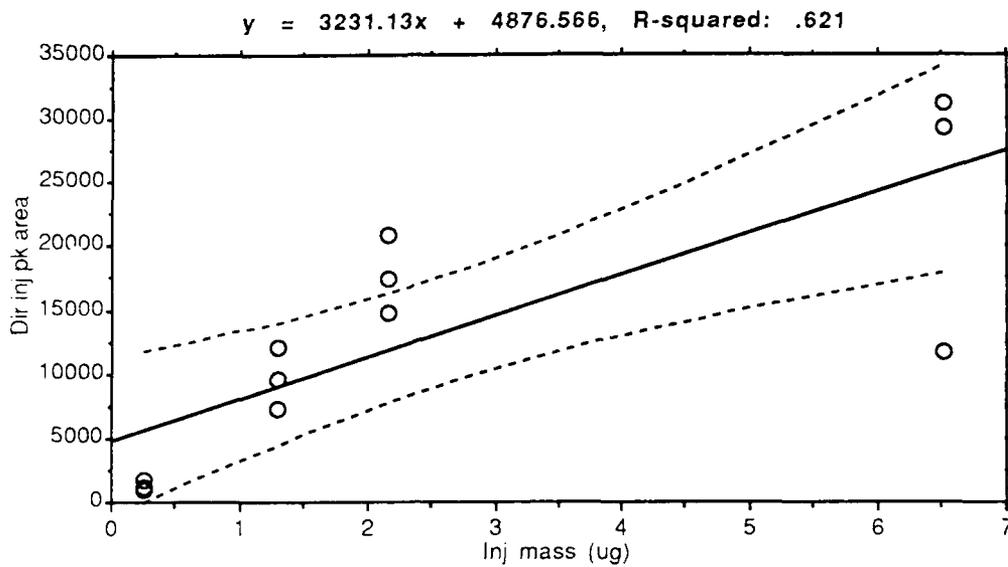


Figure A-29. Pentachlorophenol standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	4876.566				
SLOPE	3231.13	797.699	.788	4.051	.0023

Confidence Intervals Table

Parameter	95% Lower	95% Upper:	90% Lower:	90% Upper
MEAN (X,Y)	8921.024	17373.876	9709.545	16585.355
SLOPE	1453.536	5008.723	1785.181	4677.078

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF	R	R-squared:	Adj. R-squared:	Std. Error:
11	.788	.621	.583	6570.076

Analysis of Variance Table

Source	DF	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	708225936.783	708225936.783	16.407
RESIDUAL	10	431658921.747	43165892.175	p = .0023
TOTAL	11	1139884858.53		

No Residual Statistics Computed

Figure A-30. Statistical Data - pentachlorophenol standard curve.

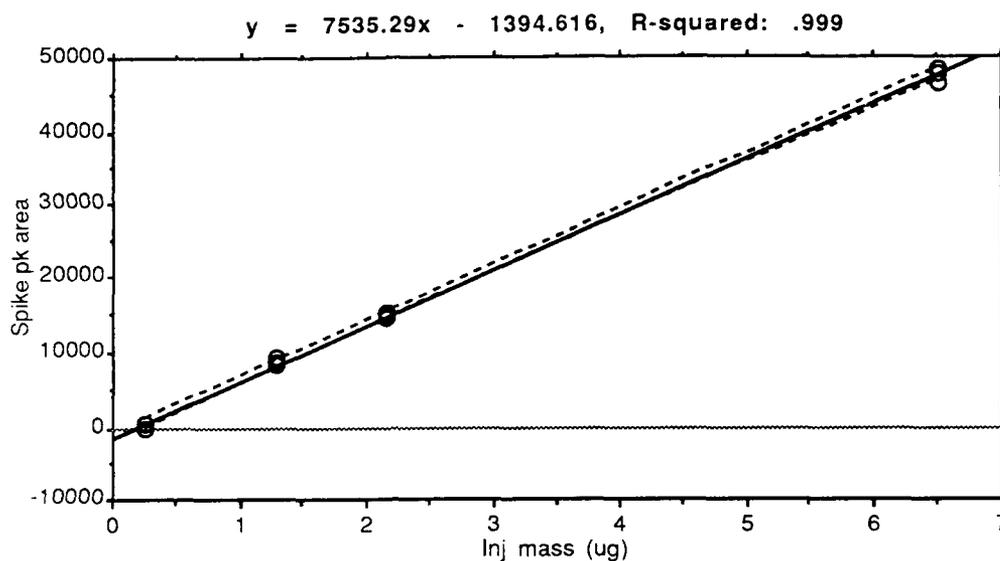


Figure A-31. Pentachlorophenol spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-1394.616				
SLOPE	7535.29	83.081	.999	90.698	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	17453.657	18334.026	17535.782	18251.901
SLOPE	7350.152	7720.427	7384.693	7685.886

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
11	.999	.999	.999	684.277

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	3.852E9	3.852E9	8226.205
RESIDUAL	10	4682345.771	468234.577	$p = 1.0000E-4$
TOTAL	11	3.856E9		

No Residual Statistics Computed

Figure A-32. Statistical Data - pentachlorophenol spike curve.

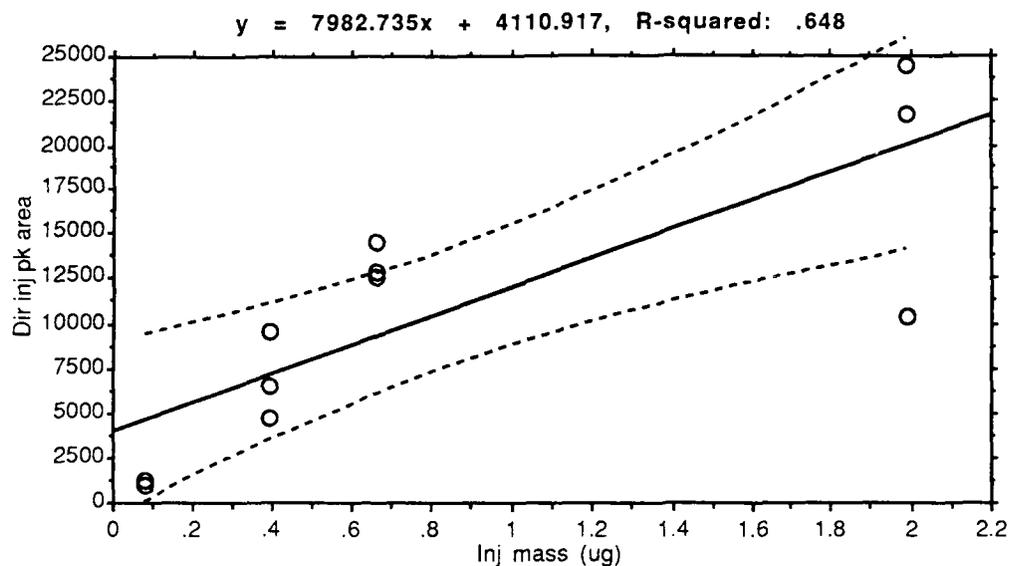


Figure A-33. Anthracene standard curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

Beta Coefficient Table

Parameter	Value	Std. Err.	Std. Value	t-Value	Probability
INTERCEPT	4110.917				
SLOPE	7982.735	1961.647	.805	4.069	.0028

Confidence Intervals Table

Parameter	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	7646.099	14092.683	8257.472	13481.31
SLOPE	3544.645	12420.825	4386.432	11579.037

Simple Regression X_1 : Inj mass (ug) Y_1 : Dir inj pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
10	.805	.648	.609	4725.206

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	369745724.103	369745734.103	16.56
RESIDUAL	9	200948182.346	22327575.816	p = .0028
TOTAL	10	570693916.449		

No Residual Statistics Computed

Figure A-34. Statistical Data - anthracene standard curve.

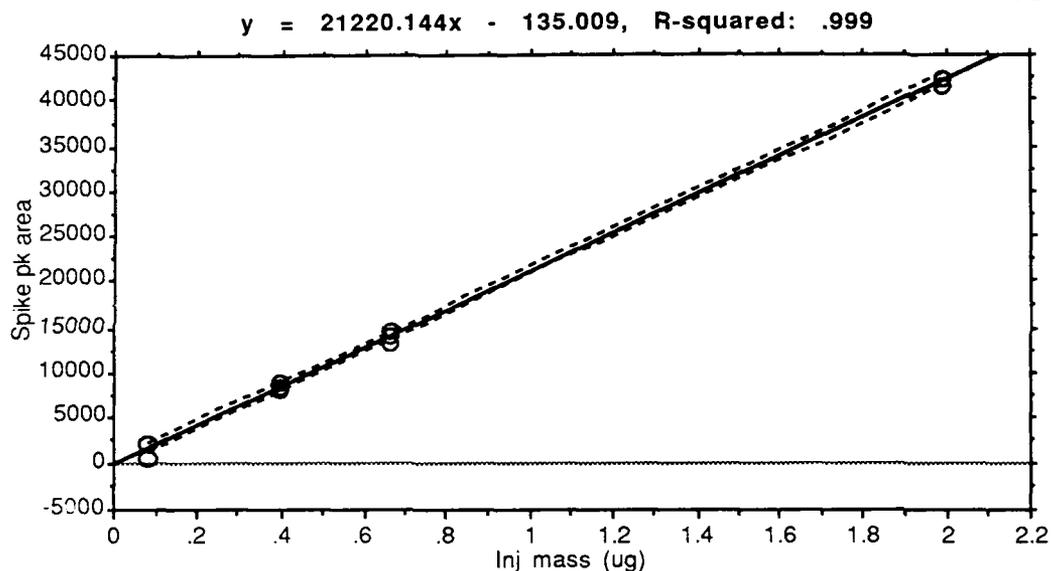


Figure A-35. Anthracene spike curve.

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

Beta Coefficient Table

Parameter:	Value:	Std. Err.:	Std. Value:	t-Value:	Probability:
INTERCEPT	-135.009				
SLOPE	21220.144	252.003	.999	84.206	1.0000E-4

Confidence Intervals Table

Parameter:	95% Lower:	95% Upper:	90% Lower:	90% Upper:
MEAN (X,Y)	17416.656	18244.817	17495.196	18166.277
SLOPE	20650.004	21790.283	20758.145	21682.143

Simple Regression X_1 : Inj mass (ug) Y_1 : Spike pk area

DF:	R:	R-squared:	Adj. R-squared:	Std. Error:
10	.999	.999	.999	607.024

Analysis of Variance Table

Source	DF:	Sum Squares:	Mean Square:	F-test:
REGRESSION	1	2612741326.14	2612741326.14	7090.629
RESIDUAL	9	3316302.706	368478.078	$p = 1.0000E-4$
TOTAL	10	2.616E9		

No Residual Statistics Computed

Figure A-36. Statistical Data - Anthracene spike curve.

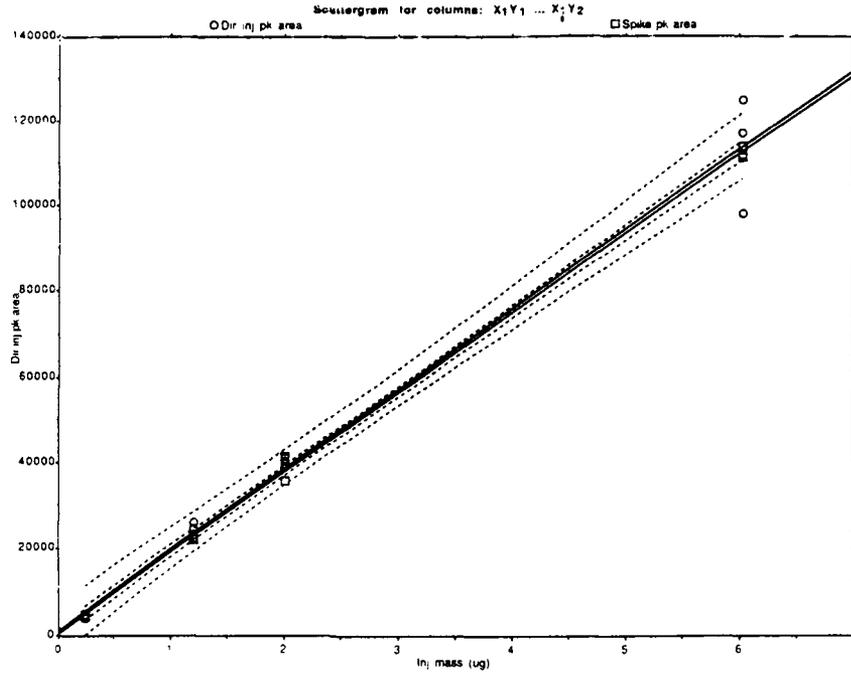


Figure A-37. Comparison of slopes for Toluene - Spikes vs direct injections.

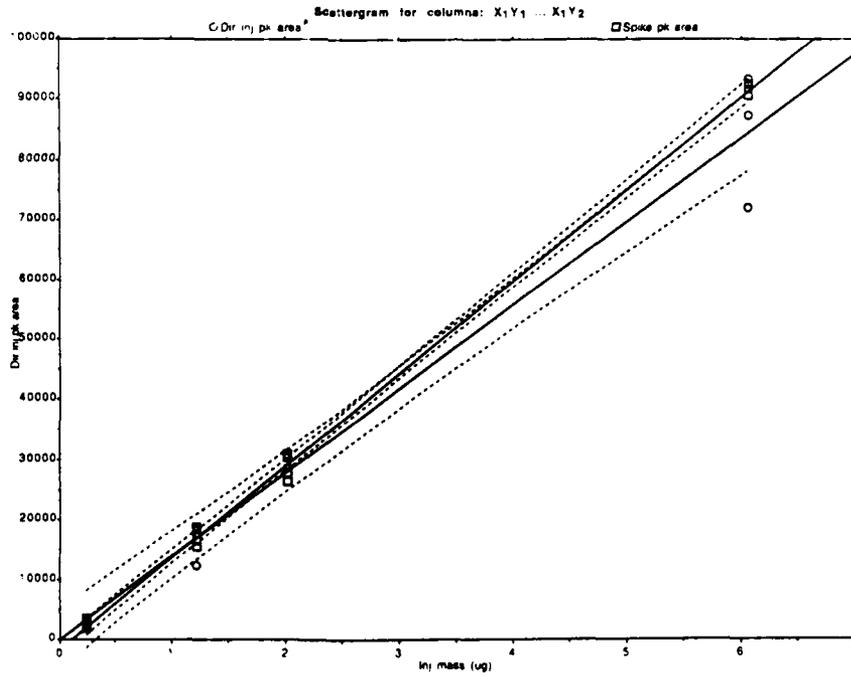


Figure A-38. Comparison of slopes for phenol - Spikes vs direct injections.

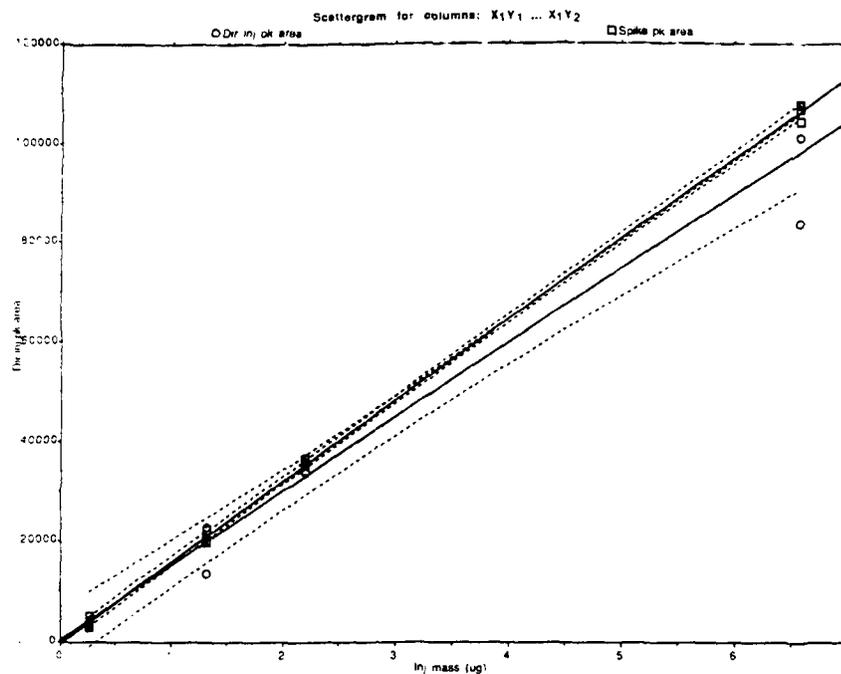


Figure A-39. Comparison of slopes for m-cresol - Spikes vs direct injections.

