AFIT/GEE/ENV/99M-11

SORPTION OF THE AIRCRAFT DEICING FLUID COMPONENT METHYL-BENZOTRIAZOLE IN SOIL

David L. Kellner, 1st Lieutenant, USAF

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THESIS

David L. Kellner, B. S., E.I.T.
1st Lieutenant, USAF
March 1999

Presented to the faculty of the Graduate School of Engineering
of the Air Force Institute of Technology
Air University
In Partial Fulfillment of the
Requirements for the Degree of
Master of Science in Environmental and Engineering Management

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Table of Content

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Dave Kellner

List of Figures

List of Tables

Abstract

The air transport industry requires deicing agents to maintain flight operations in cold weather conditions. The main type of aircraft deicing fluid (ADF) being used is Type I, composed of a propylene glycol (PG)-base, water, and several additives. Among these additives are corrosion inhibitors, wetting and thickeners; some of which are known to be toxic to microorganisms. Most of the spent ADF is closely monitored and collected for treatment or recycle; however, total capture is not possible for a variety of conditions. Therefore, investigation of suitable remediation technique for used deicing fluid is appropriate.

The goal of this research was to establish if 4(5) methyl-benzotriazole (MeBT) sorbs to various soils after the application of several concentration variations. If so, then how much and in what proportions or percentage of original concentration is sorbed. Since little research has been done on this compound, I have tried to make the best of what information is closely related to MeBT. Presented here is defining information on sorption, the definition and types of sorption isotherms, and supporting, useful reports from scientific journals and one doctoral student.

Recent studies have raised questions as to the toxicity of the deicing fluid additives, especially the corrosion inhibitor MeBT. It is known that PG exerts an oxygen demand; however, it is shown that MeBT is only slightly sorbed to the soils studied and may also degrade.

Having applied a MeBT solute to the several soils in varied concentrations, centrifuged the samples, washed the soil with methanol, and employed standard High Performance Liquid Chromatograph (HPLC) techniques, the percent of MeBT recovered from the soil and a sorption coefficient for each soil was determined.

This study demonstrated that MeBT scarcely sorbs to soil particles and sorbs only slightly better to organic material. Portions of a specific isomer are unrecoverable at lower concentrations. In most cases, nearly 100 percent of MeBT was accounted for when an initial water and subsequent methanol extraction(s) were performed.

This work parallels that of Captain Burke and will be used as reference material for Major Cornell, a doctoral student at the University of Colorado. Previous studies have indicated that MeBT degrades along with PG; this research will more clearly define what happens to MeBT after it comes in contact with soil. Proving that MeBT sorbs to soil is the first step to define a process to deal with spent ADF.

I. Introduction

1.1 Overview

Snow and ice buildup on airframes requires the air transport industry to use deicing/anti-icing agents to maintain flight operations in cold weather conditions. Commercial airports and airbases use hundreds of millions of liters of deicing fluid, approximately 52M liters of concentrated aircraft deicing fluid (ADF) are used in North America per year in an attempt to correct this safety problem [Cancilla *et al.*, 1998:3834; Sills, 1991]. In an average winter, Chicago-O'Hare International Airport alone used more than 1.5M gallons of ADF [Mericas and Wagoner, 301]. However, without this fluid the safety of air-travel would be compromised. The main type of deicing fluid currently used is SAE Type I, consisting of numerous components including water, propylene glycol (PG), and various additives. Among these additives are corrosion inhibitors, wetting agents, flame-retardants, and thickening agents; some of these are known to be toxic to microorganisms.

Other types of deicers, Type II, III, and Type IV, have a greater viscosity than Type I. They contain polymers and other additives that allow them to stick to applied surfaces resulting in longer lasting protection against ice build-up.

The use of deicing fluid is closely monitored and attempts are made to collect spent fluid; however, spent ADF is not totally captured. Over 50% can be lost due to various conditions. A substantial percentage (49% - 80%) ADF and water solution does not make it on the aircraft due to overspray or drippage. The excess ADF enters the parking apron's storm water drainage system or is collected in the bulk snow removal [Cancilla *et al.*, 1997:430; Chesterfield *et al.*].

Various treatments of used deicing/anti-icing fluid have been suggested such as land-farming or in-situ bioremediation. An understanding of the transport of ADF and the impact of the additive 4(5) methyl-benzotriazole (MeBT) is necessary to determine if bioremediation techniques can be employed effectively.

1.2 Purpose of Research

Two principle environmental concerns exist from the use of aircraft deicing fluid. First is the high oxygen demand of propylene glycol, approximately 50% to 90% of aircraft deicing fluid [Cancilla *et al.*, 1997:430; Arco]. Oxygen consumption occurs during the decomposition by bacteria. As ADF degrades, its oxygen demand is far greater than the replenishment of oxygen to the water; therefore, disrupting the environment of oxygen using organisms. This high biochemical oxygen demand (BOD), 1.68g O_2/g PG, makes treatment by municipal wastewater treatment plants an unlikely option [Halterman-O'Malley, 2-14; Cornell, 1997:2]. The second concern is the toxic nature of MeBT, a flame retardant/corrosion inhibitor in deicing/anti-icing fluid [Cancilla et al., 1998:3834].

This study investigated the sorption characteristics of MeBT with soil. Parallel study by Burke (1999) measured biodegradation of PG and MeBT using respirometry. High Performance Liquid Chromatography (HPLC) was also used to analyze MeBT. This work supported the research of Major Jeff Cornell, a Doctoral student at the University of Colorado at Boulder through the Air Force Institute of Technology. He has examined 1) toxic nature of ADF additives, 2) environmental and human health risk of ADFs overall, and 3) the design for future ADF formulations and treatments.

1.3 Primary Goals

The primary goal of this study was to determine the sorption characteristic of MeBT in various soils. This was accomplished by using several concentrations of MeBT solute in three specified soil types to measure variation in the sorption results. Several replicates of each soil type and solute concentrations were performed to ensure statistically sound data.

1.4 Scope

The scope of work follows the studies of Johnson (1997) and Halterman-O'Malley (1997) with additional references to the work of Cornell (1998). However, the research was centered on the sorption of MeBT in various soil types. Solutes from the procedures were evaluated using standard High Performance Liquid Chromatographic techniques to determine the amount of MeBT in each sample before and after the sorption process. This was used to model sorption characteristics of MeBT on the variety of soil types and to predict the effects of sorption on biodegradation and bioremediation.

1.5 Definitions

Absolute calibration – A method relating detector response to sample concentration in order to perform quantitative analysis. Standard solutions of a sample to be quantitated are prepared and equal volumes chromatographed. Peak heights or peak areas are plotted versus concentrations to produce a calibration curve.

Absorption – (1) The uptake, drinking in, or imbibing of a substance; the movement of substances into a cell; transfer of substances from one medium to another [Atlas and Bartha, 533; Fetter, 117]. (2) The process by which a compound in solution or attached to the surface of the solid particle moves into the interior of the solid particle; diffusion into the inner pore-spaces or lattice structure of the solid particle.

Acclimated – A soil that has undergone the respirometry process with exposure to MeBT and PG, the soil microcosm has shown the ability to survive in the presence of these substances.

Adsorption – Surface phenomenon, ability of a compound to clings to a solid at the solid:liquid interface [Fetter, 117].

Adsorption coefficient - (a.k.a. distribution coefficient, K_d) Ratio of the sorbed phase concentration to aqueous phase concentration. Analyte retention in HPLC is proportional to its adsorption coefficient (units: mL/g).

Aerobic - Having molecular oxygen present; process involving electron acceptors [Schwarzenbach *et al.*, 410].

Anaerobic – The absence of oxygen; able to live or grow in the absence of free oxygen, low redox potential. [Atlas and Bartha, 534; Schwarzenbach *et al.*, 410]

Aromatic compound – Carbon skeletons containing aromatic benzene ring and compounds that resemble benzene in chemical behavior. Their ring structure and stable bonds allow them to be resistant to degradation. These molecules contain delocalized clouds of resonant π-electrons and they favor substitution rather than additional reactions, both of which contribute to their stability [Schwarzenbach *et al.*, 32; Morrison, 322]

Biochemical Oxygen Demand – (BOD) Refers to the amount of dissolved oxygen required by aerobic and facultative microorganisms to stabilize organic matter in water (a.k.a. biological oxygen demand) [Atlas and Bartha, 535].

Biodegradation - The microbial mediated process of chemical breakdown of a substance to a smaller product caused by microorganisms or their enzymes [Atlas and Bartha, 535].

Chemisorption – Occurs when the solute is incorporated on a sediment or soil surface by a chemical reaction [Fetter, 117].

Completely Mixed Batch Reactor – (CMBR) Self-contained vessel in which the reactions of the sorption process will take place, conditions are the same throughout.

Deicing/Anti-icing - Spreading or spraying of a liquid agent to: (1) Melt already formed ice and snow; (2) Applied before ice and snow is present; provides a thin layer of protection.

Desorption - The process by which sorbed species are released to the surrounding environment. Desorption from the particle surface proceeds more readily than desorption from the interior of a particle.

Field Capacity - The maximum amount of water that an unsaturated zone of soil can hold against the pull of gravity [Fetter, 639]

Hydrophilic – A compound with an affinity for water. [Schwarzenbach *et al.*, 38]

Hydrophobic – A compound that repels or has a dislike for water. [Schwarzenbach *et al.*, 38]

Ion Exchange – This is where cations may be attracted to the region closest to a negatively charged (δ^-) clay-mineral surface and are held by electrostatic forces [Fetter, 117].

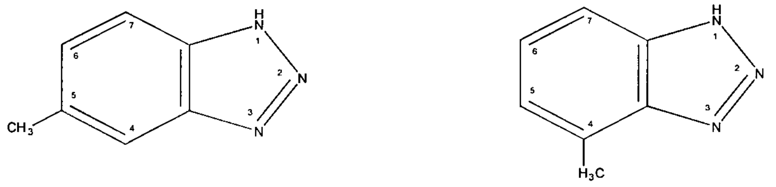
Isomer – Numerous arrangements of a given set of atoms to yield a different structure depending on the number and type of atoms [Schwarzenbach *et al.*, 9].

Isometric – *Iso*-prefix indicating equal or same. *Isometric*-Relative amount of each isomer of MeBT that composes the chemical substance; for each isomer the relative amount of each is designated by the position of the nitrogen atom on the benzene ring [Lee, 216].

Isotherm, sorption – Relationship between sorbed and solution concentrations of a compound of equilibrium and constant temperature. There are numerous types of isotherms; three referenced here are: Linear, Freundlich, and Langmuir (see Section 2.5 for further explanation) [Fetter, 117-123; Park, 661]. In adsorption, the dependence of an analyte concentration to solution is due to the surface interactions on the adsorbent surface on the equilibrium concentration of analyte in the bulk solution. The shape of the adsorption isotherm can predict the chromatographic behavior of the solute.

Methyl-benzotriazole - Compound used as a flame retardant in air transport industry, used in ADF. Pasivates the surface of metal wires and makes them less reactive to O_2 to reduce corrosion. Lower solubility in water, semi-combustible, and stable. (A.k.a. 4(5)-Methyl-benzotriazole, Tolyltriazole, MeBT, or TTZ) [Cornell et al.].

Structure:



Numbering scheme for 5-Methyl-1H-Benzotriazole. Numbering scheme for 4-Methyl-1H-Benzotriazole

Figure 1-1. The structure and nomenclature of 5-MEBT and 4-MEBT.

Natural Attenuation – Numerous processes including dilution, oxidation, and sedimentation that remove material from the environment over time.

Octanol-Water Partitioning Coefficient, (K_{ow}) – Ratio of concentrations of a compound in octanol and water at equilibrium, an indication of hydrophobicity, $C_{octanol}/C_{water}$ [Fetter, 132-133].

Organic Carbon Partitioning Coefficient, (K_{oc}) – (1) The extent to which a chemical partitions between the organic carbon and solution phases. (2) The smaller the K_{oc} value the greater the concentration of contaminant in solution. (3) K_{oc} is related to the distribution coefficient, K_d by the formula: $K_d = (K_{oc})(f_{oc})$ where K_d is an index for sorption of a given contaminant on a particular soil (at equilibrium).

(units: μg adsorbed/g OC)/(μg/mL solution)

Organic Matter Partitioning Coefficient, (K_{om}) - Extent that a chemical partitions between organic matter and solution. $K_d = K_{om}(f_{oc})$ Note: For "average" soil organic matter $f_{oc} = 0.58(f_{om})$ [(μg/g)/(μg/mL)] [Fetter, 132].

Propylene Glycol – (PG) Stable, non-toxic to mammals, humectant compound that is used in the aircraft, food, and cosmetic industries [RACB, Merck Index 12th ed.].

Structure:

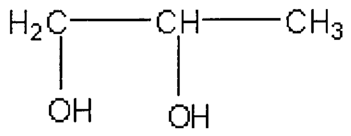


Figure 1-2. Propylediol (Propylene Glycol, PG)

Recalcitrant – A chemical that is resistant to microbial attack or degradation [Atlas and Bartha, 543].

Silicate – Soils made mainly of small quartz granules (a.k.a. sand or sandy soil) [Lee, 128].

Solubility – The maximum concentration of a contaminant that can be dissolved in water at a specific temperature.

Sorption – It is the adherence of analyte to soil, organic, or other particles. This process involves several classifications including *absorption*, *adsorption*, *chemisorption*, and *ion exchange* (see individual definitions) [Fetter, 117; Lin *et al.*, 2178].

Stationary phase – This is that part of the chromatographic system which is in equilibrium with the mobile phase, refers to phase that does not move - usually a solid.

Tautomers - Derivative of a compound, has the same basic structure with one or more compounds added on [Cornell *et al.*].

Zeolite –Clay mineral with a three-dimensional framework dawn from an open framework of $[AlO_4]^{5-}$ or $[SiO_4]^{4-}$ tetrahedra linked together (a.k.a. clay or clayey soil).

Structure:

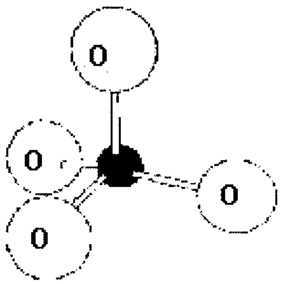


Figure 1-3: An $[AlO_4]^{5-}$ or $[SiO_4]^{4-}$ tetrahedra (primary building unit) [Lee, 128].

The tetrahedra link together leading to the formation of rings and cages (Secondary Building Units or SBU's) (a.k.a. clay or clayey soil).

II. Literature Review

2.1 Introduction

Aircraft deicing fluids may reach surface and groundwaters presenting significant long-term affects on the milieu. Only a small percentage of the ADF used at most airports and military airbases is captured and/or treated. The majority is released into the environment through surface runoff or stormwater runoff [Sills, 1991; USEPA]. The passing and subsequent enforcement of the Clean Water Act of 1987 has only recently turned public and regulatory attention to the impact that ADF has on the environment. The Environmental Protection Agency (EPA) Storm Water Discharge regulations, effective 17 December 1990, and the National Pollution Discharge Elimination System (NPDES) permit program have focused on reducing point source pollutants [Oakley and Forrest]. As a result, several large international airports, Denver IAP, Chicago O'Hare IAP, Baltimore-Washington IAP, are currently operating directly under environmental regulatory agency guidelines enforced by state or regional regulators [NRDC, Cornell *et al.*]. Two states, New York and Pennsylvania, have issued "zero-discharge" regulations concerning the glycol component of deicing fluids. The Air Force has even cut back on most cold weather flying operations that require ADF in attempts to lessen the problem [Cornell *et al.*].

Most concerns with ADF in the environment stem from the glycol content and the BOD burden it imparts. However, recent work [Pillard, 1993; Hartwell *et al.*, 1995; Fisher *et al.*, 1995; Cancilla *et al.*, 1997; Cornell, 1998] reveal that additives to ADF tend to create more toxic formulations than glycol alone. Of these studies, only Cancilla *et al.* [1997] isolated any specific compound that may be responsible for the increased toxicity observed. Two recent AFIT theses dealt with environmental impacts of aircraft deicing/anti-icing fluids [Johnson; Halterman-O'Malley, 1997].

Earlier research has concluded that MeBT is found and can be detected in subsurface water from a major North American airport [Cancilla *et al.*, 1998:3834]. What is yet to be determined is the true extent and magnitude of contamination. This requires extensive testing to accurately determine how MeBT reacts once it is released into the environment. Little is known about the environmental fate and transport MeBT. The compositions of most ADFs are proprietary and compounds are modified slightly among the manufacturers. The octanol-water partitioning coefficient (K_{ow}) and metal-binding properties of MeBT suggests that sorption to soil and organic material could significantly retard the subsurface transport rate [Cornell *et al.*]. This chapter outlines the history of ADF, discusses the composition of ADF and the main components (PG and MeBT), and gives a detailed summary of the sorption process, while looking briefly at the biodegradation relationship of PG and MeBT.

2.2 Review of ADF and the Air Force

The commercial aircraft transportation industry classifies their highly used deicing fluids as Type I or Type II. The composition of these fluids includes propylene glycol and/or ethylene glycol. Commercial fluids were designed to be primary freezing point depressants (FPD) as well as meet the performance specifications of the International Standards Organization (ISO) and the Society of Automotive Engineer (SAE).

Military deicing/anti-icing fluids were developed by the Navy and adopted for Air Force use [Chesterfield *et al.*]. These military derivative specification were developed to afford maximum corrosion protection to prevent corrosion problem in steel storage tanks and deicing trucks. Secondarily, the added benefit of aircraft and other metals protection was highly desired. However, it is important to note that the time of fluid exposure to aircraft metals is of short duration and is diluted by being mixed with water before application.

There are two types of deicing fluids that have been used by the Air Force. They are MIL-A-4823D Type I - propylene glycol base with a corrosion inhibitor and MIL-A-4823D Type II - ethylene and propylene glycol (independent or mix) with a corrosion inhibitor. The Navy is still the OPR on the specification, even though the USAF is the largest user of the fluid [HQAFCEE, July 1995].

The composition of Type I fluid is "unthickened," with a low viscosity, and Type II's composition is "thickened," and offers better anti-icing action than Type I fluid. However, Type I fluid can be applied with existing Air Force equipment while Type II fluid cannot, due to viscosity. In addition, in March 1992, Brigadier General James E. McCarthy, Air Force Civil Engineer, directed the immediate prohibition on the use of ethylene glycol (EG) in the USAF [HQAFCEE, July 1995]. EG is also listed under CERCLA as a hazardous substance and is therefore subject to the Emergency Planning and Community Right to Know Act (EPCRA) [HQAFCEE, July 1995]. By prohibiting the use of EG, the AF resorted to use the PG-based ADF [HQAFCEE, Dec 1995]. Type II anti-icing solutions are no longer necessary because the Type I ADF can be used just prior to flight [Chesterfield *et al.*].

The Air Force Material Command's Wright Laboratory has evaluated the SAE, Aerospace Material Specification (AMS) Type I FPD fluid with the intent of using it in the Air Force. The adoption action has been approved, authorizing Air Force units to use SAE/AMS Type I specification fluid, as long as it is propylene glycol-based. The change from military specification (MIL SPEC) fluid to SAE/AMS Type I fluid will require additional training. Air and ground crews will have to be well versed in the characteristics of both fluids until existing stocks of the military specification fluid are depleted. Military specification fluid is applied while Air Force aircraft are being serviced and is designed to remove snow and ice [Chesterfield *et al.*]. Within the Air Force's flight operations community, there exist differences in the understanding and interpretation of published holdover times after deicing/anti-icing.

2.3 Composition and Structure

Much of the ADF used in the United States is classified as PG-based Type I, which contains 85-90 percent propylene glycol (FPD), 1-2 percent surfactant and trace additives (provide adhesion), 0.5-0.6 percent MeBT (corrosion inhibitor and flame retardant), and water [SAE]. This section will review the characteristics of both PG and MeBT as major components of ADF.

2.3.1 Glycol

Glycols are straight-chained alcohols with two attached hydroxyl groups [Morrison, 456]. The length of the chain can vary greatly. Propylene glycol is the component of ADF that provides freeze-point depression (FPD). These solutions can push the freezing point temperatures down to -13°C to -59°C depending on concentrations [Sigma Products, MSDS]. Once in the soil, this component of ADF is nearly as, if not more, mobile than water in the subsurface transports system. This phenomenon is due to PG's high miscibility in water. Other characteristics include: highly hydrophilic, low volatility (stable indefinitely at room temperature), non-toxicity, easily biodegradable in both aerobic and anaerobic conditions, and a very high oxygen demand (ca. 1.68 g O_2/g PG degraded) [EA-Engineering, Bausmith and Neufield, Gooden, Halterman-O'Malley]. In waste treatment systems or in environmental impact assessments, the BOD exerted by PG is of primary concern.

Toxicity tests performed on flathead minnows with EG and PG are summarized in Table 2-1 below [ENSR Consulting].

MATERIAL	**COMPOSITION**	**48 HOUR LC_{50}**	**96 HOUR LC_{50}**
Ethylene Glycol	Formulated in ADF	8,541 mg/L	8,045 mg/L
Ethylene Glycol	Pure	81,950 mg/L	72,860 mg/L
Propylene Glycol	Formulated in ADF	791 mg/L	709 mg/L
Propylene Glycol	Pure	61,200 mg/L	55,860 mg/L

NOTE: LC_{50} is 50 percent mortality concentration

Table 2-1. Glycol Toxicity

Further government toxicity tests on mice indicate no real toxicological threat. Results of the study concluded that there were no treatment-related effects on pup weight, health, or development. In addition, no effect was found on the fertility of adult mice [RACB]. There was one ill-effect found with dermal exposure of PG; when applied to skin, the PG tends to replace some of the important components necessary to the skin, including water. In very high doses, PG may cause liver abnormalities or kidney damage [Network Marketing].

2.3.2 Methyl-benzotriazole

MeBT is added to ADF at a concentration of ca. 0.5% w/w to reduce the flammability hazard created when a glycol solution come into contact with metal components carrying direct current [NASA, 1968]. The ADF component MeBT is actually a mix of the two isomers, 4-methyl-benzotriazole (4-MeBT) and 5-methyl-benzotriazole (5-MeBT). In this study, the mixture of the two MeBT isomers is simply referred to as MeBT.

MeBT is a weak organic acid ($pK_a = 8.8$) which is relatively hydrophobic ($\text{Log } K_{ow} \approx 2$) and reacts strongly with some metals [Matulewicz; PMC Specialties Group; Cornell, 1998]. MeBT is a member of the benzotriazole family of compounds. Benzotriazole and their derivatives (BTs) are of great importance in organic synthesis, analytical and medicinal chemistry, and industry [Cornell, *et al.*], but there is little published information on their chemistry, toxicity, and biodegradability which is useful in assessing their likely fate in the natural environment [Cornell, *et al.*]. Following is a summary of the current literature on MeBT.

MeBT is often thought of as strictly a flame retardant when it is actually classified as a corrosion inhibitor. MeBT coats the surface of conductive wire and protects it from oxidation in the presence of glycols, thus mitigating ignition hazards. Unlike other proprietary corrosion inhibitors, MeBT is manufactured from the waste product of isocyanide formation, which makes it very inexpensive. Other corrosion inhibitors are often salts of dibasic organic acids (*e.g.* triethanolamine). Industrial uses for the corrosion inhibitors include corrosion control in metal alloy cooling water towers.

The chemical properties of MeBT (Table 2-2) suggest that MeBT is highly reactive in the environment. For example, the structure of 4-MeBT (specifically the proximity of the non-polar methyl group to the polar nitrogen ring) would suggest the 4-MeBT hydrophobic surface is smaller than that of 5-MeBT [Cornell, *et al.*]. In addition, 4-MeBT elutes earlier than 5-MeBT from a C-8 reverse-phase liquid chromatography column (often faster elution corresponds to less hydrophobicity). These facts seem to contradict solubility data that indicates 5-MeBT is more soluble in water. Further, the MeBT's solubility in water is much larger than the solubility of either individual isomer. There is no current explanation for this phenomenon. Notice in the following table, the melting point of MeBT is lower than the melting point of either individual isomer. This property is normally only found in metal alloy chemistry [Cornell, 1998].

TABLE 2-2. Physical and chemical properties of MeBT and BT [Cornell, 1998]

SUBSTANCE	Sol. - Water (wt. %)	Sol. - Min. Oil (wt. %)	pKa	Melt. Pt. (°C)	Boil. Pt. (°C)	Vap. Press. @ 20°C (mm HG)	Log K_{ow}	Sp. Gr. @ 20°C (solid)
4-Me-benzotriazole (**4-MeBT**)	0.10	N/A	8.7	145-146	N/A	N/A	N/A	N/A
5-Me-benzotriazole (**5-MeBT**)	0.18	N/A	8.7	82-83	N/A	N/A	N/A	N/A
MeBT; 55-60% 5-MeBT plus 45-50% 4-MeBT	0.55	0.01	8.7	76-87	>300	0.03 (est.)	2.17 (est)	1.36
Benzotriazole (**BT**)	1.98	0.04	8.5	98-99	>350	0.04	2.09	1.24

N/A – not available

Due to the complexity of the tautometric forms of MeBT, there appears to be no simple way to describe this chemical behavior, any attempt may result in an oversimplification of the process. A possible explanation for these phenomena is that the three tautomeric forms of each isomer act differently, yielding six molecular structures in total that must be considered [Cornell 1998].

Other characteristics of MeBT that are of interest include molecular weight of 133.16 and MeBT solubility, which is summarized in Table 2-3.

TABLE 2-3 – Solubility of MeBT

IN: WATER	**95% ETHANOL**	**METHANOL**	**ACETONE**
< 0.1 mg/mL @ 18 C	≥ 100 mg/mL @ 21° C	≥ 100 mg/mL @ 21° C	≥ 100 mg/mL @ 21° C

[NTP Chemical Repository (Radian Corporation) for Tolyltriazole]

There is no published information to suggest the mechanisms of MeBT toxicity to microorganisms. The Cornell (1998) on-going study suggests that MeBT may be an uncoupling agent for the electron transport chains. It is found that MeBT meets Lenhinger's definition of an uncoupling agent: a weak acid possessing hydrophobic properties. Uncouplers are known to disrupt the chemiosmotic potential of a cell or microbe by shuttling protons across the cell membrane against the natural flow set up by the cell. However, MeBT does not meet all the criteria and therefore cannot be considered in this category, but does necessitate the further need of study in this area [Cornell, *et al.*].

The toxicity of ADF is increased with the addition of MeBT. Cancilla [Cornell, 1998] identified triazole compounds as the fraction of ADF presenting the greatest toxicity as measured by the Microtox® assay. These Microtox® tests show three results: 1) the MeBT inhibited biodegradation of PG more than other additives, 2) the MeBT was significantly more toxic to microorganisms than other component (in the order of lowest to greatest toxicity 4-MeBT < MeBT < 5-MeBT), and 3) other additives were significantly more toxic to *C. dubia* and *P. promelas* than the MeBT, [Pillard, 312]. Chronic toxicity data for MeBT is unavailable. Limited acute toxicity data [PMC, 1996] indicates MeBT itself is moderately toxic to *Lepomis* *macrochirus* (31 mg/L 96 hr. LC_{50}.) and *Daphnia magna* (74 mg/L 48 hr. LC_{50}) [MSDS; Cornell, 1998].

The only information available on the potential environmental fate of MeBT is from US Patent 5,503,775 (1996) as referenced by Cornell [1998], which claims that, under aerobic conditions, 5-MeBT is biodegradable while 4-MeBT is recalcitrant.

Additional toxicity results of MeBT are presented as a LD_{50} range from 675 mg/kg to 1600 mg/kg with dose given orally in mice. The MeBT component significantly decreased cell growth rates and yields and inhibited the biodegradation of propylene glycol to a greater extent than the other components. When heated to decomposition this chemical emits toxic fumes. It is also an eye and lung irritant [PMC Specialties Group].

2.4 Biodegradation Concerns

In the past, the main concern regulators had with ADF discharge to the stormwater system had been the large BOD that accompanied the mixture. New research has bought to light a different problem, the biodegradation process of ADF components. Biodegradation is the most important natural or engineered treatment method for reducing the oxygen demand exerted by these discharges [Cornell, 1998]. Recent studies have set up soils enriched with microorganisms in aerobic liquid CMBRs; they propose three hypothetical conclusions that describe the relationship of PG and MeBT biodegradation:

1) Propylene Glycol biodegradation rates decrease with increased MeBT concentration
2) Cell growth rates decrease with increased MeBT concentration
3) Cell yield decreases with increased MeBT concentration [Cornell, 1998]

The biodegradation process of PG can yield intermediate products such as aldehydes and organic acids (lactic, pyruvic, or acetic acids) [MSDS - 1,2 Propanidiol; RACB]. However, these compounds, if formed, are in small quantities and are rapidly reduced to carbon dioxide and water or additional organic content. Many studies show that PG is readily degradable in soil or aquatic environments.

Noticeable degradation of MeBT was not observed in these studies or after any experiment, nor did MeBT degrade during the twelve months of feeding the enrichment culture full ADF formulations [Cornell, 1997].

This thesis effort attempts to provide one piece of the MeBT puzzle; additional information about the transport of MeBT is required before any conclusions can be made about MeBT being naturally degraded [NRDC; Cornell, 1998]. All that is available now is unpublished data, and a US Patent that proposes preferential degradation of 5-MeBT over 4-MeBT [US Patent 5,503,775]. Quantifying the effects of MeBT sorption is a necessary step before effective treatment can be considered, or before the environmental impact posed by the release of MeBT into the environment can be assessed.

2.5 Sorption

Different factors effect the fate and transport of a contaminant through water. One of these factors is the adherence of contaminant to soil, organic matter, and other materials. The sorption process includes several different classifications including absorption, adsorption, chemisorption, and ion exchange. In most cases all of these processes together are referred to as sorption. The association of a particular chemical, the sorbate, with any particular solid, the sorbent, is known as absorption (the prefix of absorption, *ab*, comes from Latin, "away from" and the suffix *sorbere* meaning, "to suck") [Fetter, 131]. The underlying principle behind this attraction results from some form of bonding between the contaminant and adsorption receptor sites on the solid. The amount of sorption that occurs in groundwater is dependent on particular characteristics of the sorbate and sorbent. It is known that the more hydrophobic the compound, the larger the fraction sorbed in soil [Maagd *et al.*, 1899]. The amount of sorption that takes place on organic matter also follows various isotherms or has varied kinetic rates.

Because of the porous nature of the soil particles, the sorbates can physically penetrate the particle and become part of the volume of the nonaqueous medium [Schwarzenbach *et al.*, 32]. Absorption is orientated in the 3-dimensional matrix. The capacity of a solid to remove a sorbate from solution is a function of the concentration of the sorbate in water (solute).

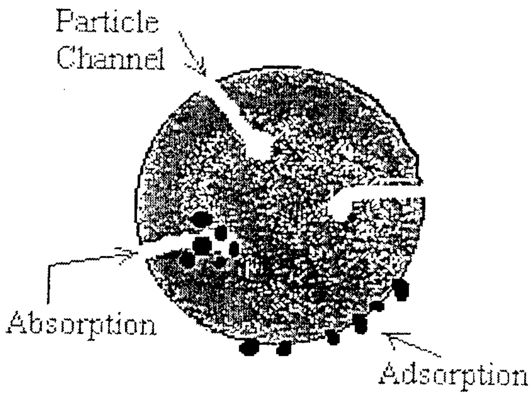


FIGURE 2-1. Soil Sorption Illustration [Ferrante, 2].

Sorption reactions generally occur over a short period of time, however if the adsorbed contaminant begins to be incorporated into the structure of the sorbent, a slower reaction, known as absorption, begins to take place. First-order rate models have been frequently used to describe sorption rate processes in transport experiments, but usually with the understanding that the first-order coefficients are approximations for physical diffusion into often undefined regions of solute immobilization [Ball and Roberts, 1238]. The sorption coefficient (K_d) is the ratio between the concentration of the compound and that of the soil [Maagd, 1900]. Alternatively, the difference between adsorption and absorption is that adsorption is the attraction between the outer surface of a solid particle and a contaminant, whereas absorption is the uptake of the contaminant into the physical structure of the solid.

Figure 2-1 shows the primary differences between intraparticle absorption versus surface adsorption. The main difference being that some contaminant particles are attracted to the outer surface of the soil particle, while others have been incorporated into the particle's structure [Ferrante and Gallagher].

2.5.1 Potential Hazards

The process of sorption can hinder the remediation of a groundwater aquifer system. Sorption tends to cause contaminants to move more slowly than the groundwater, therefore the effects must be taken into consideration when calculating how far the contaminant will travel in a given time period. There is also the tendency to underestimate the total amount of contaminant in the system. Since the contaminant may not show up on a pump test, the assumption would be that there is no more contaminant; however, there could be upwards of 35% in the system as sorbate [Yaniga]. This can drive up remediation costs and with prolonged exposure, increase risk factors.

Several factors are key to the contribution of the contaminant properties to the sorption process. The first, the solubility of a compound is inversely proportional to the amount of sorption that the solid phase can support [Yaniga]. The second factor is polarity. A polar chemical tends to dissolve easier in water than a nonpolar chemical. Therefore a polar contaminant will absorb less to a soil particle than a nonpolar one. Another factor is the viscosity of the solute. The more viscous the solute the less that it will tend to sorb to the soil particle and may have an affinity to dissolve in water [Yaniga]. The last key factor is the octanol:water partitioning coefficient. The octanol:water partitioning coefficient (K_{ow}) is a measure of the hydrophobicity or lack of affinity for water of an organic compound. The more hydrophobic a compound is, the less soluble in water it will be and the more likely it will be adsorbed to soil particles.

Several key soil factors affect the sorption rate, including the texture of the soil particles. Soil with high clay and high organic matter will tend to exhibit higher sorption than sandy, low organic soils. Clay soils tends to sorb more than sand due to small particle size, high surface area, and high surface charge. Organic matter provides sorption sites for hydrophobic compounds. The higher f_{oc} soils tend to have higher sorption capacities. The pH of the fluid can also have an affect. For example, organic acids adsorb best under acidic conditions.

Absorption isotherms provide a rational way of accounting for incomplete recoveries of sorbates from sorbent. These isotherms are plotted on a graph and are representations of the sorbed concentration (S) or mass of contaminant sorbed per unit dry mass of soil (K_d) or organic matter (K_{om}) versus the final concentration (C_f) of the contaminant. In order to use isotherms to estimate the mass adsorbed, an equilibrium must be reached between the sorbent and the sorbate and the isotherm must be considered reversible, but can be used when sorption is rate-limiting and hysteric also [Ball and Roberts, 1240].

There are numerous types of isotherms; three presented here are: Langmuir isotherms, Freundlich isotherms, and Linear isotherms. The Langmuir Isotherm contains two assumptions that usually make its use difficult in real life or a heterogeneous soil case. The assumptions are that the energy of adsorption is constant and the number of binding sites is finite. The equation for the Langmuir isotherm is:

$$S = \alpha\beta C/(1 + \alpha C)$$

where α = an absorption constant related to the binding energy (L/mg)

and β = the maximum amount of solute that can be absorbed by the solid (mg/kg) [Fetter, 133]. The Langmuir isotherm is shown in Figure 2-2A. The curvature at the end of the graph marks a point at which the receptor sites on the soil particle are full and there is no more room for additional adsorption [Schwarzenbach *et al.*, 33; Ferrante and Gallagher].

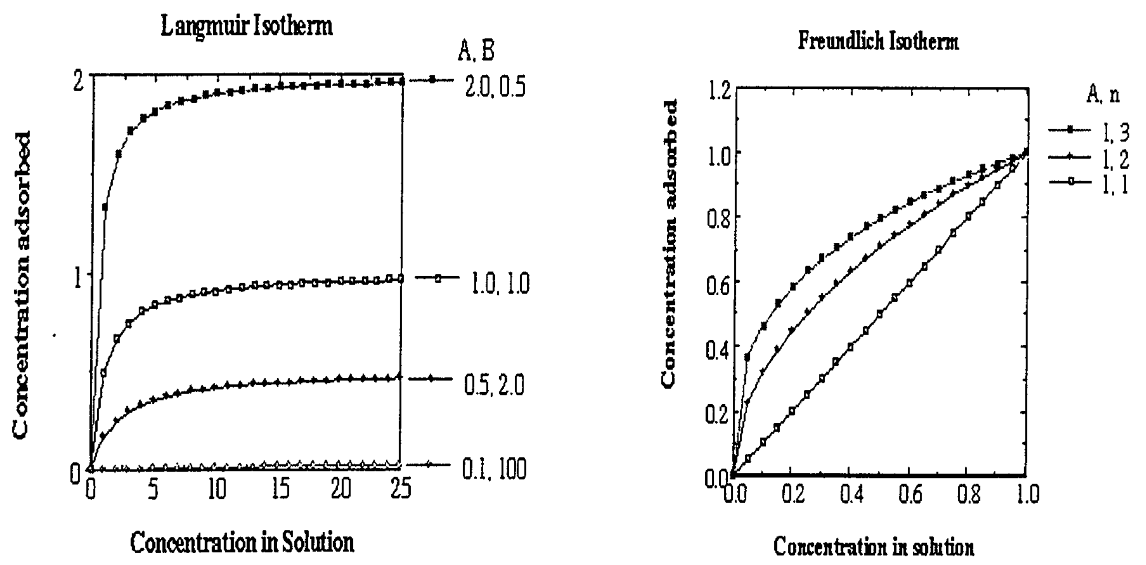


FIGURE 2-2 A & B

The Freundlich Isotherm (Figure 2-2B) is an equilibrium isotherm that is used most often in practical examples. The Freundlich equation normally results in a curved graph unless the logs of both S and C are taken. By taking the log of these terms, a straight line develops making easier to obtain the slope and intercept of the line. The equation of the Freundlich isotherm is similar to the linear isotherm, but a new exponential term (1/n) is used:

$$S = (K)C^{(1/n)}$$

where K and n are constants [Ferrante and Gallagher; Fetter, 132; Schwarzenbach *et al.*, 32].

If there is a direct, linear relationship between the amount of a solute sorbed onto a solid, C*, and the concentration of the solute, C, the absorption isotherm of C as a function of C* will plot as a straight line on a graph. The equation for the Linear isotherm is:

$$C^* = (K_d)C \rightarrow \text{where } n=1$$

The linear isotherm has only one fitting parameter (K_d) and if applicable the isotherm (by definition) must pass through zero and the regression through the origin is appropriate. The best estimate of the linear slope (K_d) is simply the average K_d of the samples [Ball and Roberts, 1240].

There are two limitation to this model; one, is that it does not limit the amount of solute that can be absorbed onto the solid and, two, with only a few points a curvilinear plot may be mistaken for a linear relationship [Fetter, 132].

2.6 Additional Research

There are several studies on halogenated organic chemicals, benzene, and methylbenzene in aquifer material, but very few have concentrated their efforts on 4(5) methyl-benzotriazole (tolyltriazole). The following section summarizes some of the research performed in areas close to MeBT.

Work done, by Duke and Stanford Universities, on long term sorption of halogenated organic chemicals by aquifer material explains the sorption effects on the Canadian Forces Base aquifer material in Borden, ON [Ball and Roberts, 1237; Brusseau, 1989].

The report includes details on the sorption isotherms for tetrachloroethene (PCE) and 1,2,4,5-tetrachlorobenzene (TeCB). It notes that the isotherms deviated from linearity when a 4 to 5 order of magnitude range in aqueous concentration was considered. However, in the dilute range (<50 μg/L), the deviation from linearity was inconsequential. Sorption of TeCB was approximately 40 times that of PCE due to the difference in the properties of the compounds [Ball and Roberts, 1247].

Ball and Roberts (1991) makes note of several things to watch out for or concentrate efforts on. One of these points is in the time for equilibrium. The time it takes halogenated organic compound to reach full sorption equilibrium can be long. In order to help shorten that time, this study compared the difference between pulverized and unpulverized soil samples from the Borden site. The increased surface area of the pulverized soil allows the system to reach equilibrium much faster than unpulverized samples, by an approximate 20:1 ratio. Pulverized samples yielded approximately 94.7% +/-2.8% recovery of TeCB. Results from this study show a good linear fit of data at low concentration of both PCE and TeCB (<100 μg/L); yet, significant deviation from linear occurs at approximately 1000 μg/L, which is less than 1% of aqueous solubility [Ball and Roberts, 1241]. Further tests with the addition of reagent-grade $CaCO_3$ to dissolve the inorganic carbonate show that there was no diminishing of the sorption capacity during this acid wash. This demonstrates that this compound does not sorb to inorganic carbonates, which can be significant in certain soil types.

Conclusions by Ball and Roberts pertain to MeBT in that they contrast the commonly held belief that the sorption capacity is inversely related to the particle size. Ball and Roberts states that to avoid bias in experiments of this duration, it is of paramount importance to avoid losses through volatilization or transformation. This study details background and methodology used to achieve credible results.

Weber and Huang (1993) describe a distribution reactivity model for sorption by soil and sediment using the interaction of a sorbate and sorbent. They investigated the time dependence of solute phase distribution relationships (PDRs) in completely mixed batch reactors. The experiments were conducted using a range of concentrations to obtain a time series of nonequilibrium PDRs for each sorbent-sorbate system. Freundlich isotherms were used to characterize the increasingly nonlinear results. An explicit account of the methodology used for the completely mixed batch reactor (CMBR), sorbent-sorbate system, and preparation is included in this report. Each step agrees with the basic known facts of this procedure.

Weber and Huang (1993) define the changes in parameters in three stages: (1) an initiation stage, (2) a logarithmic stage, and (3) an apparent equilibrium stage. It summarizes the hypothesis that there is a boundary layer around the particle that has first-order rates associated with it [Weber and Huang, 884].

The third of the related articles is on adsorption isotherms of benzene and methylbenzene. This is closest to parallel data that I have encountered. Although the methylbenzene study used vapors on activated carbon instead of soil, it is an appropriate reference [Yun, 1997].

Since activated carbon has high surface area, high surface charge, and organic consistency it makes a good material to use in the lab for sorption studies. The report contained useful information that directly relates to MeBT. A point of interest taken from the report was that the adsorption isotherms for benzene and methylbenzene were accomplished at 30°C and 70°C, slightly higher than what was used in this study. The adsorption capacity is higher for benzene than it is for methylbenzene. However, if you look at pressure, with low pressure the amount sorbed is higher for methylbenzene than for benzene. This implies that the affinity of sorption is higher for methylbenzene [Yun, 895].

Following this line of thought, benzene can be a suitable substitute for MeBT since there are no in-depth studies with MeBT at the present time. Additionally, since the log K_{ow} values of MeBT and benzene are similar (2.17 vs. 2.13) estimations for K_{oc} will be accomplished with equations derived from benzene pesticides [Fetter, 134; Karickhoff, 1984]. This will be the basis for the solute to soil mass mixture in the CMBR.

III. Methodology

3.1 Overview

This chapter illustrates the reasoning and procedures used to measure the sorption coefficient of MeBT in various soil types. A high performance liquid chromatograph (HPLC) was used to analyze the MeBT extracted from soil. Mixtures of MeBT and water were added to soils, in appropriate proportions, to simulate the potential exposure in the environment. Extraction fluid, containing water and methanol, was added to the completely mixed batch reactors to recover the MeBT. All samples were prepared under the same conditions for consistency.

3.2 Preliminary Experiments

Two preliminary tests were performed to obtain a better understanding of the experimental material. Pan evaporation and nutrient matrix experiments gave insight into the characteristics of PG and a PG/MeBT mixture, respectively. The pan evaporation experiment demonstrated the hydroscopic nature of PG, while the nutrient matrix experiment demonstrated the relationship between PG and MeBT with respect to soil microorganism growth.

3.2.1 Pan Evaporation

The pan evaporation test demonstrated the hydrophilic properties of PG. The test began by adding a small amount of PG to a pre-weighed aluminum weigh boat, 11.51 grams. The PG was exposed to the atmosphere at room temperature, approximately 19° C (67° F), to observe the evaporation rate. The viscosity of PG suggested that the liquid would take several days to evaporate. Results of the test showed differently. The PG solution gained and lost mass with the changes in atmospheric conditions. If the humidity rose, the masses in the weigh boat increased and vice versa. The liquid took some time to acclimate to the new humidity, which created a day or so lag in reaction to the change. No measurable evaporation occurred during the length of the experiment. Results of the pan evaporation are contained in Appendix C.

3.2.2 Toxicity Matrix

The second trial performed was microbial growth in a nutrient matrix. This test was to show how different concentrations of the two components in ADF under investigation, PG and MeBT, affected the growth of microbes in separate microcosms. A matrix was established with a 5-step range of each chemical, from 0 – 100 mg/L, in deionized water. Microorganisms were extracted from soil obtained from near the lab (See 3.3.2 Method of Soil Collection for details). An inorganic nutrient solution (BOD buffer) was added to the microorganisms extracted from the soil to ensure a plentiful inorganic food supply for the duration of the test. Separate 10-mL screw-top test tubes were used for each concentration intersection in the matrix. Equal volumes of PG concentration solution (4-mL) and MeBT concentration solution (4-mL) were added to the test tube. Then the same amounts (2-mL) of nutrient solute (microbes, nutrient, and water) were added to the test tubes to bring the level up to 10-mL. This mixture was then shaken to completely mix the contents. Growth of the microbes was measured with a photospectrometer. It measured the Total Suspended Solid (TSS) amount by monitoring the amount of light passed through the test tube at a wavelength of 810 nm. The more TSS or growth in the tube, the higher the count on the meter. Data from this experiment can be found in Appendix C.

3.3 Soil

Following the work of Cornell, *et al.* (1998), Johnson (1997), and Halterman-O'Malley (1997) three soil types in four configurations were used in this study. These three soils represent a range of soil types that could receive ADF applications. Soil samples were obtained from Denver International Airport (DIA), Westover Air Reserve Base (Westover), and Wright-Patterson AFB (WPAFB).

3.3.1 Purpose

Soil variations are important to this study in that a comparison matrix is constructed with the soils of interest and their mean K_d values. Four soil variations allow comparison of soil types, organic content, the exposed vs. unexposed soil difference, and the reaction to PG addition. This information allows a more complete assessment of the sorption characteristics of MeBT. This research will add to the body of knowledge for future remediation applications for ADF.

3.3.2 Method of Collection

A University of Colorado/AFIT doctoral student, Major Jeff Cornell and associates collected the DIA and Westover soils. The DIA sample was obtained from an uncontaminated site north of the C+ dam at Denver International. The soil was taken from below the root zone at a depth of approximately six inches. The soils have been analyzed in the University of Colorado's soils lab for content and consistency. A summary of the characteristics of the analysis can be found in Appendix A. The area of interest, near Bldg. 470, is one of the highest elevations on WPAFB, in a grassy open area. The sample was gathered by clearing the top 15-20 centimeters of material and collecting the next 20-30 centimeters of soil in the 0.5 square meter area. A clean metal shovel was used to free the soil and a plastic pool filter with 6-mm openings was used to sieve out the larger organic material, rocks, and general debris. Handling and processing of the samples was kept as consistent as possible to remove any process variability. Characteristics such as surface area of the collection site, depth of the site, and size distribution were not taken into consideration between sample sites.

3.3.3 Soil Types

The DIA sample is a high clay soil with medium range organic material ($\cong .0137f_{om}$). The Westover sample is a sandy soil with very little organic material (< LOD). These two soils have not been exposed to ADF in the past and have not become acclimated to it. The third soil is from WPAFB; it is high clay with a medium amount of organic material ($\cong .0287f_{om}$). The two variations with the WPAFB soil come from the fact that the original soil is an undisturbed sample with no exposure to ADF. Refer to Table 3-1 below, for soil characteristics.

Soil	Classification	Organic Content	pH*	Exposure to ADF
DIA, CO	Clay: MC=13.8	1.37±0.37%	7.5	NO
Westover ARB, MA	Sandy: MC=6.3	Below LOD assumed = 0.09%	8.0	NO
WPAFB, OH	Sandy Loam: MC=10.5%	2.87±0.15%	7.8	NO/YES**

TABLE 3-1. Soil Characteristics
MC is moisture content and is given in percent
*NOTE: pH measurements were made using a Hach pH meter
**NOTE: The soil was part of a parallel study

The WPAFB soil was also used in a parallel experiment of respirometry with exposure to varied concentrations of PG and MeBT. The soil used in this parallel experiment was evaluated and used as a soil variation for comparison in my study.

3.3.4 Analyzed Characteristics

Analyses were performed on each of the soil samples. It is important to understand the differences between samples for comparative reasons. A summary of the soil characteristics provided by the laboratory employed has been supplied in Appendix A. In cooperation with the University of Colorado at Boulder, the attributes of interest have been narrowed down to the aforementioned characteristics. Differences in these characteristics can be identified in the responses of the 4 and 5 isomers of MeBT.

3.4 Experimental Preparation

The following sections are detailed descriptions as to how each experiment was prepared and the reasoning behind the preparation. All samples and subsets were prepared as at least triplicates for statistical consistency. It was also realized, during preliminary experimentation, that the solubility of MeBT in water was enhanced by the presence of PG. This detail was utilized while creating one solution for the study.

3.4.1 Soil Preparation

Review of related literature (Ball and Roberts, 1991) shows that a pulverized soil samples provide the maximum amount of surface area for sorption to take place. However, aside from initial sieving through a 6mm screen, the samples did not receive additional treatment. The equilibration time for the soils used in this study were sufficient for the reaction to occur. It was also suggested that all samples be filtered prior to HPLC injection, to help avoid clogging of the column. As shown in Appendix B, HPLC results for the filtered samples did not differ significantly from the unfiltered samples. Therefore, unfiltered, centrifuged samples were used throughout the study.

It was important to use a consistent amount of soil and solution for each sample. This proportion was such that approximately half of the solvent is sorbed to the soil. If too much or too little is sorbed then accuracy will deteriorate [Heyse, 1998].

The amount of soil used was determined with the formula $M_s = V/K_d$, where M_s is the mass of the soil, V is the volume of solution and K_d is the sorption coefficient. I have estimated K_d for each soil type from the K_{ow} provided by the manufacturer on the MSDS and the relationship of K_d to K_{oc} via Karickhoff (see Section 2.6) [Fetter, 133; Karickhoff, 1984; Lyman and Reehl, 321]. The relationship is assumed to be similar to that of benzene for three reasons. One, it is the best available data on the chemical MeBT at the time of the study. Two, this benzene group studied by Karickhoff is the closest available equation. I chose the equation based on the log K_{ow} of benzene being very close to that of MeBT (2.17 vs. 2.13 respectively). Lastly, the range of K_{oc} (input parameter) values covered by this equation are similar. Thus, the equation $\log K_{oc} = \log K_{ow} + b$ was used. Generally $b \approx 0.2 - 0.35$ [Karickhoff, e.1979-1982]. However, in this study the equation $\log K_{oc} = 0.52 \log K_{ow} + 0.62$ was used. The conversion to K_d was accomplished by the equation $K_d = f_{oc} * K_{oc}$, where f_{oc} is the percent of organic material in the soil [Lyman and Reehl, 321]. The f_{oc} number is calculated from a f_{om} number (fraction of organic material) provide by chemical analysis $f_{oc} = 0.58*f_{om}$ [Schwarzenbach, 33]. In general, more soil was used when the organic content of the sample was lower. Specific calculations for each soil type can be found in Appendix B.

Each 40-mL screw-capped, amber glass container was rinsed with methanol and then rinsed thoroughly with distilled water. Each soil was air dried in an aluminum pan for approximately seven days. These soils were then placed in drying pans and heated to 103° for approximately 1.0 hour [Standard Methods, 2-54]. The water content for each soil type was determine by air-dried weight minus oven dried weight divided by oven dried weight. All work was accomplished using the soil's air-dried weight; however, the reports are reported on dry weight basis using the information provided in Appendix B. Therefore, in each 40-mL vial, approximately 10 grams of soil was added with a clean laboratory spoon, weighed out on an electronic scale. The appropriate amount of solution was added (see Section 3.4.2 Solute Preparation and Appendix B). Summaries of soil type and vial weights are included in Appendices E-H.

3.4.2 Solute Preparation

The range of solute concentrations for the soil study was established by the corresponding percentage of MeBT in ADF. The maximum MeBT concentration expected in the environment would be 0.5% – 0.6%. The experimental range was set at 0.01% - 0.1%, or 100ppm to 1000ppm. One producer of ADF, Octagon/Arco adds 0.05% – 0.06% MeBT to their mixture. This percentage translates into 500 mg MeBT/L deionized water obtained from dissolving laboratory grade COBRATEC TT-100™ in deionized water. Based upon that concentration, the concentration range of interest in this study was established. A calibration curve consisting of 10 mg/L, 100 mg/L, and 1000 mg/L (two orders of magnitude) standards were used. The limits of detection (LOD), upper and lower, of the HPLC were shown to be outside the concentration range used. Therefore, this range is effective. MeBT stock solution was added to the soil sample vials in a proportion to create slurry within the vial. Each soil had a different amount of solution added based upon the calculation explained in Section 3.4.1. The individual soil type solution calculations can be found in Appendix B.

3.4.3 Conditional Control for Analysis

All materials were stored under the same conditions unless otherwise indicated. The room temperature was regulated by air-conditioning, at approximately 19° C (67°F). The sample pH was not adjusted, but was monitored with a Hach unit and stayed below 8.0. The subset samples, once prepared and treated with the MeBT solute, were placed on a rotator table for complete mixing. The samples were rotated at 20 – 25 rpm until equilibrium was reached (*e.g.* statistically, no more MeBT was sorbed to the soil). This equilibrium was established experimentally by sacrificing single vials at pre-determined time intervals. Results of equilibrium tests are in Section 4.3 and Appendix B.

Concentrations of MeBT in the solute extract were compared to the known original concentration. To account for any fraction of MeBT that might have sorbed onto sorbent without being transformed, the vial was centrifuged and the water in the CMBR was sampled along with successive methanol washes of the soil. Subsequent methanol extraction and analysis should reveal the amount of MeBT lost (if any) from the bulk fluid. An isotherm was created from the results and plotted on the graph in Section 4.3 and in Appendix B.

3.4.4 Statistical Design

Since analytical chemistry is the science of making quantitative measurements, it is important that raw data be manipulated and reported correctly to give an accurate estimate of the certainty of the results [Tissue, 1996]. Three statistical evaluations were performed on the sorption coefficient results. Each soil was considered independent of the other soils tested. A balanced design, one where each treatment has the same number of trials compared with all other treatments, was achieved for this study.

The first evaluation was performed to show interaction between the soil and concentration results. A four by four matrix was created to include each of these variables. If significant interaction is identified ($p < 0.05$), the variables involved depend on each other [Ott, 906; Devore, 435]. Results of this evaluation are discussed in Section 4.3 and shown graphically in Appendix J.

Another evaluation consisted of an Analysis of Variance (Two-way ANOVA) and Pairwise Tukey analysis to look for homogeneic grouping among each independent variable. This evaluation would indicate which, if any, of the soils or concentrations acted alike in terms of their sorption coefficients. Results of these evaluations are discussed in Section 4.3 and shown in Appendix J.

Lastly, a t-test or a pairwise comparison of means was performed by Statistix® to compare high organic content to low organic content soil, clayey soil to sandy soil, ADF on an unacclimated soil, and a soil dosed with an MeBT/PG mixture to one dosed with only MeBT. Results are discussed in throughout Chapter 4 and the tables are presented in Appendix J that also summarizes the findings. The two-sample t-test was administered with a 0.05 level of significance and populations were assumed to be normal with equal variances. The null and alternate hypotheses for each of the tests were:

H_o: $\mu_a - \mu_b = 0$, the means are equal

H_a: $\mu_a - \mu_b \neq 0$, the means are not equal

The mean and standard deviation for each of the variables was determined in Statistix®. A pooled estimator, s_p^2, was calculated, which is the estimate of the common population variance.

$$s_p^2 = \frac{(n-1)*\text{Std Dev}_a^2 + (m-1)*\text{Std Dev}_b^2}{n+m-2}$$

The symbols n and m represent the sample sizes of the treatments (a and b) and Std Dev. stands for the standard deviation of the respective treatments a and b. The standard error was determined by taking the square root of the pooled estimator to yield s_p. The t statistic was then calculated from the following equation:

$$t = \frac{\overline{X}_a - \overline{X}_b}{s_p*(1/n + 1/m)}$$

This t value is compared to the t-critical value with the relationship $-t_{\alpha/2,n+m-2} \geq t$ where the –t-critical value is referenced from a pre-determined table [Ott, 260; Devour, 358 and 707]. Results were simply to accept or reject the null hypothesis depending upon the relationship of the t value to the t critical values. If the t value is $T \leq -t$ critical or $T \geq t$ critical, then we reject the null in favor of the alternate hypothesis. If T ≥ -t critical or T ≤ t critical, then we accept the null hypothesis. The full T-test is supplied in Appendix J for each set of variables.

3.5 High Performance Liquid Chromatography

Liquid chromatography (LC) relies on differences in partitioning behavior between a viscous mobile phase and a stationary phase to separate components in a solution. High-pressure pumps are used to increase efficiency of the separation. A typical schematic representation follows:

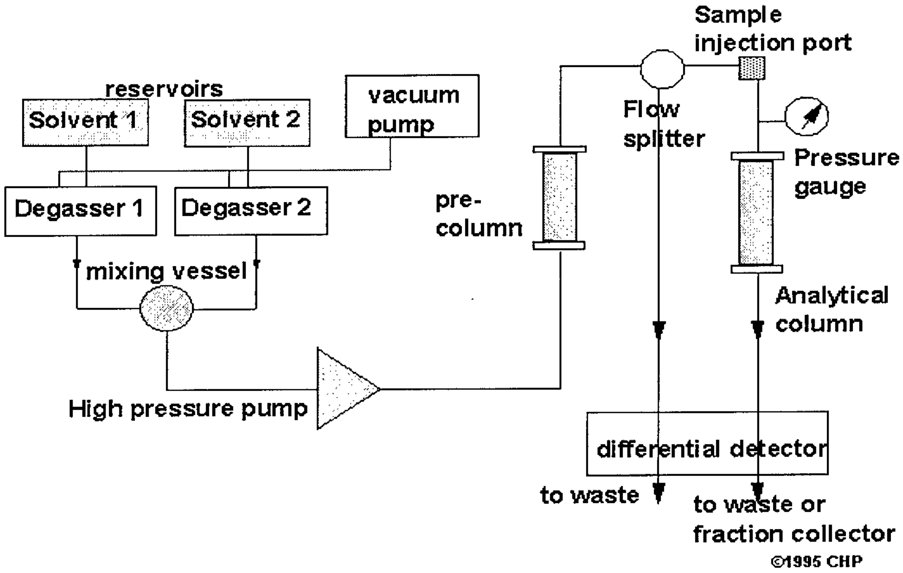


FIGURE 3-1. HPLC Schematic [Tissue].

3.5.1 Theory

Ions or molecules that are dissolved in a solvent are separated in the process. Simple liquid chromatographs consist of a column with fitted ends that holds a stationary phase. Most are made of plastic or glass that range from a few centimeters to several meters in length. HPLC columns are stainless steel tubes, typically 30-50 cm in length and 5-6 mm in diameter.

FIGURE 3-2. HPLC Column [Tissue].

The stationary phase is bonded to inert particles of 3-10 μm diameter. A slug of the compound is injected into the column and analytes are separated as they travel through the columns due to the difference in their partitioning between the mobile or liquid phase and the stationary phase of the column. Reverse-phase partition chromatography uses a relative nonpolar stationary phase and a polar mobile phase, such as methanol or methanol/water mixture. This is the most common form due to the wide range of analytes that can be dissolved in the mobile phase. In adsorption chromatography the stationary particles are made of silica, alumina or organic material. These are used in separating isomers, which can have different sorption characteristics due to steric effects in the molecule. The retention of an analyte by a column is described by the capacity factor, k', where: $k' = t_{r2} - t_{r1}/t_m$

where t_r is the time for the analyte to pass through the column and t_m is the time for mobile phase to pass through the column. In Figure 3-4, a typical separation of analytes is represented.

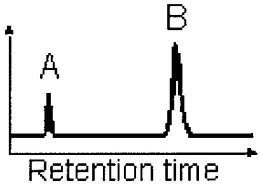


Figure 3-3. Retention Time Graph.

Usually, a relatively narrow sample band or "plug" is injected (10 - 25 μl injection volume) into the column. During the run, the sample will be spread due to the noneven flows around and inside the porous stationary particles, slow adsorption kinetics, longitudinal diffusion, and other factors. These processes together produce so called band broadening of the chromatographic zone. In general, the longer the component is retained on the column, the more broad its zone, or its peak on the chromatogram. Separation performance depends on both component retention and band broadening. Band broadening is a kinetic parameter that is dependent on the adsorbent particle size, porosity, pore size, column size, shape, and packing performance. An exact knowledge of the adsorbent surface area is very important, since retention is proportional to the surface area of the adsorbent.

3.5.2 Purpose

MeBT and sample solution were separated using isomeric-elution high-pressure liquid chromatography on a two successive ZORBAX RX-C8 columns and analyzed with an UV absorbence detector at $\lambda = 280 \mp 2$ nm. MeBT isomers and degradation byproducts of MeBT were separated by gradient elution HPLC on the ZORBAX RX-C8 column and detected similarly.

3.5.3 Procedure

MeBT was analyzed via direct aqueous injection into a Hewlett Packard 2170 high performance liquid chromatograph fitted with an ultra violet array detector. MeBT separation was achieved isocratically using two ZORBAX RX-C8 reverse phase, 250 x 4.6 mm columns at 35°C and a mobile phase comprised of two solvents: (1) 0.5-mL phosphoric acid (H_3PO_4) and 0.65-g potassium dihydrogen phosphate (KH_2PO_4) combined in water (1 L); along with (2) HPLC grade acetonitrile (ACN) (430-mL) and methanol. The solvent ratio for the HPLC pre-mobile phase began at 90:10 water:methanol and moved to 30:70 water:methanol for 0.5 hours prior to analysis. Once analysis began the ratio of eluent to methanol started at 100:0 eluent:methanol and gradually moved to 50:50 eluent:methanol at the 10-minute mark. At this point the ratio was diminished to 10:90 to flush any organic material that may have accumulated. PMC Specialties Group, Cincinnati, OH, and advice from the University of Colorado have modified this technique from an established methodology [Gruden]. The peaks for each isomer of MeBT were shown to come through at approximately 7-8 minutes with a 0.25 to 0.3-minute delay between the isomers as measured with HP Chem-Station® for LC software. All of the samples were injected at a volume of 10 μL with a HP injection autosampler [HP ChemStation®].

3.6.4 Calibration Curve

Calibration standards were prepared using a background solution of deionized water in a prepared volumetric flask (0 mg/L) and solutions of 1mg/L, 5 mg/L, 10 mg/L, 50 mg/L, 100 mg/L, 500 mg/L, and 1000 mg/L of COBRATEC TT-100™ (Tolyltriazole) in deionized water. The 1000 mg/L solution was mixed in a larger quantity (approximately 2 liters) to be diluted

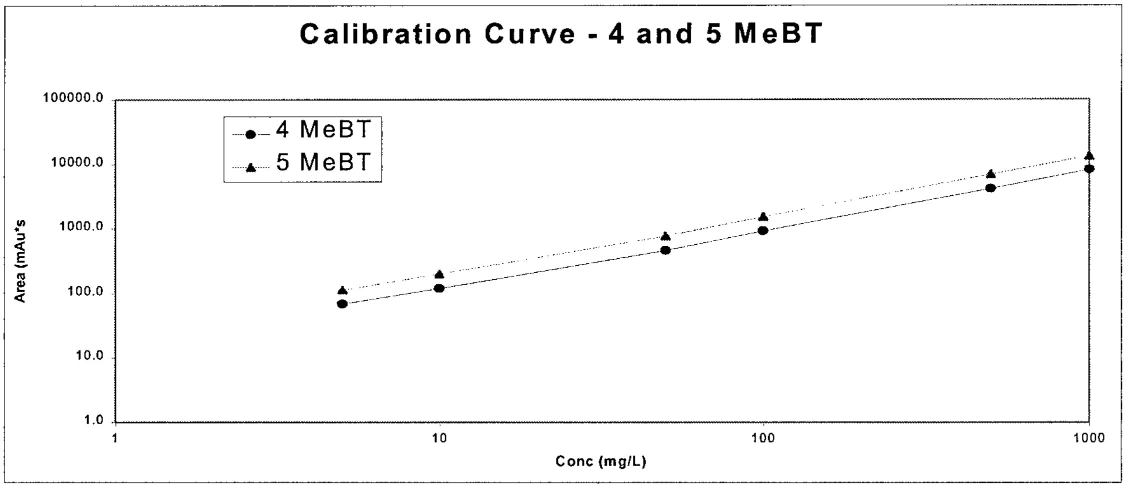


Figure 3-4. Isomer Calibration Curve.

for use in the subsequent calibration solutions for the study. Past experiments with the HPLC unit have shown the upper limit of detection (LOD) to be approximately 1200-1500 mg/L for this compound. The lower LOD was established with my mixture to be approximately 5 mg/L. The calibration curve shown in Figure 3-4 passes through the origin and is linear. Results from the calibration curve can be found in Appendix D. Note that all concentration values in this study have come as a direct result of interpolation from the calibration curve. Concentrations are reported relative to the area under the HPLC trace (example found on Figure 3-7). For a given applied concentration the resulting concentrations for each isomer will not be additive to the initial concentration analyzed. For this study, the 4-MeBT isomer is relatively stable and is not assumed to degrade; therefore, the 4 isomer can be used as a normalizing factor for comparison of the two isomers.

3.6 Data Collection

In this study, all analyses were initiated on prepared soils under controlled condition. Laboratory work must be reproducible and limit the statistical error associated with the results. By controlling the variables, like temperature, and by using replicates, the data presented is statistically sound.

The diagram (Figure 3-6) shows the sample preparation process. Equilibration was enhanced through constant mixing on a rotation table. Before sampling for analysis in the HPLC, each vial was centrifuged for approximately 20 minutes. Upon completion, the solution at the top of the vial was sampled without disturbing the soil beneath (see vial "D" in the diagram).

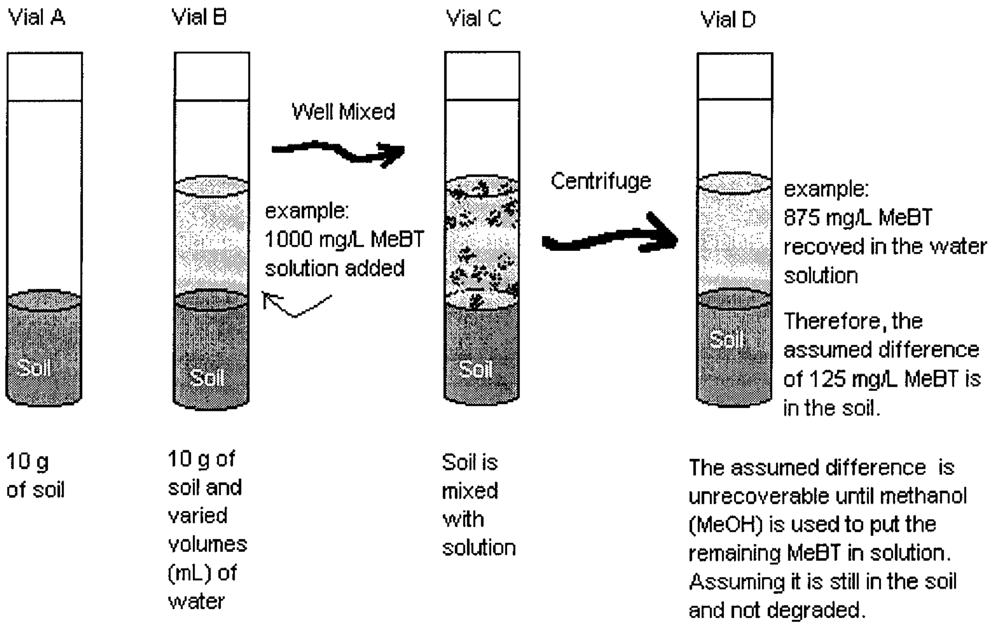


Figure 3-5. Methodology Format.

3.6.1 HPLC

The data generated from the HPLC comes in several forms; I have chosen to use the area under a curve for my study because it allows easy correlation between the concentration and HPLC results. This working curve or plot of the analytical signal is a function of the analyte amount concentrated due to the interactions on the adsorbent surface on the equilibrium concentration of analyte in the solute. Using absolute calibration, this concentration was then back calculated, by integration, from the calibration curve generated earlier. Typical HPLC results are produced in the form showed in Figure 3-6.

HP ChemStation software integrates the area under the peak or curve to get the results shown in Appendices E-G. Note that in Figure 3-6, the separation of the two isomer peaks (4-MeBT at

7.19 and 5-MeBT at 7.38 minutes, respectively) and the peak of a possible derivative of MeBT at 7.92 minutes in this diagram.

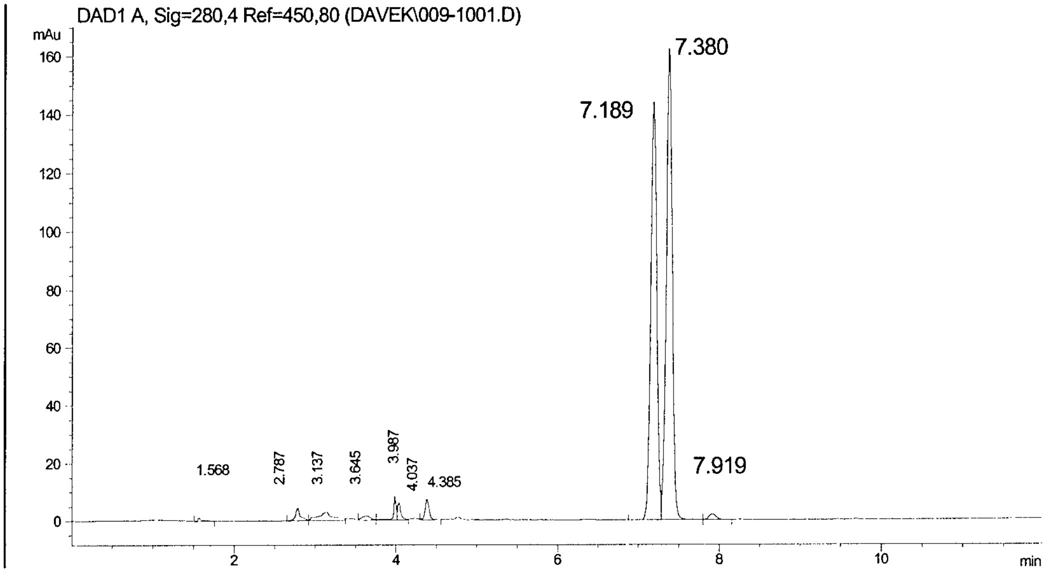


FIGURE 3-6. Typical HP ChemStation Data Result for MeBT [HP ChemStation].

Tables have been generated from all of the HPLC collected data in spreadsheet form. They can be found in Appendices E-H.

3.6.2 Quality Assurance and Quality Control (Reproducibility)

Data was generated using triplicate runs to evaluate the HPLC's performance and five replicate samples (5 bottles from the same stock) to insure that the samples were consistent within the concentration level used. Numbers are reported to at least three significant figures. Sample results were recorded and a standard deviation was taken among the five replicates to demonstrate the accuracy of the measurements. Concentrations were found by first taking the average of the individual concentration averages; then, integrating over the linear calibration curve to obtain a concentration level.

IV. Data Analysis

4.1 Overview

There were several techniques used to analyze the data generated from this study. Graphical comparisons from Excel spreadsheets were used as well as descriptive and analytical statistics from Statistix®, a statistical software package. In order to be consistent and simplify the comparison between the different techniques, a numbering system was established for each of the data sets. The soils and concentrations from this study will be referred to in this section as the following:

Wright-Patterson AFB – Untreated soil	Soil 1
Wright-Patterson AFB – Treated soil	Soil 2
Denver International Airport soil	Soil 3
Westover ARB soil	Soil 4
1000 mg/L MeBT solution	Conc. 1
100 mg/L MeBT solution	Conc. 2
10 mg/L MeBT solution	Conc. 3
Mix – approximately 100 mg/L MeBT and 1000 mg/L PG	Conc. 4

TABLE 4-1. Soil and Concentration Identification

Analyses of each soil's results are reviewed prior to the differentiation analysis. This allows a thorough look at each soil before interactive influences can affect judgment. An evaluation criterion for each soil type includes K_d results from each concentration level, how the addition of PG affected the sorption coefficient, and any anomalies encountered during the study. Each soil type and concentration was assumed to be independent of the others for this analysis. An Analysis of Variance and Tukey pairwise comparison of means tests were performed on each soil for both isomers of MeBT. Results from these analyses can be found in Appendix J under 4 MeBT and 5-MeBT respectively.