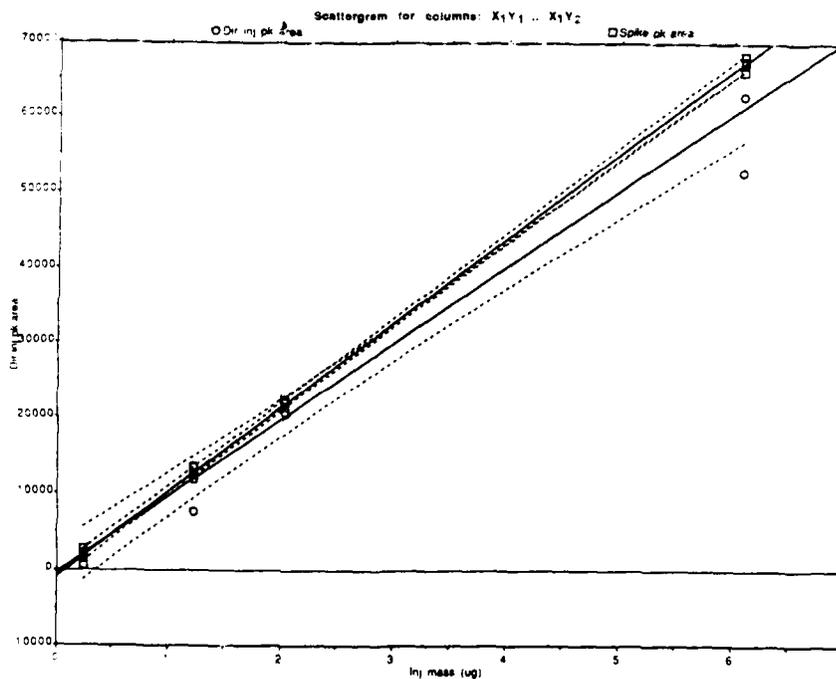


Figure A-40. Comparison of slopes for 2,6-dimethylphenol - Spikes vs direct injections.

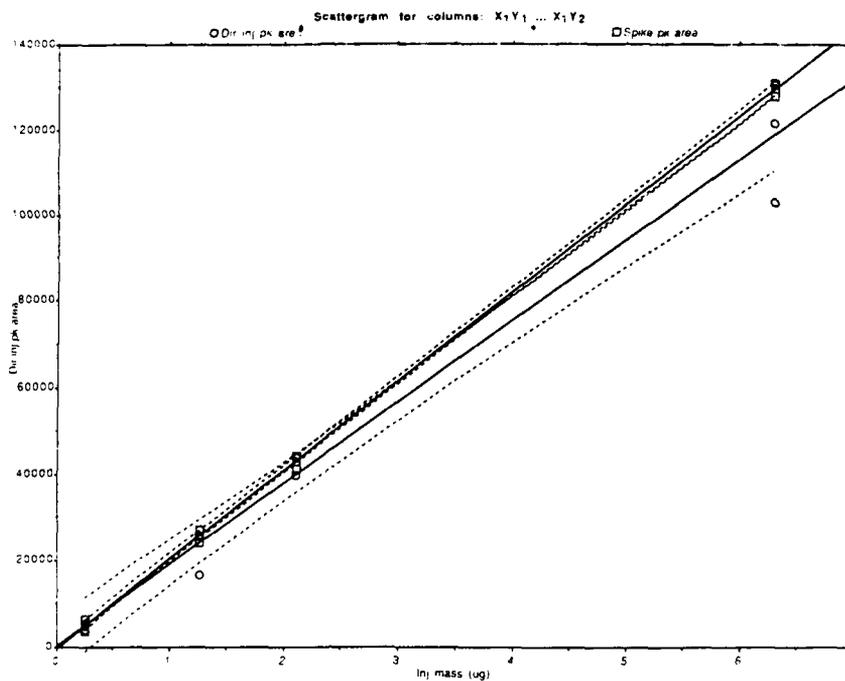


Figure A-41. Comparison of slopes for naphthalene - Spikes vs direct injections.

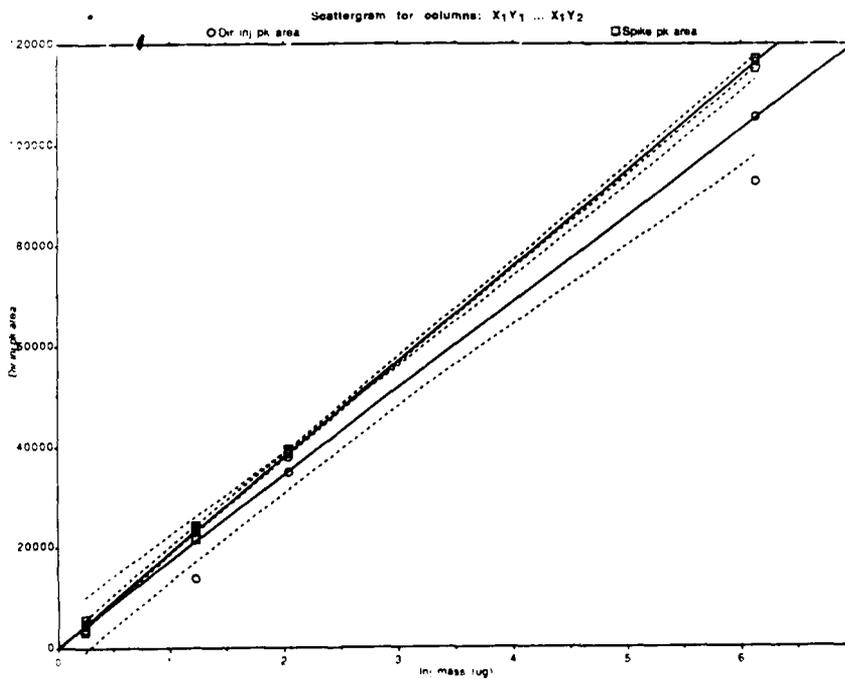


Figure A-42. Comparison of slopes for 2-methylnaphthalene - Spikes vs direct injections.

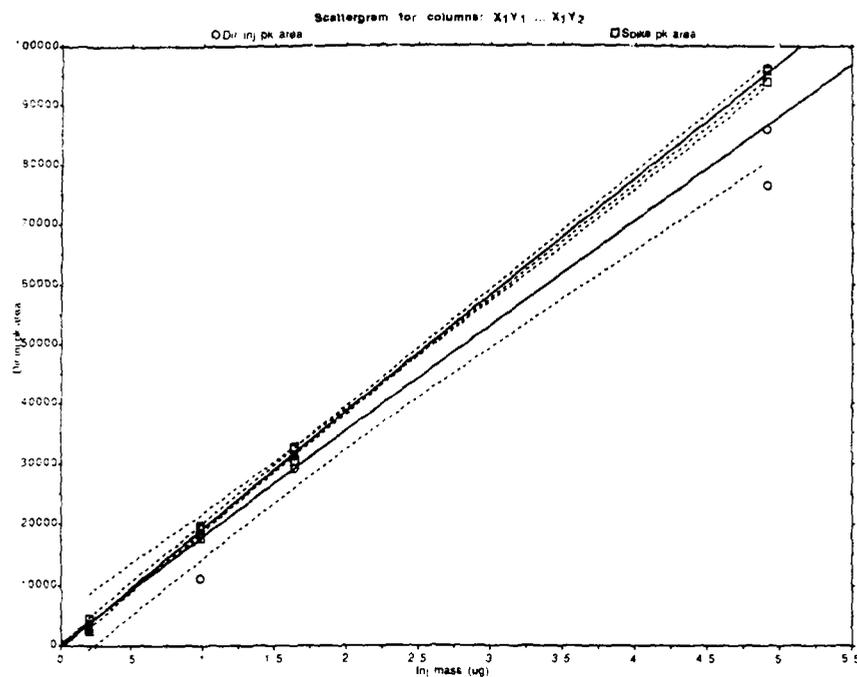


Figure A-43. Comparison of slopes for 2-ethylnaphthalene - Spikes vs direct injections.

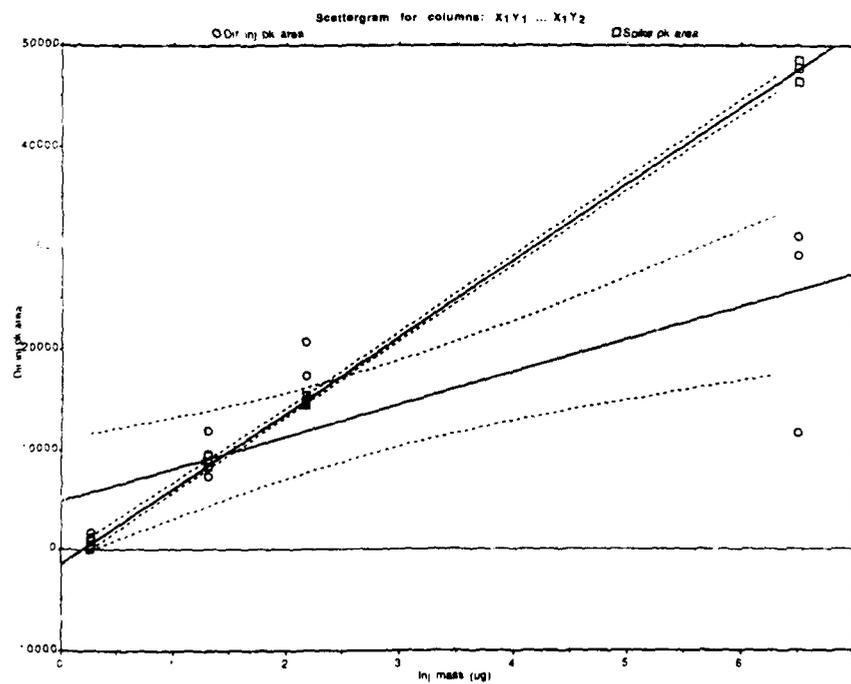


Figure A-44. Comparison of slopes for pentachlorophenol - Spikes vs direct injections.

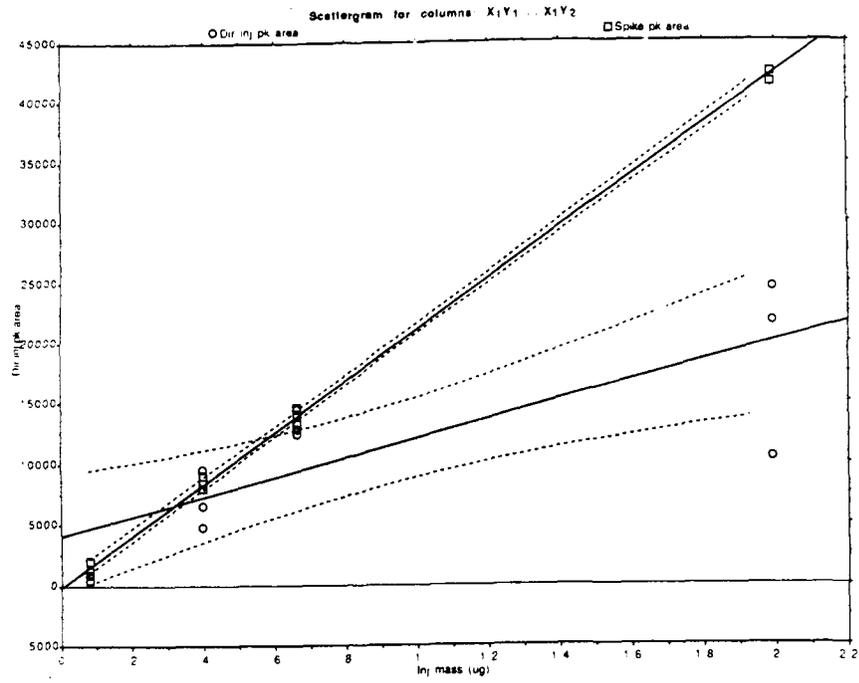


Figure A-45. Comparison of slopes for anthracene - Spikes vs direct injections.

Table A-1. Slope Comparison - Intercept Computed

Chemical	Beta (A)	Beta (B)	SE (A)	SE (B)	T
Toluene	18686.3	18596.8	833.449	236.454	0.1462
Phenol	13939.5	15339.5	682.687	197.947	-2.7854
m-Cresol	10158.7	11222.0	497.437	112.563	-2.9483
2,6-Dimethylphenol	14829.3	16204.2	734.186	145.478	-2.5978
Naphthalene	18782.1	20547.5	869.623	164.745	-2.8207
2-Methylnaphthalene	17109.3	18969.2	782.112	131.423	-3.3165
2-Ethylnaphthalene	17567.7	19452.8	833.327	161.263	-3.1409
Pentachlorophenol	3231.1	7535.3	797.699	83.081	-7.5896
Anthracene	7982.7	21220.1	1961.647	252.003	-9.4655

Table A-2. Slope Comparison - Zero Intercept

Chemical	Beta (A)	Beta (B)	SE (A)	SE (B)	T
Toluene	18956.0	18722.1	546.057	157.246	0.5822
Phenol	13931.3	14951.5	443.002	168.267	-3.0447
m-Cresol	10075.0	11001.0	323.587	95.638	-3.8809
2,6-Dimethylphenol	14933.2	16141.4	477.249	96.027	-3.5101
Naphthalene	18862.9	20505.0	564.766	107.593	-4.0393
2-Methylnaphthalene	17176.2	18956.7	507.845	85.346	-4.8897
2-Ethylnaphthalene	17663.9	19401.8	541.424	105.697	-4.4553
Pentachlorophenol	4253.9	7242.8	591.559	98.140	-7.0491
Anthracene	10781.8	21128.8	1362.722	151.231	-10.6724

Appendix B. Waste Analysis

Table B-1. Creosote Waste Analysis - Acid/Base-Neutral Extraction

Chemical	Peak Area	Mass (ug)	Diluted Conc. (ug/mL)	Waste Conc. (ug/mL)	Avg (ug/mL)	Avg (ug/g)	S. Dev (ug/mL)	95% CI (Low,High)
Naphthalene	44272.10	2.164	1082.1	28134.0	33170.9	41829.6	2361.1	31228.6 35113.2
	53607.40	2.618	1309.2	34040.2				
	53258.60	2.602	1300.8	33819.6				
	55989.60	2.734	1367.2	35547.4				
	52268.30	2.553	1276.7	33193.0				
	54003.90	2.638	1318.9	34291.1				
2-Methylnaphthalene	39672.10	2.094	1047.1	27225.1	33138.2	41788.4	3689.8	30102.9 36173.5
	47868.30	2.526	1263.2	32842.1				
	46828.60	2.472	1235.8	32129.6				
	48376.80	2.553	1276.6	33190.6				
	58136.00	3.068	1533.8	39878.8				
	48920.20	2.582	1290.9	33563.0				
2-Ethylnaphthalene	5525.56	0.293	146.7	3813.6	5045.0	6362.0	1356.6	3929.1 6161.0
	6856.91	0.362	180.9	4703.3				
	6167.14	0.326	163.2	4242.3				
	7397.87	0.390	194.8	5064.8				
	6542.21	0.346	172.8	4493.0				
	11720.30	0.612	305.9	7953.4				
Pentachlorophenol	10683.40	1.603	801.4	20837.2	22127.5	27903.5	3602.8	19163.7 25091.3
	12404.80	1.831	915.7	23807.0				
	8815.23	1.355	677.5	17614.2				
	9090.76	1.392	695.8	18089.5				
	13039.80	1.916	957.8	24902.5				
	14553.90	2.117	1058.3	27514.6				
Anthracene	12621.20	0.601	300.6	7814.8	12967.8	16378.0	5625.4	8360.2 17615.3
	15374.00	0.731	365.4	9501.2				
	12888.70	0.614	306.9	7978.7				
	32235.00	1.525	762.7	19830.7				
	18018.60	0.855	427.7	11121.4				
	35253.40	1.668	833.8	21679.8				

Note: The chemicals below were not detected in the B/N fraction.

Toluene
Phenol
m-Cresol
2,6-Dimethylphenol

Note: No chemicals were detected in the Acid fraction.