Differentiation analysis was performed by using four tests. These tests included:

1) Clayey Soil vs. Sandy Soil
2) Medium foc Content Soil vs. Low f_{oc} Content Soil
3) Acclimated Soil vs. Unacclimated Soil (on the basis of exposure to MeBT and PG)
4) Concentration Solution with PG Added vs. Solution with No PG Added

The results will be presented in graphical form, based on rejecting or accepting the null hypothesis given in Section 3.4.3, and in tabular form showing a direct comparison of the sorption coefficient values. Complete test results are included separately for each isomer in Appendix J.

4.2 Results from Preliminary Experiments

4.2.1 Pan Evaporation

Results from the pan evaporation experiment are consistent with the published data that PG is a hygroscopic compound. As the humidity in the room changed with the relative humidity from the outside, the measured amount of liquid in the pan increased or decreased accordingly. The liquid gained, on average 0.386 grams of atmospheric moisture over the course of the test period. Results from the experiment can be seen graphically in Appendix C.

4.2.2 Toxicity Matrix

A spectrophotometer, used at the completion of the test, measured the amount of growth in each vial. The amount of flock or total suspended solids (TSS) in the vial is a measure of growth; the lower the light penetration through the vial, the more flock in the vial, which was an indication that more growth had taken place. Therefore, the conclusion more TSS, more growth, and less toxicity was assumed true. Results from this toxicity experiment showed the maximum amount of growth or measured flock was realized in the 0 mg/L MeBT and 0-mg/L PG vial. Growth in a vial with only nutrient and microorganisms raises the question of what carbon source was used to produce this development. This is a question for later study.

The next several largest amounts of growth came from 100 mg/L PG row where the growth of the microbes decreased (less TSS) as the concentration of MeBT increased. Again, matching the hypothesized details of previous MeBT toxicological work [Cornell *et al.*]. This resulting matrix can be seen in Appendix C.

4.2.3 Soil Characterization

These tests consisted of a field capacity test for the WPAFB soil, a soil moisture test for each of the soils, and a sample size characterization based on published log K_{ow} value. This section includes the isotherm equilibration data for sorption and extraction. The equilibration determinations were performed on the highest f_{oc} soil and a moderate zeolite content. This soil will have the most sites available for sorption; thus, it will take the longest time to reach equilibrium (i.e. worst case).

4.3 Statistical Quantitative/Qualitative Analysis

Standards in this study were solutions containing known concentrations of analyte, MeBT. These samples provided a reference to determine unknown concentrations or to calibrate the HPLC and were used to inoculate the soils in subsequent tests. The accuracy of the measurement is how close the result comes to the true value. Determining the accuracy of a measurement requires calibration standards. This was accomplished using several concentrations to develop a calibration or working curve. Seven known concentrations were run through the HPLC to develop the calibration seen in Figure 3-4. Results of the calibration show that linearity among concentrations from 5 mg/L to 1000 mg/L MeBT is a true assessment. The Limit of Detection (LOD) is calculated to be *approximately* 5 mg/L ± 4 mg/L. Notwithstanding, measurements of lower concentrations were unreliable and for that fact, the 10-mg/L results have been eliminated from all further calculations. Calibration Curve data is provided in Appendix D along with LOD calculations.

Analysis of this data was performed on bottles taken from each soil type at each concentration over the equilibration period established in Appendix B. This sorption equilibrium test was accomplished as per Section 3.4.2; results are also in Figure 4-1. Statistical analyses were performed on the bottles, 1 hour to 216 hours, to see if the K_d values of the bottles were significantly different. It was determined that equilibrium is reached in 144 hours or 7 days.

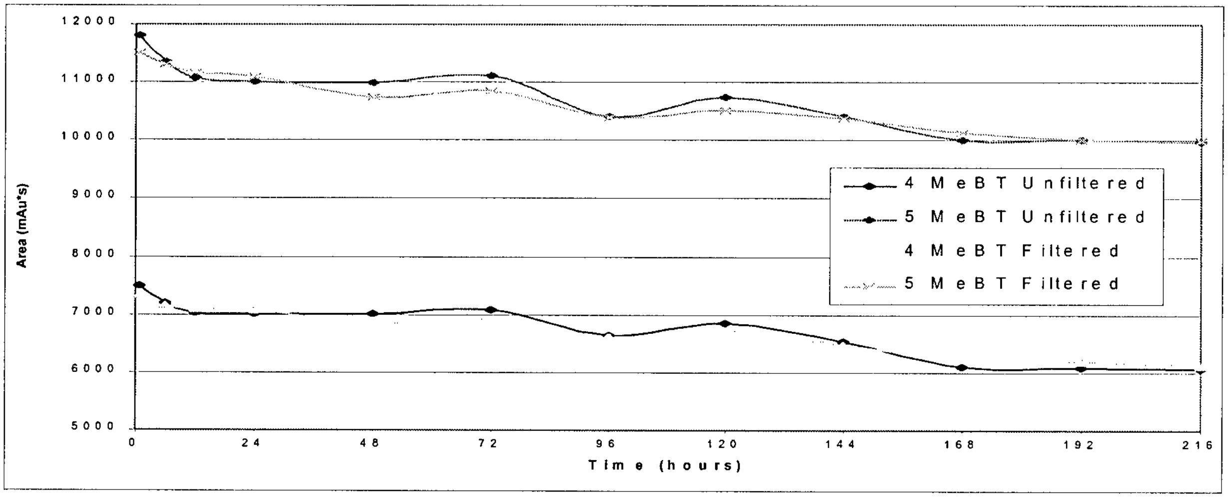


FIGURE 4-1. Establishment of Sorption Equilibrium Point

Interaction between soil types was established using Statistix®'s Two-way Analysis of Variance (ANOVA) table with soil and concentration being the variables in question. Results of the ANOVA reveal a p-value of 0.000. A p-value less than 0.05 is an indication of significant interaction between the variables. This interaction leads to the fact that there are similarities in each soil and how they reacted to the various concentrations. Results are provided in Appendix J for each isomer. Statistical reports were generated taking into account all of the resultant sorption coefficients.

4.4 Isomer Results

Both isomers of MeBT were evaluated over a range of concentrations and several soil variations. Table 4-2 provides a direct comparison of the concentration results for each soil at each

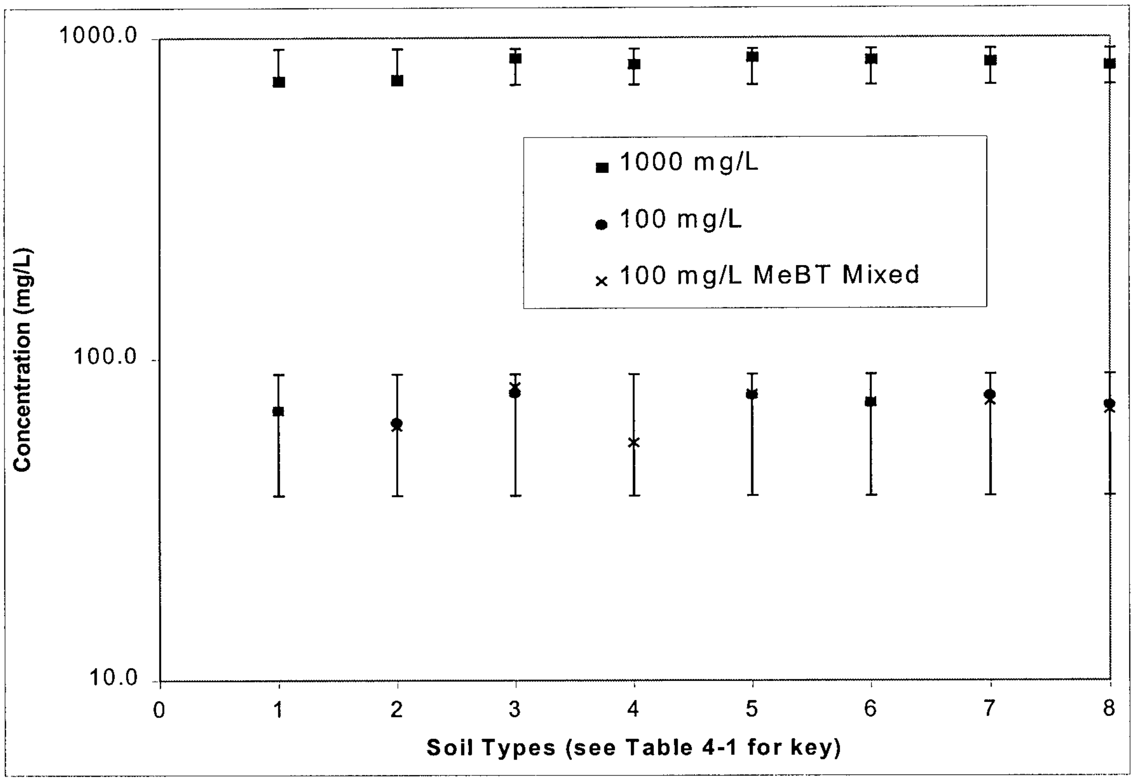
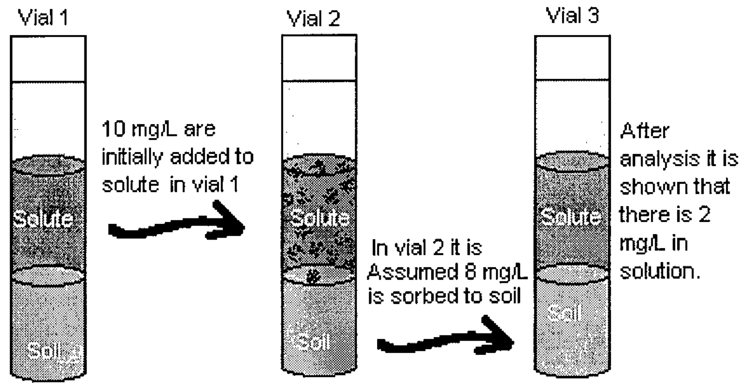


FIGURE 4-2. MeBT Isomer Recovery from All Soil Types
Note: Error bars represent one Standard Deviation among concentration group.

concentration level of solution. Direct comparison of the isomers can be seen in Figure 4-2. For the 1000 mg/L, the relationship of 4-MeBT and 5-MeBT is fairly consistent. Except for the untreated soil at 1000 mg/L, the K_d of 5-MeBT was higher than 4-MeBT; therefore it will be the basis for comparison during each of the differentiation tests. This consistency may be due to the fact that 4-MeBT is considered recalcitrant while the 5-MeBT may be degradable, and therefore somewhat unrecoverable. This unrecoverability may appear to be excess sorption, when, in fact, it is not. Figure 4-3 shows the possible paths that can occur for the MeBT.



Therefore, the 8 mg/L may be accounted for by the processes below:

- Degraded
- Sorbed
- Unrecoverable
- Lost in TSS
- Sorbed so strongly that it will not come off

FIGURE 4-3. Accounting for Unrecoverable Isomer

	Concentration				
	Soil	Isomer	1000	100	Mix
1	Untreated	4	734.7	69.0	68.7
2	Untreated	5	741.8	63.1	61.2
3	Treated	4	864.8	78.2	81.7
4	Treated	5	825.2	**0.0**	54.6
5	Westover	4	869.1	77.1	77.7
6	Westover	5	851.5	72.8	73.1
7	DIA	4	841.6	76.6	73.6
8	DIA	5	819.0	71.3	69.3

TABLE 4-2. HPLC Concentration/Soil/Isomer Results

Note 1: Bold numbers in Table 4-2 are addressed in the corresponding soil's anomaly section.

Note 2: Isomer concentration totals do not match applied concentration, see Section 3.6.4 for explanation.

4.5 Wright-Patterson Soil Results

Both of the WPAFB test soils came from the same sample set. The unacclimated or untreated soil had not been exposed to ADF in any way. The treated soil was exposed to MeBT and PG for a two-week period during testing by respirometry [Burke, 1999].

4.5.1 Wright-Patterson Soil – Untreated

This study found that for Soil 1, mean K_d results for the 4-MeBT isomer fell into two homogeneous groupings. The group of Conc. 2 and 4, and Conc. 1 were significantly different from one another. Conc. 1 had a mean K_d significantly lower than the other group.

The 5-MeBT isomer produced only three homogeneous groupings. The mean K_d of Conc. 2 was significantly higher than the other group. Conc. 1 and 4 comprise the lower mean K_d value homogeneous group.

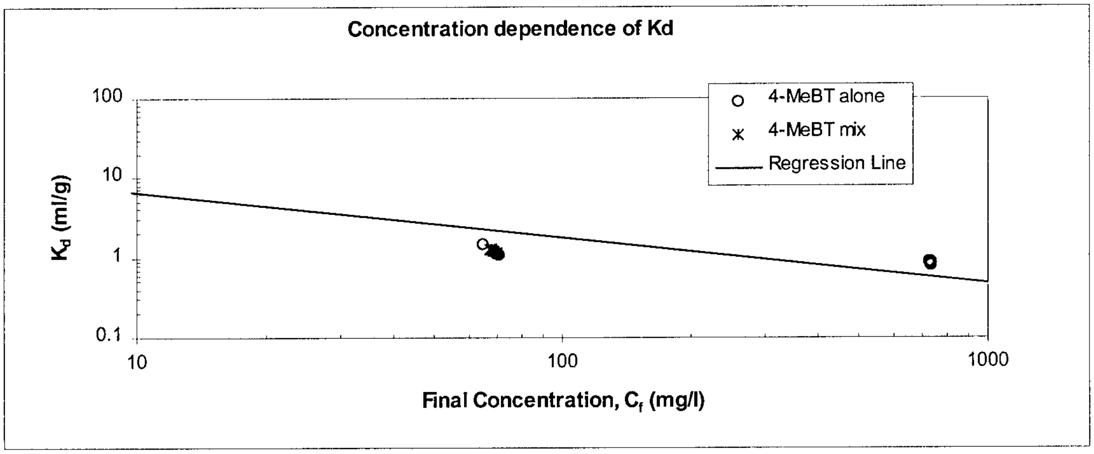


FIGURE 4-4. WPAFB Untreated Sorption Coefficient vs. Concentration – 4-MeBT

Therefore, it is assumed that Soil 1 reacts relatively the same to the various concentrations applied for both isomers. Figure 4-4 and Figure 4-5 depicts the linear regression for the concentration dependence of Kd for each isomer. Linearity is shown by the higher n value for the Freundlich isotherm: 0.859 for the 4 isomer and 0.732 for the 5 isomer. Details are in Appendix E.

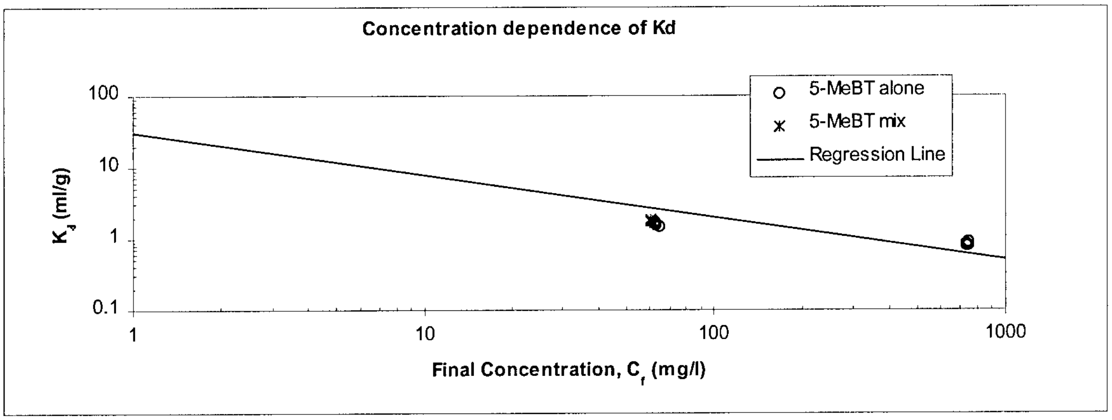


FIGURE 4-5. WPAFB Untreated Sorption Coefficient vs. Concentration – 5-MeBT

The ability to separate the 4 and 5 isomer of MeBT allows for a comparison of their means at each of the concentration levels for each soil. The 1000-mg/L concentration level for the 4 and 5 isomers show similar sorption coefficients, 0.860 vs. 0.825-mL/g, respectively. At the 100-mg/L concentration level for the 4 and 5 isomers show significantly different sorption coefficients, 1.203 vs. 330-mL/g. Finally at the 100-mg/L Mix concentration, the means of the 4 and 5 isomer are similar in direction but not in magnitude (1.219 vs. 1.744-mL/g, respectively). A summary of these results is in Table 4-3.

Specifically looking at Conc.2 and Conc. 4 for Soil 1, the study reveals that there is no significant difference between the two concentrations for the 4 isomer (1.203 vs. 1.219-mL/g). This is also evident by the homogeneous grouping of the two means. The same results were not achieved for the 5-MeBT isomer. This relationship suggests that there is no difference how Soil 1 sorbs 100-mg/L of MeBT with or without the addition of PG for the 4 isomer, but there is a difference in the 5 isomer. Results are shown in Appendix J, also refer to Table 4-3 for a summary of means sorption results and Figure 4-6 for a graphical display.

Two anomalies exist for Soil 1. First, the *high* sorption coefficients for the 10-mg/L samples, both 4 and 5-MeBT, are inconsistent with the sorption pattern established in this study. At the low end concentration level, the nonlinear portion of the calibration curve could have adversely affected the results. Secondly, the 5 isomer, in 3 of the 4 concentrations, has a higher sorption coefficient than the 4 isomer.

Untreated	Kd-4 (mL/g)	Kd-5 (mL/g)
Conc. 1	0.860	0.825
Conc. 2	1.203	1.645
Conc. 4	1.219	1.735

TABLE 4-3. WPAFB Untreated Average Sorption Coefficient Results.

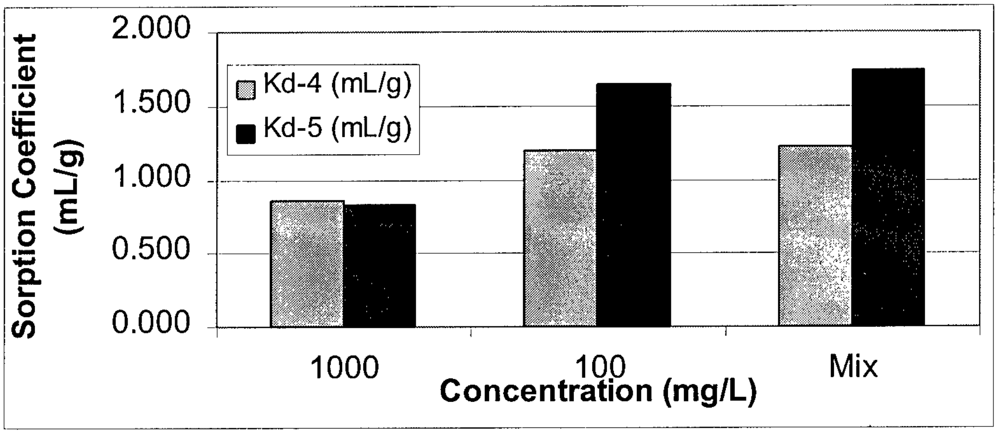


FIGURE 4-6. WPAFB Untreated Soil Sorption Results.

4.5.2 Wright-Patterson Soil – Treated

The sorption coefficient results for the 4 isomer in Soil 2 shows three homogeneous grouping of means. Conc. 2 was the highest at 0.706-mL/g, next was Conc. 4 at 0.521-mL/g, followed by Conc. 1 at 0.350-mL/g. With Soil 2 the 5-MeBT isomer produced a separate group for each concentration indicating that each concentration is sorbed differently. The means range is from

Conc. 2 at 44.5-mL/g to Conc. 1 at 0.512-mL/g. Results are presented in Table 4-4 and Figure 4-9. Figure 4-7 and Figure 4-8 depicts a linear regression for the concentration dependence of K_d, each group of coefficients is graphed on these figures. Results show a good linear fit for the 4-MeBT isomer with n = 0.708, but a poor linear relationship for the 5-MeBT isomer with n = 0.125.

Focusing attention to Conc. 2 and Conc. 4 under the 4 isomer, we find that the means are not statistically similar since they are put into two homogeneously different groups. Refer to Test 4, Section 4.11 for specific results of this comparison. For the 5 isomer, the same phenomenon exists. Refer to Table 4-4 and Figure 4-9, respectively, for a summary of mean sorption data.

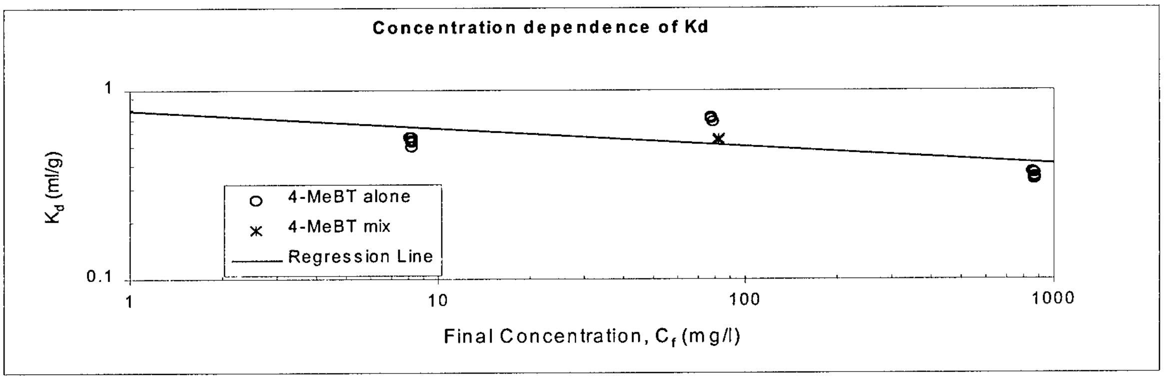


FIGURE 4-7. WPAFB Treated Sorption Coefficient vs. Concentration – 4-MeBT

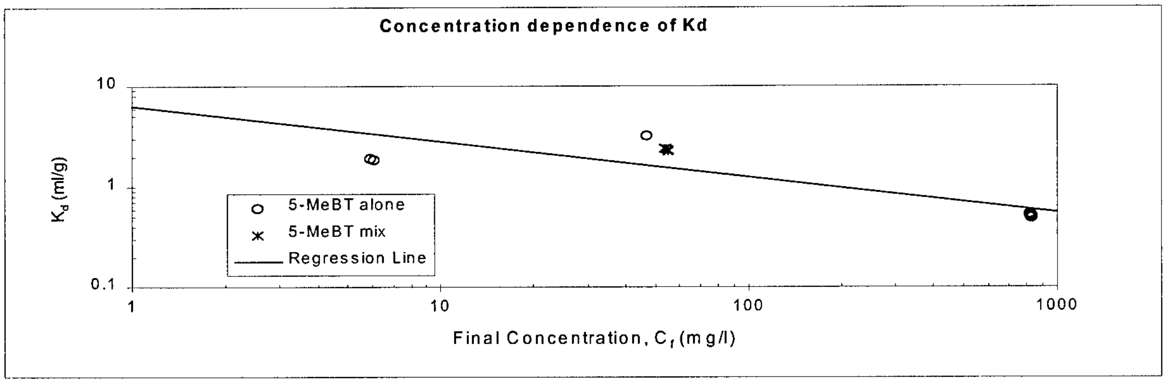


FIGURE 4-8. WPAFB Treated Sorption Coefficient vs. Concentration – 5-MeBT

Again, the anomaly discovered in Soil 2 was the relatively *high* sorption coefficient of the 10-mg/L concentration solution for the 5 isomer (mean K_d value of 3.225-mL/g). In addition, the 5 isomer for the Conc. 2 and 3 does not show significant sorption after equilibrium is reached. This could be from the unrecoverable condition described in Section 4.4. Refer to Appendix F for HPLC results and note the appearance of an additional peak with higher retention time when the 5 isomer is unrecoverable. In this case too, each 5 isomer had a higher sorption coefficient than the 4 isomer.

Treated	Kd-4 (mL/g)	Kd-5 (mL/g)
Conc. 1	0.350	0.512
Conc. 2	0.706	**44.50**
Conc. 4	0.547	2.325

TABLE 4-4. WPAFB Treated Average Sorption Coefficient Results.

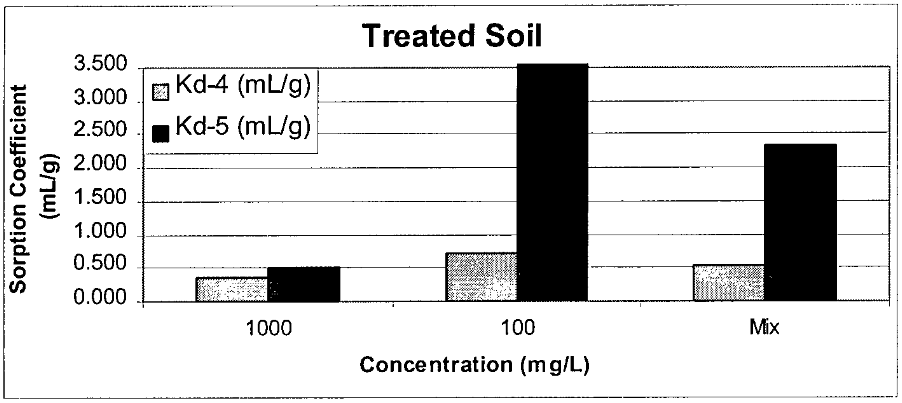


FIGURE 4-9. WPAFB Treated Soil Sorption Results.

4.6 Denver International Airport (DIA) Soil Results

The sorption coefficients for the 4-MeBT isomer on Soil 3 show three homogeneous groups. Conc. 3 is has the highest K_d at 2.840-mL/g, followed by Conc. 4 at 0.208-mL/g, with the lowest K_d at Conc. 1 equal to 0.044 mL/g. The 5 isomer had two homogeneous groups. Conc. 4 and 2 have the highest sorption coefficient at 0.291 and 0.255-mL/g respectively, followed by the lowest mean K_d value of Conc. 1 at 0.075-mL/g. Results are contained in Table 4-5 and Figure 4-12.

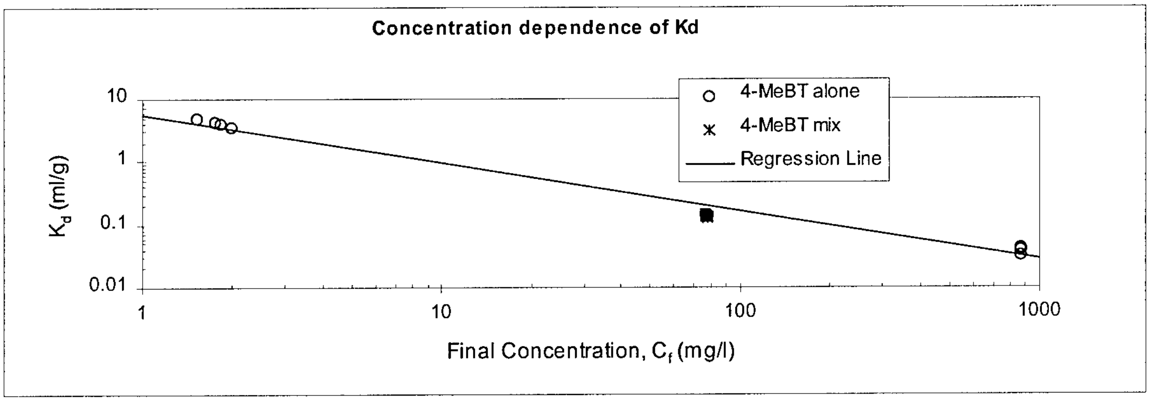


FIGURE 4-10. DIA Sorption Coefficient vs. Concentration – 4-MeBT

Figure 4-10 and Figure 4-11 depicts a linear regression for the concentration dependence of K_d, each group of coefficients is graphed on these figures. Results show an excellent linear fit.

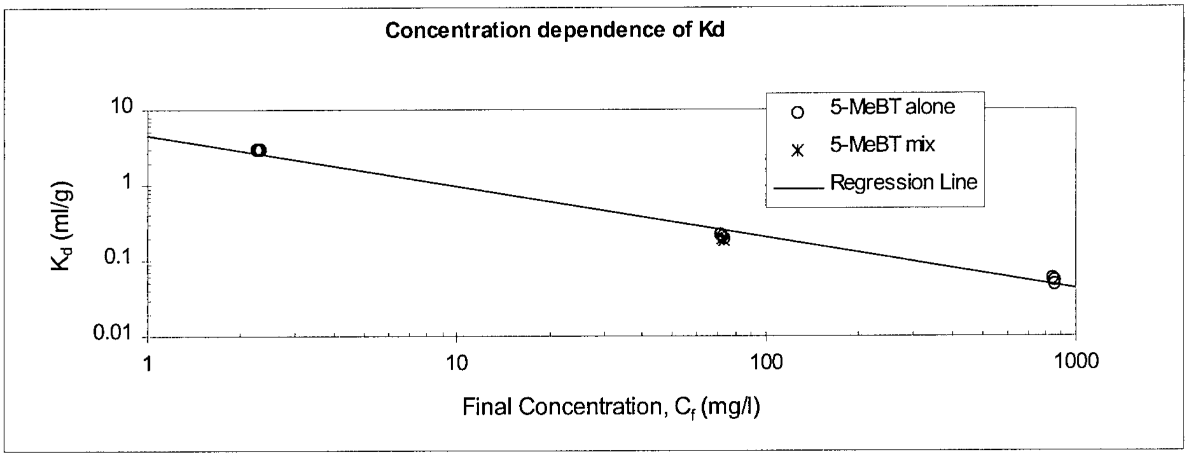


FIGURE 4-11. DIA Sorption Coefficient vs. Concentration – 5-MeBT

The Conc. 2 and 4 result show the relationship between the addition of PG and when no PG added. With Conc. 2 and Conc. 4 being significantly different for 4-MeBT, there is a difference between PG added and not adding PG to the solution while for the 5-MeBT there is also a difference when PG is added. See Table 4-5 for a comparison.

Soil 3 with 5-MeBT has been placed into two homogeneous groups. Conc. 1, 2, and 4 are statistically the same with values of 0.0754, 0.2550, and 0.2906-mL/g respectively. Conc. 3 is higher at a K_d value of 5.0206-mL/g. The results (Table 4-5 and Figure 4-12) show that the addition of PG to the solution had little affect on the sorption coefficient of 5-MeBT.

DIA	Kd-4 (mL/g)	Kd-5 (mL/g)
Conc. 1	0.044	0.075
Conc. 2	0.160	0.255
Conc. 4	0.208	0.291

Table 4-5. DIA Soil Average Sorption Coefficient Results.

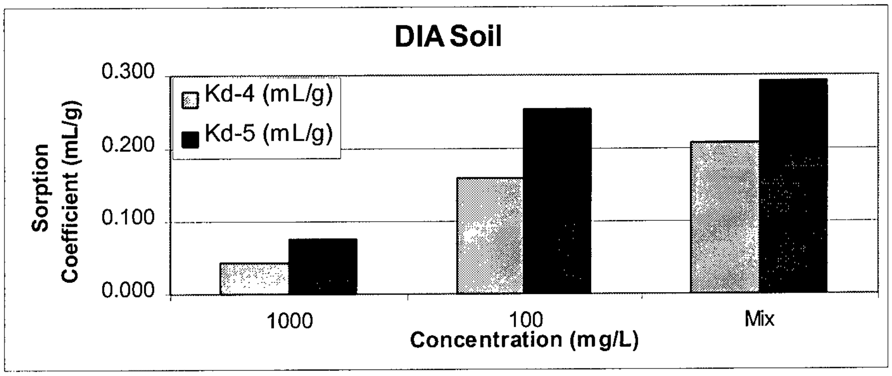


Figure 4-12. DIA Soil Sorption Results.

4.7 Westover ARB Soil Results

The Tukey Comparison of Means has separated both the 4 and the 5 isomers into three homogeneous groups. The 4 isomer ranges from 0.148-mL/g to a low of 0.036-mL/g, with the grouping of Conc. 4 and Conc. 2 in the middle with values of 0.197 and 0.146-mL/g, respectively. The 5-isomer grouping has a high K_d value of 2.970 mL/g and a low of 0.056 mL/g, with the same grouping the middle. Refer to Table 4-6 for a summary of average sorption coefficient data. Figure 4-15 contains a graphical representation of the sorption data.

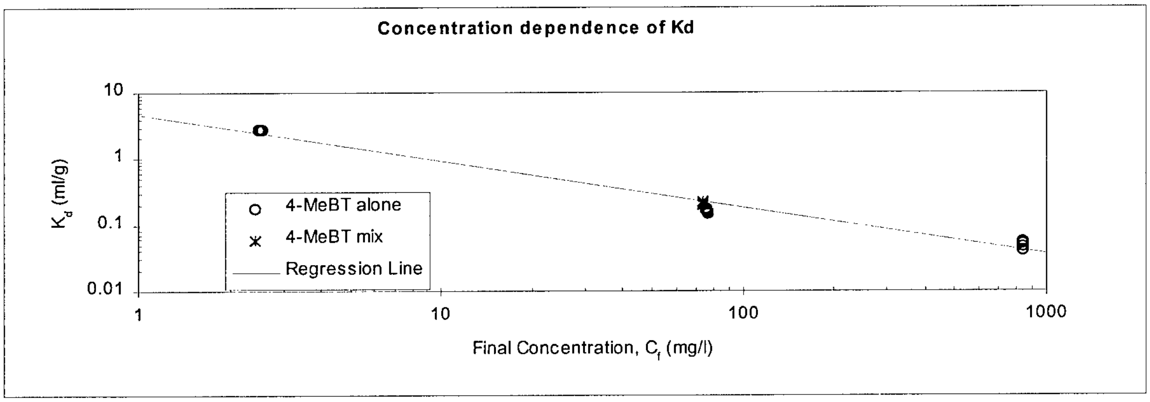


FIGURE 4-13. Westover ARB Sorption Coefficient vs. Concentration – 4-MeBT

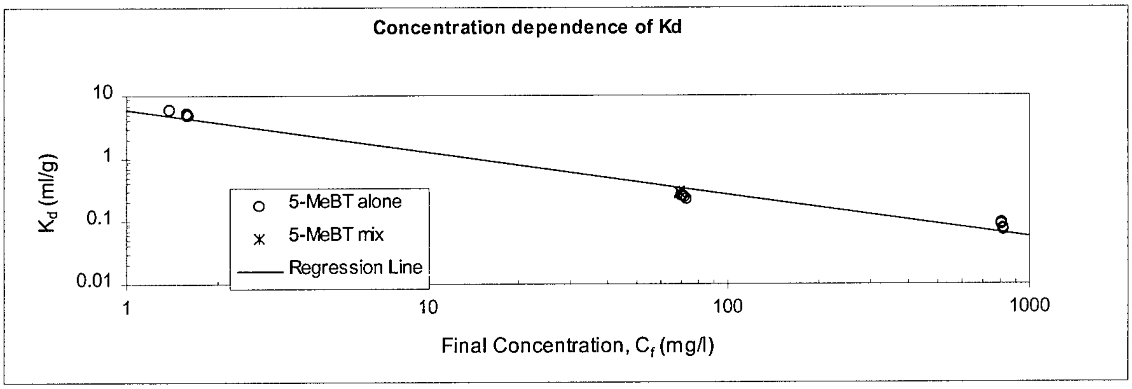


FIGURE 4-14. Westover ARB Sorption Coefficient vs. Concentration – 5-MeBT

The comparison of Conc. 2 (No PG added) and Conc. 4 (PG added) show the same result for both the 4 and the 5 isomer. Both isomers have mean K_d values for Conc. 4 and Conc. 2 that are statistically equal. Details for this are shown in Section 4.11 and are presented in tabular form in Table 4-6 and graphically in Figure 4-15.

Again, the K_d value of Conc. 3 is significantly higher, for both the 4 and the 5 isomer, than the other concentrations in this soil type. Additionally, the 5 isomer is higher in sorption coefficient value than the 4 isomer, except in Conc. 3 and 4 where they are equal. Moreover, the low value of the sorption coefficient for Conc. 1 is below 0.100-mL/g. This and Soil 3's Conc. 1 are the only ones to drop below 0.100-mL/g. In addition, the 5 isomer for the Conc. 3 does not show a significant concentration level after equilibrium is reached. This could be from the unrecoverable condition described in Section 4.4. Refer to Appendix H for HPLC results and note the appearance of an additional peak with higher retention time when the 5 isomer is unrecoverable.

Westover	Kd-4 (mL/g)	Kd-5 (mL/g)
1000	0.036	0.051
100	0.148	0.203
Mix	0.136	0.193

TABLE 4-6. Westover ARB Soil Average Sorption Coefficient Results.

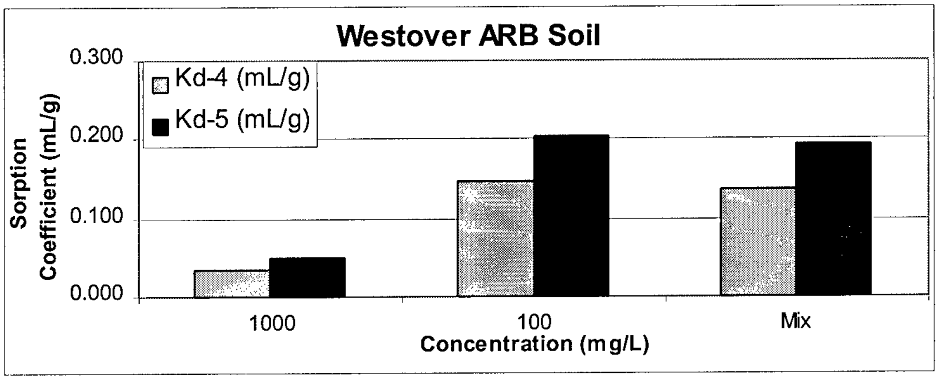


FIGURE 4-15. Westover ARB Sorption Results.

4.8 Soil Type Differentiation

The first statistical comparison was conducted to determine if there was a significant difference between the mean sorption coefficients for a sandy soil (Soil 4) and the mean K_d values of a clayey soil (Soil 3). This comparison was accomplished using a two-sample t-test as described in Section 3.4.3. As shown in Figure 4-16 (4-MeBT) and Figure 4-17 (5-MeBT), the t value obtained, indicated by the stem line and circle, fell between the t critical values ($t_{crit} = t_{.025}$ and $t_{.975}$) for the 4 isomer and outside for the 5 isomer. This indicates that the null hypothesis proposed in Section 3.4.3 should be accepted for the 4 isomer; therefore, the mean sorption coefficients for Soil 3 and Soil 4 are to be considered equal. The null is rejected for the 5 isomer and indicates that the means of the soils are not equal and the sorption is decreased with the sandy soil vs. clayey. Table 4-7 and Figure 4-18 summarizes the average sorption coefficient results for both soils.

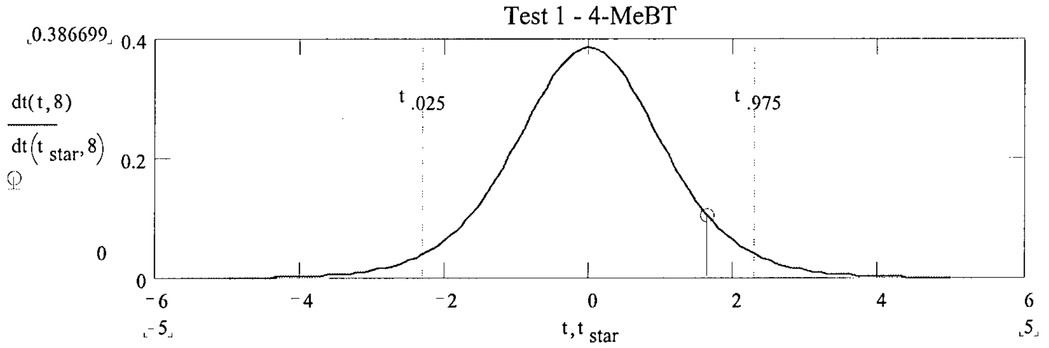


FIGURE 4-16. Test 1 t-test Results for 4-MeBT – Soils 3 & 4.

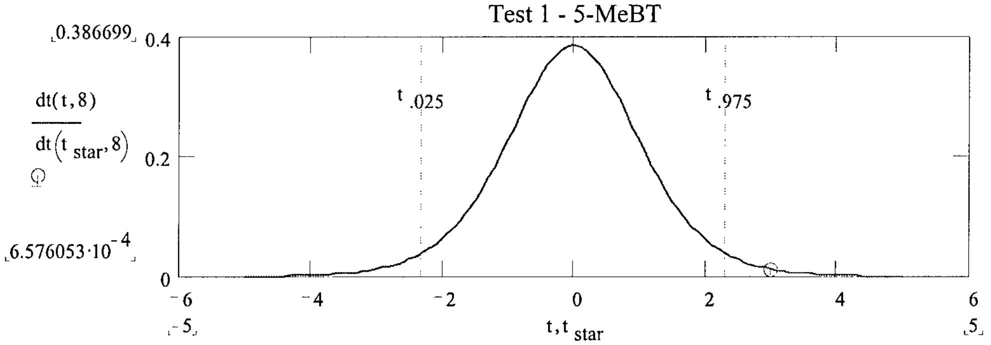


FIGURE 4-17. Test 1 t-test Results for 5-MeBT – Soils 3 & 4.

Soil Type Differentiation		
	Kd-4 (mL/g)	**Kd-5 (mL/g)**
Soil 3	0.160	0.075
Soil 4	0.148	0.051

TABLE 4-7. Average Sorption Coefficients for Soil Type Differentiation.

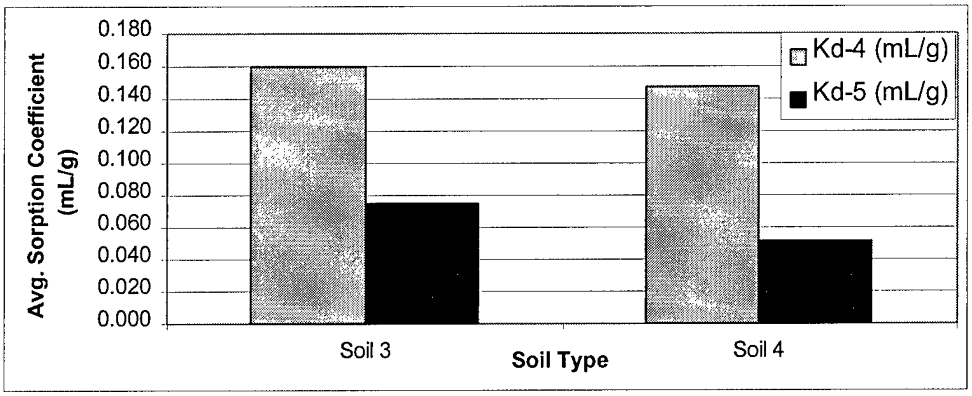


FIGURE 4-18. Average Sorption Coefficients for Soil Type Differentiation.

4.9 Organic Content Differentiation

The second statistical comparison was conducted to determine if there was a significant difference between a medium organic content soil (Soil 1) and a soil with virtually no organic content (Soil 4) with regard to MeBT sorption. A two-sample t-test was used to calculate a t value for this comparison. Figure 4-19 and Figure 4-20 depicts the results of the T-test for both the 4 and 5 isomers. The null hypothesis in Section 3.4.3 will be rejected for both isomers since the t value does not fall between the t critical values. Organic content clearly increased sorption of MeBT. Reference Table 4-8 and Figure 4-21 for a direct comparison summary of the mean K_d values.

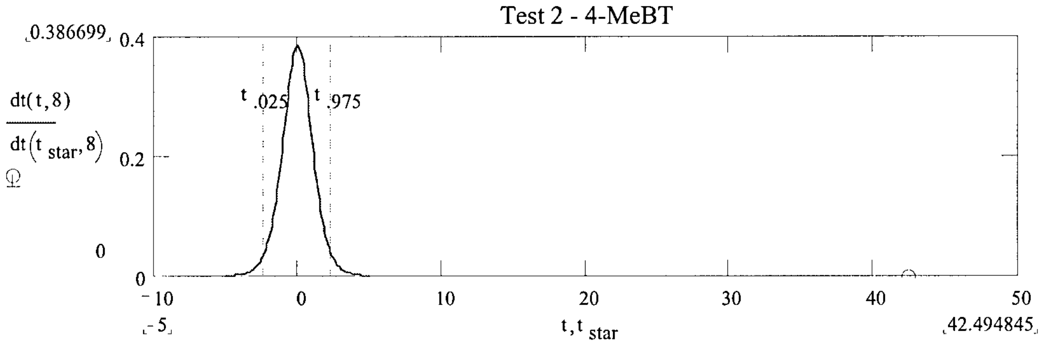


FIGURE 4-19. Test 2 t-test Results for 4-MeBT – Soils 1 & 4.

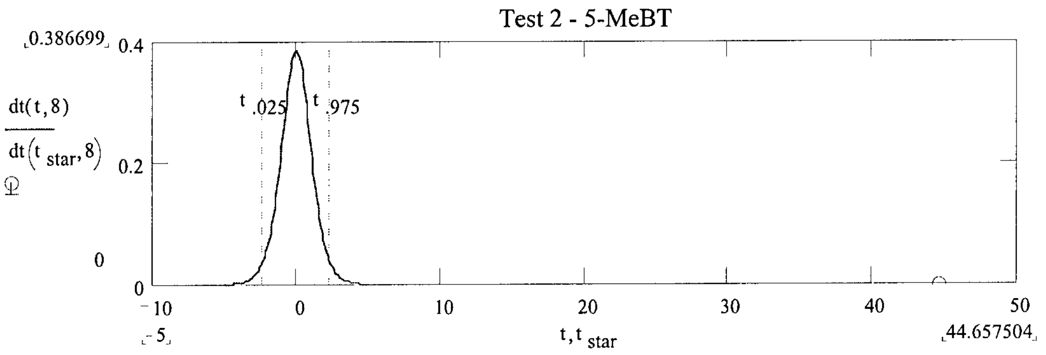


FIGURE 4-20. Test 2 t-test Results for 5-MeBT – Soils 1 & 4.

Organic Differentiation		
	Kd-4 (mL/g)	Kd-5 (mL/g)
Soil 1	0.860	0.825
Soil 4	0.036	0.051

TABLE 4-8. Average Sorption Coefficients for Organic Content Differentiation.

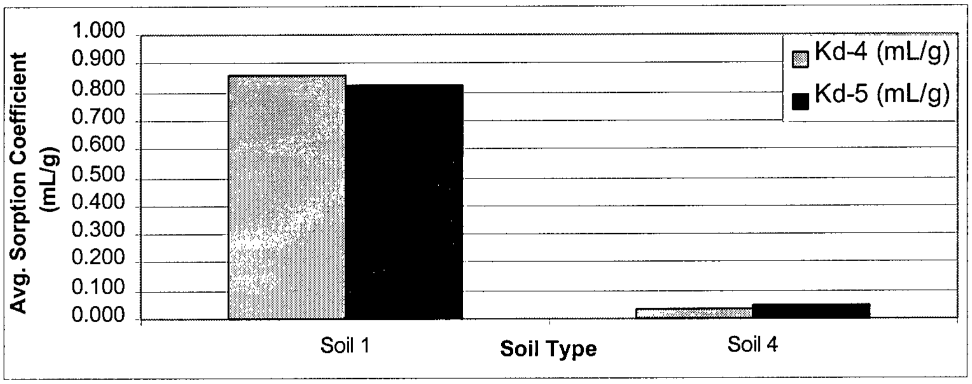


FIGURE 4-21. Average Sorption Coefficients for Organic Content Differentiation.

4.10 Acclimation Differentiation

The third statistical comparison was conducted to determine if there was a significant difference between the mean sorption coefficients for a soil that was exposed to a solution of MeBT and PG (Soil 2) and a soil that was previously unexposed to these compounds (Soil 1). To make this comparison, a two-sample t-test was employed. The result of the statistical tests determined a t value for comparison. Given the null hypothesis in Section 3.4.3 and the t critical value established from the degrees of freedom, Figure 4-22 and Figure 4-23 were created. These graphs show the t value outside the t critical values; therefore, the null hypothesis is rejected and the means of the two soils are not equal. Table 4-9 is a summary of average sorption data and Figure 4-24 is a graphical representation of the same information.

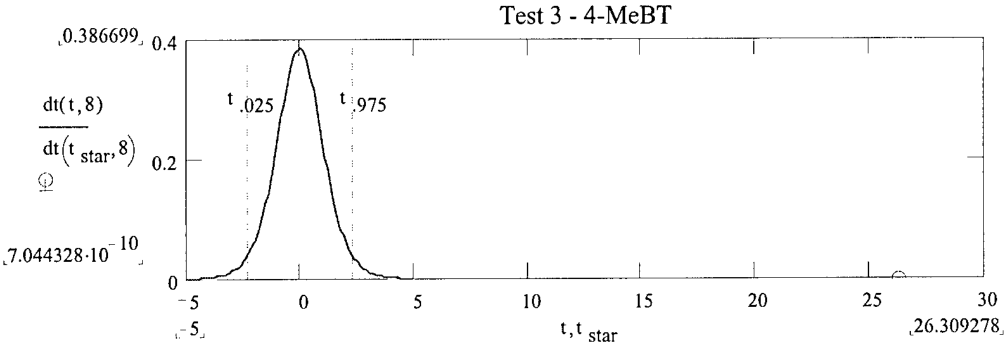


FIGURE 4-22. Test 3 t-test Results for 4-MeBT – Soils 1 & 2.

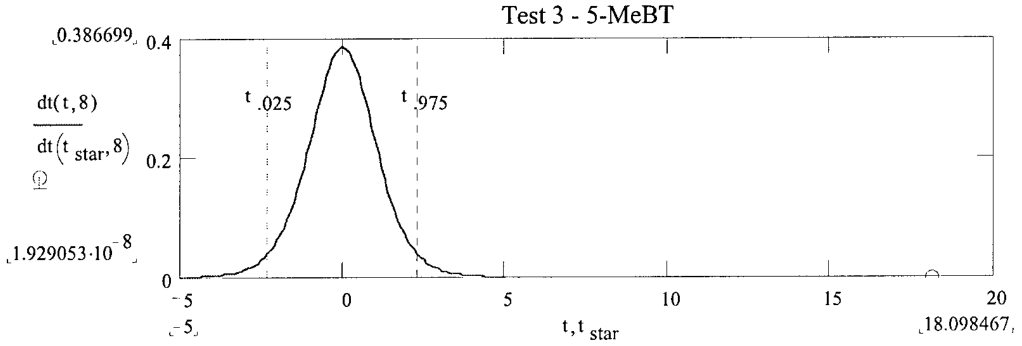


FIGURE 4-23. Test 3 t-test Results for 5-MeBT – Soils 1 & 2.

Soil Type Differentiation		
	Kd-4 (mL/g)	Kd-5 (mL/g)
Soil 1	0.860	0.825
Soil 2	0.350	0.512

TABLE 4-9. Average Sorption Coefficients for Acclimation Differentiation.

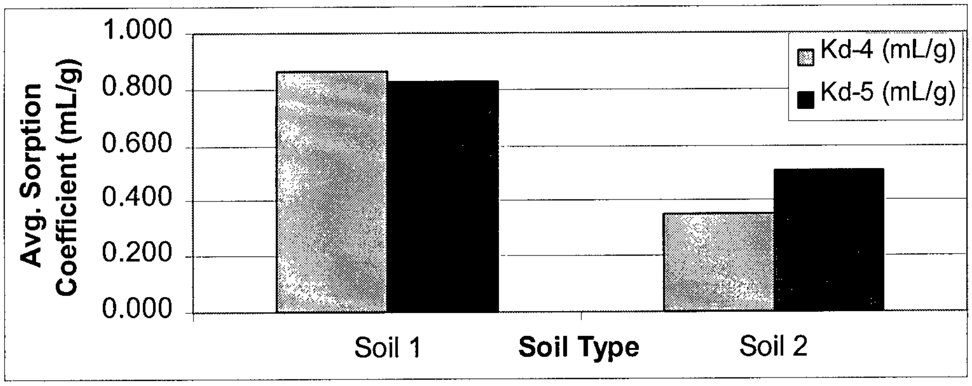


FIGURE 4-24. Average Sorption Coefficients for Acclimation Differentiation.

4.11 Propylene Glycol Additive Soil Differentiation

The fourth statistical comparison was conducted to determine if there was a significant difference between the mean K_d value for soils dosed with a combination of MeBT and PG (Concentration 4 – approximately 100 mg/L MeBT and 1000 mg/L PG) and the same soils dosed with only a solution of MeBT only (Concentration 2 – 100 mg/L MeBT). A two-sample t-test was conducted. Again, referencing the hypothesis in Section 3.4.3 and using the degrees of freedom for this comparison, a t value was established. Figure 4-25 and 4-26 show the results of the t-test respectively for each isomer. The results show that the null hypothesis should be accepted for the 4-MeBT because the t value is between the t critical values and rejected for the 5-MeBT isomer t value placement outside the t-critical range. This account would suggest there is no difference in the mean sorption coefficient of a solution containing PG or one without PG for the 4-MeBT and a significant difference in sorption of the added PG concentration for the 5-MeBT. Additionally, Table 4-10 and Figure 4-27 provides a direct comparison summary of average sorption data for each soil. Notice the *trend* for each soil is almost identical.

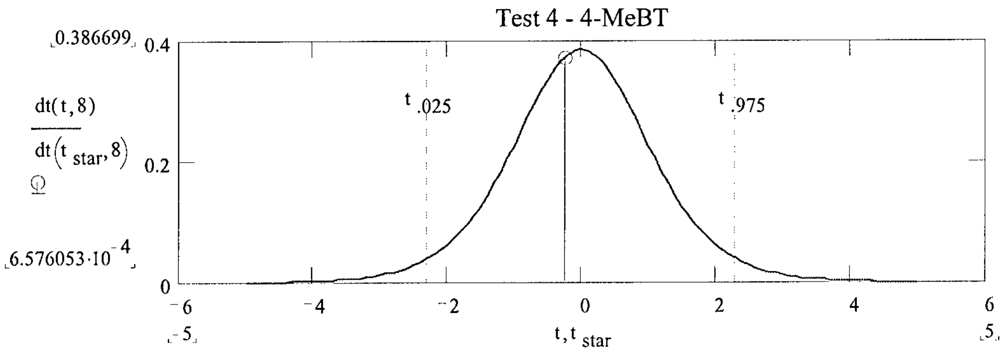


FIGURE 4-25. Test 4 t-test Results for 4-MeBT – Conc. 2 & 4.

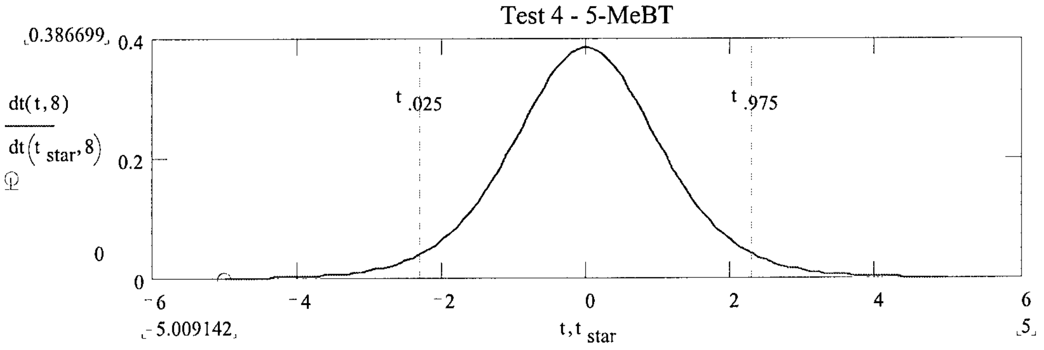


FIGURE 4-26. Test 4 t-test Results for 5-MeBT – Conc. 2 & 4.

Soil Type Differentiation								
	Soil 1-4	**Soil 1-5**	**Soil 2-4**	**Soil 2-5**	**Soil 3-4**	**Soil 3-5**	**Soil 4-4**	**Soil 4-5**
Conc. 2	1.203	330.000	0.433	44.500	0.160	0.255	0.148	0.203
Conc. 4	1.219	1.735	0.377	2.325	0.208	0.291	0.136	0.193

TABLE 4-10. Average Sorption Coefficients for PG Additive Soil Differentiation.

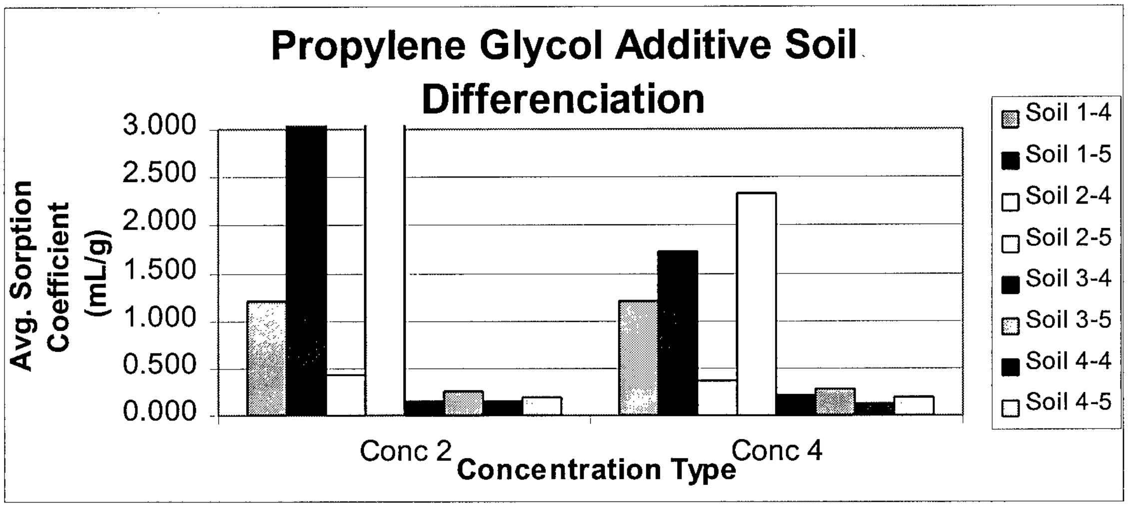


FIGURE 4-27. Average Sorption Coefficient for PG Additive Soil Differentiation.

4.12 Adjustments

This study was based on several assumptions that have large consequences, if incorrect. The conclusions in Chapter 5 are based upon these assumptions and the best information available at the time of study.

The first assumption was that the K_{ow} or octanol:water partitioning coefficient provided by the manufacturer is accurate. This study began by using the MSDS log K_{ow} value for preliminary calculations. If the log K_{ow} provided was incorrect, calculations based upon it will be off by that proportion. Examples include the volume of solute added to soil sample and the theoretical sorption coefficient. Note that Section 5.1 touches on the differences in K_{ow}'s between theoretical and achieved and a chart of experimental K_{ow}'s is included in Appendix I. A discrepancy can be found that may be attributed to the manufacturer or the difference in reagent grade and proprietary grade product.

The next assumption I have made is in regards to the sorption equilibrium isotherm results. The isotherms were developed over a 216-hour (9-day) period at which time it appeared that the HPLC resultant areas had leveled out or reached equilibrium. It is possible that this was a temporary stagnation point and sorption of MeBT in these soils may take weeks if not years. The time frame for this study made it impractical to lengthen the time scale for sorption isotherms.

The results of most 10-mg/L concentration runs are inconsistent with the trends established by other concentrations applied. This could have arisen from the fact that the calibration curve goes non-linear at approximately 7 mg/L. I assume that the non-linear point comes at the limit of detection (5-mg/L) and does not affect the results at the 10-mg/L point. However, inconsistent values at the 10-mg/L level may support the non-linear assumption. For this reason the 10 mg/L data was virtually eliminated from consideration in this study.

The final assumption that I have made in this study is the use of benzene as a substitute for MeBT in the calculation of the initial K_{oc} and soil mass. MeBT has an aromatic ring as part of its structure. The log K_{ow} of benzene and MeBT are similar at 2.17 and 2.13 respectively. Taking into account the second of these assumptions, this information was the best available at the time of the study. Use of toluene was considered because of the similar structure; however, this formula calculated out so little solute added to the soil that a saturated condition was not attainable for this study. A slurry or saturated condition would not have been achieved within the vial.

V. Conclusions and Recommendations

5.1 Conclusion

Results of this study help define the transport of MeBT in subsurface soils. Although limited in scope, this study describes the likely behavior of MeBT in a water-saturated soil environment. This section will begin with the major findings and continue with conclusions from each of the four tests performed during this study and finally address all other findings that have arisen.

- In the range of concentrations examined in this study (100 to 1000 mg/L), MeBT had an effective range of sorption coefficients from 0.03 to 1.45-mL/g for the 4-MeBT and 0.04 to 3.24-mL/g for the 5-MeBT.
- The two isomers, 4-MeBT and 5-MeBT, showed different sorption characteristics--the 5 isomer was consistently higher.
- Soil previously exposed to PG and MeBT, in most cases, shows approximately 50% less sorption than the unexposed, clean soil.
- The application of an additional organic material, propylene glycol, along with MeBT made no difference in the sorption of MeBT on any soil with the 4 isomer.
- Samples exposed to 5-MeBT for at least two weeks showed reduced 5-MeBT amounts and an additional peak in HPLC traces. This suggests biodegradation may occur in the 5 isomer.

5.1.1 Statistical Evaluation of Laboratory Results

The first of the four statistical tests performed for this study was a comparison of clayey soil vs. sandy soil. Samples from Denver International Airport and Westover Air Reserve Base were used. This test concluded that resultant mean sorption coefficients were equal for the 4-MeBT;

therefore, with 95% confidence, it can be said that there is no difference in how these particular clayey and sandy soils sorb 4-MeBT isomer. However, with 95% confidence, there is a significant difference in how these soils sorb 5-MeBT.

Test 2 for this study involved the comparison of a medium organic content (f_{oc}) soil vs. a soil that had virtually no organic content. Soil samples from Wright-Patterson Air Force Base and Westover ARB was used. Test 2 concluded that at all concentration levels applied, difference sorption coefficients were achieved for both the 4 and 5 isomer of MeBT. Thus, with 95% confidence, it can be said that soils with higher organic contents sorb more MeBT than those soils with low f_{oc}.

Test 3 compared the difference between a soil that had not been exposed to ADF or MeBT prior to this study and a soil that had been acclimated to MeBT and PG through a respirometry study. This test concluded that there is a large difference in how each soil sorbed the MeBT. The soil that had no exposure prior to the study had the larger of the two sorption coefficients. This phenomenon was noted for both the 4 and 5 isomer of MeBT.

The final test data results from all soils types comparing the 100-mg/L MeBT solution and 100-mg/L MeBT with 1000-mg/L propylene glycol (Mix) solution indicate that there is seemingly no difference if PG is added to the mix or if it is not added to the mix for the 4-MeBT isomer. However, the 5-MeBT indicates a significant difference in the mean sorption coefficient for the two concentrations. Reviewing the 5-MeBT, it is possible that microorganisms in the acclimated soils (Soil 2 or Treated Soil) are able to degrade the 5-MeBT isomer, thus lowering the concentration.

5.1.2 Significant Conclusions from Statistical Results

The K_d values obtained for the majority of soil types and concentrations would tend to reinforce the conclusion that MeBT does not sorb well to the soils in this study. There are certain combinations of concentrations and soil types that lead to higher sorption coefficients. These are explained in Section 4.4. These results represent low concentrations near the limit of detection and the non-linear portion of the HPLC; results may have been skewed because of this situation. Further analyses at low concentrations are necessary to support my findings.

Using the K_d values obtained during analysis, I have back-calculated log K_{ow} values for the 4 and 5 MeBT isomers. I have concluded that the published log K_{ow} values appear to be too high. Results in Appendix I reveal that few K_{ow} value approach the published value of 2.17. However, the calculation used for the log K_{ow} values is based on assumptions and cannot be relied upon; this conclusion is only speculative.

One possible reason for this discrepancy could come be differences of laboratory grade MeBT and reagent grade MeBT (see Section 4.12). It was assumed that the product used throughout my study was pure tolyltriazole; however, the laboratory grade identifier suggests that impurities may exist which could cause the difference in K_{ow}.

Another speculative conclusion for the log K_{ow} difference is the reporting process. Log K_{ow} values in this study come from isometric calculations. The K_{ow} value that has been published comes from unaltered methyl-benzotriazole.

As alluded to in Section 4.4, the 4-MeBT has a higher sorption coefficient than 5-MeBT (except for the untreated soil at 1000 mg/L). An explanation for this situation is included in Section 4.4 and reinforces areas presented in the literature review section. I would conclude that the 4-MeBT would move rather freely through the subsurface with little to slow it down, while the 5-MeBT is influenced by other factors, rendering it unrecoverable at times.

Lastly, as shown in the literature review section, the sorption coefficient is inversely related to the particle size of the soil. MeBT is a contradiction to that claim by Ball [Ball and Roberts, 1991].

5.2 Follow-on Research

This research involves the compound of interest, MeBT. The ultimate future to this subject is to find out what to do with ADF in the environment. In order to get there, numerous questions must be answered. The transport result with sorption is just one of many phases. Several areas are open to further interpretation, not only with MeBT, but ADF in general.

5.2.1 Analysis of Other ADF Components

There are numerous additives in ADF that allow it to perform in cold weather. MeBT has been the first to be studied in any depth. Further research can be done using another component of ADF and its relationship to PG and MeBT. A good working relationship with a manufacturer of ADF would be helpful to understand exactly what goes into ADF and the proportions in which they are mixed.

5.2.2 Breakdown of MeBT *in-situ*

An attempt can be made to isolate microorganisms that utilize MeBT aerobically as a sole substrate for growth. If the isolation is successful, experiments will then be conducted to investigate the biodegradation rates of MeBT by the isolated organisms.

5.2.3 Environment Variation Study

It is important to understand how this compound reacts under all environmental situations. The latest studies look at this compound under very specific conditions. Further research is necessary to determine how MeBT reacts under environmental changes. Such changes include temperature (-10 C- 5 C) and pH (5.0 – 9.0 or greater).

5.2.4 HPLC identification of MeBT degradation products

In several of the HPLC results, there was a small, but significant spike beyond the retention time window of interest. In most cases it was accompanied by a substantial decrease in 5-MeBT concentration. It is not known what this spike is or how to isolate it; furthermore, it is not known if it is exactly related to the decrease in the 5-MeBT isomer. Further research is necessary to determine if there is a correlation between the decrease in the 5-MeBT isomer and the area of the new spike. Ensure abiotic conditions are achieved for this portion.

5.2.5 Repeat this study

An effort can be accomplished along the same concepts as this study; however, the major emphasis would be on the metal binding properties of MeBT instead of focusing on the organic content binding. The metal binding alternative could give better information as to the difference in the K_{ow} factors.

Appendix A

Soil Analysis Report

University of Colorado at Boulder

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Colorado State University
Soil, Water and Plant Testing Laboratory
Natural & Environmental Sciences Bldg - A319
Fort Collins, CO 80523

(970) 491-5061 FAX: 491-2930

DATE RECEIVED: 12-14-1998
DATE PARTIAL REPORTED: 01-22-1999
DATE REPORTED: 02-16-1999

BILLING:

RESEARCH SOIL ANALYSIS

8-Dec-98

Lab #	Sample ID #	paste		Lime Estimate	%	AB-DTPA Extract						
						ppm						
		pH	EC mmhos/cm		OM	NO_3-N	P	K	Zn	Fe	Mn	Cu
R3392	Afit # 1	7.8	1.2	Medium	2.7	3.3	5.3	91.7	2.44	50.0	2.89	2.93
R3393	Afit # 2	7.7	0.9	Medium	2.9	6.2	4.9	92.0	2.63	51.7	2.76	3.15
R3394	Afit # 3	7.8	0.8	Medium	3.0	6.2	5.6	99.2	2.70	50.2	2.63	2.89

Lab #	Sample ID #	%			Texture	%
		Sand	Silt	Clay		TOC
R3392	Afit # 1	48	36	16	Loam	1.61
R3393	Afit # 2	48	36	16	Loam	1.82
R3394	Afit # 3	49	35	16	Loam	1.78

Appendix B

Caculation of:

Solution Concentration
Moisture Content
Individual Sample Sizes
Sorption Equilibrium Isotherm
Extraction Isotherm
Filtered Sample Comparison

Field Capacity Calculations

Mass of Soil = Ms = **100.01** grams

Mass of Water Absorbed in Soil Mw = **19.1** grams
Achieve 100% FC

FC = Mw/Ms
= 0.191
= **19.1%**

Dry Soil Weight Calulations

WPAFB					
Air- Dried Sample Weight	100.02	100.01	100.01 g		
Weight after heat/decant	90.32	91.05	90.27 g		
					AVG
Water Content	10.7%	9.8%	10.8%		**10.5%**
DIA					
Air- Dried Sample Weight	100.01	100.01	100.002 g		
Weight after heat/decant	88.12	87.56	87.98 g		
					AVG
Water Content	13.5%	14.2%	13.7%		**13.8%**
Westover					
Air- Dried Sample Weight	100.00	100.00	100.01 g		
Weight after heat/decant	94.3	93.82	94.1 g		
					AVG
Water Content	6.0%	6.6%	6.3%		**6.3%**

Solute Concentration - MeBT

Product Used:
Tolyltriazole (Solid)
Cobratec TT-100
Laboratory Grade

$$1000 \text{ mg/L} = \frac{1 \text{ gram MeBT}}{1 \text{ Liter Deionized Water}}$$

Solute Concentration - PG

Product Used:
Propylene Glycol (Aqueous)
Mallinckrodt, OR 1925
Laboratory Grade - 1,2 Propanediol

$$1000 \text{ mg/L} = \frac{5 \text{ grams of Liquid PG}}{5000 \text{ mL Deionized Water}}$$

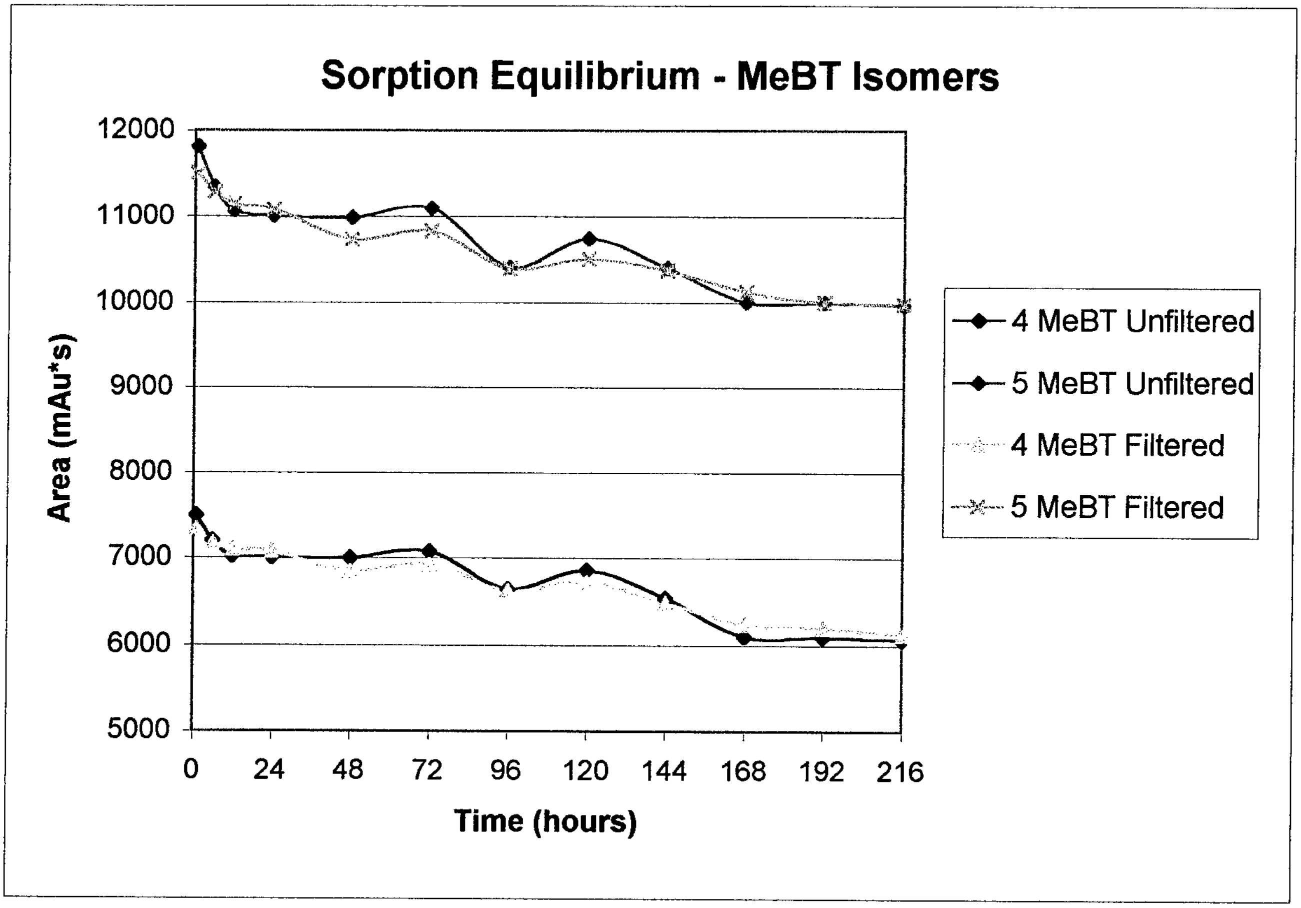
1000 mg/L

		4 MeBT		**5 MeBT**		**4 MeBT**		**5 MeBT**	
	Starting (Hrs)	Retention Time (Avg.)	Area	Retention Time (Avg.)	Area	Retention Time (Avg.)	Area	Retention Time (Avg.)	Area
	1	7.020	7495.6	7.208	11814.4	6.996	7340.7	7.179	11505.6
	6	6.969	7198.6	7.157	11350.1	6.947	7177.1	7.128	11294.7
	12	6.954	7022.4	7.138	11072.9	6.944	7099.3	7.125	11152.9
1 day	24	**6.948**	**7011.2**	**7.116**	**11009.5**	6.972	7074.6	7.155	11083.9
2 days	48	7.019	7004.7	7.207	10990.5	6.994	6852.0	7.179	10740.5
3 days	72	7.063	7076.4	7.252	11101.3	6.995	6923.9	7.184	10836.3
4 days	96	7.021	6646.2	7.210	10411.4	7.001	6629.4	7.198	10396.4
5 days	120	7.087	6862.6	7.276	10747.1	7.045	6728.9	7.234	10509.7
6 days	144	7.065	6542.3	7.253	10403.8	7.028	6489.1	7.210	10374.5
7 days	168	7.036	6103.7	7.222	10009.1	6.992	6238.2	7.179	10126.8
8 days	192	7.042	6089.4	7.238	9996.6	6.999	6197.3	7.188	10001.7
9 days	216	7.027	6065.5	7.211	9967.0	6.983	6119.7	7.172	9982.9
		7.021	6759.88	7.207	10739.48	6.991	6739.18	7.178	10667.16