Table B-2. Creosote Waste Analysis - Purge and Trap of MeOH Extract

Chemical	m	b	Peak Area	Mass (ug)	Conc. (ug/mL)	Avg (ug/mL)	S. Dev. (ug/mL)
Toluene	1856.62	0.070	4.61	4.41	5.56	0.20	3.509
	1800.50	0.067	4.21				5.315
Phenol	1010.83	0.178	11.8	12.02	15.16	0.27	10.837
	1273.87	0.196	12.3				13.207
m-Cresol	7667.71	0.771	50.8	55.60	70.11	4.77	34.307
	9793.10	0.961	60.4				76.894
2,6-Dimethylphenol	6070.53	0.393	25.9	28.95	36.51	3.03	15.411
	7945.58	0.509	32.0				42.496

Appendix C. Air Sampling Data

Table C-1. Toluene air sampling data

Flask	Time	Spiked Area	Unspiked Area	Mass (ug)	Pump (mL/min)	Flow (L/cm ² -sec)	Flux 1/SQRT(t)
m = 18596.76 120 mass 0.241 b = 554.76 1000 mass 2.011 1120 mass 2.252							
1	0.17	26621.0		1.161	1	30.1	9.05E-05
1	0.17		21794.5	1.142	2	29.9	8.97E-05
1	1.18	52406.8		0.536	1	30.1	4.18E-05
1	1.18		13438.4	0.693	2	29.9	5.44E-05
1	5.17		3597.8	0.164	2	29.9	1.28E-05
1	10.17	47281.0		0.261	1	30.1	2.03E-05
1	10.17		2495.6	0.104	2	29.9	8.19E-06
1	50.50		848.2	0.016	2	39.5	9.38E-07
(Only 0, 1, and 5 hr data were used)							
2.449 Flask 1 Regression Output:							
2.449 Constant 9.637E-06							
0.919 Std Err of Y Est 1.057E-05							
0.919 R Squared 0.9233966							
0.440 No. of Observations 5							
Degrees of Freedom 3							
X Coefficient(s) 3.359E-05							
Std Err of Coef. 5.585E-06							
2	0.17	16760.8		0.630	3	29.7	4.98E-05
2	0.17		21604.4	1.132	4	30.1	8.83E-05
2	1.18	62628.6		1.086	3	29.7	8.58E-05
2	1.18		10464.5	0.533	4	30.1	4.16E-05
2	5.17		3117.9	0.138	4	30.1	1.07E-05
2	10.17		1238.6	0.037	4	30.1	2.87E-06
2	50.50	40107.1		0.116	3	69	3.94E-06
2	50.50		4355.7	0.204	4	41.2	1.16E-05
2	100.17	40066.0		0.114	3	53.8	4.96E-06
2.449 Flask 2 Regression Output:							
2.449 Constant 2.976E-05							
0.919 Std Err of Y Est 3.211E-05							
0.919 R Squared 0.2673443							
0.440 No. of Observations 5							
Degrees of Freedom 3							
X Coefficient(s) 1.776E-05							
Std Err of Coef. 1.697E-05							
3	0.17	14981.2		0.535	5	30.3	4.14E-05
3	0.17		18264.6	0.952	6	30.5	7.33E-05
3	1.18	44754.9		0.125	5	30.3	9.67E-06
3	5.17		7705.2	0.384	6	30.5	2.96E-05
3	10.17	49627.6		0.387	5	30.3	3.00E-05
3	10.17		4121.2	.92	6	30.5	1.48E-05
3	100.17	41060.0		0.167	5	62.9	6.24E-06
2.449 Flask 3 Regression Output:							
2.449 Constant 8.622E-06							
0.919 Std Err of Y Est 2.175E-05							
0.440 R Squared 0.5558488							
No. of Observations 4							
Degrees of Freedom 2							
X Coefficient(s) 1.909E-05							
Std Err of Coef. 1.207E-05							
1	5.17	42393.4		-0.002	1	30.1	-1.73E-07
1	50.50	7266.7		-1.650	1	48.8	-7.94E-05
1	100.17	NV		-2.041	1	60.5	-7.92E-05
2	100.17		0.0	-0.030	2	44.3	-1.58E-06
2	5.17	40312.1		-0.114	3	29.7	-9.02E-06
2	10.17	4771.7		-2.025	3	29.7	-1.60E-04
2	100.17		0.0	-0.030	4	52	-1.35E-06
3	1.18		NV	-0.030	6	30.5	-2.30E-06
3	5.17		NV	-2.282	5	30.3	-1.77E-04
3	50.50	25589.8		-0.665	5	60.5	-7.59E-05
3	50.50		0.0	-0.030	6	46.2	-1.52E-06
3	100.17		0.0	-0.030	6	55.9	-1.25E-06

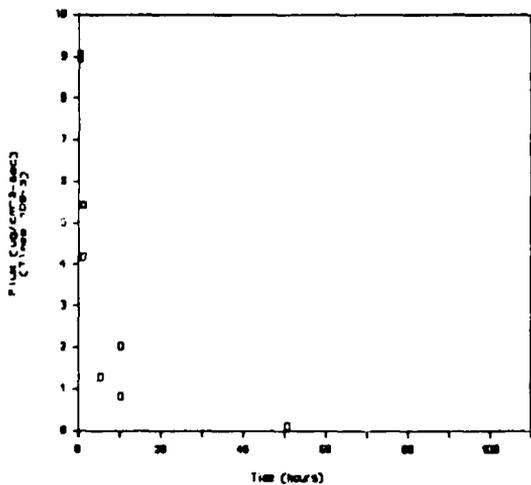


Figure C-1. Mass flux rate vs time for Toluene - Flask 1.

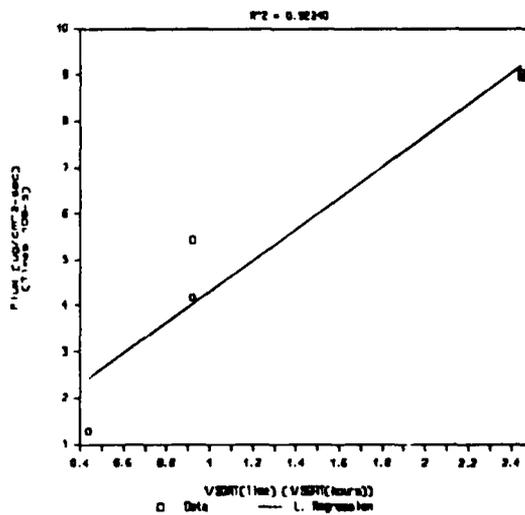


Figure C-2. Mass flux rate vs 1/t^{1/2} for toluene - Flask 1.

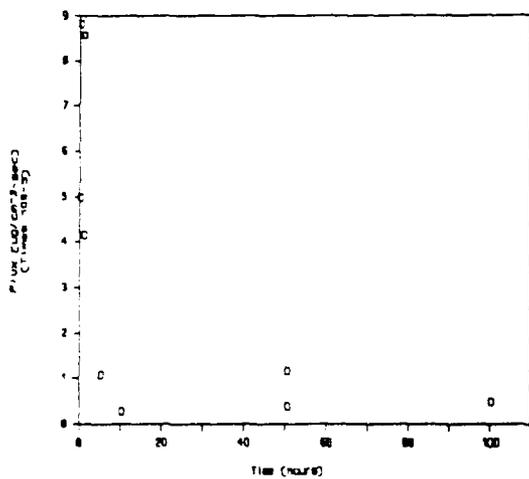


Figure C-3. Mass flux rate vs time for toluene - Flask 2.

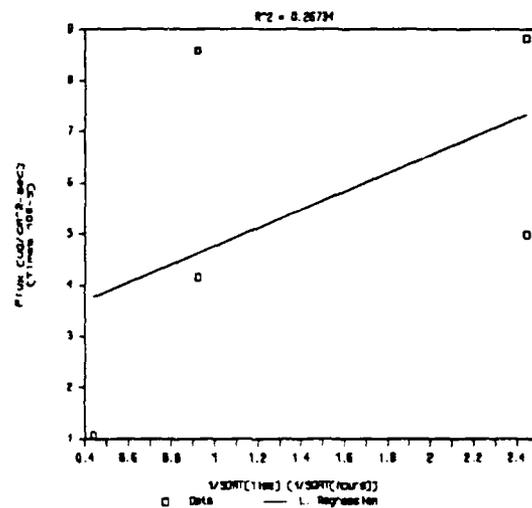


Figure C-4. Mass flux rate vs $1/t^{1/2}$ for toluene - Flask 2.

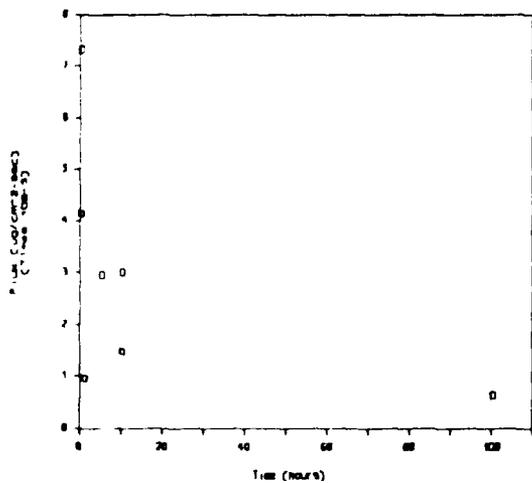


Figure C-5. Mass flux rate vs time for toluene - Flask 3.

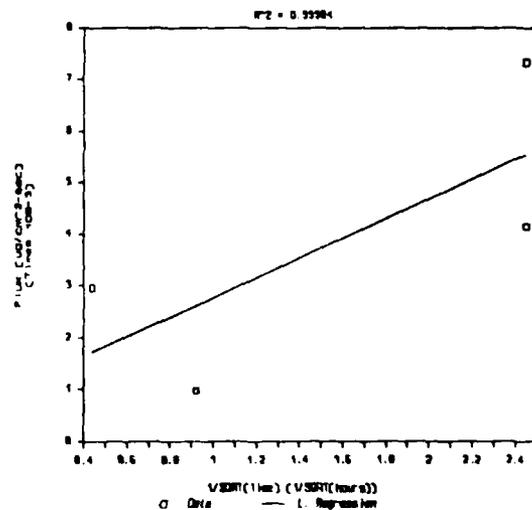


Figure C-6. Flux vs. $1/t^{0.5}$ relationship for Toluene in Flask 3.

Table C-2. Phenol air sampling data

Flask	Time	Spiked Area	Unspiked Area	Mass (ug)	Pump (mL/min)	Flow (ug/cm ² -sec)	Flux 1/SQRT(t)	
a = 15339.49 120 mass 0.243 b = -1725.11 1000 mass 2.024 1120 mass 2.267								
(Only 0, 1, and 5 hr data were used)								
1	0.17	11969.0		0.650	1	30.1	5.07E-05	2.449
1	0.17		3894.9	0.366	2	29.9	2.88E-05	2.449
1	1.18	41789.9		0.570	1	30.1	4.44E-05	0.919
1	1.18		11506.9	0.863	2	29.9	6.77E-05	0.919
1	5.17		4593.2	0.412	2	29.9	3.23E-05	0.440
1	10.17	43183.5		0.661	1	30.1	5.15E-05	
1	10.17		5536.6	0.473	2	29.9	3.72E-05	
1	50.50		4744.2	0.422	2	39.5	2.51E-05	
1	100.17		1541.1	0.213	2	44.3	1.13E-05	
Flask 1 Regression Output: Constant 4.861E-05 Std Err of Y Est 1.777E-05 R Squared 0.0261706 No. of Observations 5 Degrees of Freedom 3 X Coefficient(s) -2.666E-06 Std Err of Coef. 9.390E-06								
2	0.17	6010.8		0.261	3	29.7	2.07E-05	2.449
2	0.17		4407.1	0.400	4	30.1	3.12E-05	2.449
2	1.18	51503.9		1.203	3	29.7	9.51E-05	0.919
2	1.18		7999.1	0.634	4	30.1	4.94E-05	0.919
2	5.17		6139.7	0.513	4	30.1	4.00E-05	0.440
2	10.17		6578.9	0.541	4	30.1	4.22E-05	
2	50.50		7867.9	0.625	4	41.2	3.56E-05	
2	100.17	37055.2		0.504	3	53.8	2.20E-05	
2	100.17		2818.7	0.296	4	52	1.34E-05	
Flask 2 Regression Output: Constant 7.207E-05 Std Err of Y Est 2.734E-05 R Squared 0.3227114 No. of Observations 5 Degrees of Freedom 3 X Coefficient(s) -1.728E-05 Std Err of Coef. 1.445E-05								
3	0.17	13761.2		0.767	5	30.3	5.94E-05	2.449
3	0.17		6022.4	0.505	6	30.5	3.89E-05	2.449
3	1.18	38529.9		0.357	5	30.3	2.77E-05	0.919
3	1.18		6721.3	0.551	6	30.5	4.24E-05	0.919
3	5.17		12275.2	0.913	6	30.5	7.02E-05	0.440
3	10.17	42908.4		0.643	5	30.3	4.98E-05	
3	10.17		10539.0	0.800	6	30.5	6.15E-05	
3	50.50	51534.7		1.448	5	60.5	5.62E-05	
3	50.50		11061.0	0.834	6	46.2	4.24E-05	
3	100.17	36412.2		0.462	5	62.9	1.72E-05	
3	100.17		5126.1	0.447	6	55.9	1.88E-05	
Flask 3 Regression Output: Constant 5.030E-05 Std Err of Y Est 1.950E-05 R Squared 0.0101256 No. of Observations 5 Degrees of Freedom 3 X Coefficient(s) -1.805E-06 Std Err of Coef. 1.030E-05								
1	5.17	31137.2		-0.125	1	30.1	-9.72E-06	
1	50.50	9580.4		-1.287	1	48.8	-6.19E-05	
1	100.17	NV		-1.912	1	60.5	-7.42E-05	
2	5.17	30954.3		-0.137	3	29.7	-1.08E-05	
2	10.17	15542.2		-1.141	3	29.7	-9.02E-05	
2	50.50	NV		-1.912	3	69	-6.50E-05	
3	5.17	NV		-2.155	5	30.3	-1.67E-04	

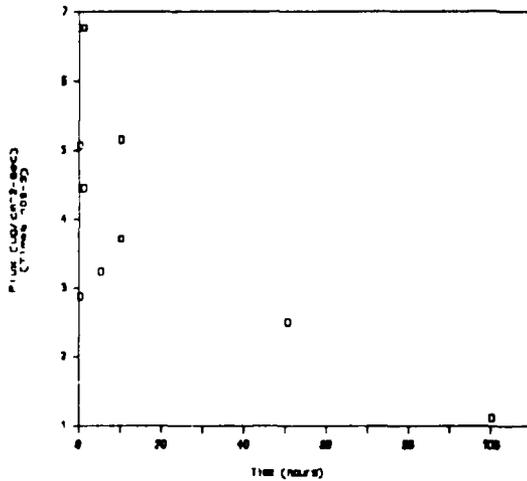


Figure C-7. Mass flux vs time for phenol - Flask 1.

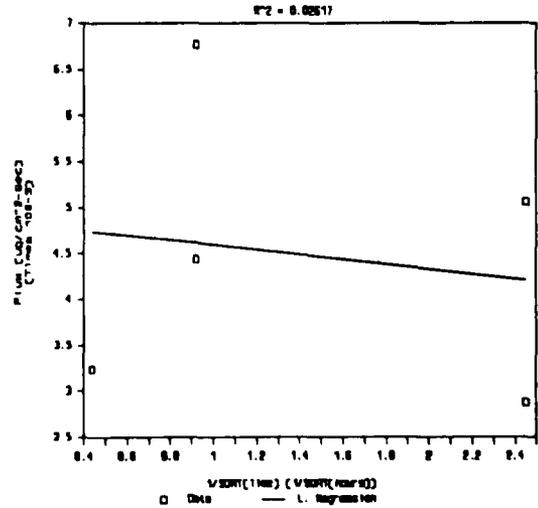


Figure C-8. Mass flux rate vs $1/t^{1/2}$ for phenol - Flask 1.

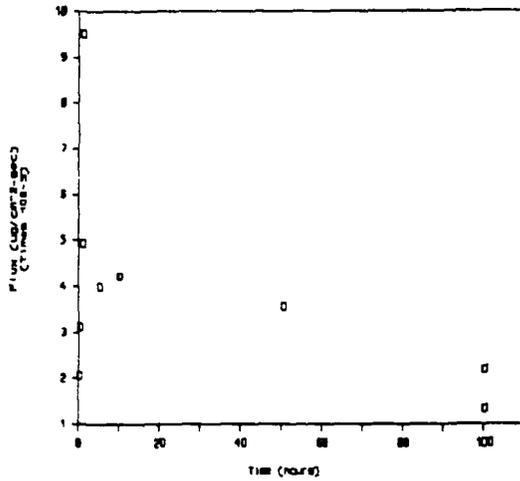


Figure C-9. Mass flux rate vs time for phenol - Flask 2.

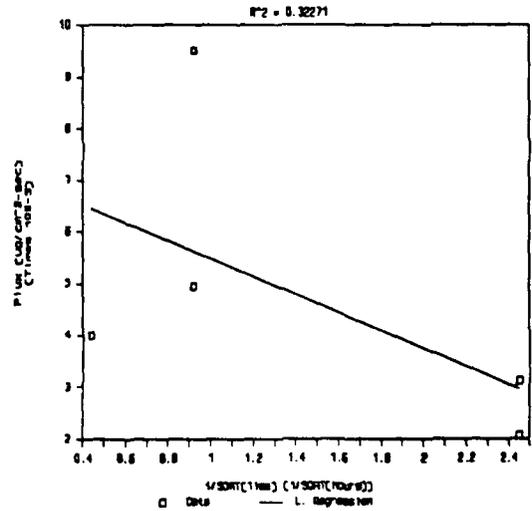


Figure C-10. Mass flux rate vs $1/t^{1/2}$ for phenol - Flask 2.

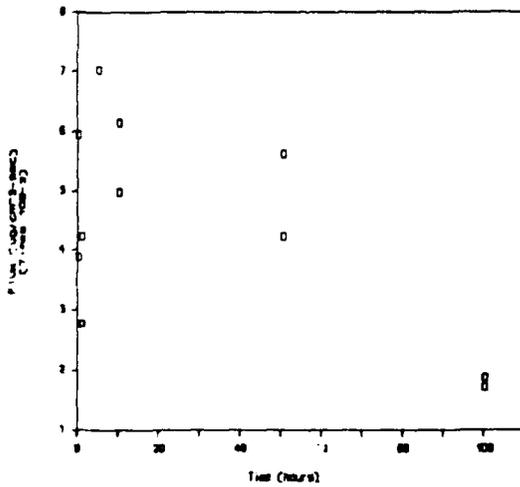


Figure C-11. Mass flux rate vs time for phenol - Flask 3.

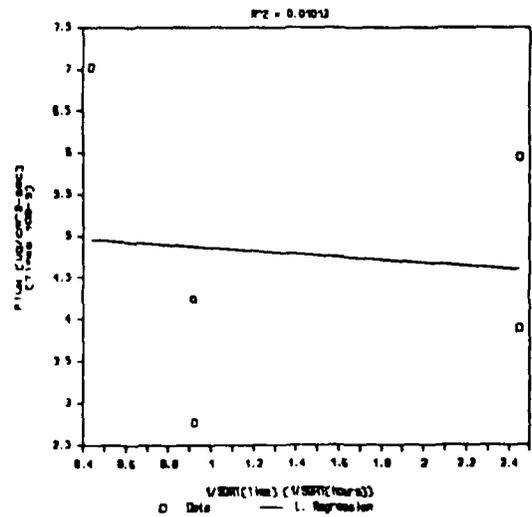


Figure C-12. Mass flux rate vs $1/t^{1/2}$ for phenol - Flask 3.

Table C-3. m-Cresol air sampling data

Flask	Time	Spiked Area	Unspiked Area	Mass	Pump	Flow (mL/min)	Flux (ug/cm ² -sec)	Flux 1/SQRT(t)
m = 11221.96 120 mass 0.244 b = -985.992 1000 mass 2.030 1120 mass 2.274								
(Only 0, 1, and 5 hr data were used)								
1	0.17	8434.6		0.595	1	30.1	4.64E-05	2.449
1	0.17		1569.4	0.228	2	29.9	1.79E-05	2.449
1	1.18	26281.7		0.156	1	30.1	1.22E-05	0.919
1	1.18		3066.2	0.361	2	29.9	2.83E-05	0.919
1	5.17	28593.7		0.362	1	30.1	2.82E-05	0.440
1	5.17		1588.8	0.229	2	29.9	1.80E-05	0.440
1	10.17		3607.6	0.409	2	29.9	3.21E-05	
1	50.50		2152.2	0.280	2	39.5	1.66E-05	
Flask 1 Regression Output:								
								1.845E-05
								1.247E-05
								0.1658532
								6
								4
								5.298E-06
								5.940E-06
2	0.17	2049.2		0.026	3	29.7	2.09E-06	2.449
2	0.17		1049.9	0.181	4	29.9	1.42E-05	2.449
2	1.18	32709.0		0.729	3	29.7	5.76E-05	0.919
2	1.18		3927.2	0.438	4	30.1	3.41E-05	0.919
2	5.17		3576.2	0.407	4	30.1	3.17E-05	0.440
2	10.17		2955.6	0.351	4	30.1	2.74E-05	0.440
2	50.50		6441.0	0.662	4	41.2	3.77E-05	
2	100.17	32338.4		0.940	3	53.8	4.10E-05	
2	100.17		8236.7	0.822	4	52.0	3.71E-05	
Flask 2 Regression Output:								
								5.295E-05
								1.529E-05
								0.6075606
								5
								3
								-1.742E-05
								8.081E-06
3	0.17	9127.2		0.657	5	30.3	5.09E-05	2.449
3	0.17		1108.6	0.187	6	30.5	1.44E-05	2.449
3	1.18	34906.4		0.924	5	30.3	7.16E-05	0.919
3	1.18		1588.2	0.229	6	30.5	1.77E-05	0.919
3	5.17		3018.5	0.357	6	30.5	2.75E-05	0.440
3	10.17	25552.2		0.091	5	30.3	7.04E-06	0.440
3	10.17		5766.2	0.602	6	30.5	4.63E-05	
3	50.50	44768.3		2.047	5	60.5	7.94E-05	
3	50.50		9450.1	0.930	6	46.2	4.73E-05	
3	100.17	33372.8		1.032	5	62.9	3.85E-05	
3	100.17		7555.9	0.761	6	55.9	3.20E-05	
1	10.17	20361.0		-0.377	1	30.1	-2.90E-05	
1	50.50	7596.0		-1.265	1	48.8	-6.09E-05	
1	100.17	NV		-1.942	1	60.5	-7.54E-05	
1	100.17		0.0	0.088	2	44.3	4.66E-06	
2	5.17	22000.0		-0.226	3	29.7	-1.78E-05	
2	10.17	4244.0		-1.808	3	29.7	-1.43E-04	
2	50.50	NV		-1.942	3	69.0	-6.61E-05	
3	5.17	NV		-2.186	5	30.3	-1.69E-04	

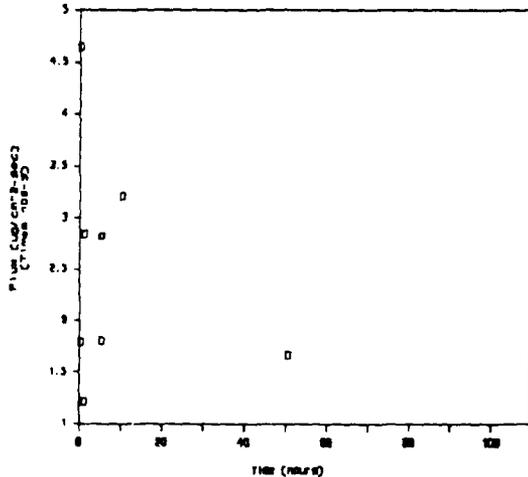


Figure C-13. Mass Flux vs time for m-cresol - Flask 1.

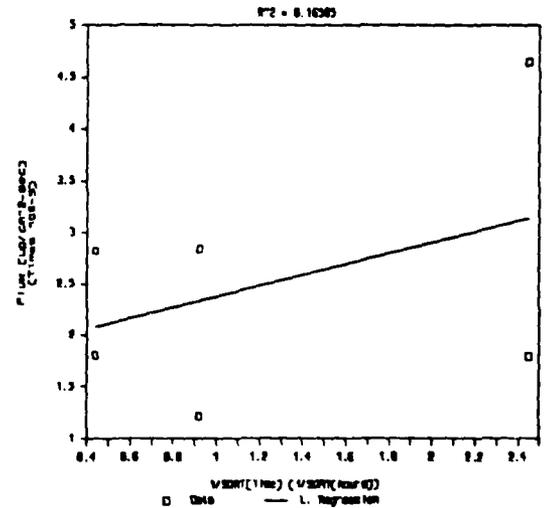


Figure C-14. Mass flux rate vs 1/t^{1/2} for m-cresol - Flask 1.

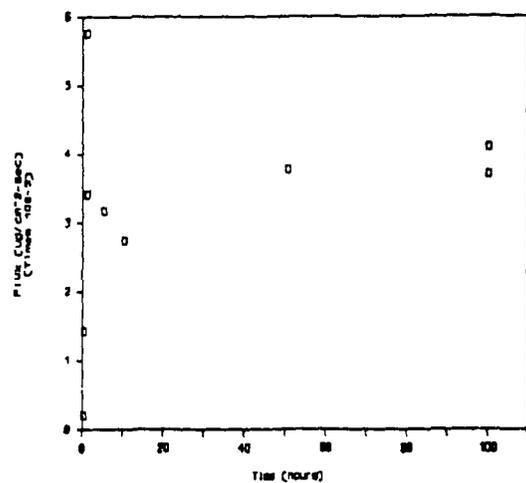


Figure C-15. Mas flux rate vs time for m-cresol - Flask 2.

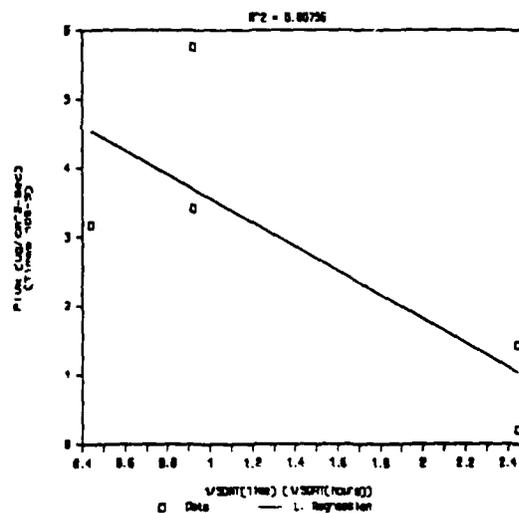


Figure C-16. Mass flux rate vs $1/t^{1/2}$ for m-cresol - Flask 2.

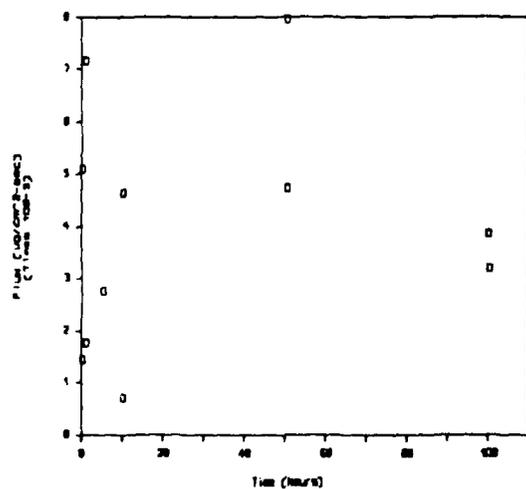


Figure C-17. Mass flux rate vs time for m-cresol - Flask 3.

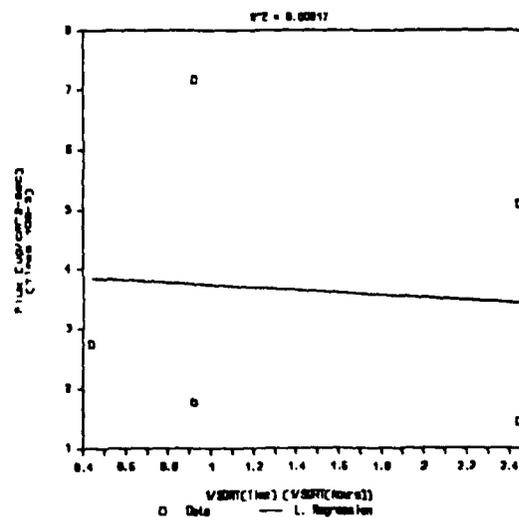


Figure C-18. Mass flux rate vs $1/t^{1/2}$ for m-cresol - Flask 3.

Table C-4. 2,6-Dimethylphenol air sampling data

2,6-Dimethylphenol									
		m = 16204.202 120 mass		0.263					
		b = -301.376 1000 mass		2.193					
		1120 mass		2.456					
Flask	Time	Spiked Area	Unspiked Area	Mass	Pump	Flow (mL/min)	Flux (ug/cm ² -sec)	1/SQRT(t)	
1	0.17	15580.3		0.717	1	30.1	5.59E-05	2.449	(Only 0, 1, and 5 hr data were used)
1	0.17		4250.7	0.281	2	29.9	2.21E-05	2.449	Flask 1 Regression Output:
1	1.18	52071.9		0.776	1	30.1	6.05E-05	0.919	Constant 8.120E-05
1	1.18		14223.9	0.896	2	29.9	7.04E-05	0.919	Std Err of Y Est 2.608E-05
1	5.17	61510.4		1.359	1	30.1	1.06E-04	0.440	R Squared 0.3246291
1	5.17		8197.0	0.524	2	29.9	4.12E-05	0.440	No. of Observations 6
									Degrees of Freedom 4
1	10.17	59566.7		1.239	1	30.1	9.66E-05		
1	10.17		12056.5	0.763	2	29.9	5.99E-05		X Coefficient(s) -1.723E-05
1	50.50		13355.2	0.843	2	39.5	5.01E-05		Std Err of Coef. 1.242E-05
1	100.17		17841.5	1.120	2	44.3	5.93E-05		
2	0.17	8322.4		0.269	3	29.7	2.13E-05		2.449 Flask 2 Regression Output:
2	0.17		3067.5	0.208	4	30.1	1.62E-05		Constant 8.569E-05
2	1.18	68429.9		1.786	3	29.7	1.41E-04		Std Err of Y Est 4.521E-05
2	1.18		10572.2	0.671	4	30.1	5.23E-05		R Squared 0.2383270
2	5.17	46111.8		0.408	3	29.7	3.23E-05		No. of Observations 6
2	5.17		13693.4	0.864	4	30.1	6.74E-05		Degrees of Freedom 4
2	10.17		13705.5	0.864	4	30.1	6.74E-05		
2	50.50		22258.9	1.392	4	41.2	7.93E-05		X Coefficient(s) -2.410E-05
2	100.17	73483.2		2.360	3	53.8	1.03E-04		Std Err of Coef. 2.154E-05
2	100.17		20903.0	1.309	4	52.0	5.91E-05		
3	0.17	9241.1		0.326	5	30.3	2.52E-05		2.449 Flask 3 Regression Output:
3	0.17		10482.9	0.666	6	30.5	5.12E-05		Constant 1.330E-04
3	1.18	75255.0		2.207	5	30.3	1.71E-04		Std Err of Y Est 5.874E-05
3	1.18		5942.8	0.385	6	30.5	2.97E-05		R Squared 0.3378527
3	5.17		23278.6	1.455	6	30.5	1.12E-04		No. of Observations 5
3	10.17	55132.2		0.965	5	30.3	7.48E-05		Degrees of Freedom 3
3	10.17		21220.0	1.328	6	30.5	1.02E-04		
3	50.50	91371.5		3.464	5	60.5	1.34E-04		X Coefficient(s) -3.841E-05
3	50.50		31329.6	1.952	6	46.2	9.92E-05		Std Err of Coef. 3.105E-05
3	100.17	58128.9		1.413	5	62.9	5.27E-05		
3	100.17		31061.6	0.835	6	55.8	8.13E-05		
1	50.50	4046.6		-1.925	1	48.8	-9.26E-05		
1	100.17	NV		-2.174	1	60.5	-8.44E-05		
2	10.17	29231.9		-0.633	3	29.7	-5.01E-05		
2	50.50	NV		-2.174	3	69.0	-7.40E-05		
3	5.17	NV		-2.437	5	30.3	-1.89E-04		

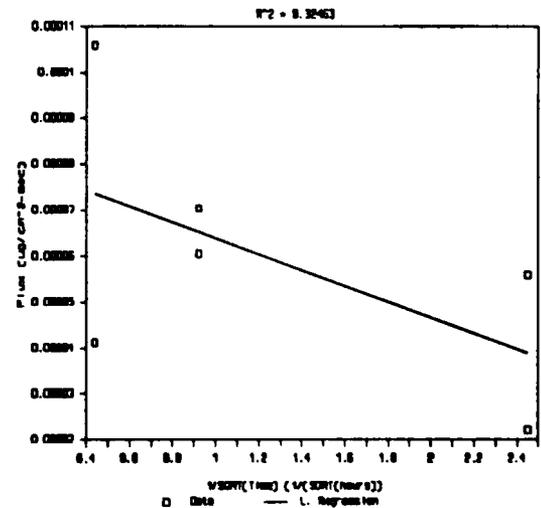
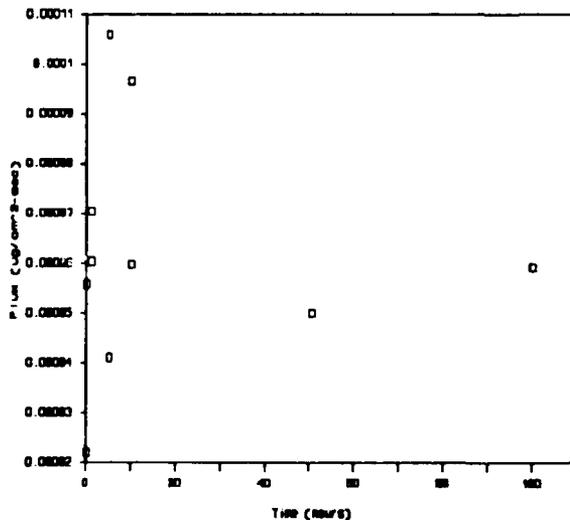


Figure C-19. Mass flux rate vs time for 2,6-dimethylphenol Flask 1.

Figure C-20. Mass flux rate vs 1/t^{1/2} for 2,6-dimethylphenol - Flask 1.

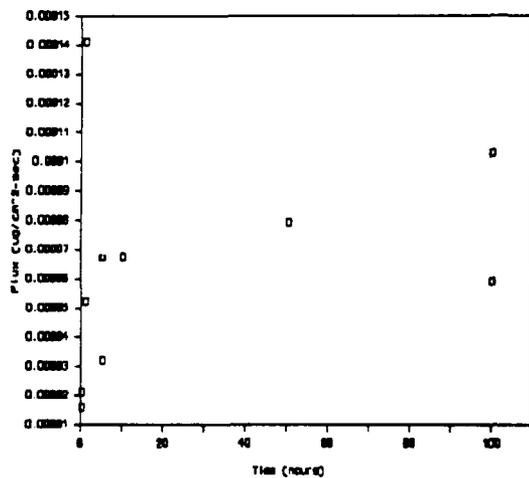


Figure C-21. Mass flux rate vs time for 2,6-dimethylphenol - Flask 2.

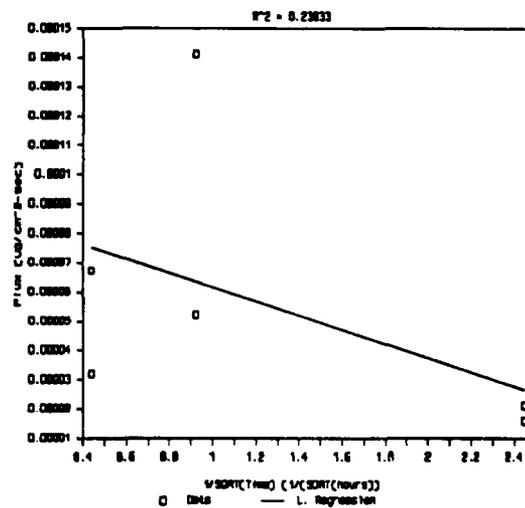


Figure C-22. Mass flux rate vs $1/t^{1/2}$ for 2,6-dimethylphenol - Flask 2.