Bold Numbers were adjusted for one run that was abnormal (Avg. of two runs)

Example:

Avg of three runs	7.351	7.249	7.228	7.276	Time
	10740.4	10752.3	10748.5	10747.07	Area



Mass of the Soil:Solute Calculation

MeBT K_{ow} 147.90 manufacturer

log K_{ow} 2.17

Approximation from benzene

$\log K_{om} = 0.52 \log K_{ow} + 0.62$

log K_{om} 1.748

K_{om} 56.03

$K_{oc} = 1.724 * K_{om}$

K_{oc} 96.59

f_{om} for soil **0.02867** (by percent)

$f_{oc} = .58 * f_{om}$

f_{oc} **0.017**

$Kd = f_{oc} * K_{oc}$

Kd = 1.606

Mass of soil

Ms = Vol. of solution/Kd

Vol. of solution = **16.06 mL**

Ms = **10.0 g**

Mass of the Soil:Solute Calculation

MeBT K_{ow} 147.90
log K_{ow} 2.17

Approximation from benzene
log K_{om} = 0.52 log K_{ow} + 0.62
log K_{om} 1.748
K_{om} 56.03

K_{oc} = 1.724*K_{om}
K_{oc} 96.59

f_{om} for soil **0.0287** (by percent)
f_{oc} = .58*f_{om}
f_{oc} **0.017**

Kd = f_{oc}*K_{oc}
Kd 1.608 **<---Theoretical Sorption Coefficient**

Mass of soil
Ms = Vol of solution/Kd
Vol of solution = **16.08 mL**
Ms **10 g**

Mass of the Soil:Solute Calculation

MeBT K_{ow}	147.90
log K_{ow}	2.17

Approximation from benzene

log K_{om} = 0.52 log K_{ow} + 0.62

log K_{om}	1.748
K_{om}	56.03

K_{oc} = 1.724*K_{om}

K_{oc}	96.59

f_{om} for soil **0.0137** (by percent)

f_{oc} = .58*f_{om}

f_{oc}	**0.008**

Kd = f_{oc}*K_{oc}

Kd 0.767 **<---Theoretical Sorption Coefficient**

Mass of soil

Ms = Vol of solution/Kd

Vol of solution = **7.67 mL**

Ms **10 g**

Mass of the Soil:Solute Calculation

MeBT K_{ow} 147.90
log K_{ow} 2.17

Approximation from benzene
$\log K_{om} = 0.52 \log K_{ow} + 0.62$
log K_{om} 1.748
K_{om} 56.03

$K_{oc} = 1.724{*}K_{om}$
K_{oc} 96.59

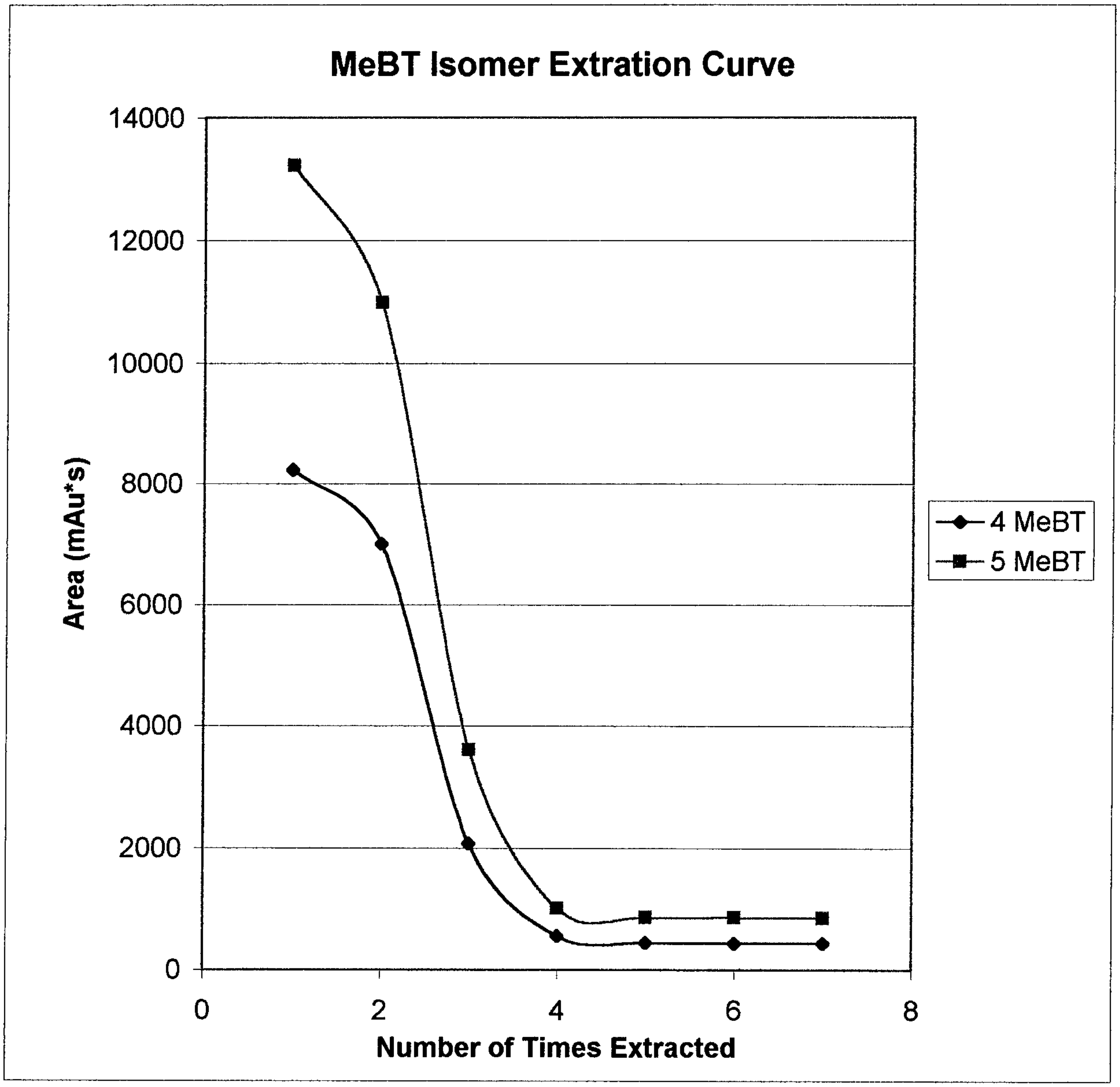
f_{om} for soil **0.009** (by percent, below LOD)
$f_{oc} = .58{*}f_{om}$
f_{oc} **0.005**

$Kd = f_{oc}{*}K_{oc}$
Kd 0.504 **<---Theoretical Sorption Coefficient**

Mass of soil
Ms = Vol of solution/Kd
Vol of solution = **5.04 mL**
Ms = **10 g**

1000 mg/L	0		**8225.7**		**13224.4**	4 MeBT	5 MeBT
Water	0.5	7.019	7004.7	7.207	10990.5	15%	17%
1 Meth	1 hr	7.026	2069.1	7.215	3606.9	75%	73%
2 Meth	6 hr	7.025	562.6	7.211	1015.3	93%	92%
3 Meth	24 hr	7.018	441.7	7.205	865.9	95%	93%
4 Meth	48 hr	7.011	439.6	7.201	857.2	95%	94%
5 Meth	72 hr	7.007	433.8	7.198	852.4	95%	94%
Percent MeBT Recoved			**94.73%**		**93.55%**		

Bold numbers obtained from calibration curve - 10/31/98



Appendix B

Filtered Sample Comparison

	Filtered Sample							
1000 mg/L	Retention Time	4 - Area (mAu*s)	4 Average	4 Peak Std Dev	Retention Time	5 - Area (mAu*s)	5 Average	5 Peak Std Dev
	8.456	7390.9			8.951	12416.6		
	8.345	7383.1			8.853	12385.7		
	8.295	7370.7			8.742	12380		
	8.152	7361.4			8.681	12375.2		
	8.108	7369.6	7375.14	11.73597	8.511	12379.5	12387.4	16.7447

Avg. Time 8.2712

Avg. Time 8.7476

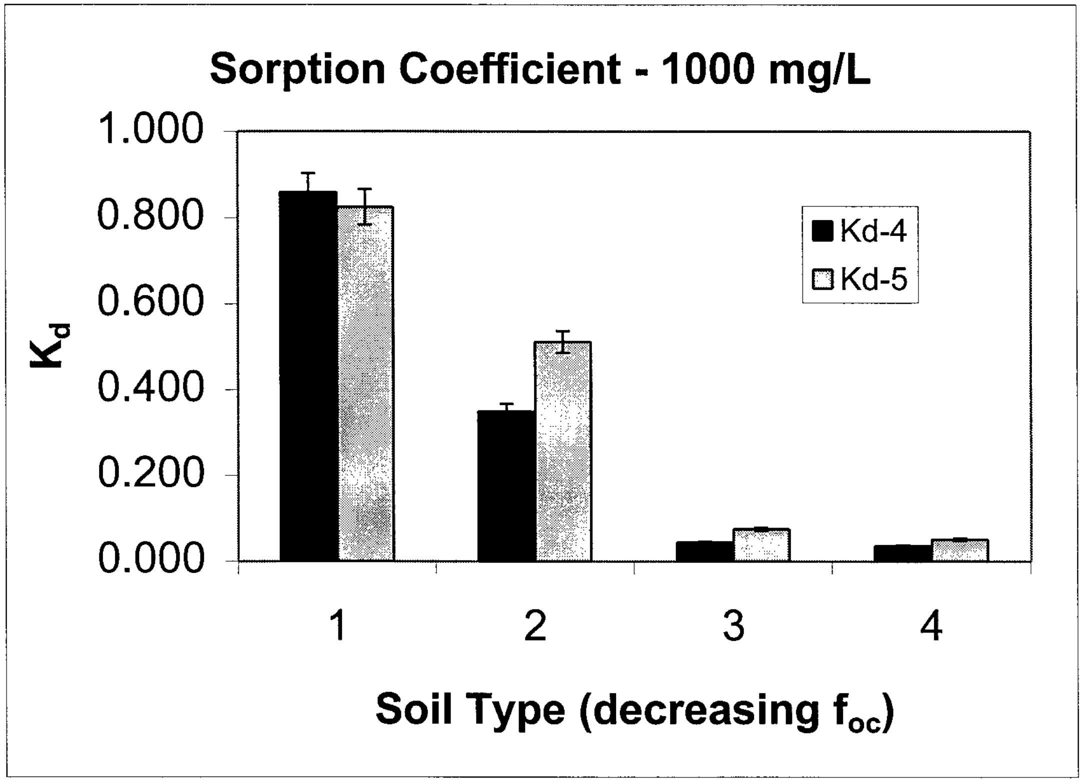
Difference from unfiltered 1000 mg/L sample

4 MeBT	5 MeBT
850.52	836.96
Difference **10.3%**	Difference **6.3%**

1000 mg/L - Average Kd values

		foc	Kd-4	Kd-5
1	Untreate	5.25%	0.860	0.825
2	Treated	5.25%	0.350	0.512
3	DIA	1.37%	0.044	0.075
4	Westove	0.90%	0.036	0.051

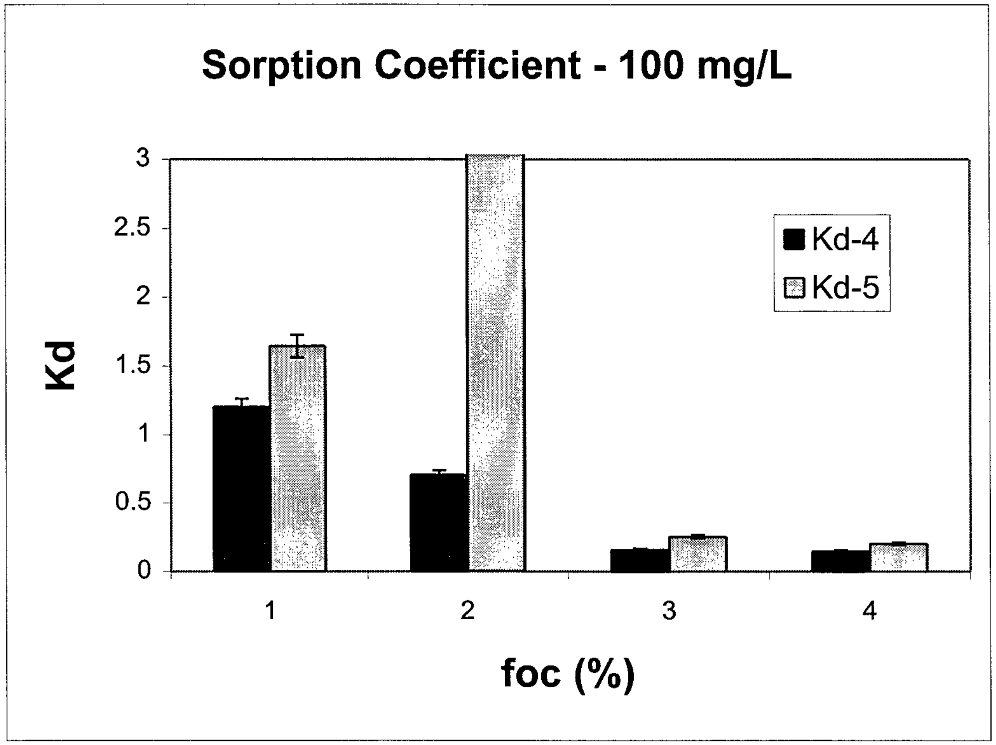
Brackets indicate 5% window within isomer type
Numbers reflect average Kd values



100 mg/L - Average Kd values

		foc	Kd-4	Kd-5
1	Untreate	5.25%	1.203	1.645
2	Treated	5.25%	0.706	**44.5**
3	DIA	1.37%	0.160	0.255
4	Westove	0.90%	0.148	0.203

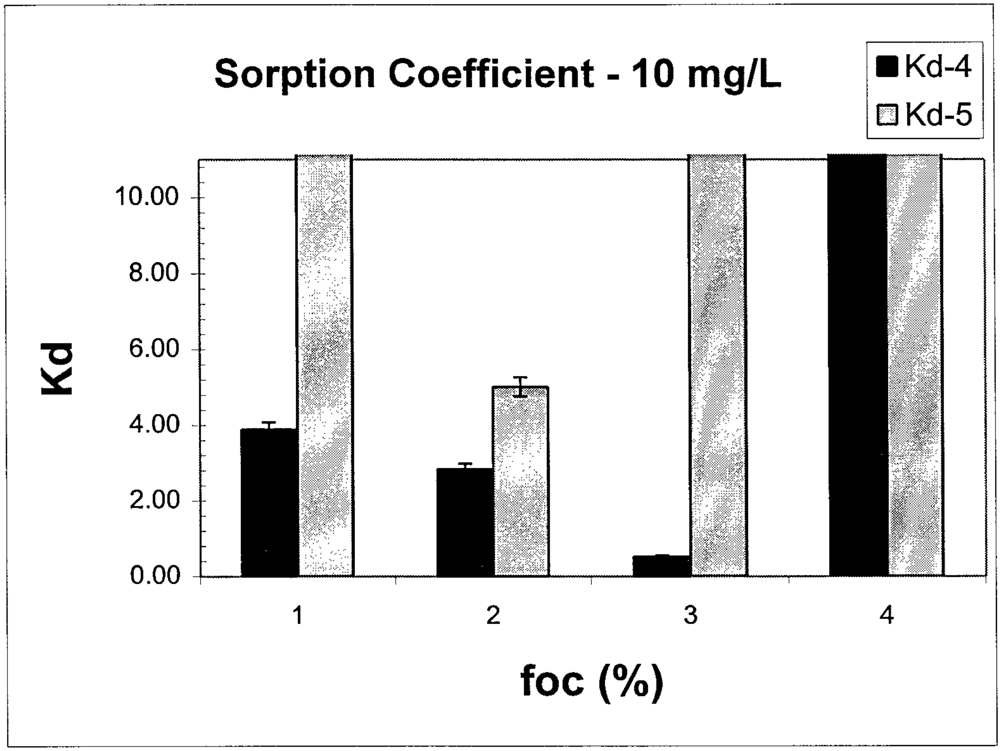
Brackets indicate 5% window within isomer type
Numbers reflect average Kd values



10 mg/L

		foc	Kd-4	Kd-5
1	Westove	0.90%	3.89	9401
2	DIA	1.37%	2.84	5.02
3	Treated	5.25%	0.5	16860
4	Untreate	5.25%	32.8	55.2

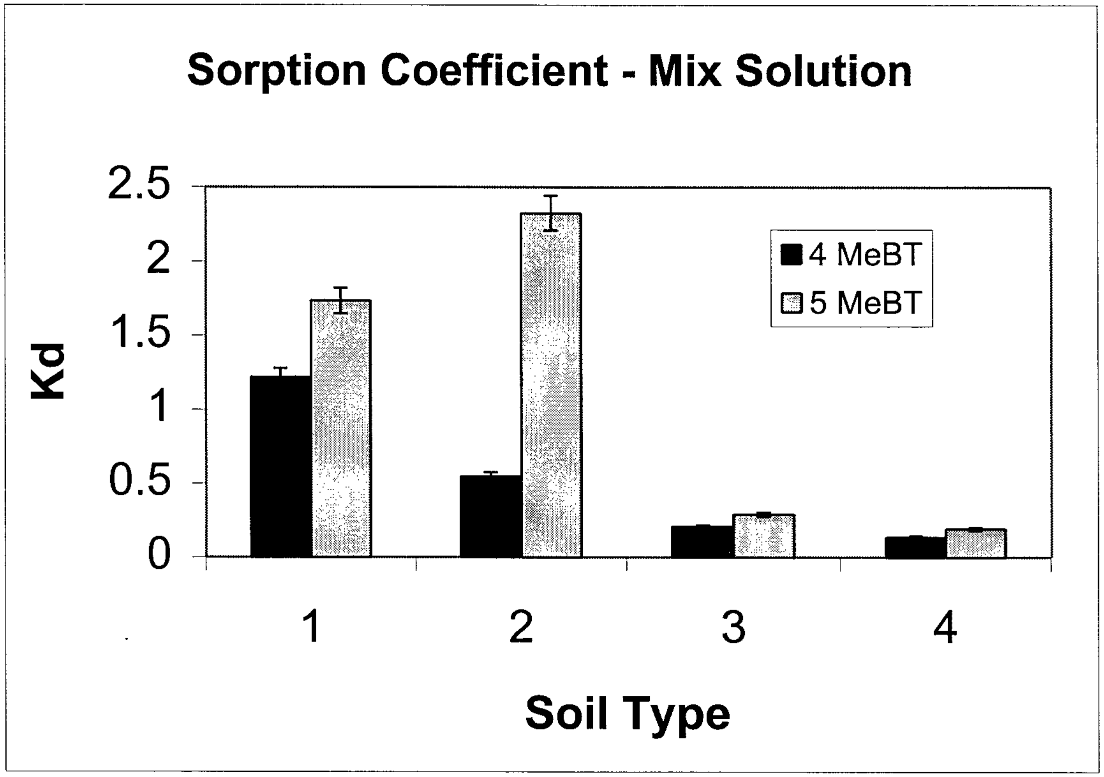
Brackets indicate 5% window within isomer type
Numbers reflect average Kd values



100 mg/L MeBT - 1000 mg/L PG (Mix)

		foc	Kd-4	Kd-5
1	Untreate	5.25%	1.219	1.735
2	Treated	5.25%	0.547	2.325
3	DIA	1.37%	0.208	0.291
4	Westove	0.90%	0.136	0.193

Brackets indicate 5% window within isomer type
Numbers reflect average Kd values

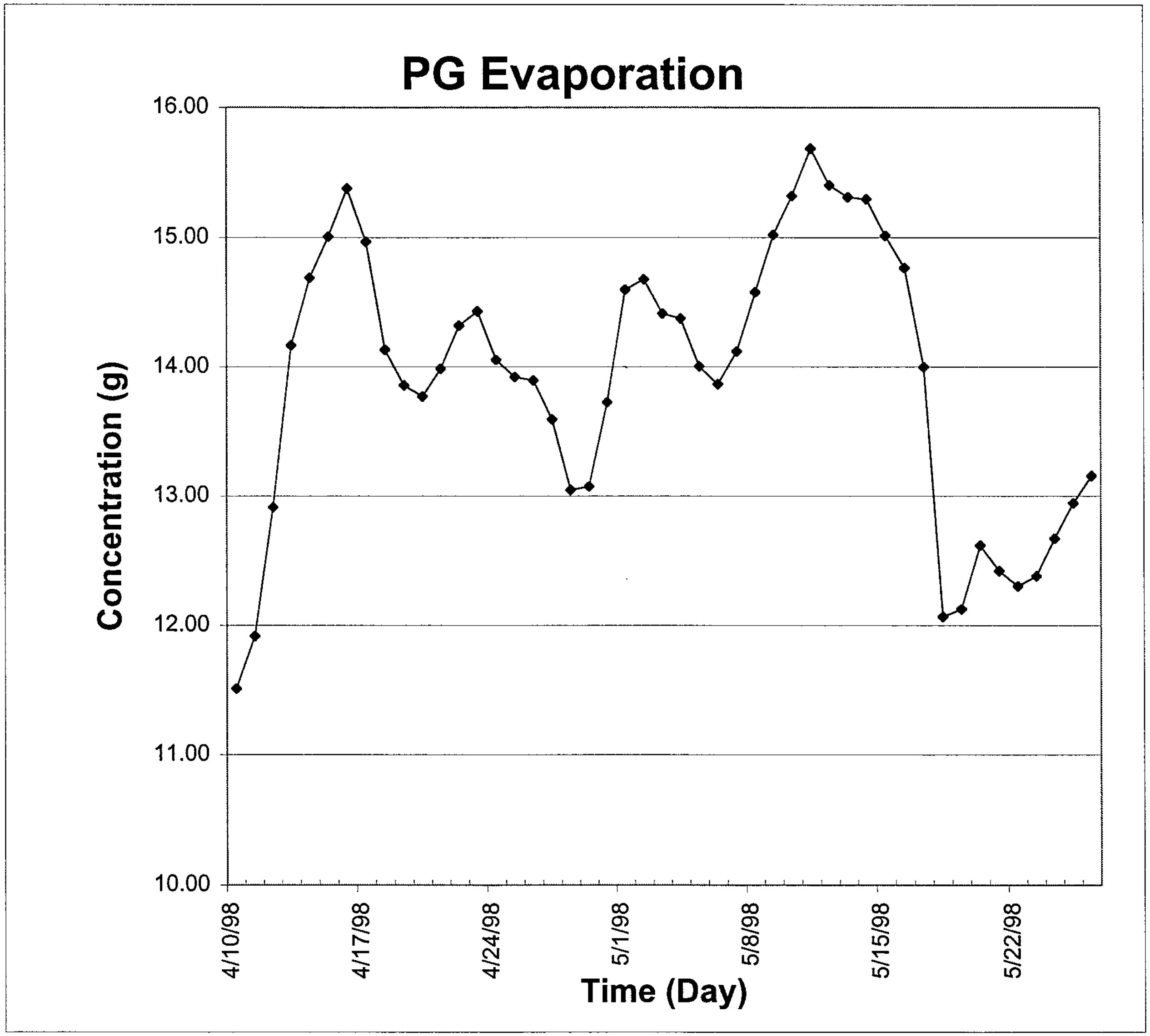


Appendix C

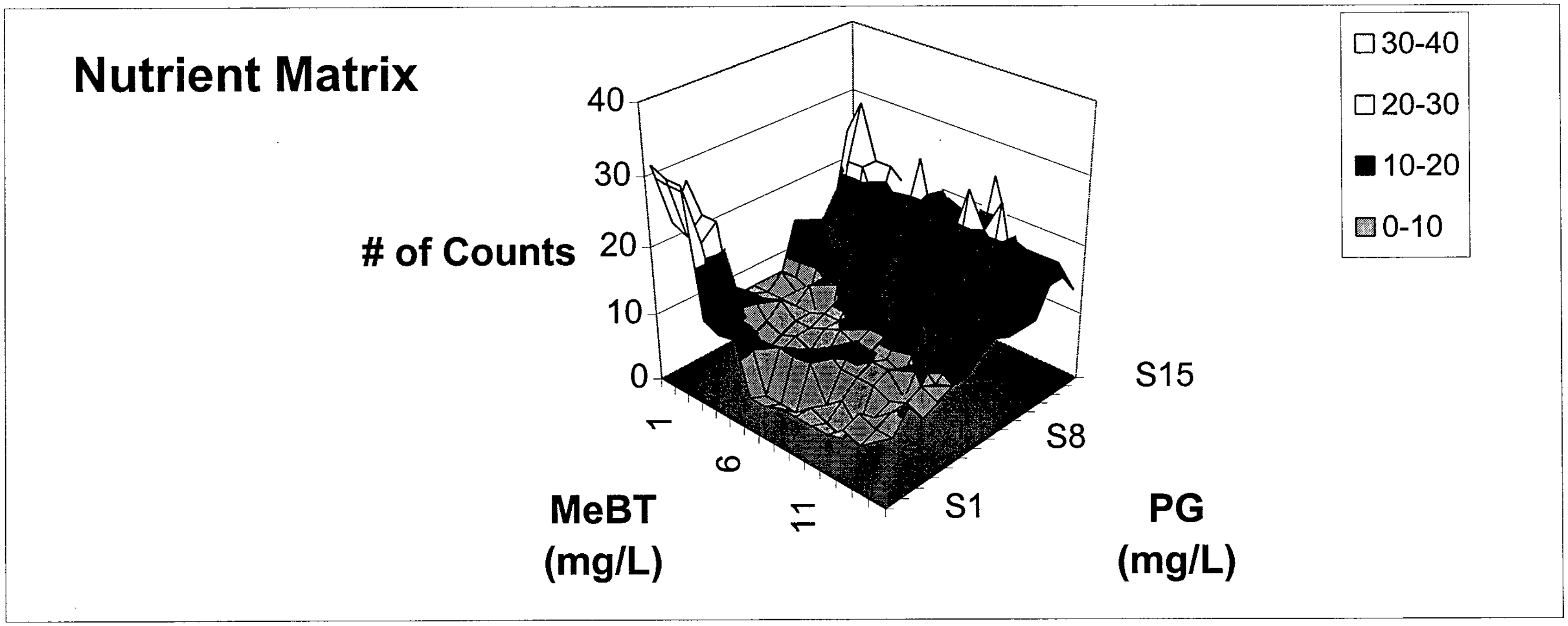
Preliminary Experiments

for PG and MeBT

DATE	TIME	WEIGHT	DIFF
10-Apr	1015	11.508	
11-Apr	1200	11.915	0.407
12-Apr	1600	12.912	0.997
13-Apr	1200	14.164	1.252
14-Apr	1300	14.686	0.522
15-Apr	1830	15.005	0.319
16-Apr	1400	15.377	0.372
17-Apr	1000	14.965	-0.412
18-Apr	1600	14.132	-0.833
19-Apr	1100	13.856	-0.276
20-Apr	1600	13.771	-0.085
21-Apr	1100	13.986	0.215
22-Apr	1615	14.318	0.332
23-Apr	1530	14.429	0.111
24-Apr	1630	14.055	-0.374
25-Apr	1400	13.92	-0.135
26-Apr	1130	13.895	-0.025
27-Apr	1145	13.593	-0.302
28-Apr	1630	13.046	-0.547
29-Apr	1700	13.074	0.028
30-Apr	1200	13.725	0.651
1-May	930	14.595	0.87
2-May	1100	14.676	0.081
3-May	1300	14.412	-0.264
4-May	1445	14.374	-0.038
5-May	1500	14.002	-0.372
6-May	1700	13.866	-0.136
7-May	1100	14.118	0.252
8-May	1800	14.576	0.458
9-May	1300	15.02	0.444
10-May	1500	15.318	0.298
11-May	1700	15.683	0.365
12-May	1100	15.4	-0.283
13-May	1800	15.311	-0.089
14-May	1400	15.295	-0.016
15-May	1200	15.012	-0.283
16-May	2100	14.765	-0.247
17-May	1100	13.998	-0.767
18-May	1600	12.066	-1.932
19-May	1800	12.123	0.057
20-May	1700	12.617	0.494
21-May	1600	12.419	-0.198
22-May	2200	12.302	-0.117



	MeBT														
PG	**0 mg/L**			**0.1 mg/L**			**1 mg/L**			**10 mg/L**			**100 mg/L**		
0 mg/L	32	31	31	13	12	14	5	5	6	6	6	6	8	7	9
	23	22	22	13	10	12	4	4	4	6	5	4	9	8	8
	28	24	24	11	11	9	10	11	10	5	7	4	7	9	11
0.1 mg/L	11	10	10	7	6	7	8	9	11	9	9	9	8	9	8
	10	11	11	8	7	8	7	7	7	12	10	10	7	10	9
	8	9	9	10	8	8	9	10	9	9	9	8	11	9	10
1 mg/L	8	8	8	8	8	9	9	11	10	10	12	11	11	11	10
	8	10	8	10	1	10	12	11	11	11	12	11	12	11	12
	8	8	7	10	10	10	12	11	12	12	10	10	12	12	13
10 mg/L	15	14	13	14	11	12	12	13	15	12	14	14	12	11	12
	14	15	12	11	11	11	13	13	11	13	12	11	11	12	12
	13	11	11	12	12	12	13	12	11	13	13	12	12	13	12
100 mg/L	15	22	22	16	20	18	18	16	17	25	20	25	13	13	16
	25	30	22	22	20	25	15	13	15	16	14	15	15	14	16
	20	19	18	17	20	15	19	18	14	25	17	16	16	16	13



Appendix D

Calibration Curve Data

for MeBT Isomers

Calibration Curve Data **10/31/98**
2 Columns, ACN, 2 Peaks

Standard oncentrati	Replicate	Retention Time	4 - Area (mAu*2)	4 Average	4 Peak Std Dev	Retention Time	5 - Area (mAu*2)	5 Average	5 Peak Std Dev
1000 mg/L	1	7.891	8237.7			8.115	13252.6		
	2	7.798	8229.2			8.031	13229.9		
	3	7.790	8219.3			8.004	13208.3		
	4	7.783	8221.3			7.997	13216.9		
	5	7.777	8220.8	8225.7	7.76	7.990	13214.1	13224.4	17.66
500 mg/L	1	7.770	4170.7			7.984	6933.8		
	2	7.761	4165.5			7.974	6925.7		
	3	7.753	4165.3			7.966	6922.6		
	4	7.751	4165.1			7.963	6921.8		
	5	7.750	4164.8	4166.3	2.48	7.959	6920.2	6924.8	5.40
100 mg/L	1	7.745	919.0			7.959	1538.8		
	2	7.742	917.6			7.956	1536.9		
	3	7.733	917.4	918.0	0.87	7.947	1535.2	1537.0	1.80
50 mg/L	1	7.725	461.2			7.939	773.5		
	2	7.718	460.6			7.932	771.8		
	3	7.709	459.7	460.5	0.75	7.922	771.0	772.1	1.28
10 mg/L	1	7.701	119.6			7.916	200.2		
	2	7.695	119.8			7.908	201.6		
	3	7.685	120.4	119.9	0.42	7.897	201.4	201.1	0.76
5 mg/L	1	7.638	68.1			7.846	113.4		
	2	7.630	67.6			7.837	113.0		
	3	7.622	68.4			7.828	113.8		
	4	7.614	68.7			7.819	114.2		
	5	7.607	68.5	68.3	0.43	7.811	113.6	113.6	0.45
1 mg/L	1	7.678	42.4			7.892	70.7		
	2	7.668	41.4			7.881	70.0		
	3	7.661	41.9			7.873	70.6		
	4	7.653	41.7			7.862	70.1		
	5	7.648	41.3	41.7	0.44	7.855	70.3	70.3	0.30
0 mg/L	1		4.8				40.0		
	2		5.0				5.0		
	3		4.0				23.0		
	4		6.2				16.5		
	5		4.1	4.8	0.9		18.0	20.5	12.74

Avg Retention Time, **7.714** Avg Retention Time, 5 = **7.926**
Retention Time Difference = **0.213**

Variance at low concentration
Var = Std Dev^2
Var = 195.53
Std Dev = 13.98

Limit of Detection, LOD
LOD = 3 * Std Dev
LOD = 41.95
slope = 8.182

4 MeBT LOD of appro **5.127** **mg/L**

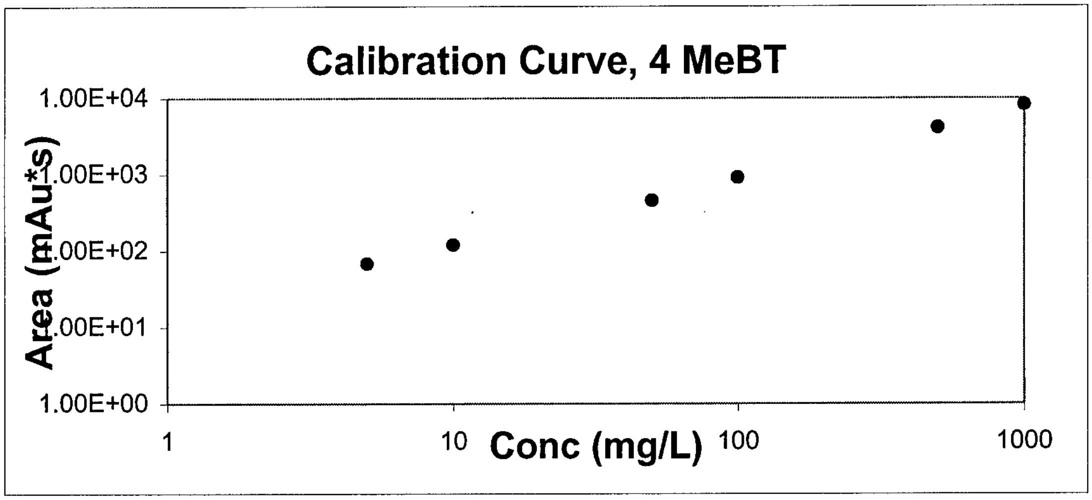
Variance at low concentration
Var = Std Dev^2
Var = 519.97
Std Dev = 22.80

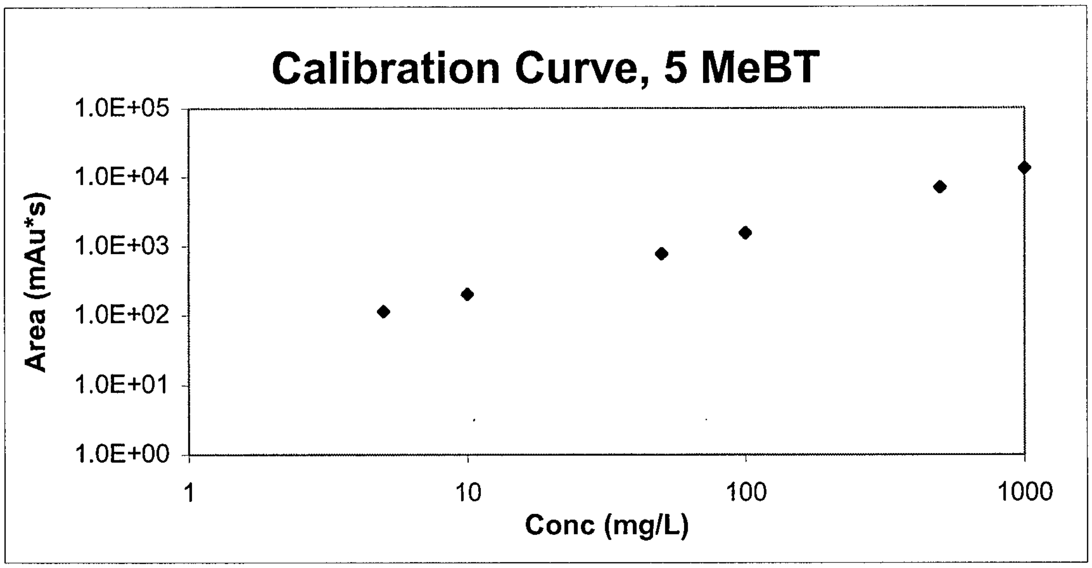
Limit of Detection, LOD
LOD = 3 * Std Dev
LOD = 68.41
slope = 13.19

5 MeBT LOD of appro **5.186** **mg/L**

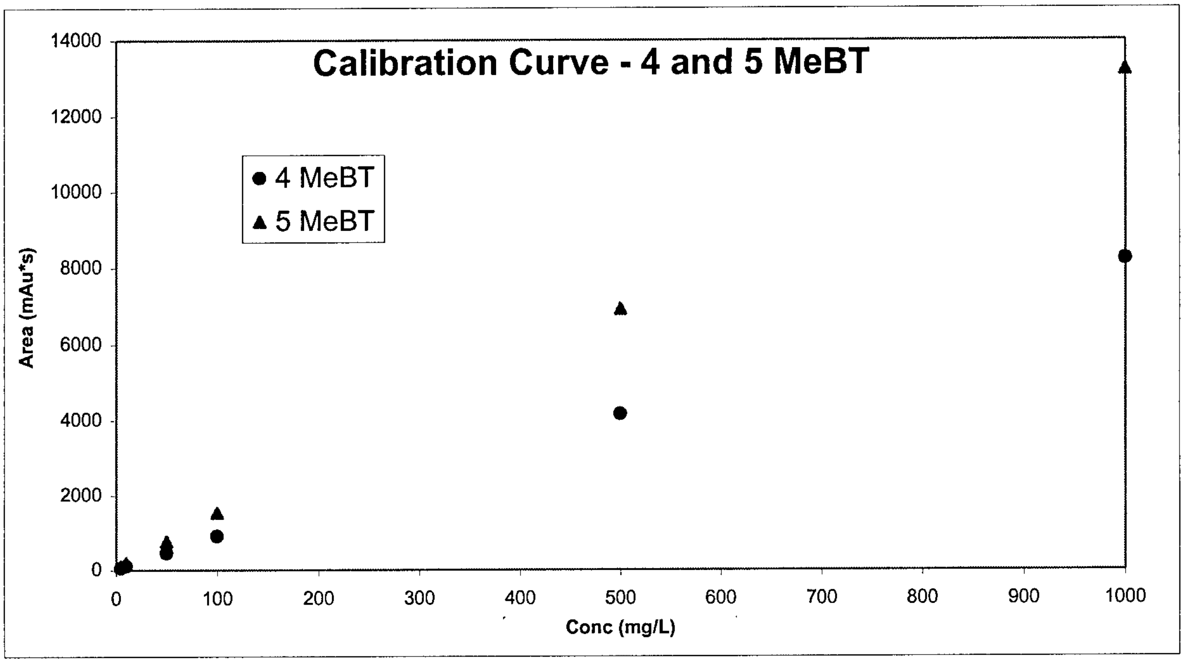
		4	4	5	5
	Standard	Avg	3 Std Dev	Avg	3 Std Dev
	1000	8225.7	23.27	13224.4	52.97
	500	4166.3	7.45	6924.8	16.21
	100	918.0	2.62	1537.0	5.40
	50	460.5	2.26	772.1	3.83
	10	119.9	1.25	201.1	2.27
Below LOD	5	68.3	1.29	113.6	1.35
Below LOD	1	41.7	1.32	70.3	0.91
Below LOD	0	4.8	2.7	20.5	38.21

R Square 0.999907





			High	Low	Close			High	Low	Close
	4	4	4	4	4	5	5	5	5	5
Standard	Std Dev	3 sigma	+3 sigma	-3 sigma	Avg	Std Dev	3 sigma	+3 sigma	-3 sigma	Avg
1000	7.76	23.27	8248.9	8202.4	8225.7	17.66	52.97	13277.3	13171.4	13224.4
500	2.48	7.45	4173.7	4158.8	4166.3	5.40	16.21	6941.0	6908.6	6924.8
100	0.87	2.62	920.6	915.4	918.0	1.80	5.40	1542.4	1531.6	1537.0
50	0.75	2.26	462.8	458.2	460.5	1.28	3.83	775.9	768.3	772.1
10	0.42	1.25	121.2	118.7	119.9	0.76	2.27	203.3	198.8	201.1
5	0.43	1.29	69.6	67.0	68.3	0.45	1.35	115.0	112.3	113.6
1	0.44	1.32			41.7	0.30				70.3
0	0.9	2.65			4.8	12.74				20.5



Appendix E

Wright-Patterson AFB Soil

Untreated Sample Analysis

Appendix E

Wright-Patterson AFB Soil

4- MeBT

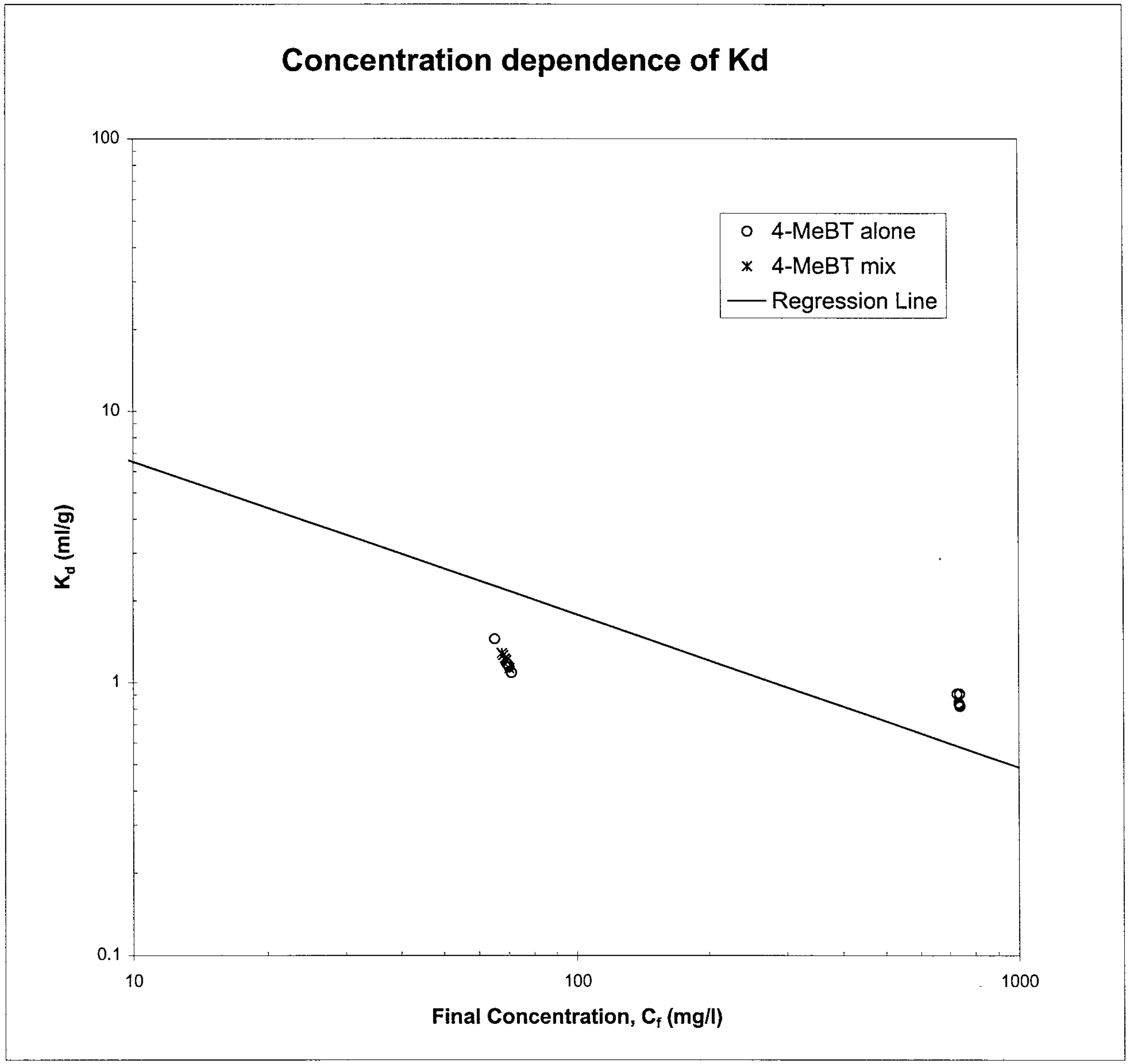
4-MeBT Data

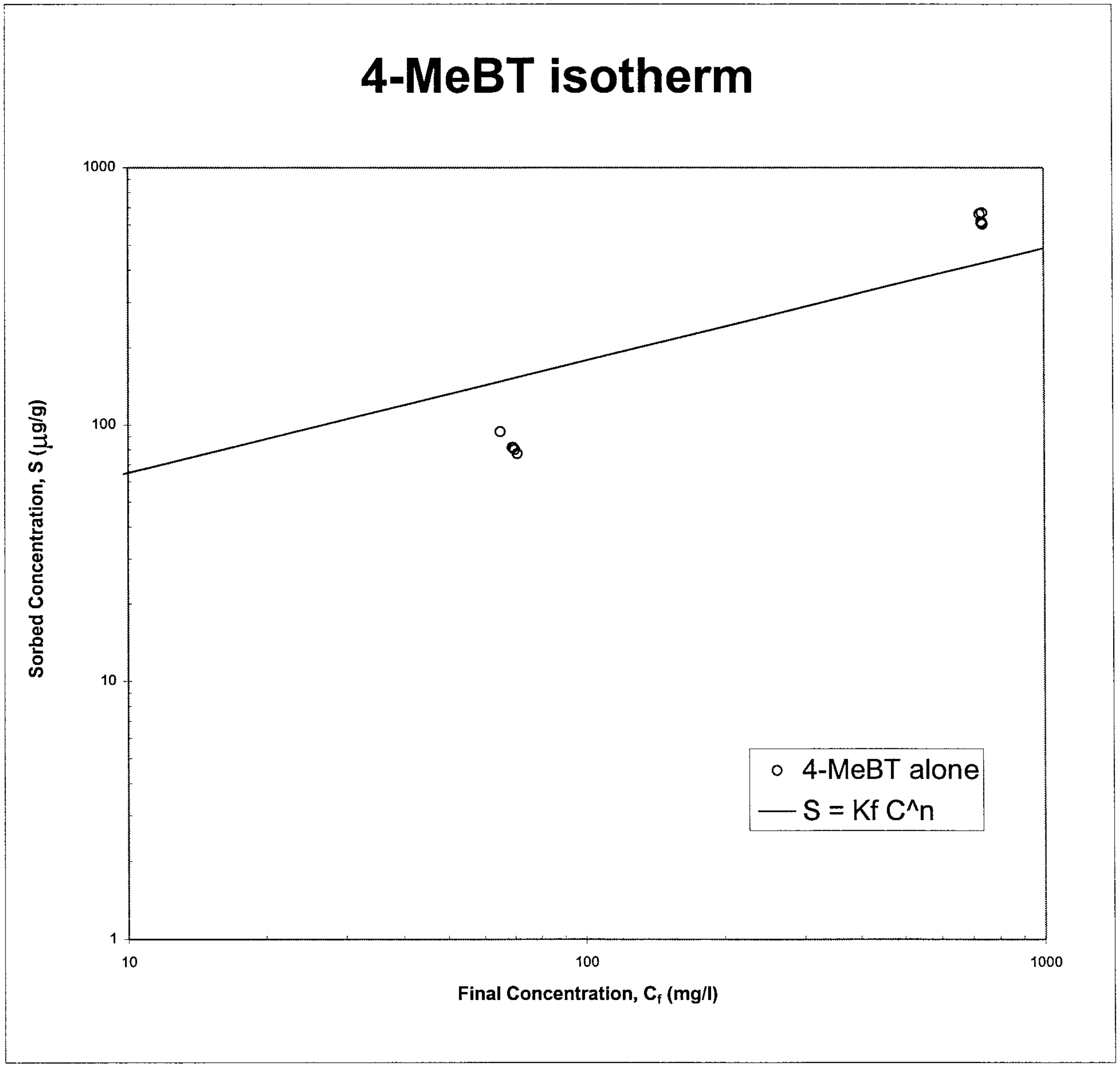
Moisture Content of soil 0.105

Outliers identified in bold

	all data	with 10 mg/L		
slope	0.8587	0.4373	n =	0.859
intercept	0.3385	1.3754	Kf =	2.180
r^2	0.9948	0.8883		

Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	28.181	38.187	10.006	61.775	57.695	738.63	9.055	24.539	961.25	603.289	0.817	2.78053	2.86843
1000	Bottle 2	28.309	38.318	10.009	63.981	59.845	736.87	9.058	26.614	964.26	668.132	0.907	2.82486	2.86739
1000	Bottle 3	28.453	38.468	10.015	62.056	59.129	735.77	9.063	24.540	961.22	610.421	0.830	2.78563	2.86674
1000	Bottle 4	28.080	38.087	10.007	61.715	57.549	733.93	9.056	24.579	961.31	617.132	0.841	2.79038	2.86565
1000	Bottle 5	28.287	38.291	10.004	62.819	57.725	728.04	9.053	25.479	962.69	660.366	0.907	2.81978	2.86216
100	Bottle 1	28.327	38.333	10.006	64.78	63.068	69.63	9.055	27.398	96.53	81.389	1.169	1.91056	1.8428
100	Bottle 2	28.180	38.181	10.001	64.594	62.793	70.09	9.051	27.363	96.53	79.928	1.140	1.9027	1.84566
100	Bottle 3	28.164	38.171	10.007	64.644	62.803	71.07	9.056	27.424	96.53	77.106	1.085	1.88709	1.85169
100	Bottle 4	28.316	38.319	10.003	64.504	62.487	65.11	9.052	27.136	96.50	94.085	1.445	1.97352	1.81365
100	Bottle 5	27.923	37.932	10.009	64.135	62.165	69.29	9.058	27.154	96.50	81.563	1.177	1.91149	1.84067
10	Bottle 1	27.421	37.424	10.003	63.934	61.603	0.82	9.052	27.461	9.65	26.797	32.680	1.42809	-0.0862
10	Bottle 2	27.877	37.878	10.001	64.202	62.449	0.83	9.051	27.274	9.65	26.584	32.029	1.42462	-0.0809
10	Bottle 3	27.316	37.324	10.008	64.252	62.428	0.84	9.057	27.879	9.66	27.146	32.317	1.43371	-0.0757
10	Bottle 4	27.816	37.823	10.007	64.252	62.414	0.77	9.056	27.380	9.65	26.856	34.877	1.42904	-0.1135
10	Bottle 5	27.656	37.656	10.000	63.885	62.003	0.82	9.050	27.179	9.65	26.520	32.342	1.42358	-0.0862
100	Mix 1	28.296	38.298	10.002	64.633	62.651	70.23	9.052	27.285	96.52	79.240	1.128		
100	Mix 2	27.853	37.856	10.003	64.030	62.264	67.59	9.052	27.125	96.50	86.612	1.281		
100	Mix 3	28.185	38.192	10.007	64.635	62.815	69.05	9.056	27.394	96.53	83.121	1.204		
100	Mix 4	27.960	37.968	10.008	64.242	62.371	68.59	9.057	27.225	96.51	83.917	1.223		
100	Mix 5	27.916	37.919	10.003	64.171	62.400	68.03	9.052	27.203	96.51	85.569	1.258		
							1				23.737	23.737		
							1000				486.81	0.487		


Concentration dependence of Kd
100
10
1
0.1
K_d (ml/g)
10
100
1000
Final Concentration, C_f (mg/l)
○ 4-MeBT alone
✱ 4-MeBT mix
— Regression Line


4-MeBT isotherm
Sorbed Concentration, S (µg/g)
1000
100
10
1
Final Concentration, C_f (mg/l)
10
100
1000
○ 4-MeBT alone
— S = Kf C^n

Appendix E

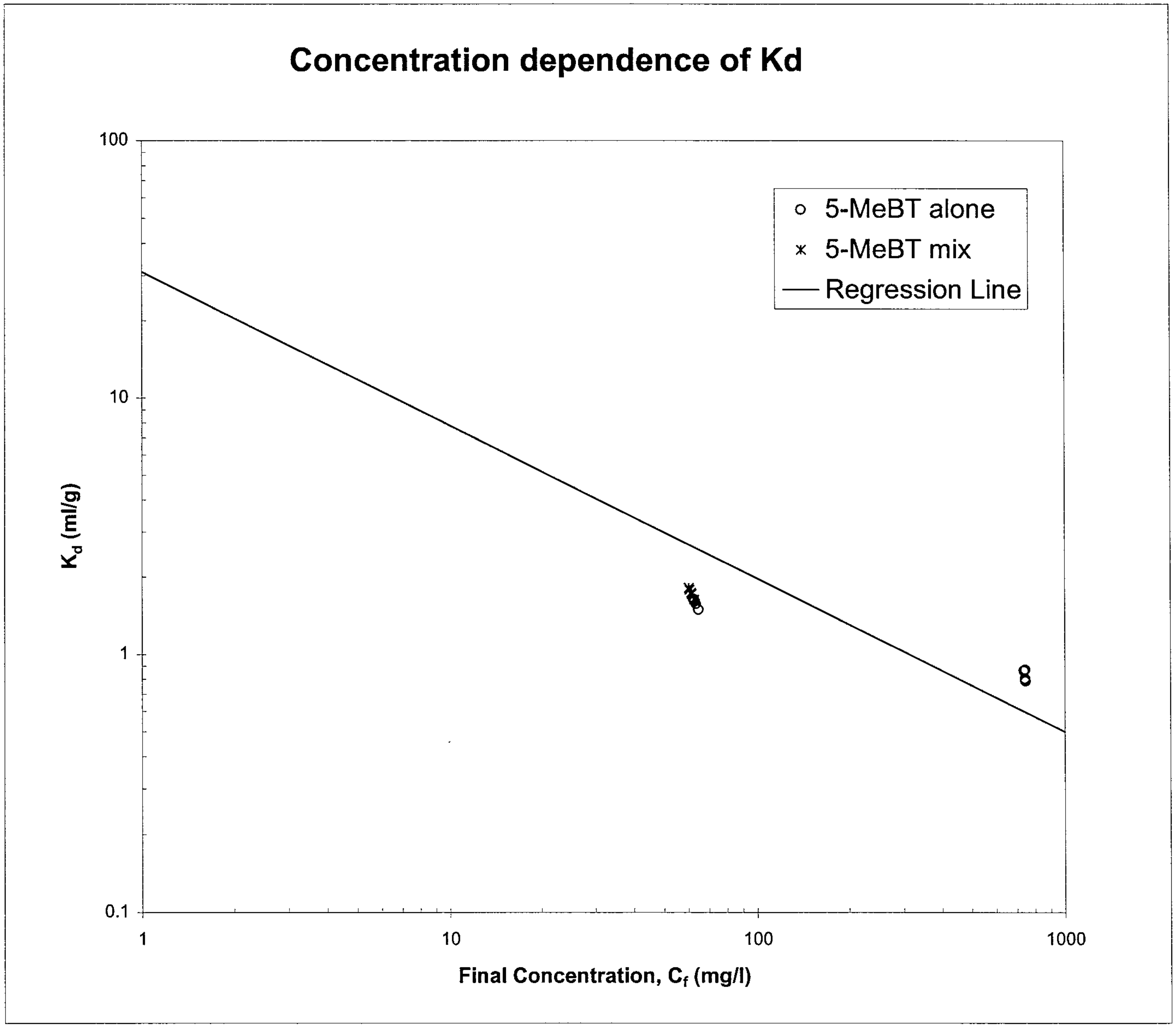
Wright-Patterson AFB Soil

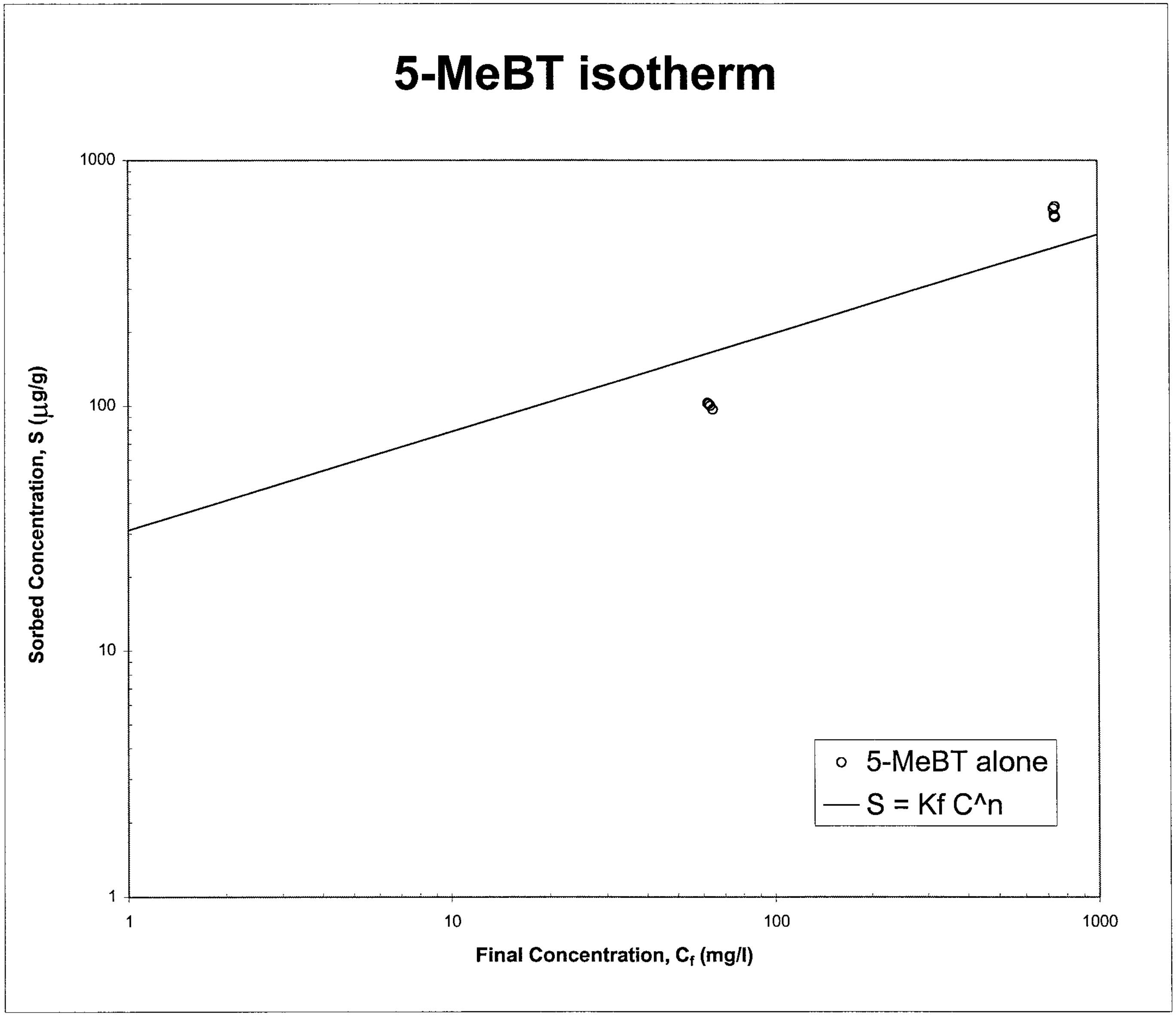
5-MeBT

5-MeBT Data
Moisture Content of soil 0.105
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.7325	0.402	n =	0.732
intercept	0.6839	1.491	Kf =	4.829
r^2	0.9983	0.922		

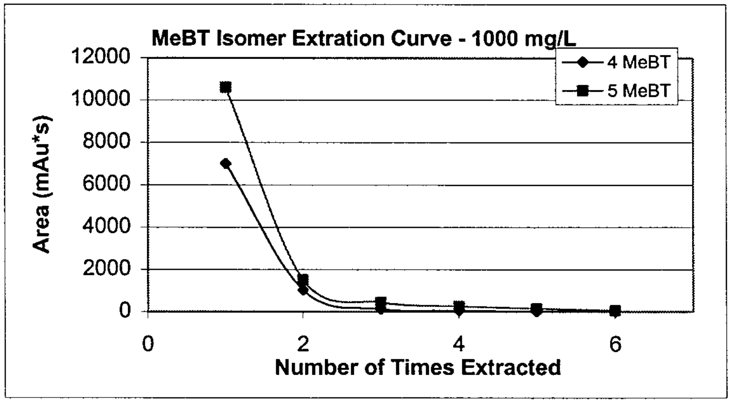
Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	28.181	38.187	10.006	61.775	57.695	744.8	9.055	24.539	961.25	586.569	0.788	2.76832	2.87204
1000	Bottle 2	28.309	38.318	10.009	63.981	59.845	743.81	9.058	26.614	964.26	647.740	0.871	2.8114	2.87146
1000	Bottle 3	28.453	38.468	10.015	62.056	59.129	742.16	9.063	24.540	961.22	593.120	0.799	2.77314	2.8705
1000	Bottle 4	28.080	38.087	10.007	61.715	57.549	741.46	9.056	24.579	961.31	596.695	0.805	2.77575	2.87009
1000	Bottle 5	28.287	38.291	10.004	62.819	57.725	736.75	9.053	25.479	962.69	635.854	0.863	2.80336	2.86732
100	Bottle 1	28.327	38.333	10.006	64.78	63.068	62.91	9.055	27.398	96.53	101.721	1.617	2.00741	1.79872
100	Bottle 2	28.180	38.181	10.001	64.594	62.793	63.48	9.051	27.363	96.53	99.913	1.574	1.99962	1.80264
100	Bottle 3	28.164	38.171	10.007	64.644	62.803	64.65	9.056	27.424	96.53	96.548	1.493	1.98474	1.81057
100	Bottle 4	28.316	38.319	10.003	64.504	62.487	62.31	9.052	27.136	96.50	102.479	1.645	2.01063	1.79456
100	Bottle 5	27.923	37.932	10.009	64.135	62.165	62.37	9.058	27.154	96.50	102.308	1.640	2.00991	1.79498
10	Bottle 1	27.421	37.424	10.003	63.934	61.603	0.53	9.052	27.461	9.65	27.677	52.221	1.44212	-0.2757
10	Bottle 2	27.877	37.878	10.001	64.202	62.449	0.51	9.051	27.274	9.65	27.548	54.016	1.44009	-0.2924
10	Bottle 3	27.316	37.324	10.008	64.252	62.428	0.54	9.057	27.879	9.66	28.069	51.980	1.44823	-0.2676
10	Bottle 4	27.816	37.823	10.007	64.252	62.414	0.46	9.056	27.380	9.65	27.793	60.419	1.44393	-0.3372
10	Bottle 5	27.656	37.656	10.000	63.885	62.003	0.48	9.050	27.179	9.65	27.541	57.378	1.43999	-0.3188
100	Mix 1	28.296	38.298	10.002	64.633	62.651	62.65	9.052	27.285	96.52	102.089	1.630		
100	Mix 2	27.853	37.856	10.003	64.030	62.264	60.52	9.052	27.125	96.50	107.796	1.781		
100	Mix 3	28.185	38.192	10.007	64.635	62.815	61.34	9.056	27.394	96.53	106.443	1.735		
100	Mix 4	27.960	37.968	10.008	64.242	62.371	61.44	9.057	27.225	96.51	105.410	1.716		
100	Mix 5	27.916	37.919	10.003	64.171	62.400	60.20	9.052	27.203	96.51	109.098	1.812		
							1				30.98	30.984		
							1000				498.43	0.498		


Concentration dependence of Kd
5-MeBT alone
5-MeBT mix
Regression Line
100
10
1
0.1
K_d (ml/g)
1
10
100
1000
Final Concentration, C_f (mg/l)


5-MeBT isotherm
Sorbed Concentration, S (μg/g)
1000
100
10
1
1
10
100
1000
Final Concentration, C_f (mg/l)
○ 5-MeBT alone
— S = Kf C^n

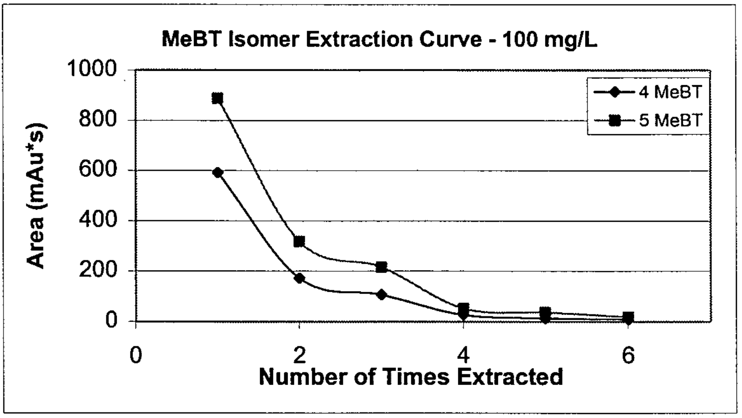
1000 mg/L	0		8225.7		13224.4	4 MeBT	5 MeBT
Water	0.5	7.019	6994.7	7.207	10598.5	85%	80%
1 Meth	1 hr	7.026	1015.6	7.215	1523.7	12%	12%
2 Meth	6 hr	7.025	121.8	7.211	437.1	1%	3%
3 Meth	24 hr	7.018	55.7	7.205	261.8	1%	2%
4 Meth	48 hr	7.011	20.1	7.201	149.6	0%	1%
5 Meth	72 hr	7.007	12.5	7.198	62.1	0%	0%
Sum Recovered			8220.4		13032.8		
Percent MeBT Recovered			**99.94%**		**98.55%**		

		Refilled	Difference
Empty	28.287		
w/ Soil only	38.291		
Soil Weight (air-dried)	10.004		
w/ Soil and MeBT mix	62.819		
After Initial Extraction	57.725		5.094
of water/MeBT		63.294	
1 Meth	42.314	60.872	20.980
2 Meth	43.111	61.554	17.761
3 Meth	43.872	61.217	17.682
4 Meth	43.457	61.641	17.760
5 Meth	43.377	61.521	18.264
6 Meth	43.689		17.832



100 mg/L	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.072	591.8	7.264	887.4	64%	58%
1 Meth	1 hr	7.028	171.9	7.214	318.3	19%	21%
2 Meth	6 hr	7.223	105.6	7.439	215.7	12%	14%
3 Meth	24 hr	7.072	26.4	7.268	52.0	3%	3%
4 Meth	48 hr	7.148	13.1	7.299	37.1	1%	2%
5 Meth	72 hr	7.102	8.5	7.231	17.6	1%	1%
Sum Recovered			917.3		1528.1		
Percent MeBT Recovered			**99.92%**		**99.42%**		

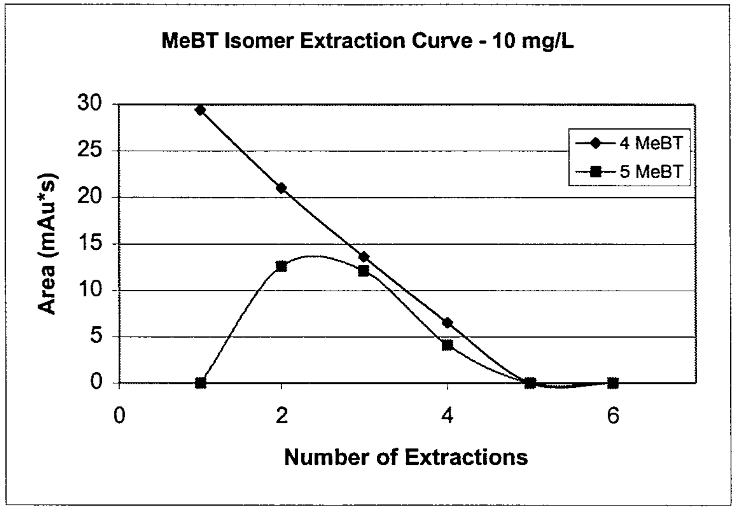
		Refilled	Difference
Empty	27.923		
w/ Soil only	37.932		
Soil Weight (air-dried)	10.009		
w/ Soil and MeBT mix	64.135		
After Initial Extraction	62.165		1.97
of water/MeBT		64.267	
1 Meth	62.473	64.512	1.794
2 Meth	62.653	64.399	1.859
3 Meth	62.431	64.133	1.968
4 Meth	62.298	64.774	1.835
5 Meth	62.905		1.869



10 mg/L	0		119.9		201.1	4 MeBT	5 MeBT
Water	0.5	7.142	29.4	7.35	0.0	25%	0%
1 Meth	1 hr	7.118	21.0	7.307	12.6	18%	6%
2 Meth	6 hr	7.203	13.6	7.402	12.1	11%	6%
3 Meth	24 hr	7.189	6.5	7.382	4.1	5%	2%
4 Meth	48 hr	7.135	0	7.35	0	0%	0%
5 Meth	72 hr	7.135	0	7.35	0	0%	0%
Sum Recovered			70.5		28.8		
Percent MeBT Recovered			**58.80%**		**14.32%**		

Additional Spike a	Water	7.869	9.1
	Meth 1	7.899	5.0

		Refilled	Difference
Empty	27.656		
w/ Soil only	37.656		
Soil Weight (air-dried)	10.000		
w/ Soil and MeBT mix	63.885		
After Initial Extraction	62.003		1.882
of water/MeBT		64.509	
1 Meth	62.448	64.371	2.061
2 Meth	62.595	64.011	1.776
3 Meth	62.100	64.229	1.911
4 Meth	62.348	64.094	1.881
5 Meth	62.150		1.944



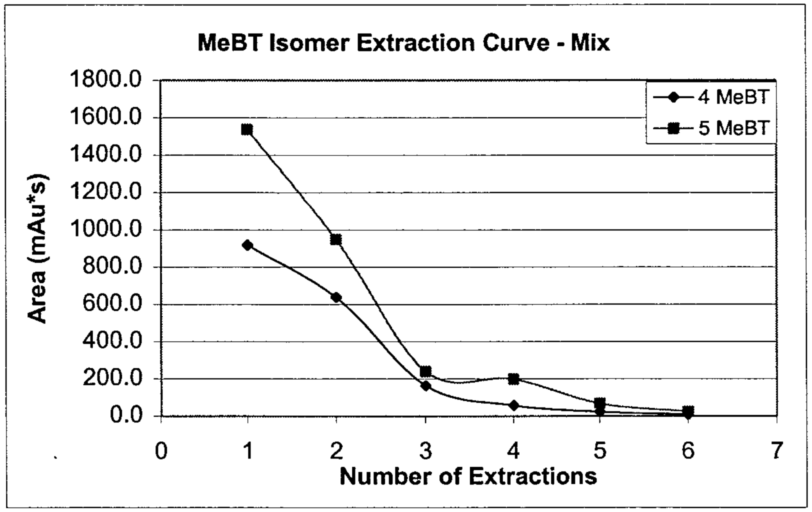
0 mg/L	0		4.8		20.5	4 MeBT	5 MeBT
Water	0.5	7.135	0.00	7.35	0.00	0%	0%
1 Meth	1 hr	7.135	0.00	7.35	0.00	0%	0%
2 Meth	6 hr	7.135	0.00	7.35	0.00	0%	0%
3 Meth	24 hr	7.135	0.00	7.35	0.00	0%	0%
4 Meth	48 hr	7.135	0.00	7.35	0.00	0%	0%
5 Meth	72 hr	7.135	0.00	7.35	0.00	0%	0%
Sum Recovered			0.00		0.00		
Percent MeBT Recovered			**0.00%**		**0.00%**		