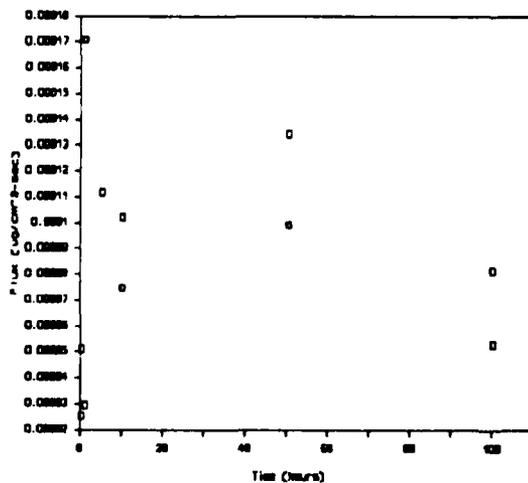


Figure C-23. Mass flux rate vs time for 2,6-dimethylphenol - Flask 3.

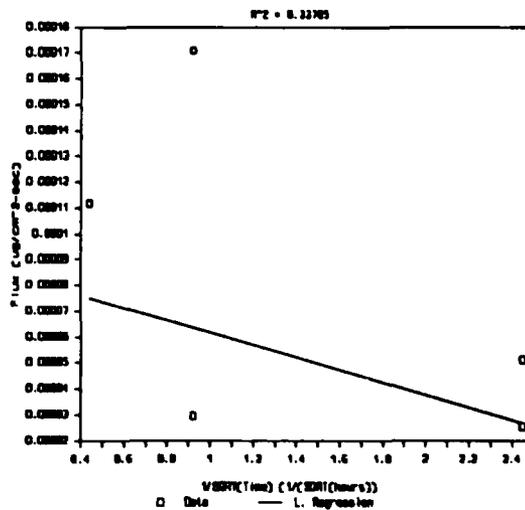


Figure C-24. Mass flux rate vs $1/t^{1/2}$ for 2,6-dimethylphenol - Flask 3.

Table C-5. Naphthalene air sampling data

Naphthalene		m = 20547.51 120 mass 0.252		b = -195.863 1000 mass 2.102		1120 mass 2.354			
Flask	Time	Spiked Area	Unspiked Area	Mass	Pump (mL/min)	Flow (ug/cm ² -sec)	Flux 1/SQRT(t)		
1	0.17	14088.7		0.443	1	30.1	3.46E-05	(Only 0, 1, and 5 hr data were used)	
1	0.17		4243.9	0.216	2	29.9	1.70E-05	2.449 Flask 1 Regression Output:	
1	1.18	61370.9		0.642	1	30.1	5.01E-05	2.449 Constant 2.344E-04	
1	1.18		42103.2	2.059	2	29.9	1.62E-04	0.919 Std Err of Y Est 8.918E-05	
1	5.17	134117.0		4.183	1	30.1	3.26E-04	0.919 R Squared 0.5269716	
1	5.17		34875.7	1.707	2	29.9	1.34E-04	0.440 No. of Observations 6	
1	10.17	158681.0		5.378	1	30.1	4.19E-04	0.440 Degrees of Freedom 4	
1	10.17		44334.6	2.167	2	29.9	1.70E-04	X Coefficient(s) -8.968E-05	
1	50.50	111399.0		3.329	1	48.8	1.60E-04	Std Err of Coef. 4.248E-05	
1	50.50		201316.0	9.807	2	39.5	5.83E-04		
1	100.17	307275.0		14.964	2	44.3	7.93E-04		
2	0.17	8869.0		0.189	3	29.7	1.50E-05	2.449 Flask 2 Regression Output:	
2	0.17		4060.1	0.207	4	30.1	1.62E-05	2.449 Constant 3.772E-04	
2	1.18	117878.0		3.392	3	29.7	2.68E-04	0.919 Std Err of Y Est 7.639E-05	
2	1.18		26768.5	1.312	4	30.1	1.02E-04	0.919 R Squared 0.8147986	
2	5.17	133529.0		4.154	3	29.7	3.28E-04	0.440 No. of Observations 6	
2	5.17		97363.2	4.748	4	30.1	3.70E-04	0.440 Degrees of Freedom 4	
2	10.17	164494.0		5.661	3	29.7	4.47E-04		
2	10.17		79532.7	3.880	4	30.1	3.03E-04	X Coefficient(s) -1.527E-04	
2	50.50	325930.0		15.872	4	41.2	9.04E-04	Std Err of Coef. 3.639E-05	
2	100.17	441976.0		19.417	3	53.8	8.47E-04		
2	100.17		364276.0	17.738	4	52.0	8.01E-04		
3	0.17	10342.1		0.261	5	30.3	2.02E-05	2.449 Flask 3 Regression Output:	
3	1.18	92965.1		2.131	5	30.3	1.65E-04	0.919 Constant 8.339E-04	
3	1.18		20085.8	0.987	6	30.5	7.60E-05	0.919 Std Err of Y Est 5.237E-04	
3	5.17	136208.0		15.399	6	30.5	1.19E-03	0.440 R Squared 0.4005563	
3	10.17	151070.0		5.008	5	30.3	3.88E-04	No. of Observations 4	
3	10.17		184592.0	8.993	6	30.5	6.92E-04	Degrees of Freedom 2	
3	50.50	845788.0		39.070	5	60.5	1.52E-03		
3	50.50		443957.0	21.616	6	46.2	1.10E-03	X Coefficient(s) -3.996E-04	
3	100.17	686525.0		31.319	5	62.9	1.17E-03	Std Err of Coef. 3.457E-04	
3	100.17		578795.0	28.178	6	55.9	1.18E-03		
1	100.17	NV		-2.092	1	60.5	-8.12E-05		
2	50.50	NV		-2.092	3	69.0	-7.12E-05		
3	0.17		NV	0.010	6	30.5	7.34E-07		
3	5.17		NV	-2.344	5	30.3	-1.82E-04		

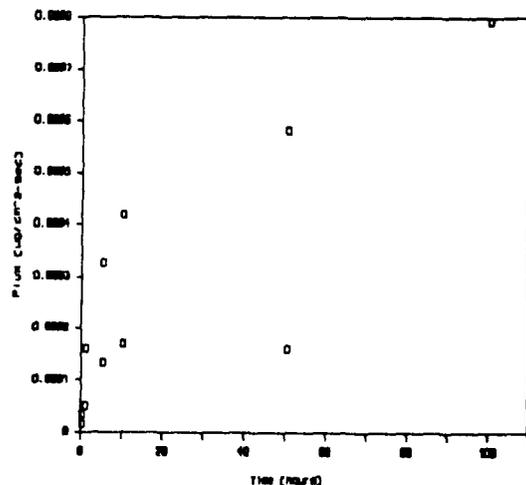
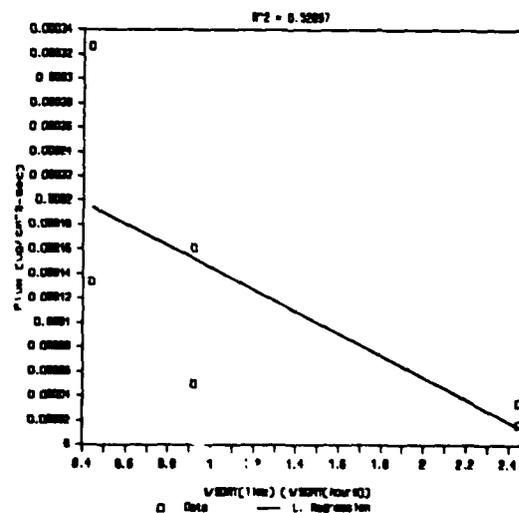


Figure C-25. Mass flux rate vs time for naphthalene - Flask 1.

Figure C-26. Mass flux vs $1/t^{1/2}$ for naphthalene - Flask 1.

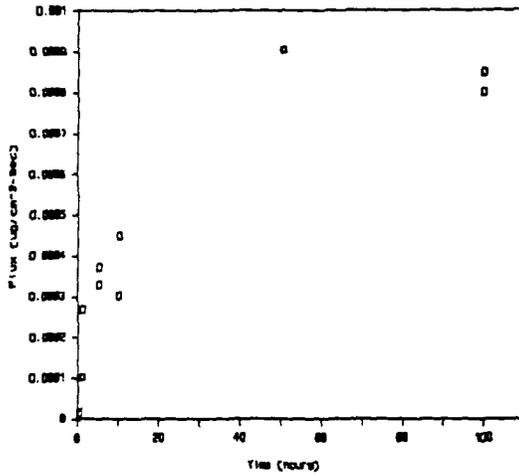


Figure C-27. Mass flux rate vs time for naphthalene - Flask 2.

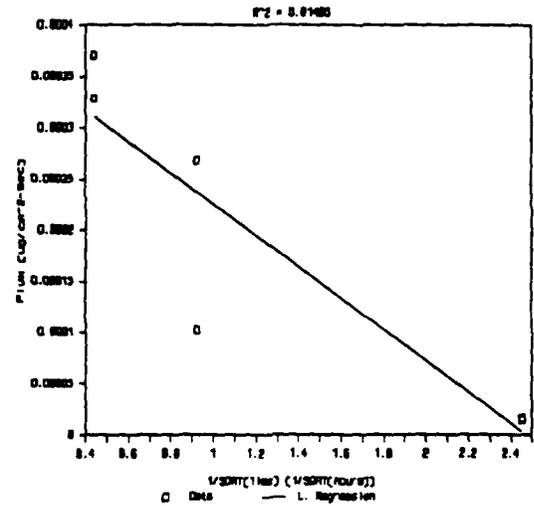


Figure C-28. Mass flux rate vs $1/t^{1/2}$ for naphthalene - Flask 2.

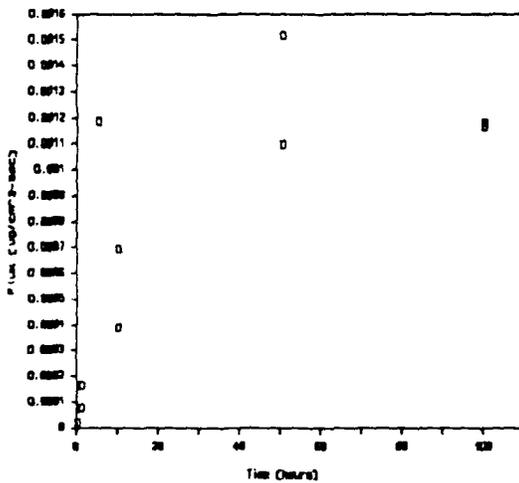


Figure C-29. Mass flux rate vs time for naphthalene - Flask 3.

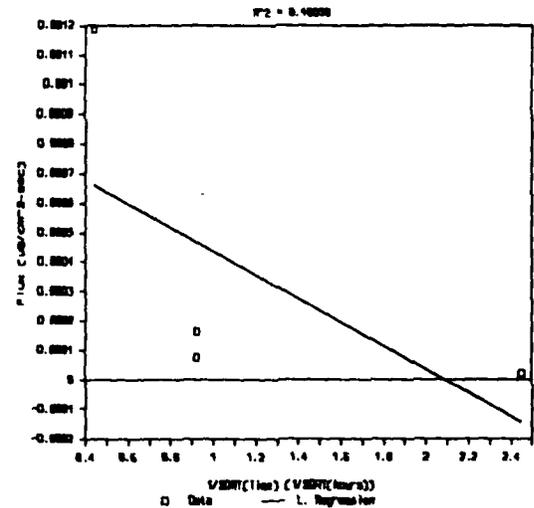


Figure C-30. Mass flux vs $1/t^{1/2}$ for naphthalene - Flask 3.

Table C-6. 2-Methylnaphthalene air sampling data

Flask	Time	Spiked Area	Unspiked Area	Mass	Pump (mL/min)	Flow (ug/cm ² -sec)	Flux 1/SQRT(t)	
m = 18969.168 120 mass 0.245 b = -53.827 1000 mass 2.045 1120 mass 2.290								
1	0.17	9546.6		0.261	1	30.1	2.04E-05	(Only 0, 1, and 5 hr data were used)
1	0.17		778.8	0.044	2	29.9	3.45E-06	2.449 Flask 1 Regression Output:
1	1.18	48917.6		0.292	1	30.1	2.27E-05	2.449 Constant 4.124E-05
1	1.18		3874.9	0.207	2	29.9	1.63E-05	0.919 Std Err of Y Est 2.520E-05
1	5.17	61661.3		0.963	1	30.1	7.51E-05	0.919 R Squared 0.7248797
1	5.17		2593.5	0.140	2	29.9	1.10E-05	0.440 No. of Observations 6
1	10.17	54349.3		0.578	1	30.1	4.51E-05	0.440 Degrees of Freedom 4
1	10.17		2606.4	0.140	2	29.9	1.10E-05	X Coefficient(s) -1.293E-05
1	50.50		1197.7	0.066	2	39.5	3.92E-06	Std Err of Coef. 1.201E-05
1	100.17		175201.0	9.239	2	44.3	4.90E-04	
2	0.17	6406.1		0.096	3	29.7	7.55E-06	2.449 Flask 2 Regression Output:
2	0.17		634.4	0.036	4	30.1	2.83E-06	2.449 Constant 9.517E-05
2	1.18	58034.8		0.772	3	29.7	6.10E-05	0.919 Std Err of Y Est 3.136E-05
2	1.18		2460.8	0.133	4	30.1	1.03E-05	0.919 R Squared 0.6305485
2	5.17	61577.8		0.959	3	29.7	7.58E-05	0.440 No. of Observations 6
2	5.17		28196.1	1.489	4	30.1	1.16E-04	0.440 Degrees of Freedom 4
2	10.17		5079.4	0.271	4	30.1	2.11E-05	
2	50.50		30466.7	1.609	4	41.2	9.17E-05	X Coefficient(s) -3.903E-05
2	100.17		286195.0	13.045	3	53.8	5.69E-04	Std Err of Coef. 1.494E-05
2	100.17		220127.0	11.607	4	52.0	5.24E-04	
3	0.17	7783.0		0.168	5	30.3	1.30E-05	2.449 Flask 3 Regression Output:
3	1.18	73058.5		1.564	5	30.3	1.21E-04	0.919 Constant 2.681E-04
3	1.18		1419.7	0.078	6	30.5	5.98E-06	0.919 Std Err of Y Est 1.506E-04
3	5.17		87413.4	4.611	6	30.5	3.55E-04	0.440 R Squared 0.4300812
3	10.17		61530.1	0.957	5	30.3	7.41E-05	No. of Observations 4
3	10.17		13084.1	0.693	6	30.5	5.33E-05	Degrees of Freedom 2
3	50.50		504438.0	24.550	5	60.5	9.53E-04	
3	50.50		24935.8	1.317	6	46.2	6.69E-05	X Coefficient(s) -1.221E-04
3	100.17		426267.0	20.429	5	62.9	7.62E-04	Std Err of Coef. 9.939E-05
3	100.17		390824.0	20.606	6	55.9	8.65E-04	
1	50.50	28952.7		-0.516	1	48.8	-2.48E-05	
1	100.17	NV		-2.042	1	60.5	-7.92E-05	
2	10.17	9875.6		-1.767	3	29.7	-1.40E-04	
2	50.50	NV		-2.042	3	69.0	-6.95E-05	
3	0.17		NV	0.003	6	30.5	2.18E-07	
3	5.17		NV	-2.287	5	30.3	-1.77E-04	

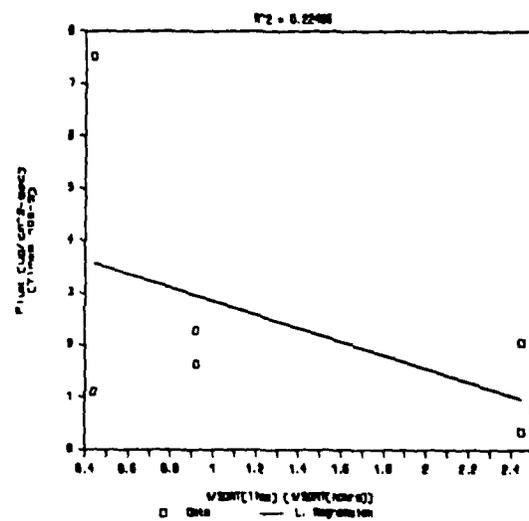
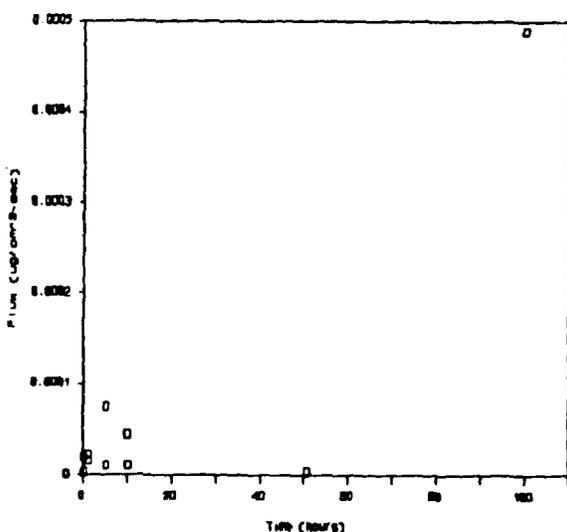


Figure C-31. Mass flux rate vs time for 2-methylnaphthalene - Flask 1.