		Refilled	Difference
Empty	26.167		
w/ Soil only	36.172		
Soil Weight (air-dried)	10.005		
w/ Soil and MeBT mix	62.594		
After Initial Extraction	58.456		4.138
of water/MeBT			
1 Meth			0.000
2 Meth			0.000
3 Meth			0.000

Mix	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.268	637.5	7.461	949.0	69%	62%
1 Meth	1 hr	7.249	162.5	7.447	239.3	18%	16%
2 Meth	6 hr	7.254	56.6	7.453	198.7	6%	13%
3 Meth	24 hr	7.251	22.3	7.45	65.4	2%	4%
4 Meth	48 hr	7.244	8.9	7.448	23.1	1%	2%
5 Meth	72 hr					0%	0%
Sum Recovered			887.83		1475.5		
Percent MeBT Recovered			**96.71%**		**96.00%**		

Additional Spike a Water
Meth 1

Empty	27.916	Refilled	Difference
w/ Soil only	37.919		
Soil Weight (air-dried)	10.003		
w/ Soil and MeBT mix	64.171		
After Initial Extraction	62.400		1.771
of water/MeBT		64.248	
1 Meth	61.411	64.190	2.837
2 Meth	62.276	64.236	1.914
3 Meth	62.196		2.040



1000 mg/L

Runs	4 MeBT			5 MeBT			
1	7.036	6103.7	738.63	7.222	10009.1	744.80	
2	7.042	6089.4	736.87	7.238	9996.6	743.81	
3	7.027	6080.5	735.77	7.211	9975.8	742.16	
4	7.026	6065.5	733.93	7.184	9967.0	741.46	
5	7.021	6017.7	728.04	7.157	9907.8	736.75	
avg	7.031	**6071.36**		7.202	**9971.26**		
conc.			**734.65**			**741.80**	Interpolated from calibration curve
Standard Deviation		33.05			39.18		
Average of 4 & 5 MeBT				**738.22**			

100 mg/L

Runs	4 MeBT			5 MeBT			
1	7.661	640.12	69.63	8.266	969.65	62.91	
2	7.736	644.71	70.09	7.946	978.26	63.48	
3	7.701	653.33	71.07	7.908	996.18	64.65	
4	7.675	598.78	65.11	7.881	960.36	62.31	
5	7.644	637.02	69.29	7.849	961.38	62.37	
avg	7.683	**634.79**		7.970	**973.17**		
conc.			**69.038**			**63.144**	Interpolated from calibration curve
Standard Deviation		21.05			14.76		
Average of 4 & 5 MeBT				**0.00**			

10 mg/L

Runs	4 MeBT			5 MeBT				Other	
1	7.247	35.03	0.82	7.439	47.02	0.53		8.346	6.24
2	7.232	35.49	0.83	7.424	45.99	0.51		8.337	6.39
3	7.217	35.66	0.84	7.409	47.23	0.54		8.307	7.32
4	7.204	33.16	0.77	7.395	43.20	0.46		8.300	7.19
5	7.191	35.39	0.82	7.382	44.17	0.48		8.276	7.65
avg	7.218	**34.95**		7.410	**45.52**				
conc.			**0.816**			**0.504**	Interpolated from calibration curve		
Standard Deviation		1.02			1.77				
Average of 4 & 5 MeBT				**0.00**					

100 mg/L MeBT / 1000 mg/L PG

Runs	4 MeBT			5 MeBT				Other	
1	7.184	645.57	70.23	7.376	965.62	62.65			
2	7.181	621.46	67.59	7.372	933.01	60.52			
3	7.183	634.77	69.05	7.374	945.53	61.34			
4	7.184	630.61	68.59	7.375	947.09	61.44		7.904	7.00
5	7.186	625.49	68.03	7.377	928.19	60.20		7.900	7.40
avg	7.184	**631.58**		7.375	**943.89**				
conc.			**68.698**			**61.23**	Interpolated from calibration curve		
Standard Deviation		9.31			14.58				
Average of 4 & 5 MeBT				**0.00**					

Below LOD

Appendix F

Wright-Patterson AFB Soil

Treated Sample Analysis

Appendix F

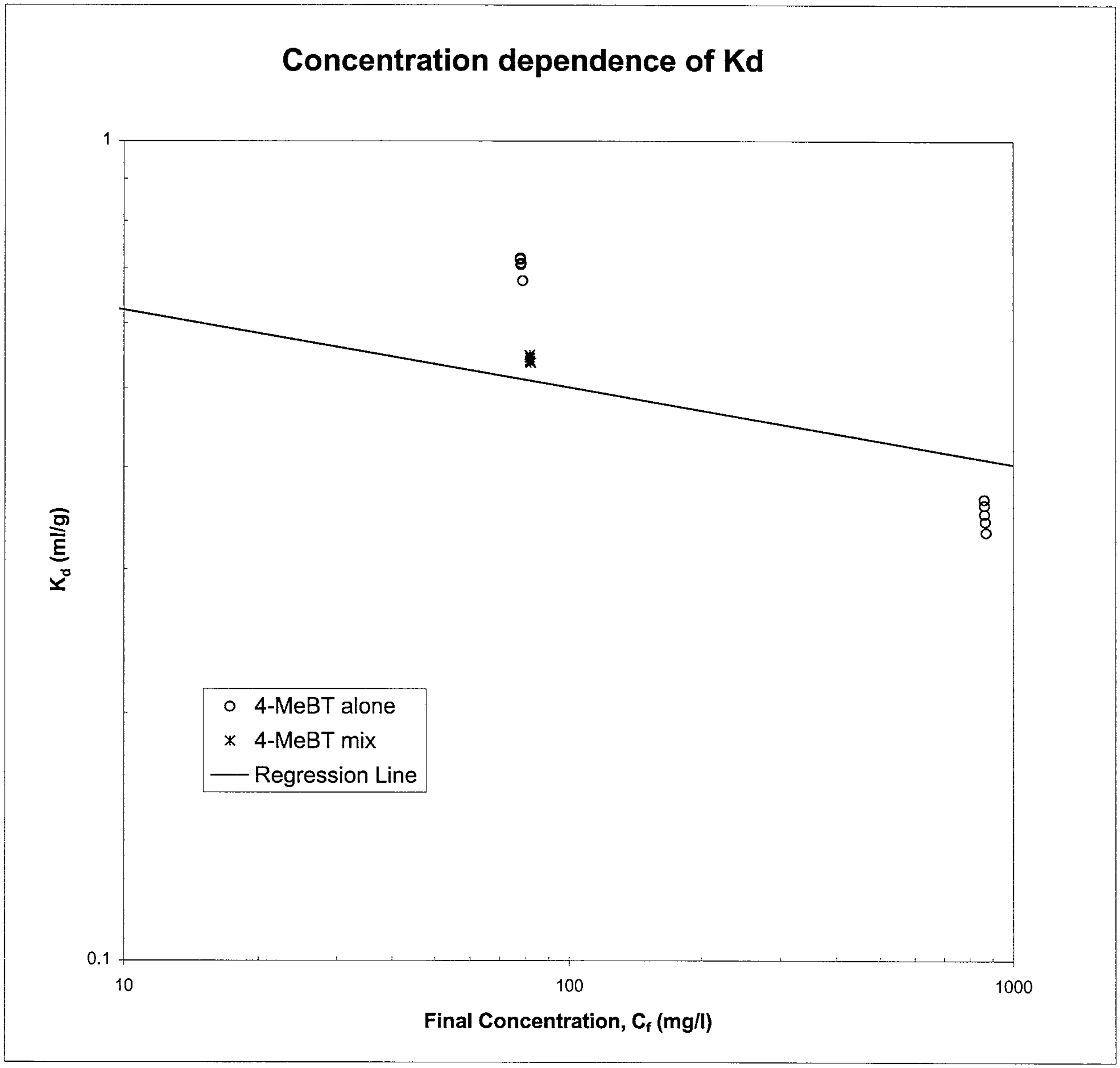
Wright-Patterson AFB Soil

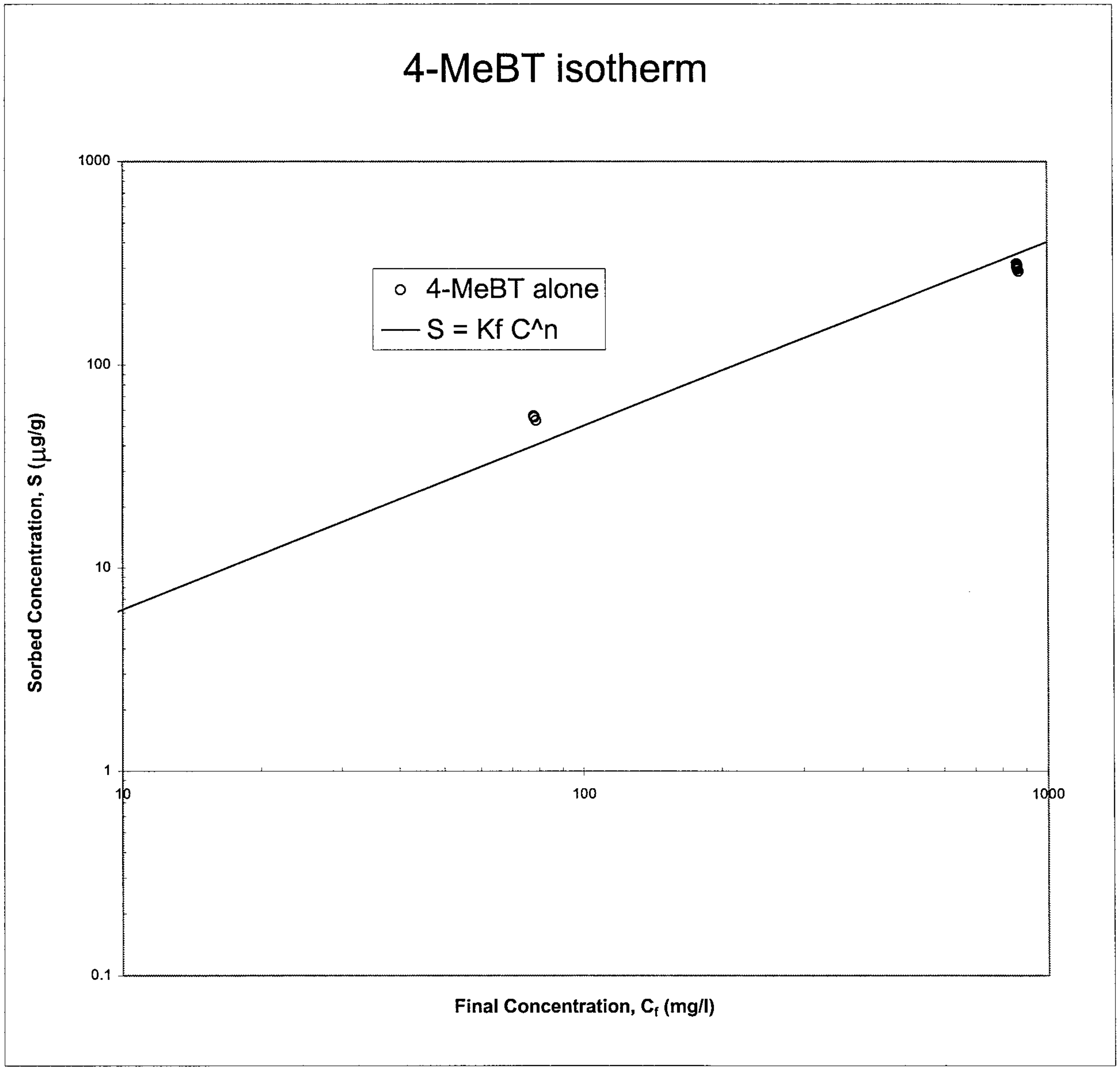
4-MeBT

4-MeBT Data
Moisture Content of soil 0.105
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.7075	0.9055	**n =**	0.7075
intercept	0.4028	-0.1113	**Kf =**	2.528
r^2	0.9990	0.9826		

Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	28.066	38.068	10.002	64.183	62.341	863.67	9.052	27.065	964.88	302.644	0.350	2.48093	2.93635
1000	Bottle 2	27.799	37.806	10.007	64.054	62.239	866.17	9.056	27.199	965.04	296.942	0.343	2.47267	2.93760
1000	Bottle 3	28.092	38.092	10.000	64.564	62.715	861.52	9.050	27.422	965.35	314.616	0.365	2.49778	2.93527
1000	Bottle 4	28.285	38.293	10.008	64.756	62.849	862.96	9.057	27.414	965.31	309.796	0.359	2.49108	2.93599
1000	Bottle 5	28.170	38.177	10.007	64.652	62.811	869.78	9.056	27.426	965.33	289.364	0.333	2.46144	2.93941
100	Bottle 1	28.264	38.264	10.000	64.730	62.831	78.2	9.050	27.416	96.53	55.543	0.710	1.74463	1.89321
100	Bottle 2	28.057	38.066	10.009	64.442	62.639	77.97	9.058	27.327	96.52	55.963	0.718	1.7479	1.89193
100	Bottle 3	28.352	38.352	10.000	64.739	62.936	78.87	9.050	27.337	96.52	53.329	0.676	1.72696	1.89691
100	Bottle 4	27.947	37.949	10.002	64.330	62.521	78.2	9.052	27.331	96.52	55.325	0.707	1.74293	1.89321
100	Bottle 5	28.502	38.506	10.004	64.929	63.198	77.95	9.053	27.374	96.53	56.170	0.721	1.7495	1.89182
10	Bottle 1	28.176	38.176	10.000	65.959	64.114	8.22	9.050	28.733	9.67	4.602	0.560	0.6629	0.91487
10	Bottle 2	27.916	37.919	10.003	64.375	62.615	8.20	9.052	27.407	9.65	4.400	0.537	0.64341	0.91381
10	Bottle 3	28.295	38.295	10.000	64.356	62.912	8.25	9.050	27.011	9.65	4.173	0.506	0.62048	0.91645
10	Bottle 4	28.066	38.066	10.000	64.645	62.869	8.15	9.050	27.529	9.65	4.578	0.562	0.66064	0.91116
10	Bottle 5	27.041	37.048	10.007	63.638	61.805	8.23	9.056	27.541	9.65	4.333	0.526	0.63677	0.91540
100	Mix 1	27.748	37.755	10.007	64.079	62.321	81.88	9.056	27.275	96.51	44.073	0.538		
100	Mix 2	27.557	37.561	10.004	63.966	62.181	81.89	9.053	27.356	96.53	44.221	0.540		
100	Mix 3	27.852	37.852	10.000	64.071	62.281	81.7	9.050	27.169	96.50	44.440	0.544		
100	Mix 4	27.665	37.672	10.007	64.291	62.492	82.09	9.056	27.570	96.55	44.024	0.536		
100	Mix 5	27.305	37.308	10.003	63.808	61.980	81.75	9.052	27.451	96.54	44.841	0.549		
							1				0.7740	0.774		
							1000				402.93	0.403		


Concentration dependence of Kd
K_d (ml/g)
1
0.1
10
100
1000
Final Concentration, C_f (mg/l)
4-MeBT alone
4-MeBT mix
Regression Line


4-MeBT isotherm
○ 4-MeBT alone
— S = Kf C^n
Sorbed Concentration, S (μg/g)
1000
100
10
1
0.1
10
100
1000
Final Concentration, C_f (mg/l)

Appendix F

Wright-Patterson AFB Soil

5-MeBT

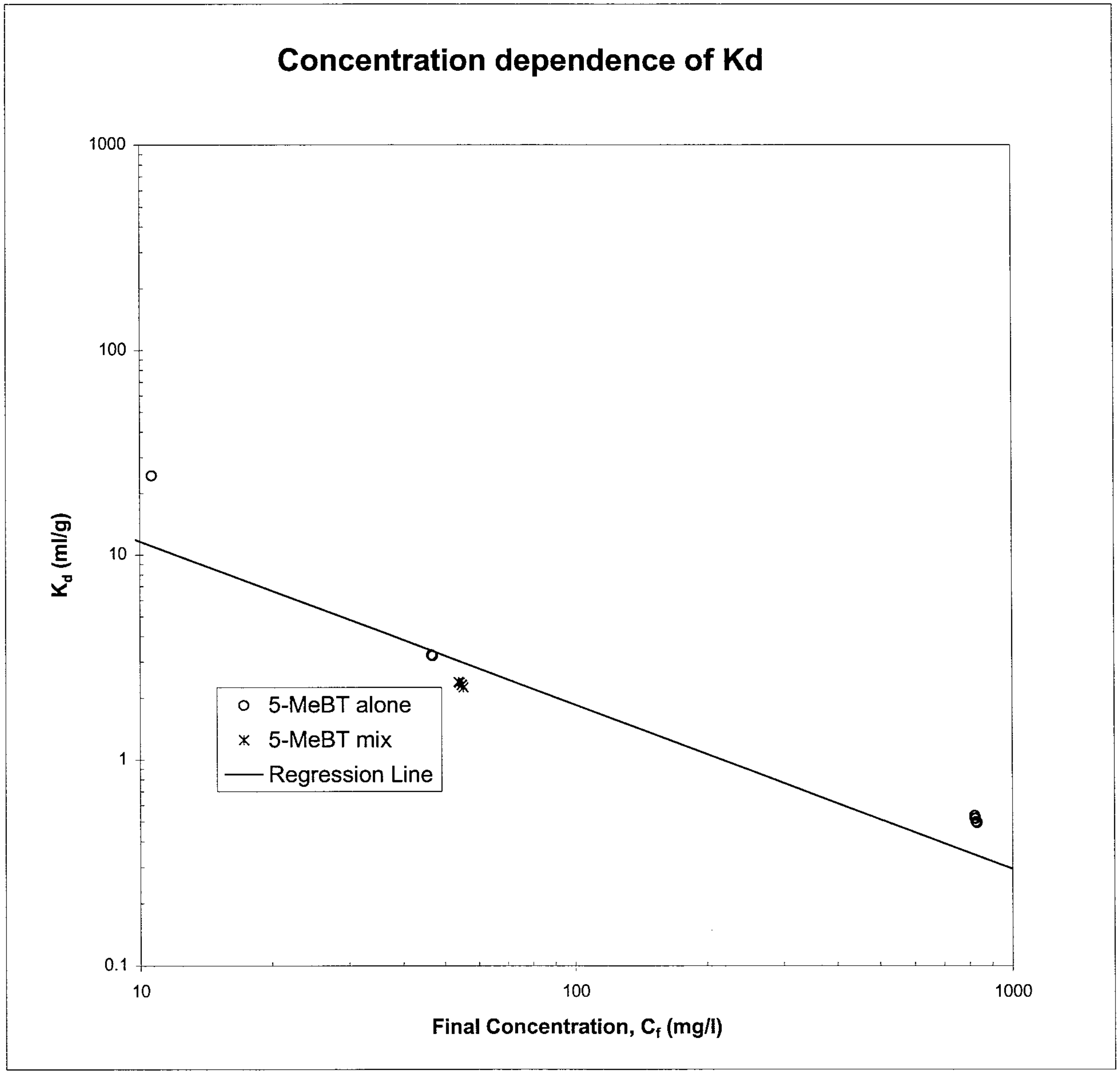
5-MeBT Data

Moisture Content of soil 0.105

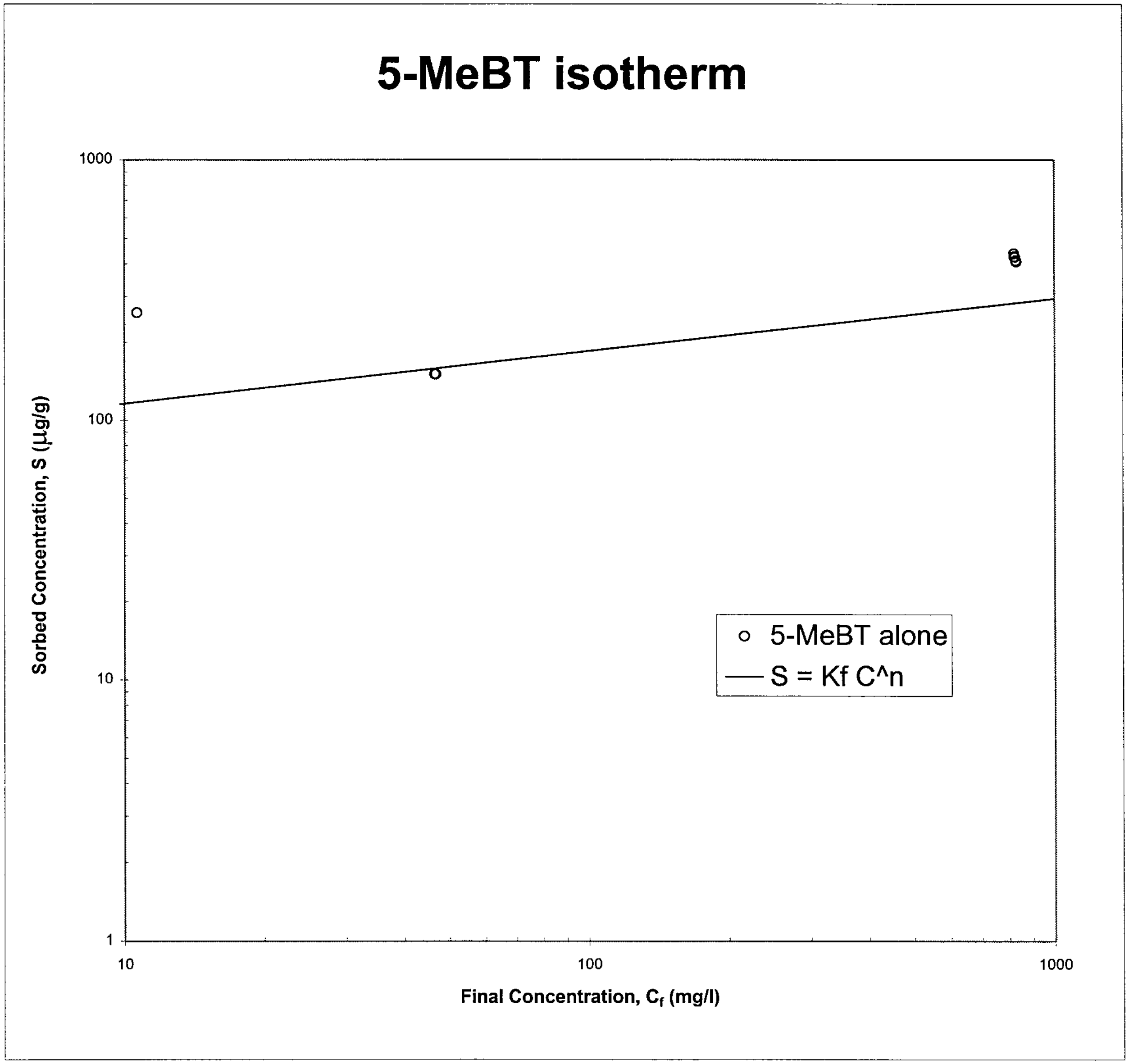
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.1253	0.2019	**n =**	0.1253
intercept	2.1925	1.8627	**Kf =**	155.79
r^2	0.3625	0.4744		

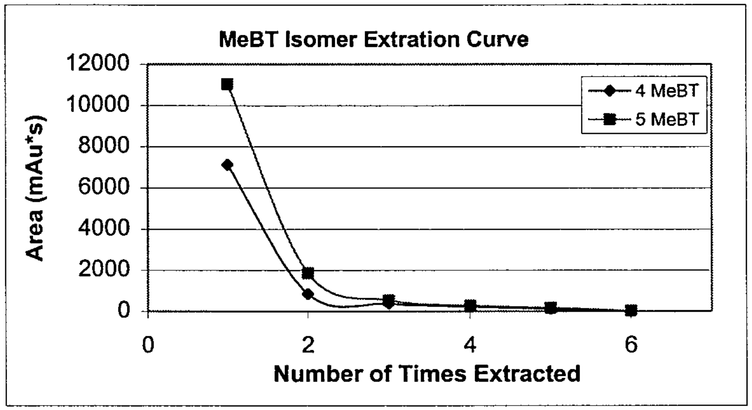
Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	28.066	38.068	10.002	64.183	62.341	821.99	9.052	27.065	964.88	427.273	0.520	2.63071	2.91487
1000	Bottle 2	27.799	37.806	10.007	64.054	62.239	827.7	9.056	27.199	965.04	412.482	0.498	2.6154	2.91787
1000	Bottle 3	28.092	38.092	10.000	64.564	62.715	820.84	9.050	27.422	965.35	437.883	0.533	2.64136	2.91426
1000	Bottle 4	28.285	38.293	10.008	64.756	62.849	825.02	9.057	27.414	965.31	424.634	0.515	2.62801	2.91646
1000	Bottle 5	28.170	38.177	10.007	64.652	62.811	830.51	9.056	27.426	965.33	408.290	0.492	2.61097	2.91934
100	Bottle 1	28.264	38.264	10.000	64.730	62.831	46.86	9.050	27.416	96.53	150.487	3.211	2.1775	1.6708
100	Bottle 2	28.057	38.066	10.009	64.442	62.639	1.52	9.058	27.327	96.52	286.607	188.557	2.45729	0.18184
100	Bottle 3	28.352	38.352	10.000	64.739	62.936	10.64	9.050	27.337	96.52	259.435	24.383	2.41403	1.02694
100	Bottle 4	27.947	37.949	10.002	64.330	62.521	46.69	9.052	27.331	96.52	150.470	3.223	2.17745	1.66922
100	Bottle 5	28.502	38.506	10.004	64.929	63.198	46.59	9.053	27.374	96.53	150.989	3.241	2.17895	1.66829
10	Bottle 1	28.176	38.176	10.000	65.959	64.114	6.08	9.050	28.733	9.67	11.396	1.874	1.05676	0.7839
10	Bottle 2	27.916	37.919	10.003	64.375	62.615	5.89	9.052	27.407	9.65	11.393	1.934	1.05664	0.77012
10	Bottle 3	28.295	38.295	10.000	64.356	62.912	0.01	9.050	27.011	9.65	28.782	5756	1.45913	-2.301
10	Bottle 4	28.066	38.066	10.000	64.645	62.869	0.13	9.050	27.529	9.65	28.990	232	1.46224	-0.9031
10	Bottle 5	27.041	37.048	10.007	63.638	61.805	0.00	9.056	27.541	9.65	29.361	195740	1.46777	-3.8239
100	Mix 1	27.748	37.755	10.007	64.079	62.321	53.84	9.056	27.275	96.51	128.523	2.387		
100	Mix 2	27.557	37.561	10.004	63.966	62.181	54.13	9.053	27.356	96.53	128.100	2.367		
100	Mix 3	27.852	37.852	10.000	64.071	62.281	55.21	9.050	27.169	96.50	123.969	2.245		
100	Mix 4	27.665	37.672	10.007	64.291	62.492	54.91	9.056	27.570	96.55	126.769	2.309		
100	Mix 5	27.305	37.308	10.003	63.808	61.980	54.71	9.052	27.451	96.54	126.836	2.318		
							1				72.90	72.90		
							1000				293.96	0.294		



Concentration dependence of Kd

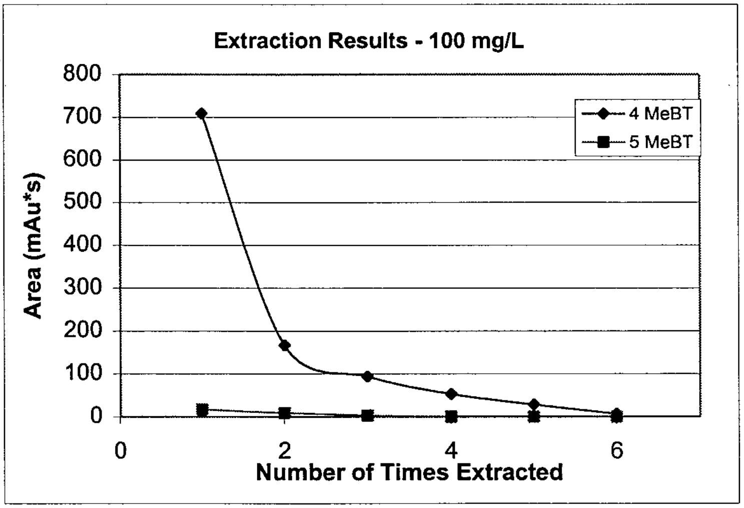

5-MeBT isotherm
Sorbed Concentration, S (µg/g)
1000
100
10
1
10
100
1000
Final Concentration, C_f (mg/l)
○ 5-MeBT alone
— S = Kf C^n

1000 mg/L	0		8225.7		13224.4	4 MeBT	5 MeBT
Water	0.5	6.765	7125.9	7.011	11036.8	87%	83%
1 Meth	1 hr	6.755	848.1	6.989	1863.5	10%	14%
2 Meth	6 hr	6.739	372.8	6.968	543.0	5%	4%
3 Meth	24 hr	6.724	231.4	6.949	279.4	3%	2%
4 Meth	48 hr	6.719	127.3	6.936	165.1	2%	1%
5 Meth	72 hr	6.711	15.5	6.924	35.4	0%	0%
Sum Recovered			8721.0		13923.2		
Percent MeBT Recovered			**106.02%**		**105.28%**		


MeBT Isomer Extration Curve

Empty	28.170	Refilled	Difference
w/ Soil only	38.177		
Soil Weight (air-dried)	10.007		
w/ Soil and MeBT mix	64.652		
After Initial Extraction	62.811		1.841
of water/MeBT		63.294	
1 Meth	62.023	63.584	1.271
2 Meth	61.435	63.645	2.149
3 Meth	61.941	63.359	1.704
4 Meth	61.254	63.698	2.105
5 Meth	61.882	63.386	1.816
6 Meth	61.342		2.044

100 mg/L	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.051	708.4	7.254	17.4	77%	1%
1 Meth	1 hr	7.035	166.3	7.243	9.2	18%	1%
2 Meth	6 hr	7.046	93.2	7.222	3.3	10%	0%
3 Meth	24 hr	7.038	52.6	7.216	0.0	6%	0%
4 Meth	48 hr	7.034	28.1	7.210	0.0	3%	0%
5 Meth	72 hr	7.029	6.7	7.204	0.0	1%	0%
Sum Recovered			1055.3		29.9		
Percent MeBT Recovered			**114.96%**		**1.95%**		


Extraction Results - 100 mg/L

Empty	28.502	Refilled	Difference
w/ Soil only	38.506		
Soil Weight (air-dried)	10.004		
w/ Soil and MeBT mix	64.929		
After Initial Extraction	63.198		1.731
of water/MeBT		63.955	
1 Meth	62.584	63.821	1.371
2 Meth	61.960	63.706	1.861
3 Meth	62.222	64.029	1.484
4 Meth	62.156	63.832	1.873
5 Meth	63.010		0.822

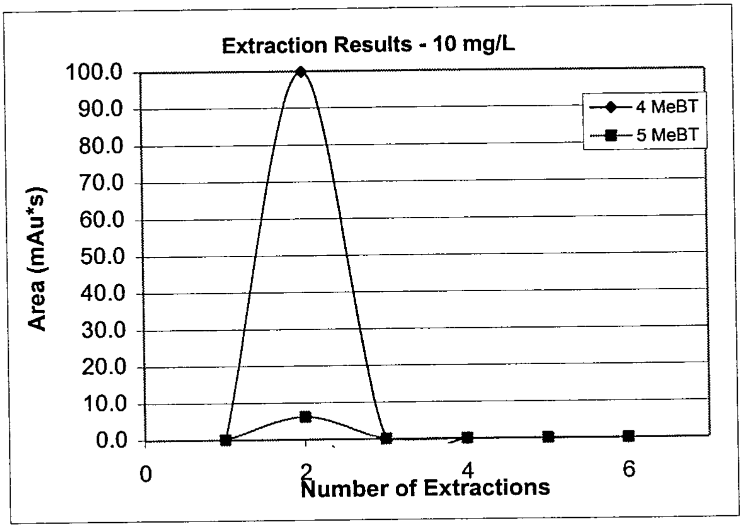
10 mg/L	0		119.9		201.1	4 MeBT	5 MeBT
Water	0.5	7.135	0.0	7.350	0.0	0%	0%
1 Meth	1 hr	7.134	99.83	7.321	6.1	83%	3%
2 Meth	6 hr	7.135	0	7.35	0.0	0%	0%
3 Meth	24 hr	7.135	0	7.35	0	0%	0%
4 Meth	48 hr	7.135	0	7.35	0	0%	0%
5 Meth	72 hr	7.135	0	7.35	0	0%	0%
Sum Recovered			99.8		6.1		
Percent MeBT Recovered			**83.26%**		**3.03%**		

Additional spike a	Water	7.948	131.9
and one at	Water	8.803	7.2
	Meth 1	8.696	23.4
	Meth 1	9.613	13.7
	Meth 2	7.651	27.2

		Refilled	Difference
Empty	27.041		
w/ Soil only	37.048		
Soil Weight (air-dried)	10.007		
w/ Soil and MeBT mix	63.638		
After Initial Extraction	61.805		1.833
of water/MeBT		63.804	
1 Meth	62.413	63.991	1.391
2 Meth	62.288	64.112	1.703
3 Meth	62.567	64.684	1.545
4 Meth	62.606	63.863	2.078
5 Meth	62.918	63.456	0.945
6 Meth	62.451		1.005

0 mg/L	0		4.8		20.5	4 MeBT	5 MeBT
Water	0.5	7.264	820.3	7.475	398.7	17090%	1945%
1 Meth	1 hr	7.264	254.1	7.474	211.9	5294%	1034%
2 Meth	6 hr	7.263	107.3	7.472	136.4	2235%	665%
3 Meth	24 hr	7.261	42.2	7.471	79.2	879%	386%
4 Meth	48 hr	7.261	20.6	7.469	34.1	429%	166%
5 Meth	72 hr					0%	0%
Sum Recovered			1244.5		860.3		
Percent MeBT Recovered			**25927%**		**4197%**		

No Additional spike

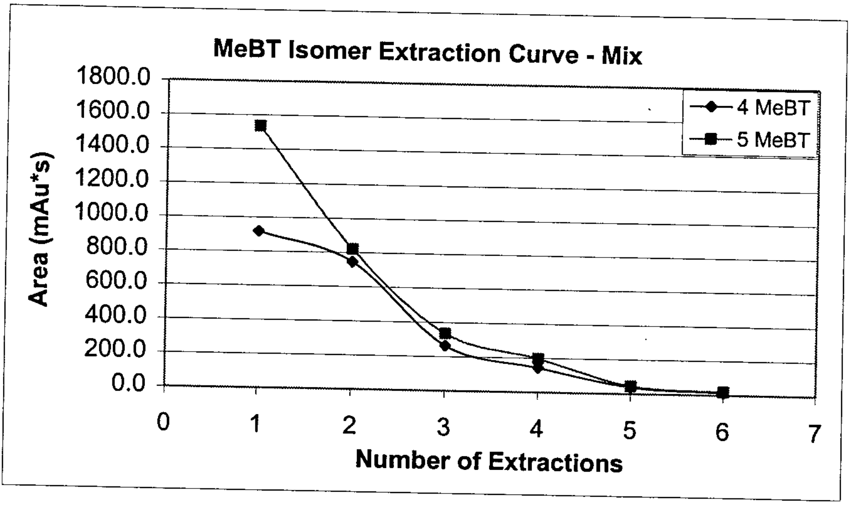


	Refilled	Difference
Empty		
w/ Soil only		
Soil Weight (air-dried)		
w/ Soil and MeBT mix		
After Initial Extraction of water/MeBT		0
1 Meth		0.000
2 Meth		0.000
3 Meth		0.000
4 Meth		0.000
5 Meth		0.000
6 Meth		0.000

Mix	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.244	744.4	7.449	820.4	81%	53%
1 Meth	1 hr	7.254	264.5	7.452	334.4	29%	22%
2 Meth	6 hr	7.253	142.8	7.452	196.2	16%	13%
3 Meth	24 hr	7.252	38.1	7.449	43.7	4%	3%
4 Meth	48 hr	7.250	12.3	7.445	18.8	1%	1%
5 Meth	72 hr					0%	0%
Sum Recovered			1202.1		1413.5		
Percent MeBT Recovered			**130.95%**		**91.96%**		