Figure C-32. Mass flux rate vs 1/t^{1/2} for 2-methylnaphthalene - Flask 1.

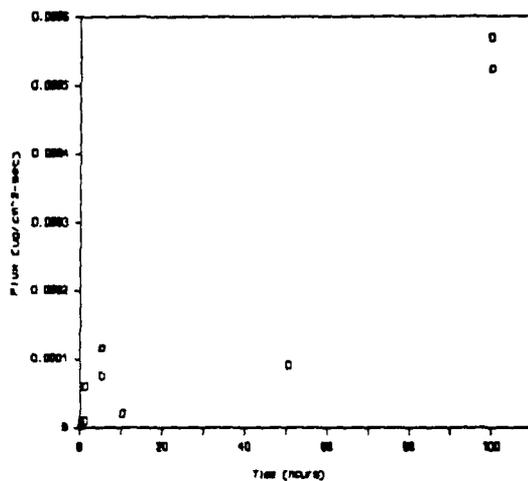


Figure C-33. Mass flux rate vs time for 2-methylnaphthalene - Flask 2.

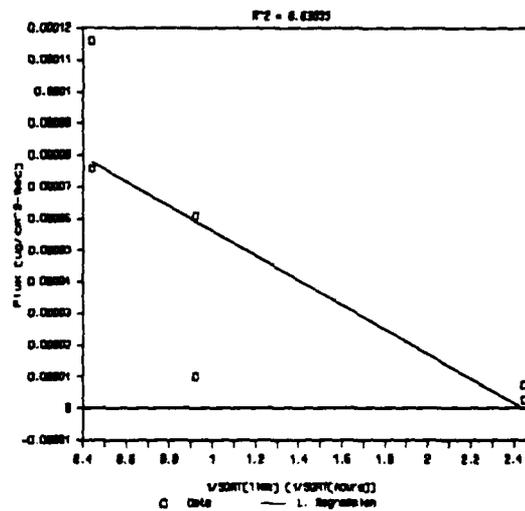


Figure C-34. Mass flux rate vs $1/t^{1/2}$ for 2-methylnaphthalene - Flask 2.

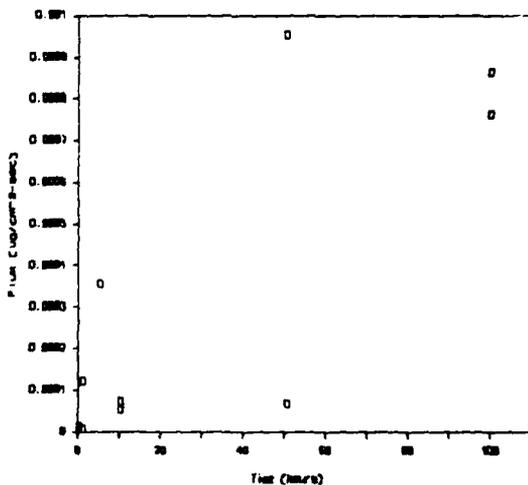


Figure C-35. Mass flux rate vs time for 2-methylnaphthalene - Flask 3.

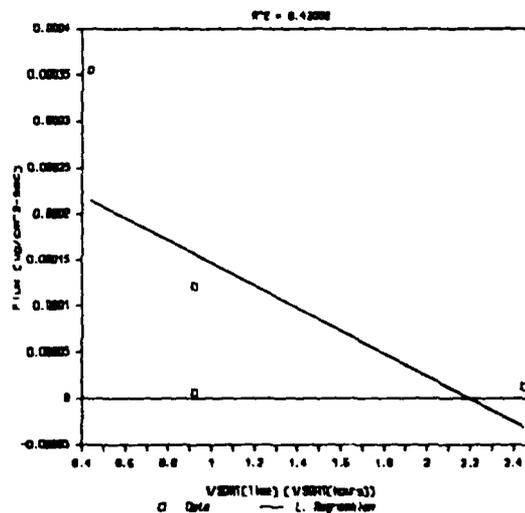


Figure C-36. Mass flux rate vs $1/t^{1/2}$ for 2-methylnaphthalene - Flask 3.

Appendix D. Soil Extraction

Table D-1. Tissumizer losses

Chemical	-----Std mixed with soil----->						<-----Std without soil----->					
	Sample	Peak Area	Mass (ug)	Avg Mass (ug)	Calc'd Mass (ug)	Delta %	Sample	Peak Area	Mass (ug)	Avg Mass (ug)	Calc'd Mass (ug)	Delta %
Flask 1												
Toluene	1	125106.0	6.697	6.601533	9.3	-28.7	4	89116.5	4.762	5.856847	9.3	-36.7
	1	121538.0	6.506				4	129830.0	6.951			
	2	120573.0	6.454	6.617450	9.3	-28.5	5	115174.0	6.163	6.617665	9.3	-28.5
Phenol	2	126663.0	6.781				5	132070.0	7.072			
	3	109254.0	5.845	6.205362	9.3	-33.0	6	126170.0	6.755	7.126006	9.3	-23.0
	3	122655.0	6.566		Avg ->	-30.1	6	139981.0	7.497		Avg ->	-29.4
	1	79914.2	5.322	5.261550	6.9	-24.2	4	65483.7	4.381	4.952221	6.9	-28.6
	1	78054.6	5.201				4	82995.2	5.523			
	2	79218.0	5.277	5.329675	6.9	-23.2	5	84017.5	5.590	5.654761	6.9	-18.5
m-Cresol	2	80840.8	5.383				5	86014.6	5.720			
	3	75546.6	5.037	5.113419	6.9	-26.3	6	81535.4	5.428	5.772392	6.9	-16.8
	3	77877.7	5.189		Avg ->	-24.6	6	92105.5	6.117		Avg ->	-21.3
	1	57343.7	5.198	5.215850	7.0	-25.1	4	47351.7	4.307	4.902167	7.0	-29.6
	1	57748.5	5.234				4	60700.2	5.497			
	2	58524.0	5.303	5.308303	7.0	-23.7	5	61676.9	5.584	5.654348	7.0	-18.8
2,6-Dimethylphenol	2	58643.2	5.314				5	63256.9	5.725			
	3	55300.5	5.016	5.038961	7.0	-27.6	6	59440.0	5.385	5.723591	7.0	-17.8
	3	55821.6	5.062		Avg ->	-25.5	6	67047.9	6.063		Avg ->	-22.0
	1	92563.5	5.731	5.706465	7.5	-24.1	4	75741.0	4.693	5.330097	7.5	-29.1
	1	91771.2	5.682				4	96396.2	5.967			
	2	93122.5	5.765	5.789743	7.5	-23.0	5	97879.6	6.059	6.142659	7.5	-18.3
Naphthalene	2	93911.1	5.814				5	100572.0	6.225			
	3	87836.0	5.439	5.490278	7.5	-27.0	6	94244.5	5.835	6.202689	7.5	-17.5
	3	89492.4	5.541		Avg ->	-24.7	6	106172.0	6.571		Avg ->	-21.7
	1	112743.0	5.496	5.421864	7.2	-24.8	4	90960.5	4.436	5.052051	7.2	-29.9
	1	109677.0	5.347				4	116262.0	5.668			
	2	111441.0	5.433	5.509442	7.2	-23.6	5	118388.0	5.771	5.836781	7.2	-19.0
2-Methylnaphthalene	2	114578.0	5.586				5	121083.0	5.902			
	3	106094.0	5.173	5.251017	7.2	-27.1	6	114535.0	5.584	5.963584	7.2	-17.3
	3	109305.0	5.329		Avg ->	-25.2	6	130147.0	6.343		Avg ->	-22.1
	1	107360.0	5.663	5.489425	7.0	-21.7	4	83115.7	4.384	5.056451	7.0	-27.9
	1	100792.0	5.316				4	108610.0	5.728			
	2	101404.0	5.349	5.418546	7.0	-22.7	5	108075.0	5.700	5.739093	7.0	-18.2
2-Ethylnaphthalene	2	104059.0	5.489				5	109549.0	5.778			
	3	97366.2	5.136	5.200867	7.0	-25.8	6	104945.0	5.535	5.915458	7.0	-15.6
	3	99838.4	5.266		Avg ->	-23.4	6	119370.0	6.296		Avg ->	-20.6
	1	84324.2	4.344	4.260986	5.6	-24.1	4	68105.7	3.510	3.959535	5.6	-29.3
	1	81090.5	4.178				4	85969.9	4.429			
	2	82723.5	4.262	4.329835	5.6	-22.9	5	88372.6	4.552	4.572871	5.6	-18.5
Pentachlorophenol	2	85369.8	4.398				5	89176.2	4.594			
	3	79936.3	4.119	4.165101	5.6	-25.8	6	85110.3	4.385	4.703349	5.6	-16.2
	3	81747.9	4.212		Avg ->	-24.3	6	97514.8	5.022		Avg ->	-21.3
	1	34387.6	4.749	4.862343	7.4	-34.6	4	26246.9	3.668	4.170571	7.4	-43.9
	1	36101.5	4.976				4	33816.8	4.673			
	2	36502.3	5.029	5.486174	7.4	-26.2	5	37238.9	5.127	4.831959	7.4	-35.0
Anthracene	2	43388.3	5.943				5	32792.3	4.537			
	3	39075.6	5.371	5.031838	7.4	-32.3	6	32533.1	4.503	5.006173	7.4	-32.7
	3	33967.9	4.693		Avg ->	-31.1	6	40123.6	5.510		Avg ->	-37.2
	1	105063.0	4.957	1.938875	2.4	-19.2	4	305.4	1.446	1.691605	2.4	-29.5
	1	41008.2	1.939				4	40967.8	1.937			
	2	39106.5	1.849	1.874914	2.4	-21.9	5	42829.6	2.025	1.951068	2.4	-18.7
Anthracene	2	40195.4	1.901				5	39704.3	1.877			
	3	37279.1	1.763	1.782485	2.4	-25.7	6	38321.5	1.812	1.994569	2.4	-16.9
	3	38100.1	1.802		Avg ->	-22.3	6	46058.6	2.177		Avg ->	-21.7

One Factor ANOVA-Repeated Measures for X₁ ... X₂

Source:	df:	Sum of Squares:	Mean Square:	F-test:	P value:
Between subjects	107	104.312	.975	.135	1
Within subjects	108	777.496	7.199		
treatments	1	676.632	676.632	717.798	1.0E-4
residual	107	100.863	.943		
Total	215	881.808			

Reliability Estimate: for- All treatments: -.635 Single Treatment: -.761

1

One Factor ANOVA-Repeated Measures for X₁ ... X₂

Group:	Count:	Mean:	Std. Dev.:	Std. Error:
Toluene Results	108	5.04	1.29	.124
Treatment	108	1.5	.502	.048

2

One Factor ANOVA-Repeated Measures for X₁ ... X₂

Comparison:	Mean Diff.:	Fisher PLSD:	Scheffe F-test:	Dunnnett t:
Toluene Re... vs. Treatment	3.54	.262*	717.798*	26.792

* Significant at 95%

3

Figure D-1. Analysis of variance for extraction efficiencies with soil vs without soil.

Table D-2. Naphthalene soil extraction data

Time	Peak Area	Mass* (ug)	Conc (mg/L)	Chemical	Soil	Soil Conc (mg/g)	Avg Conc. (mg/g)
				Mass (mg)	Mass (g)		
Flask 1							
0	47857.7	3.110	1555.0	15.55	20.3	0.766	0.756
0	46605.8	3.029	1514.4	15.14	20.3	0.746	
10	43167.8	2.806	1403.2	14.03	20.5	0.684	0.676
10	42142.4	2.740	1370.0	13.70	20.5	0.668	
50	38684.6	2.516	1258.1	12.58	21.1	0.596	0.573
50	35612.4	2.317	1158.7	11.59	21.1	0.549	
100	26075.0	1.700	850.1	8.50	20.9	0.407	0.403
100	25547.3	1.666	833.0	8.33	20.9	0.399	
Flask 2							
0	46958.3	3.052	1525.9	15.26	20.4	0.748	0.714
0	42629.0	2.772	1385.8	13.86	20.4	0.679	
10	37387.5	2.432	1216.2	12.16	21.0	0.579	0.598
10	39828.9	2.590	1295.2	12.95	21.0	0.617	
50	31261.1	2.036	1017.9	10.18	21.0	0.485	0.510
50	34587.8	2.251	1125.6	11.26	21.0	0.536	
100	24782.2	1.617	808.3	8.08	20.8	0.389	0.396
100	25722.6	1.677	838.7	8.39	20.8	0.403	
Flask 3							
0	38712.5	2.518	1259.0	12.59	21.1	0.597	0.604
0	39605.5	2.576	1287.9	12.88	21.1	0.610	
10	43294.8	2.815	1407.3	14.07	21.2	0.664	0.732
10	52213.7	3.392	1695.9	16.96	21.2	0.800	
50	35696.1	2.323	1161.4	11.61	20.1	0.578	0.545
50	31640.0	2.060	1030.2	10.30	20.1	0.513	
100	40391.0	2.627	1313.3	13.13	24.1	0.545	0.506
100	34587.5	2.251	1125.5	11.26	24.1	0.467	

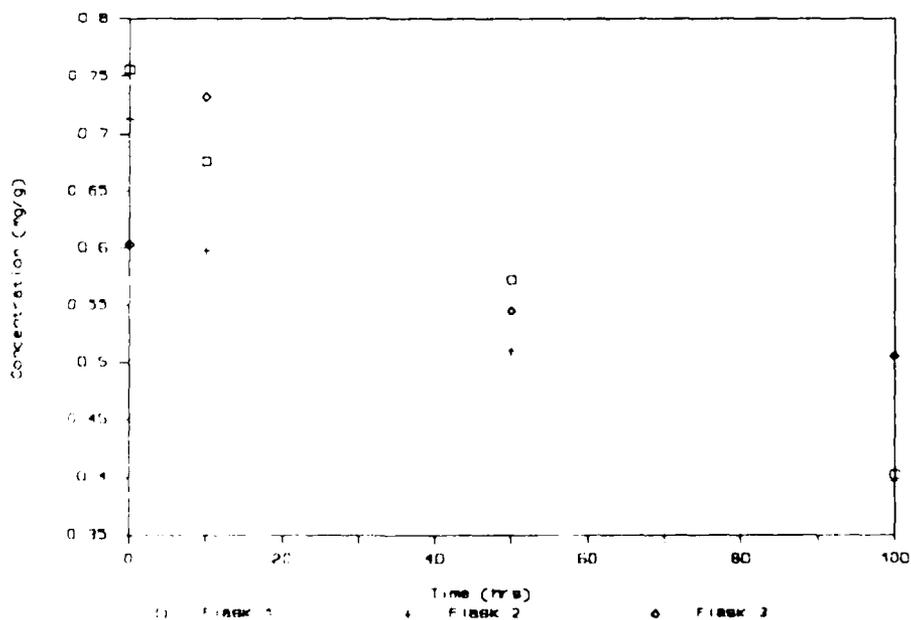


Figure D-2. Soil concentration of naphthalene vs time.

Table D-3. 2-Methylnaphthalene soil extraction data

Time	Peak Area	Mass* (ug)	Conc (mg/L)	Chemical	Soil	Soil Conc (mg/g)	Avg Conc. (mg/g)
				Mass (mg)	Mass (g)		
0	218660.0	15.052	7526.1	75.26	20.3	3.707	3.794
0	228886.0	15.756	7878.0	78.78	20.3	3.881	
10	233934.0	16.103	8051.7	80.52	20.5	3.928	3.738
10	211358.0	14.550	7274.8	72.75	20.5	3.549	
50	200959.0	13.834	6917.0	69.17	21.1	3.278	3.374
50	212763.0	14.646	7323.2	73.23	21.1	3.471	
100	187602.0	12.915	6457.4	64.57	20.9	3.090	3.176
100	198138.0	13.640	6819.9	68.20	20.9	3.263	
Flask 2							
0	261008.0	17.967	8983.3	89.83	20.4	4.404	3.990
0	211925.0	14.589	7294.3	72.94	20.4	3.576	
10	201605.0	13.878	6939.2	69.39	21.0	3.304	3.386
10	211556.0	14.563	7281.6	72.82	21.0	3.467	
50	183136.0	12.607	6303.7	63.04	21.0	3.002	3.028
50	186377.0	12.830	6415.2	64.15	21.0	3.055	
100	192969.0	13.284	6642.0	66.42	20.8	3.193	3.130
100	185297.0	12.756	6378.0	63.78	20.8	3.066	
Flask 3							
0	205519.0	14.148	7073.9	70.74	21.1	3.353	3.278
0	196376.0	13.519	6759.3	67.59	21.1	3.203	
10	231138.0	15.911	7955.5	79.55	21.2	3.753	4.087
10	272336.0	18.746	9373.1	93.73	21.2	4.421	
50	185112.0	12.743	6371.7	63.72	20.1	3.170	3.193
50	187806.0	12.929	6464.4	64.64	20.1	3.216	
100	267808.0	18.435	9217.3	92.17	24.1	3.825	3.560
100	230779.0	15.886	7943.1	79.43	24.1	3.296	

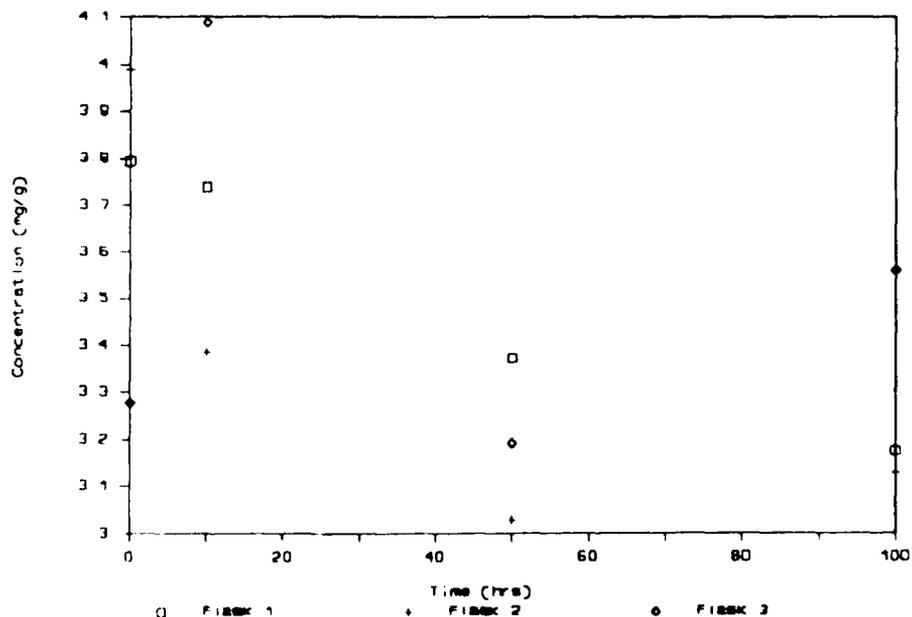
**Figure D-3.** Soil concentration of 2-methylnaphthalene.

Table D-4. 2-Ethyl-naphthalene soil extraction data

Time	Peak Area	Mass* (ug)	Conc (mg/L)	Chemical	Soil	Soil Conc (mg/g)	Avg Conc. (mg/g)
				Mass (mg)	Mass (g)		
Flask 1							
0	130598.0	8.881	4440.5	44.40	20.3	2.187	2.262
0	139517.0	9.487	4743.3	47.43	20.3	2.337	
10	140941.0	9.583	4791.7	47.92	20.5	2.337	2.223
10	127103.0	8.644	4321.8	43.22	20.5	2.108	
50	124449.0	8.463	4231.7	42.32	21.1	2.006	2.051
50	130098.0	8.847	4423.5	44.23	21.1	2.096	
100	122490.0	8.330	4165.2	41.65	20.9	1.993	2.045
100	128894.0	8.765	4382.6	43.83	20.9	2.097	
Flask 2							
0	147237.0	10.011	5005.4	50.05	20.4	2.454	2.316
0	130669.0	8.886	4442.9	44.43	20.4	2.178	
10	120896.0	8.222	4111.0	41.11	21.0	1.958	2.032
10	130097.0	6.847	4423.5	44.23	21.0	2.106	
50	113623.0	7.728	3864.1	38.64	21.0	1.840	1.850
50	114863.0	7.812	3906.2	39.06	21.0	1.860	
100	127028.0	8.639	4319.3	43.19	20.8	2.077	2.020
100	120060.0	8.165	4082.7	40.83	20.8	1.963	
Flask 3							
0	121083.0	8.235	4117.4	41.17	21.1	1.951	1.939
0	119511.0	8.128	4064.0	40.64	21.1	1.926	
10	143817.0	9.779	4889.3	48.89	21.2	2.306	2.458
10	162794.0	11.067	5533.7	55.34	21.2	2.610	
50	115283.0	7.841	3920.5	39.20	20.1	1.950	1.948
50	114951.0	7.818	3909.2	39.09	20.1	1.945	
100	168441.0	11.451	5725.4	57.25	24.1	2.376	2.199
100	143315.0	9.745	4872.3	48.72	24.1	2.022	

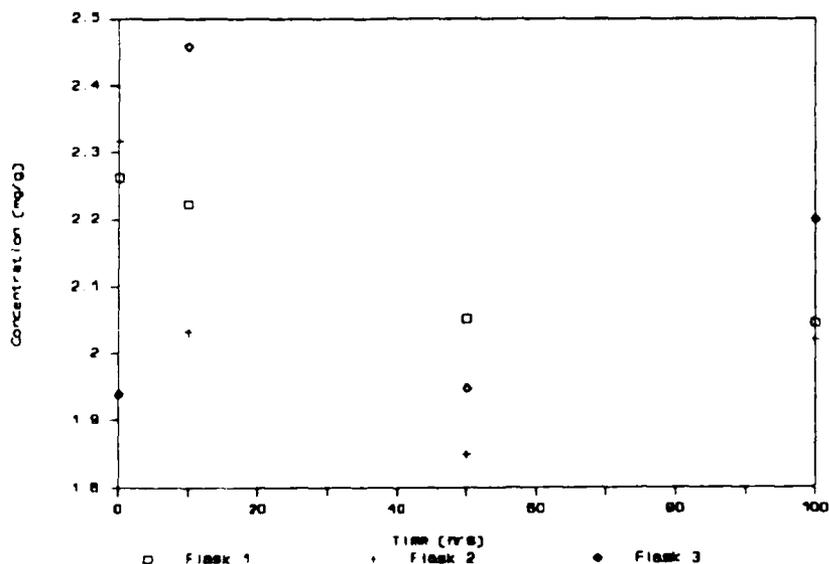
**Figure D-4.** Concentration of 2-ethyl-naphthalene in soil.

Table D-5. Pentachlorophenol soil extraction data

Time	Peak Area	Mass* (ug)	Conc (mg/L)	Chemical	Soil	Soil Conc (mg/g)	Avg Conc. (mg/g)
				Mass (mg)	Mass (g)		
0	8021.8	1.814	906.8	9.07	20.3	0.447	0.583
0	13781.0	2.923	1461.5	14.61	20.3	0.720	
10	7023.7	1.621	810.7	8.11	20.5	0.395	0.401
10	7253.2	1.666	832.8	8.33	20.5	0.406	
50	6033.8	1.431	715.4	7.15	21.1	0.339	0.354
50	6699.8	1.559	779.5	7.80	21.1	0.369	
100	10267.9	2.246	1123.2	11.23	20.9	0.537	0.508
100	8970.7	1.996	998.2	9.98	20.9	0.478	
Flask 2							
0	15349.5	3.225	1612.5	16.13	20.4	0.790	0.855
0	18068.8	3.749	1874.4	18.74	20.4	0.919	
10	11765.8	2.535	1267.4	12.67	21.0	0.604	0.629
10	12891.9	2.752	1375.9	13.76	21.0	0.655	
50	8406.8	1.888	943.9	9.44	21.0	0.449	0.457
50	8752.4	1.954	977.2	9.77	21.0	0.465	
100	10557.7	2.302	1151.1	11.51	20.8	0.553	0.452
100	6182.6	1.459	729.7	7.30	20.8	0.351	
Flask 3							
0	7370.1	1.688	844.1	8.44	21.1	0.400	0.460
0	10009.7	2.197	1098.3	10.98	21.1	0.521	
10	29512.5	5.953	2976.5	29.77	21.2	1.404	1.079
10	15206.3	3.198	1598.8	15.99	21.2	0.754	
50	10496.8	2.290	1145.2	11.45	20.1	0.570	0.474
50	6495.5	1.520	759.9	7.60	20.1	0.378	
100	8923.0	1.987	993.6	9.94	24.1	0.412	0.378
100	7230.7	1.661	830.7	8.31	24.1	0.345	

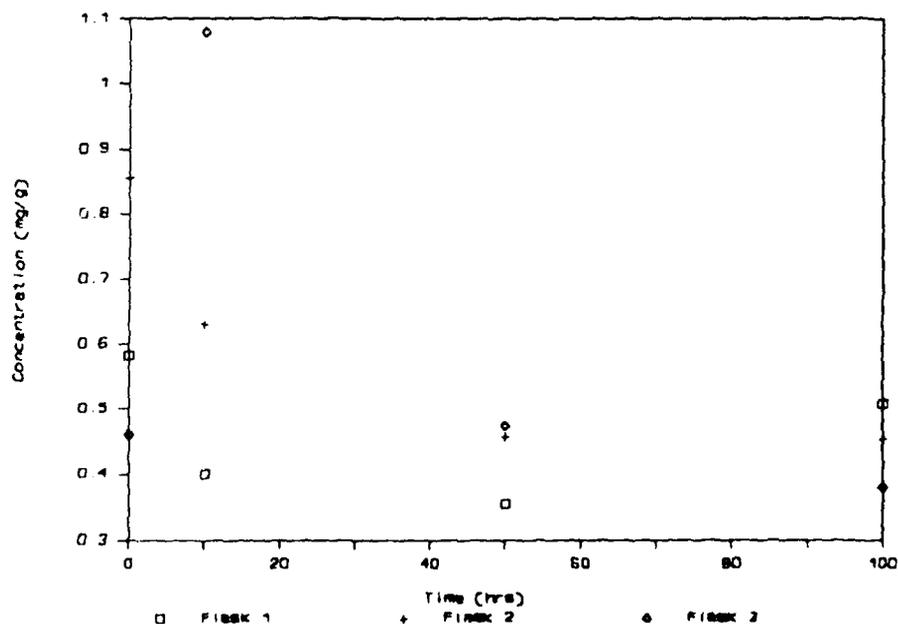


Figure D-5. Concentration of pentachlorophenol in soil.

Table D-6. Anthracene soil extraction data

Time	Peak Area	Mass* (ug)	Conc (mg/L)	Chemical Mass (mg)	Soil Mass (g)	Soil Conc (mg/g)	Avg Conc. (mg/g)
0	12318.3	0.755	377.6	3.78	20.3	0.186	0.204
0	14717.9	0.901	450.4	4.50	20.3	0.222	
10	12337.7	0.756	378.2	3.78	20.5	0.185	0.184
10	12219.4	0.749	374.6	3.75	20.5	0.183	
50	10866.5	0.667	333.6	3.34	21.1	0.158	0.159
50	10941.5	0.672	335.9	3.36	21.1	0.159	
100	12822.6	0.786	392.9	3.93	20.9	0.188	0.194
100	13679.5	0.838	418.9	4.19	20.9	0.200	
Flask 2							
0	14865.5	0.910	454.9	4.55	20.4	0.223	0.221
0	14634.9	0.896	447.9	4.48	20.4	0.220	
10	11689.5	0.717	358.6	3.59	21.0	0.171	0.188
10	14033.9	0.859	429.7	4.30	21.0	0.205	
50	15335.7	0.938	469.1	4.69	21.0	0.223	0.229
50	16155.5	0.988	494.0	4.94	21.0	0.235	
100	17819.3	1.089	544.5	5.44	20.8	0.262	0.224
100	12631.1	0.774	387.1	3.87	20.8	0.186	
Flask 3							
0	11753.9	0.721	360.5	3.61	21.1	0.171	0.184
0	13513.6	0.828	413.9	4.14	21.1	0.196	
10	13935.8	0.853	426.7	4.27	21.2	0.201	0.206
10	14629.9	0.895	447.7	4.48	21.2	0.211	
50	13996.6	0.857	428.5	4.29	20.1	0.213	0.175
50	8938.9	0.550	275.2	2.75	20.1	0.137	
100	13745.3	0.842	420.9	4.21	24.1	0.175	0.167
100	12552.6	0.770	384.8	3.85	24.1	0.160	

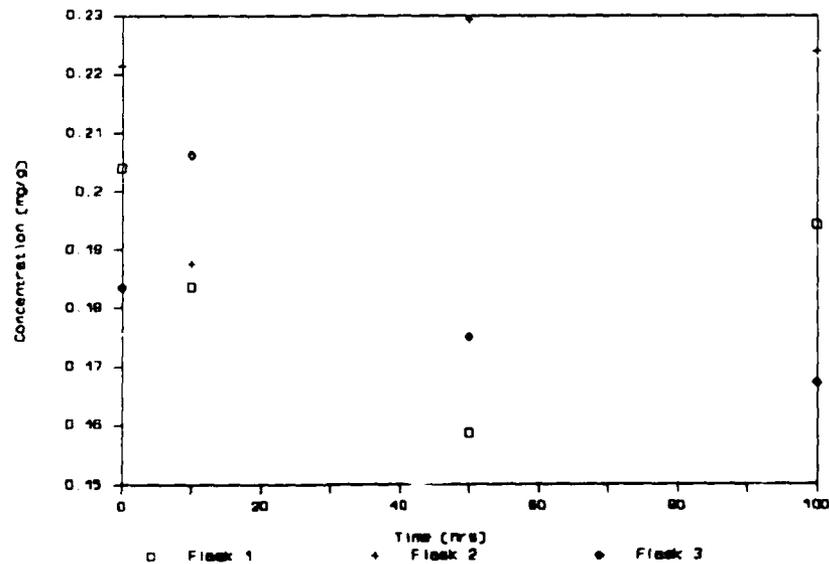


Figure D-6. Concentration of anthracene in soil.

Appendix E. Comparison of soil
extraction and flux data

Table E-1. Comparison of soil concentrations to mass lost by volatilization - naphthalene.

Time	Soil Mass (g)	Flux (ug/cm ² -sec)	dMA (mg)	Concentration	
				Calc'd (mg/g)	Soil ext. (mg/g)
Flask 1					
0	262.8	2.576E-05		0.756	0.756
0.17	262.8	1.059E-04	2.803E-05	0.755	
1.18	262.8	2.301E-04	4.365E-04	0.755	
5.17	262.8	2.948E-04	2.672E-03	0.751	
10.17	242.3	3.715E-04	4.257E-03	0.746	0.676
50.50	221.2	7.929E-04	6.002E-02	0.745	0.573
100.17	200.3	2.948E-04	6.904E-02	0.745	0.403
				% loss	2.94
Flask 2					
0	278.5	1.555E-05		0.714	0.714
0.17	278.5	1.852E-04	4.277E-05	0.713	
1.18	278.5	3.493E-04	6.945E-04	0.712	
5.17	278.5	3.750E-04	3.687E-03	0.707	
10.17	257.5	9.043E-04	8.175E-03	0.696	0.598
50.50	236.5	8.240E-04	8.909E-02	0.695	0.511
100.17	215.7	3.750E-04	7.611E-02	0.695	0.396
				% loss	5.81
Flask 3					
0	262.6	2.021E-05		0.604	0.604
0.17	262.6	1.205E-04	2.998E-05	0.603	
1.18	262.6	1.185E-03	1.696E-03	0.601	
5.17	262.6	5.401E-04	8.783E-03	0.586	
10.17	241.4	1.307E-03	1.180E-02	0.566	0.598
50.50	221.3	1.176E-03	1.280E-01	0.565	0.511
100.17	197.2	5.401E-04	1.089E-01	0.565	0.396
				% loss	18.63

Table E-2. Comparison of soil concentrations to mass lost by volatilization - 2-methylnaphthalene.

Time	Soil Mass (g)	Flux (ug/cm ² -sec)	dMA (mg)	Concentration	
				Calc'd (mg/g)	Soil ext. (mg/g)
0	262.8			3.794	3.794
0.17	262.8	1.190E-05	0.0005	3.794	
1.18	262.8	1.950E-05	0.0040	3.794	
5.17	262.8	4.305E-05	0.0318	3.794	
10.17	242.3	2.804E-05	0.0454	3.794	3.738
50.50	221.2	3.921E-06	0.1647	3.793	3.374
100.17	200.3	4.896E-04	3.1323	3.779	3.176
				% loss	2.5
Flask 2					
0	278.5			3.990	3.990
0.17	278.5	5.191E-06	0.0002	3.990	
1.18	278.5	3.569E-05	0.0053	3.990	
5.17	278.5	9.597E-05	0.0670	3.990	
10.17	257.5	2.110E-05	0.0748	3.989	3.386
50.50	236.5	9.167E-05	0.5813	3.987	3.028
100.17	215.6	5.466E-04	4.0512	3.970	3.130
				% loss	2.3
Flask 3					
0	262.6			3.278	
0.17	262.6	1.303E-05	0.0006	3.278	
1.18	262.6	6.358E-05	0.0100	3.278	
5.17	262.6	3.549E-04	0.2130	3.277	
10.17	241.4	6.370E-05	0.2675	3.276	4.087
50.50	221.3	5.097E-04	2.9559	3.264	3.193
100.17	197.2	8.139E-04	8.4015	3.226	3.560
				% loss	-18.4677

Appendix F. Model parameters

Table F-1. Measured values of parameters used in the Thibodeaux-Hwang-AEER model.

Chemical	Log(K _{ow})	D _s (cm ² /sec)	Solubility (mol/L)	Vapor Press (atm)	H (atm L/mol)	Source
Anthracene (C ₁₄ H ₁₀)		.0421*	4.21E-07	5.04E-05 2.58E-07‡ 8.04E-04	1.65	Thibodeaux (1979) Sims et al (1988) Sonnefeld (1983) Mahmood & Sims (1986) Verscheuren Leo, Hansch, Elkins (1971) Mackay (1982)
m-Cresol (C ₇ H ₈ O)	4.45 4.45 4.45 4.34		4.21E-07 7.24E-06		1.77E-02 1.23E-03	Nirmalakhandan, Speece (1988) Nirmalakhandan, Speece (1988) Loehr, Krishnamoorthy (1988) Verscheuren Leo, Hansch, Elkins (1971) Verscheuren Verscheuren
1,5-Dimethylnaphthalene (C ₁₂ H ₁₂)	1.96		2.32E-01	5.26E-05‡		Leo, Hansch, Elkins (1971) Verscheuren
2,3-Dimethylphenol (C ₈ H ₁₀ O)	1.96, 2.01		2.17E-01‡	1.58E-04~ 6.58E-03σ		Nirmalakhandan, Speece (1988) Sonnefeld et al (1983)
2,4-Dimethylphenol			5.36E-01£	1.98E-01	3.71E-01	Nirmalakhandan, Speece (1988)
2,5-Dimethylphenol			2.03E-01			IRP Toxicology Guide Loehr, Krishnamoorthy (1988)
2,6-Dimethylphenol	2.30		1.21E-02‡	8.82E-05‡	6.70E-03‡	
3,4-Dimethylphenol	2.41		6.50E-02			Verscheuren Leo, Hansch, Elkins (1971)
3,5-Dimethylphenol	2.36 2.36					Verscheuren Leo, Hansch, Elkins (1971)
1-Ethyl-naphthalene (C ₁₂ H ₁₂)	2.35					Verscheuren
2-Ethyl-naphthalene	2.35			2.48E-05 3.36E-05 1.72E-09‡		Leo, Hansch, Elkins (1971) Mackay et al (1982) Mackay et al (1982) Sims et al (1988)
1-Methylnaphthalene (C ₁₁ H ₁₀)			1.83E-04			Verscheuren Nirmalakhandan, Speece (1988) Mackay et al (1982) Mackay
2-Methylnaphthalene	3.86			9.21E-05	2.68E-01	Mackay et al (1982) Mackay et al (1982) Verscheuren
Naphthalene (C ₁₀ H ₈)	3.01, 3.45 3.30 3.37		2.34E-04 2.47E-04‡ 2.34E-04	7.15E-05 1.31E-03 6.96E-05‡	4.82E-01	IRP Toxicology Guide Mahmood & Sims (1986)

Table F-1. (continued)

Chemical	Log(K _{ow})	D _s (cm ² /sec)	Solubility (mol/L)	Vapor Press (atm)	H (atm L./mol)	Source
Naphthalene (cont)	3.01, 3.37, 3.45	.0513* 0.577	2.68E-04	1.14E-04 1.08E-04	4.25E-01 4.83E-01	Leo, Hansch, Elkins (1971) Thibodeaux (1979) Rubio, Nieto, Vives (1983) Mackay et al (1982)
Pentachlorophenol (C ₅ HCl ₅ O)	3.59 5.01 5.12 5.12 5.01	0.086~	1.88E-05* 5.26E-05† 5.30E-05	6.47E-05‡ 1.03E-04	4.16E-01 2.80E-03‡	Sims et al (1988) Sonnefeld (1983) Caldwell (1984) Nirmalakhandan, Speece (1988) Mackay et al (1982) Verscheuren IRP Toxicology Guide Loehr, Krishnamoorthy (1988) Mackay et al (1982)
Phenol (C ₆ H ₆ O)	1.46 1.46 1.46 1.46, 1.48		5.26E-05‡ 1.31E-04⊂ 3.19E-04⊂ 9.92E-01 8.93E-01‡ 8.71E-01⊂	1.45E-07‡ 1.45E-07‡ 6.96E-04‡ 2.63E-04‡	7.00E-04‡	Verscheuren Verscheuren Verscheuren Loehr, Krishnamoorthy (1988) IRP Toxicology Guide Verscheuren Leo, Hansch, Elkins (1971) Mackay et al (1982)
Tetrachlorophenol (C ₆ H ₂ Cl ₄ O)	4.42			2.60E-04 1.32E-03?	3.97E-04	Verscheuren Nirmalakhandan, Speece (1988) Schellenberg
Toluene (C ₇ H ₈)	2.69		5.59E-03	7.90E-02¶ 5.26E-01§		Verscheuren Verscheuren Chiou, Schmedding (1982) Sims et al. (1986)
				2.90E-02	6.74	Nirmalakhandan, Speece (1988)

* @ 0°C
 † @ 15°C
 ‡ @ 20°C
 ~ @ 30°C
 ? @ 40°C
 ⊂ @ 50°C
 ⊂ @ 70°C
 σ @ 76°C
 £ @ 100°C
 ¶ @ 190°C
 § @ 250°C

Table F-2. Estimated values of parameters used in Thibodeaux-Hwang AERR model.

Chemical	MW	M _r	VB	DBa	(f/σ)	T _b (*K)	(e/k)ba	T*	Omega	V'b	B'	(sigma)ab
Toluene	92.10	0.0454	111.14	0.0804	384.15	441.77	186.34	1.50	1.17	118.2	0.0021	4.75
Phenol	94.11	0.0451	96.16	0.0852	454.85	523.08	202.77	1.47	1.21	103.4	0.0021	4.62
m-Cresol	108.15	0.0438	116.62	0.0773	475.35	546.65	207.28	1.44	1.22	125.6	0.0021	4.81
2,6-Dimethylphenol	122.17	0.0423	135.11	0.0717	485.15	557.92	209.41	1.42	1.23	136.7	0.0021	4.89
Naphthalene	128.19	0.0423	140.44	0.0702	491.15	564.82	210.70	1.42	1.23	147.6	0.0021	4.97
2-Methylnaphthalene	142.20	0.0416	160.90	0.0655	513.15	590.12	215.37	1.38	1.24	169.8	0.0021	5.12
2-Ethyl-naphthalene	156.23	0.0409	181.36	0.0616	531.15	610.82	219.11	1.36	1.25	192.0	0.0021	5.25
Pentachlorophenol	266.34	0.0383	183.76	0.0592	582.15	669.47	229.39	1.30	1.27	207.9	0.0021	5.34
Anthracene	178.24	0.0401	190.20	0.0592	627.15	721.22	238.09	1.25	1.30	196.7	0.0021	5.28

DB (g/cc)	DP (g/cc)	St	Moisture	S ₁	S ₂	D'a cnvrsion
1.04 Ma/A	95160	2.67 hp	0.610 A (cm ²)	70.9	288.15 1>(*100000)	1.787 (N e/m ²)
					298.15 2(*100000)	1.837 (N e/m ²)

COMPOUND	DMA (25°C) (cm ² /sec)	D'a (cm ² /sec)	C1o (g/cm ²)	Ma/A (g/cm ²)	Log(kow)	ksw	S (mol/L)	P (atm)	HA (atm ² /mol)	HC (g/cc)/(g/cc)	HC' (g/cc)/(g/cc)	Ca* (g/cm ³)	DBa (ML)	te (sec)	te (days)
Toluene	0.0660	2.46E-02	4.41	5.29E-01	2.69	5.61E+02	5.39E-03	2.90E-02	3.19E+00	2.12E-01	3.78E-04	1.67E-03	0.0860	2.45E+04	0.3
Phenol	0.0874	2.30E-02	12	1.44E+00	1.46	2.99E+00	8.71E-01	2.63E-04	3.02E-04	1.23E-03	4.13E-06	4.98E-03	0.0874	2.21E+06	25.3
m-Cresol	0.0750	1.98E-02	56	6.67E+00	1.96	2.51E+01	2.17E-01	5.26E-05	2.42E-04	9.91E-06	3.93E-07	2.20E-03	0.0750	2.56E+06	296.0
Naphthalene	0.0722	1.90E-02	29	3.47E+00	2.36	1.38E+02	1.70E-03	3.78E-04	2.22E-01	9.09E-03	6.60E-05	1.91E-03	0.0750	1.61E+05	11.9
2-Methylnaphthalene	0.0668	1.76E-02	33200	3.97E+03	3.01	2.19E+03	2.34E-04	1.00E-04	4.27E-01	1.75E-02	7.98E-06	2.63E-01	0.0722	1.38E+06	16.0
2-Ethyl-naphthalene	0.0625	1.65E-02	5040	6.05E+02	3.86	8.15E+04	1.89E-04	9.21E-05	5.03E-01	2.06E-02	2.52E-07	8.33E-03	0.0668	4.73E+07	5.47E+02
Pentachlorophenol	0.0573	1.51E-02	22100	2.65E+03	4.21	3.62E+05	3.55E-04	3.36E-05	9.46E-02	3.87E-03	1.07E-08	5.39E-05	0.0625	1.19E+09	1.36E+04
Anthracene	0.0591	1.56E-02	13000	1.56E+03	5.01	1.09E+07	2.26E-05	1.45E-07	2.76E-03	1.13E-04	1.03E-11	2.29E-07	0.0573	1.34E+12	1.36E+07
					4.45	1.00E+06	5.04E-05	5.04E-05	6.96E+00	2.85E-01	2.83E-07	3.68E-03	0.0591	4.77E+07	5.52E+02

Table F-3. Mass flux rates calculated by Thibodeaux Hwang AERR Model.

Time (hrs)	Toluene	Phenol	m-Cresol	2,6-DMP	Naphthalene	2-Mennaph	2-EUnaph	PCP	Anthracene
0.17	6.901E-05	1.980E-05	2.694E-05	1.765E-04	6.915E-02	1.179E-02	3.16E-04	4.671E-05	4.615E-03
1.10	2.597E-05	7.450E-06	1.014E-05	6.643E-05	2.602E-02	4.438E-03	1.246E-04	1.757E-05	1.716E-03
5.17	1.256E-05	3.602E-06	4.902E-06	3.212E-05	1.258E-02	2.146E-03	6.206E-05	8.498E-06	8.136E-04
6.01	1.098E-05	3.131E-06	4.288E-06	2.809E-05	1.102E-02	1.872E-03	5.690E-05	7.432E-06	7.344E-04
10.00	2.622E-06	3.568E-06	2.338E-05	2.338E-05	9.156E-03	1.562E-03	4.733E-05	6.184E-06	6.111E-04
15.00	1.722E-05	2.661E-05	9.547E-05	5.951E-02	1.172E-02	3.649E-04	6.743E-05	8.857E-06	8.512E-04
20.00	2.275E-06	4.918E-06	1.765E-05	1.100E-02	1.175E-03	6.743E-05	8.857E-06	8.512E-04	8.512E-04
30.00	1.700E-06	3.522E-06	1.264E-05	7.872E-03	1.558E-03	4.802E-05	6.342E-06	6.095E-04	6.095E-04
40.00	1.423E-06	2.554E-06	9.162E-06	5.711E-03	1.129E-03	3.502E-05	4.598E-06	4.419E-04	4.419E-04
50.00	1.265E-06	1.896E-06	6.803E-06	4.779E-03	8.386E-04	2.902E-05	3.848E-06	3.698E-04	3.698E-04
50.50	8.418E-06	1.571E-05	3.377E-05	4.452E-02	1.229E-02	2.600E-05	3.414E-06	3.281E-04	3.281E-04
70.00	1.326E-06	3.593E-06	4.464E-06	5.885E-03	1.623E-03	3.986E-04	5.290E-05	4.808E-03	4.808E-03
80.00	1.165E-06	2.601E-06	3.232E-06	4.261E-03	1.175E-03	3.268E-05	6.992E-06	6.355E-04	6.355E-04
90.00	1.032E-06	1.926E-06	2.393E-06	3.155E-03	9.870E-04	3.814E-05	5.062E-06	4.601E-04	4.601E-04
100.00	9.871E-07	1.842E-06	2.288E-06	3.017E-03	8.702E-04	3.187E-05	4.230E-06	3.845E-04	3.845E-04
100.17	1.169E-05	1.762E-06	2.734E-05	2.887E-03	7.961E-04	2.700E-05	3.504E-06	3.257E-04	3.257E-04
100.17	1.169E-05	1.762E-06	2.734E-05	3.413E-02	1.295E-02	4.422E-04	5.940E-05	5.076E-03	5.076E-03

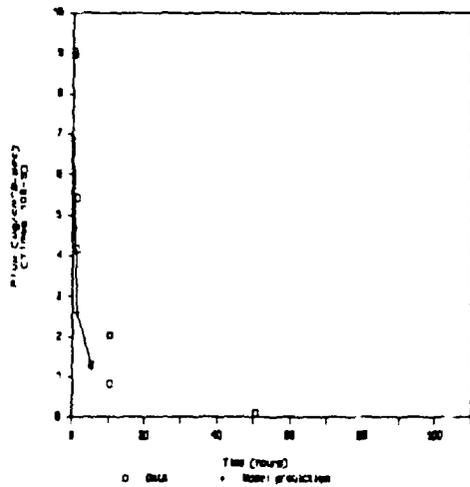


Figure F-1. Comparison of model prediction against measured flux rates for toluene (Flask 1 only).

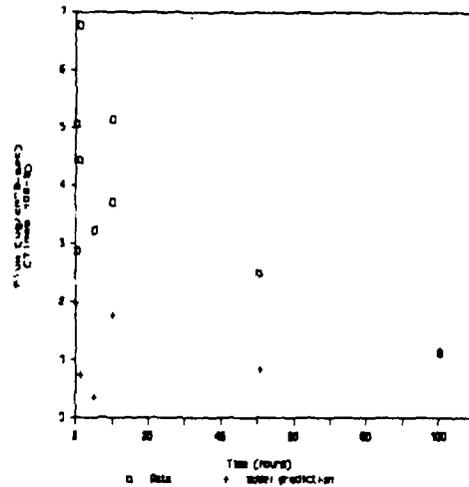


Figure F-2. Comparison of model prediction to measured flux values for phenol (Flask 1 only).

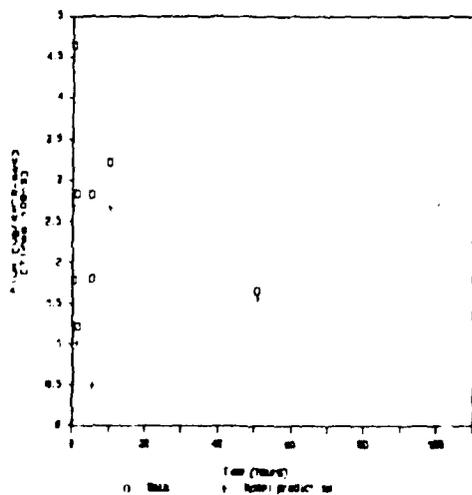


Figure F-3. Comparison of model prediction to measured flux rates for m-cresol (Flask 1 only).

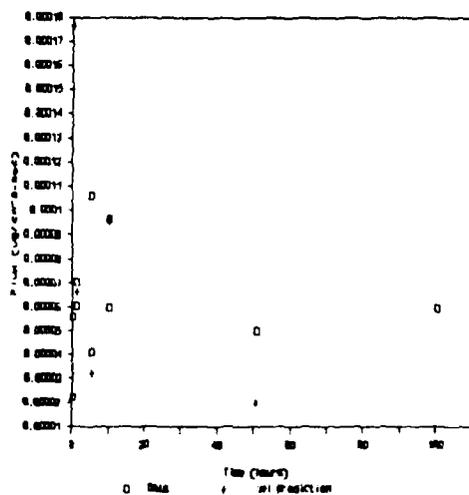


Figure F-4. Comparison of model prediction to measured flux rates for 2,6-dimethylphenol (Flask 1 only).

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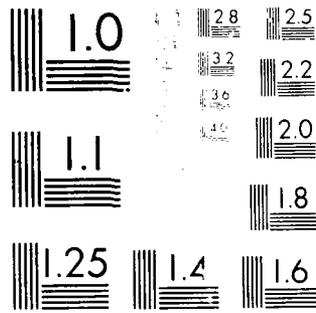
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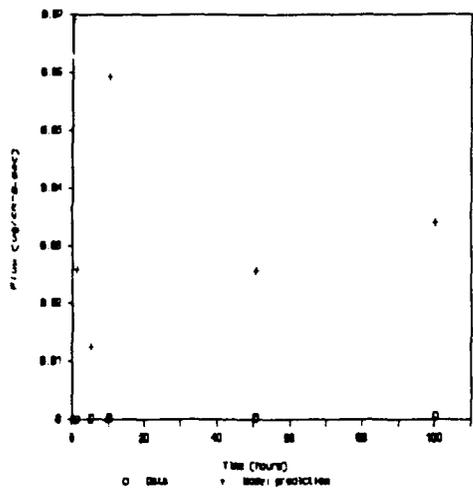


Figure F-5. Comparison of model predictions to measured flux rates for naphthalene (Flask 1 only).

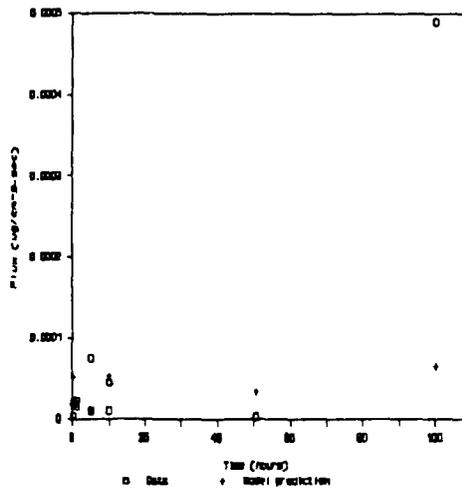


Figure F-6. Comparison of model prediction to measured flux rates for 2-methylnaphthalene (Flask 1 only).