Additional spike a Water 8.227 12.5

		Refilled	Difference
Empty	27.305		
w/ Soil only	37.308		
Soil Weight (air-dried)	10.003		
w/ Soil and MeBT mix	63.808		
After Initial Extraction	61.980		1.828
of water/MeBT		64.240	
1 Meth	62.163	64.333	2.077
2 Meth	62.214	63.961	2.119
3 Meth	61.898	64.12	2.063
4 Meth	62.541		1.579



HPLC Results

1000 mg/L

Runs	4 MeBT			5 MeBT			
1	7.372	7118.9	863.67	7.569	10981.6	821.99	
2	7.356	7139.2	866.17	7.553	11053.6	827.70	
3	7.337	7101.4	861.52	7.534	10967.2	820.84	
4	7.301	7113.1	862.96	7.506	11019.8	825.02	
5	7.278	7168.5	869.78	7.473	11088.9	830.51	
avg	7.329	**7128.22**		7.527	**11022.22**		
conc.			**864.82**			**825.21**	Interpolated from calibration curve
Standard Deviation		26.35			50.28		
Average of 4 & 5 MeBT				**0.00**			

100 mg/L

Runs	4 MeBT			5 MeBT				Other	
1	7.344	718.50	78.20	8.461	17.38	0.00		7.925	11.02
2	7.323	716.39	77.97	8.436	18.06	0.00		7.923	11.16
3	7.301	724.66	78.87	8.410	17.70	0.00		7.923	11.07
4	7.283	718.57	78.20	8.387	18.06	0.00		7.922	11.11
5	7.264	716.28	77.95	8.364	17.99	0.00		7.921	11.23
avg	7.303	**718.88**		8.412	**17.84**				
conc.			**78.24**			**0.00**	Interpolated from calibration curve		
Standard Deviation		3.41			0.30				
Average of 4 & 5 MeBT				**0.00**					

10 mg/L

Runs	4 MeBT			5 MeBT				Other	
1	7.149	101.56	8.22	7.895	6.31	0.00		7.896	6.13
2	7.148	102.34	8.30	7.896	6.47	0.00		7.893	6.48
3	7.148	101.79	8.25	7.892	6.47	0.00		7.896	6.47
4	7.149	100.81	8.15	7.895	6.84	0.00		7.892	6.59
5	7.147	102.63	8.33	7.894	6.59	0.00		7.895	6.84
avg	7.148	**101.83**		7.894	**6.54**				
conc.			**8.25**			**0.00**	Interpolated from calibration curve		
Standard Deviation		0.71			0.20				
Average of 4 & 5 MeBT				**0.00**					

100 mg/L MeBT / 1000 mg/L PG

Runs	4 MeBT			5 MeBT				Other	
1	7.187	752.18	81.88	7.378	830.89	53.84		7.916	12.85
2	7.188	752.27	81.89	7.379	835.28	54.13		7.919	13.03
3	7.188	744.78	81.07	7.379	851.76	55.21		7.916	12.41
4	7.189	754.11	82.09	7.381	847.23	54.91		7.919	12.38
5	7.189	751.02	81.75	7.380	844.21	54.71		7.918	12.53
avg	7.188	**750.87**		7.379	**841.87**				
conc.			**81.736**			**54.56**	Interpolated from calibration curve		
Standard Deviation		3.58			8.60				
Average of 4 & 5 MeBT				**0.00**					

Below LOD

Appendix G

Denver International Airport Soil

Sample Analysis

Appendix G

Denver International Airport Soil

4 MeBT

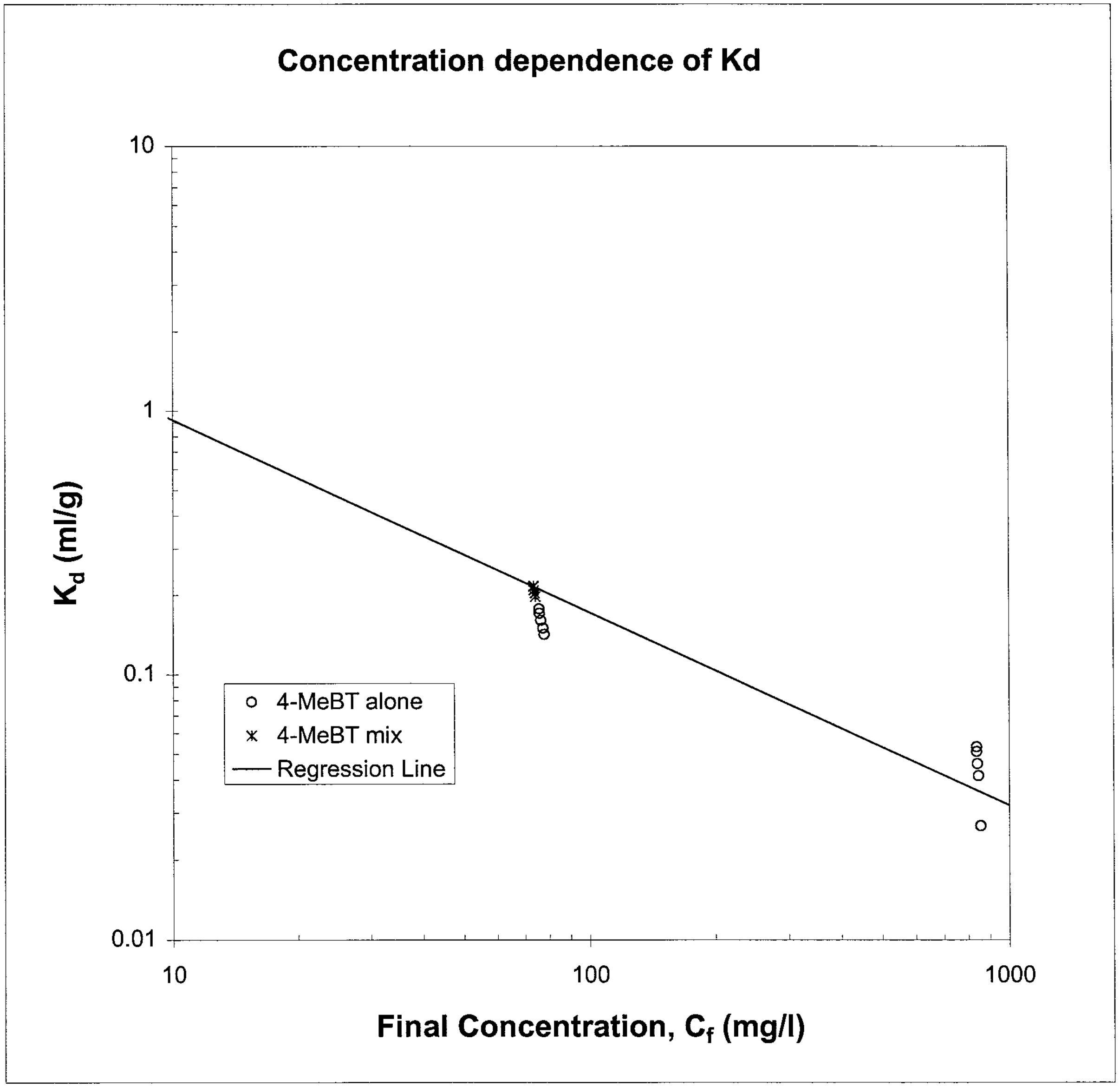
4-MeBT Data

Moisture Content of soil 0.138

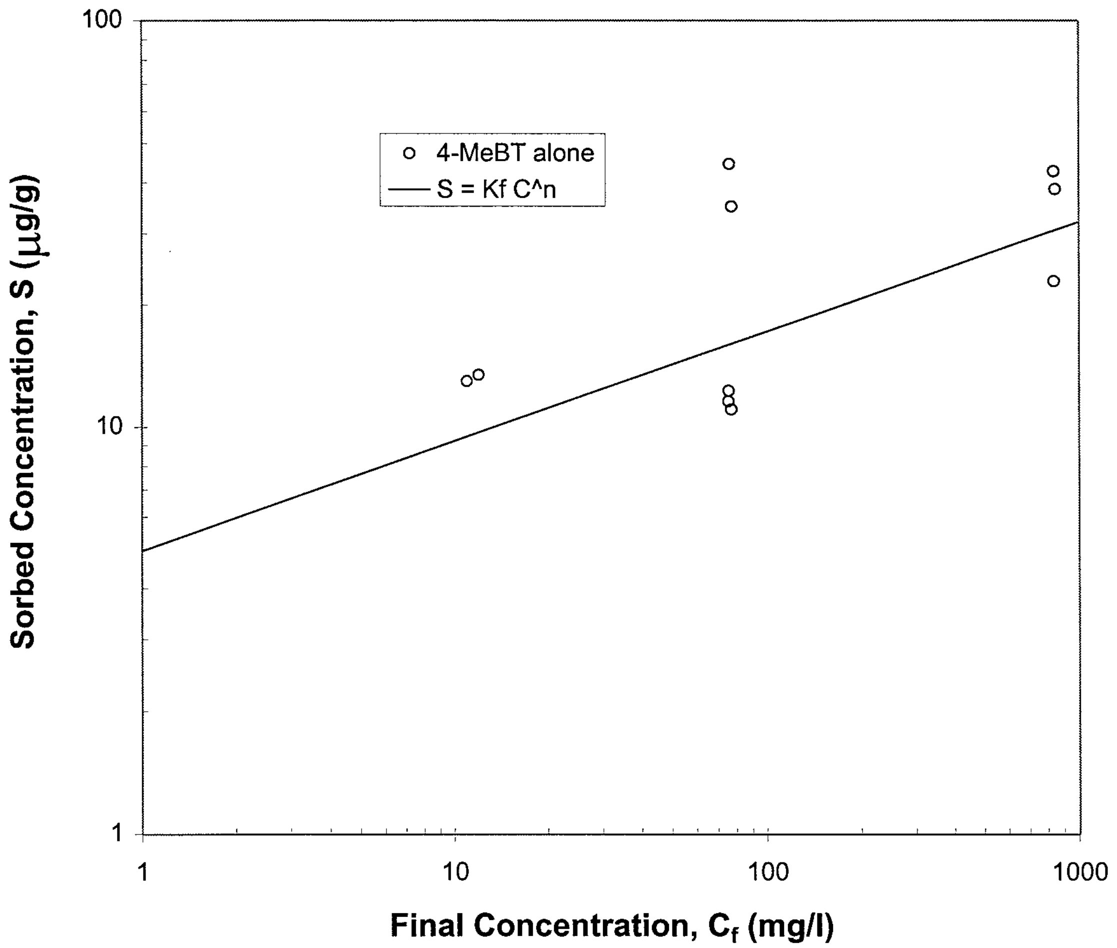
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.4471	0.2703	n =	0.447
intercept	0.2454	0.6944	Kf =	1.759
r^2	0.8995	0.8791		

Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	w/ Soil and MeBT	After Initial Extractio	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	27.983	37.988	10.005	46.476	44.697	854.17	8.792	9.701	874.94	22.916	0.027	1.36015	2.93154
1000	Bottle 2	28.417	38.418	10.001	46.826	45.070	838.69	8.788	9.621	873.94	38.592	0.046	1.58649	2.9236
1000	Bottle 3	27.933	37.936	10.003	46.379	44.542	835.51	8.790	9.656	874.38	42.696	0.051	1.63039	2.92195
1000	Bottle 4	27.893	37.901	10.008	46.429	44.603	843.82	8.794	9.742	875.42	35.002	0.041	1.5441	2.92625
1000	Bottle 5	28.047	38.047	10.000	46.596	44.815	835.75	8.787	9.762	875.77	44.461	0.053	1.64798	2.92208
100	Bottle 1	27.914	37.917	10.003	46.524	44.634	77.75	8.790	9.820	87.65	11.057	0.142	1.04365	1.8907
100	Bottle 2	28.083	38.088	10.005	46.589	44.738	76.40	8.792	9.714	87.51	12.276	0.161	1.08907	1.88309
100	Bottle 3	27.674	37.683	10.009	46.291	44.083	77.28	8.795	9.822	87.64	11.572	0.150	1.06339	1.88807
100	Bottle 4	28.018	38.024	10.006	46.555	44.656	75.86	8.793	9.744	87.55	12.953	0.171	1.11237	1.88001
100	Bottle 5	27.461	37.465	10.004	46.072	44.336	75.62	8.791	9.820	87.65	13.435	0.178	1.12822	1.87864
10	Bottle 1	28.123	38.128	10.005	46.875	45.073	2.57	8.792	9.960	8.78	7.038	2.738	0.84742	0.40993
10	Bottle 2	27.977	37.980	10.003	46.554	44.785	2.34	8.790	9.787	8.76	7.149	3.055	0.85424	0.36922
10	Bottle 3	27.591	37.598	10.007	46.216	44.372	2.48	8.793	9.832	8.77	7.028	2.834	0.84681	0.39445
10	Bottle 4	28.175	38.179	10.004	46.921	45.117	2.52	8.791	9.955	8.78	7.091	2.814	0.85069	0.4014
10	Bottle 5	27.692	37.695	10.003	46.337	44.578	2.52	8.790	9.855	8.77	7.006	2.780	0.84549	0.4014
100	Mix 1	27.986	37.986	10.000	46.388	44.616	73.41	8.787	9.615	87.39	15.293	0.208		
100	Mix 2	27.613	37.615	10.002	46.021	44.345	74.05	8.789	9.619	87.39	14.600	0.197		
100	Mix 3	27.847	37.856	10.009	46.370	44.665	73.93	8.795	9.728	87.52	15.034	0.203		
100	Mix 4	27.791	37.800	10.009	46.357	44.587	73.38	8.795	9.771	87.58	15.772	0.215		
100	Mix 5	27.429	37.433	10.004	46.001	44.262	73.33	8.791	9.781	87.60	15.874	0.216		
							1				4.948	4.948		
							1000				32.014	0.032		


Concentration dependence of Kd
K_d (ml/g)
10
1
0.1
0.01
10
100
1000
Final Concentration, C_f (mg/l)
○ 4-MeBT alone
⁎ 4-MeBT mix
—— Regression Line

4-MeBT isotherm



Appendix G

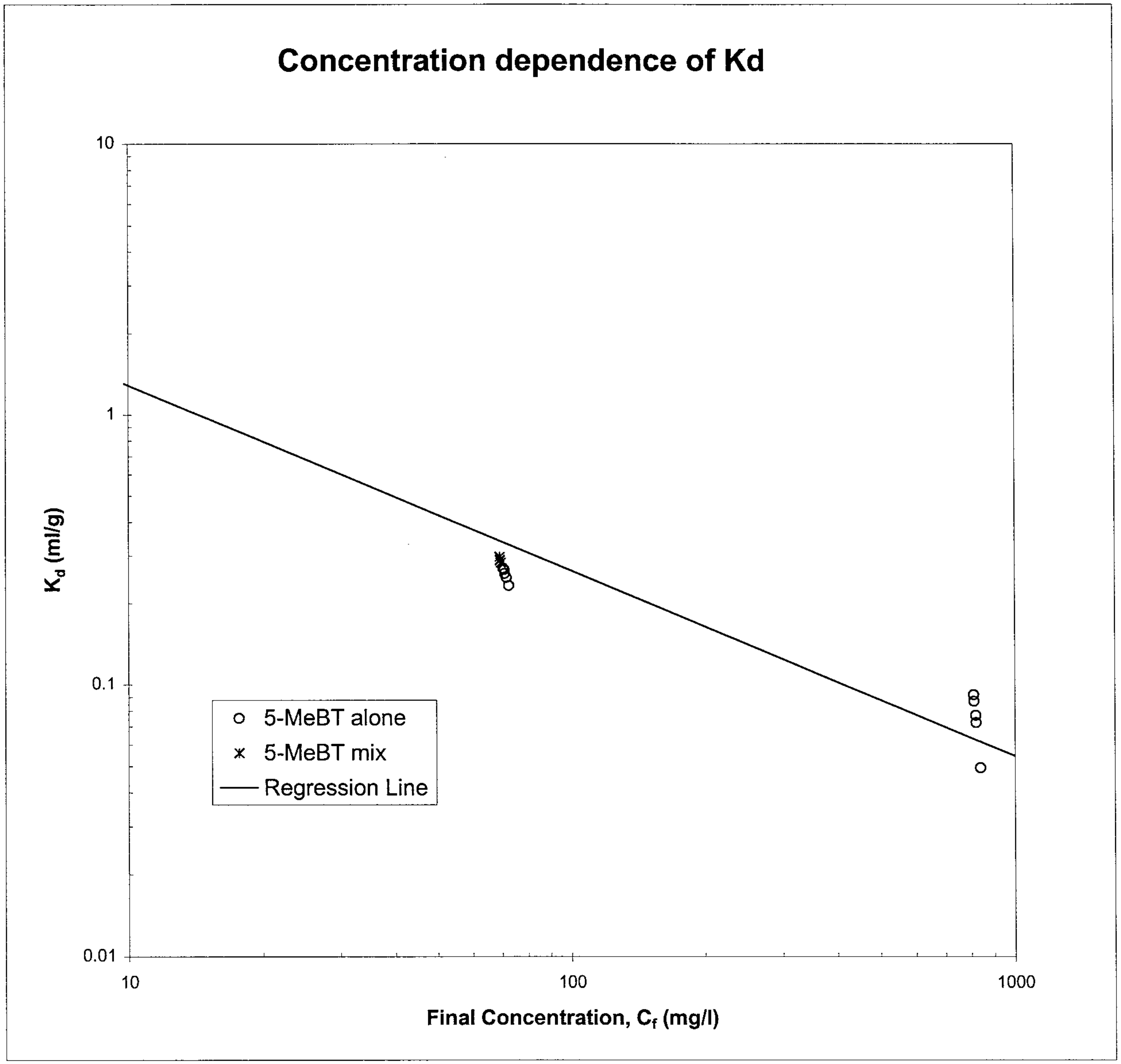
Denver International Airport Soil

5 MeBT

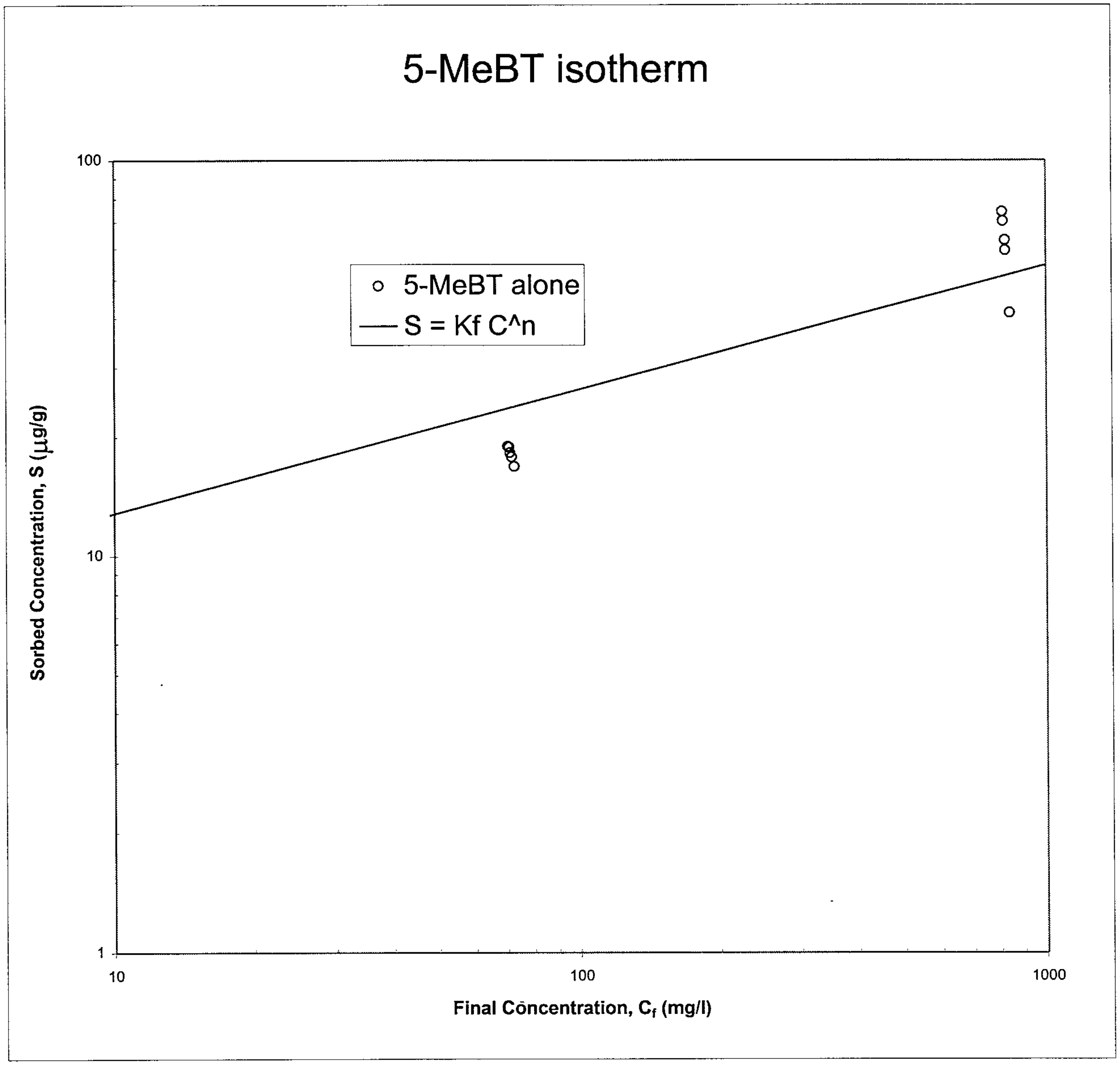
5-MeBT Data
Moisture Content of soil 0.138
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.4915	0.3140	n =	0.491
intercept	0.3487	0.7943	Kf =	2.232
r^2	0.9382	0.9238		

Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	27.983	37.988	10.005	46.476	44.697	837.55	8.792	9.701	874.94	41.256	0.049	1.61548	2.92301
1000	Bottle 2	28.417	38.418	10.001	46.826	45.070	819.75	8.788	9.621	873.94	59.326	0.072	1.77324	2.91368
1000	Bottle 3	27.933	37.936	10.003	46.379	44.542	810.40	8.790	9.656	874.38	70.280	0.087	1.84683	2.9087
1000	Bottle 4	27.893	37.901	10.008	46.429	44.603	818.53	8.794	9.742	875.42	63.016	0.077	1.79945	2.91303
1000	Bottle 5	28.047	38.047	10.000	46.596	44.815	808.96	8.787	9.762	875.77	74.222	0.092	1.87053	2.90793
100	Bottle 1	27.914	37.917	10.003	46.524	44.634	71.67	8.790	9.820	87.65	17.850	0.249	1.25163	1.85534
100	Bottle 2	28.083	38.088	10.005	46.589	44.738	70.36	8.792	9.714	87.51	18.950	0.269	1.27761	1.84733
100	Bottle 3	27.674	37.683	10.009	46.291	44.083	72.54	8.795	9.822	87.64	16.865	0.232	1.22698	1.86058
100	Bottle 4	28.018	38.024	10.006	46.555	44.656	71.04	8.793	9.744	87.55	18.295	0.258	1.26233	1.8515
100	Bottle 5	27.461	37.465	10.004	46.072	44.336	70.76	8.791	9.820	87.65	18.864	0.267	1.27562	1.84979
10	Bottle 1	28.123	38.128	10.005	46.875	45.073	1.95	8.792	9.960	8.78	7.740	3.969	0.88874	0.29003
10	Bottle 2	27.977	37.980	10.003	46.554	44.785	1.39	8.790	9.787	8.76	8.207	5.904	0.91416	0.14301
10	Bottle 3	27.591	37.598	10.007	46.216	44.372	1.60	8.793	9.832	8.77	8.012	5.007	0.90372	0.20412
10	Bottle 4	28.175	38.179	10.004	46.921	45.117	1.59	8.791	9.955	8.78	8.144	5.122	0.91083	0.2014
10	Bottle 5	27.692	37.695	10.003	46.337	44.578	1.58	8.790	9.855	8.77	8.060	5.101	0.90635	0.19866
100	Mix 1	27.986	37.986	10.000	46.388	44.616	69.18	8.787	9.615	87.39	19.922	0.288		
100	Mix 2	27.613	37.615	10.002	46.021	44.345	69.48	8.789	9.619	87.39	19.601	0.282		
100	Mix 3	27.847	37.856	10.009	46.370	44.665	69.37	8.795	9.728	87.52	20.077	0.289		
100	Mix 4	27.791	37.800	10.009	46.357	44.587	69.08	8.795	9.771	87.58	20.549	0.297		
100	Mix 5	27.429	37.433	10.004	46.001	44.262	69.16	8.791	9.781	87.60	20.514	0.297		
							1				6.227	6.227		
							1000				54.499	0.054		

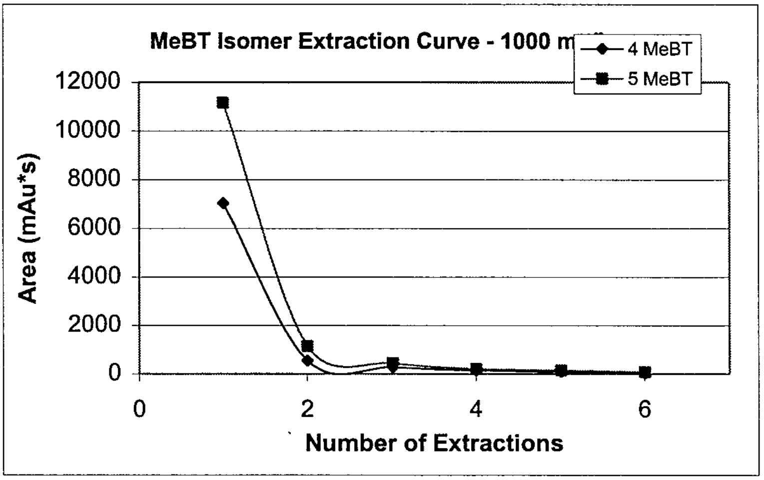


Concentration dependence of Kd


5-MeBT isotherm
○ 5-MeBT alone
— S = Kf C^n
Sorbed Concentration, S (µg/g)
100
10
1
10
100
1000
Final Concentration, C$_f$ (mg/l)

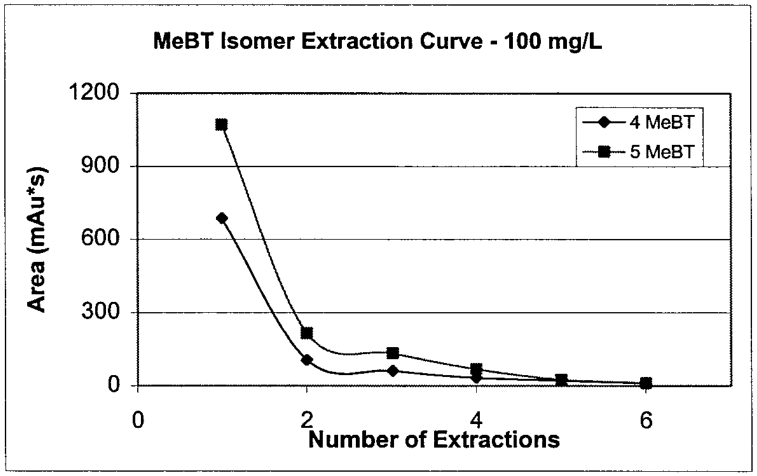
1000 mg/L	0		8225.7		13224.4	4 MeBT	5 MeBT
Water	0.5	6.966	7029.4	7.145	11161.8	85%	84%
1 Meth	1 hr	6.761	554.1	6.931	1147.2	7%	9%
2 Meth	6 hr	6.752	277.9	6.922	441.7	3%	3%
3 Meth	24 hr	6.750	142.9	6.919	209.2	2%	2%
4 Meth	48 hr	6.744	97.8	6.914	138.2	1%	1%
5 Meth	72 hr	6.731	45.6	6.91	72.4	1%	1%
Sum Recovered			8147.7		13170.5		
Percent MeBT Recovered			**99.05%**		**99.59%**		

Empty	28.047	Refilled	Difference
w/ Soil only	38.047		
Soil Weight (air-dried)	10.000		
w/ Soil and MeBT mix	46.596		
After Initial Extraction	44.815		1.781
of water/MeBT		46.156	
1 Meth	44.360	46.612	1.796
2 Meth	44.849	46.541	1.763
3 Meth	44.716	46.083	1.825
4 Meth	44.369	46.354	1.714
5 Meth	44.455		1.899



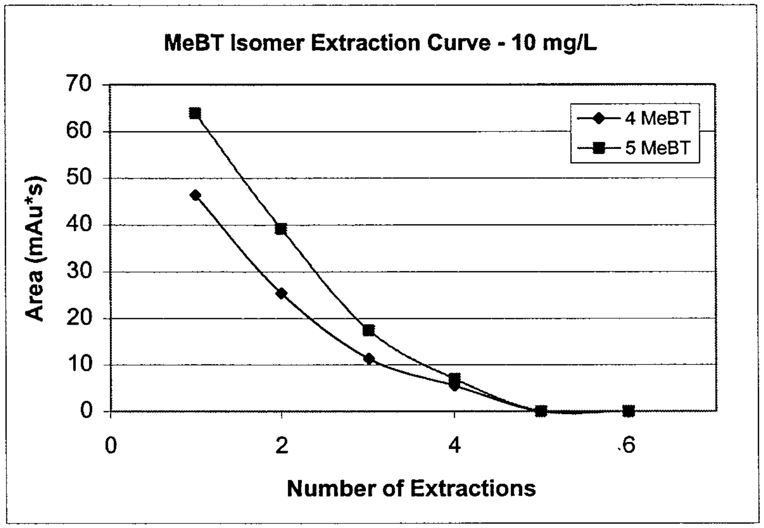
100 mg/L	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.055	686.3	7.241	1071.7	75%	70%
1 Meth	1 hr	7.045	105.6	7.229	214.6	12%	14%
2 Meth	6 hr	7.044	61.8	7.230	132.6	7%	9%
3 Meth	24 hr	7.040	32.7	7.223	67.3	4%	4%
4 Meth	48 hr	7.038	20.6	7.221	25.1	2%	2%
5 Meth	72 hr	7.036	10.4	7.218	11.9	1%	1%
Sum Recovered			917.4		1523.2		
Percent MeBT Recovered			**99.93%**		**99.10%**		

Empty	27.461	Refilled	Difference
w/ Soil only	37.465		
Soil Weight (air-dried)	10.004		
w/ Soil and MeBT mix	46.072		
After Initial Extraction	44.336		1.736
of water/MeBT		46.554	
1 Meth	44.381	46.359	2.173
2 Meth	44.414	46.523	1.945
3 Meth	44.652	46.691	1.871
4 Meth	44.698	46.578	1.993
5 Meth	44.385		2.193



10 mg/L	0		119.9		201.1	4 MeBT	5 MeBT
Water	0.5	7.156	46.4	7.346	63.9	39%	32%
1 Meth	1 hr	7.145	25.4	7.334	39.2	21%	19%
2 Meth	6 hr	7.159	11.3	7.352	17.5	9%	9%
3 Meth	24 hr	7.141	5.5	7.346	7.0	5%	3%
4 Meth	48 hr	7.135	0	7.35	0	0%	0%
5 Meth	72 hr	7.135	0	7.35	0	0%	0%
Sum Recovered			88.6		127.6		
Percent MeBT Recovered			**73.89%**		**63.45%**		
Additional spike a	Water	7.894	6.2				
	Meth 1	7.896	3.0				

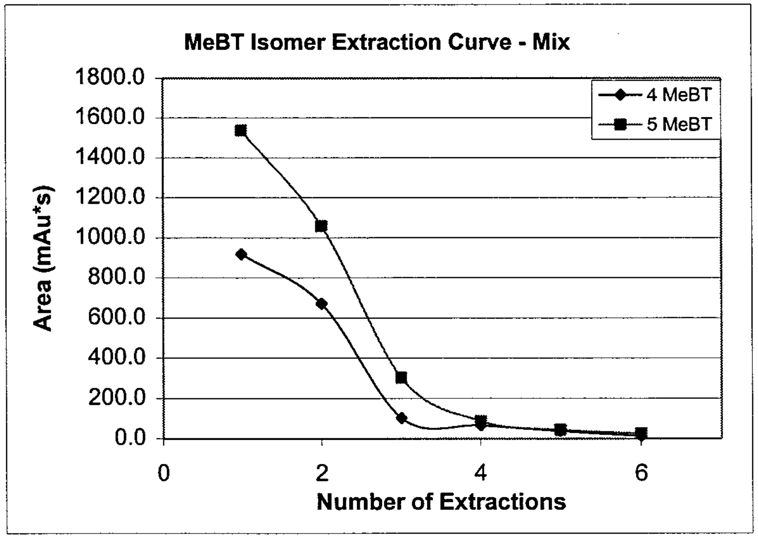
		Refilled	Difference
Empty	27.692		
w/ Soil only	37.695		
Soil Weight (air-dried)	10.003		
w/ Soil and MeBT mix	46.337		
After Initial Extraction	44.578		1.759
of water/MeBT		46.648	
1 Meth	44.857	45.959	1.791
2 Meth	44.114	46.223	1.845
3 Meth	44.452	46.138	1.771
4 Meth	44.501	46.161	1.637
5 Meth	44.499		1.662



Mix	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.311	671.2	7.513	1057.4	73%	69%
1 Meth	1 hr	7.272	101.2	7.472	301.5	11%	20%
2 Meth	6 hr	7.261	65.3	7.460	85.2	7%	6%
3 Meth	24 hr	7.255	36.4	7.457	43.0	4%	3%
4 Meth	48 hr	7.251	12.5	7.453	24.7	1%	2%
5 Meth	72 hr					0%	0%
Sum Recovered			886.6		1511.8		
Percent MeBT Recovered			**96.58%**		**98.36%**		

No Additional spike

		Refilled	Difference
Empty	27.429		
w/ Soil only	37.433		
Soil Weight (air-dried)	10.004		
w/ Soil and MeBT mix	46.001		
After Initial Extraction	44.262		1.739
of water/MeBT		46.152	
1 Meth	44.291	46.265	1.861
2 Meth	43.989	45.932	2.276
3 Meth	44.097	46.115	1.835
4 Meth	44.352		1.763



0 mg/L	0		**4.8**		**20.5**	4 MeBT	5 MeBT
Water	0.5		0.0		0.0	0%	0%
1 Meth	1 hr		0.0		0.0	0%	0%
2 Meth	6 hr		0.0		0.0	0%	0%
3 Meth	24 hr					0%	0%
4 Meth	48 hr					0%	0%
5 Meth	72 hr					0%	0%
Sum Recovered			0		0		
Percent MeBT Recovered			**0.00%**		**0.00%**		

No Additional spike - Zero result after background subtraction

Empty	Refilled	Difference
w/ Soil only		
Soil Weight (air-dried)		
w/ Soil and MeBT mix		
After Initial Extraction		0.00
of water/MeBT		
1 Meth		0.000
2 Meth		0.000
3 Meth		0.000
4 Meth		0.000

1000 mg/L

Runs	4 MeBT			5 MeBT			
1	9.825	7041.7	854.17	10.517	11177.7	837.55	
2	9.758	6905.4	838.69	10.424	10942.4	819.75	
3	7.497	6890.2	835.51	7.702	10835.6	810.40	
4	7.465	6957.7	843.82	7.667	10938.0	818.53	
5	7.444	6892.2	835.75	7.644	10817.5	808.96	
avg	8.398	**6937.44**		8.791	**10942.24**		
conc.			**841.59**			**819.04**	Interpolated from calibration curve
Standard Deviation		64.39			143.52		
Average of 4 & 5 MeBT				**830.31**			

100 mg/L

Runs	4 MeBT			5 MeBT			
1	7.613	714.47	77.75	7.817	1103.56	71.67	
2	7.583	702.03	76.40	7.787	1083.62	70.36	
3	7.553	710.10	77.28	7.756	1116.93	72.54	
4	7.525	697.26	75.86	7.726	1093.98	71.04	
5	7.497	694.92	75.62	7.696	1089.74	70.76	
avg	7.554	**703.76**		7.756	**1097.57**		
conc.			**76.58**			**71.27**	Interpolated from calibration curve
Standard Deviation		8.34			13.03		
Average of 4 & 5 MeBT				**73.93**			

10 mg/L

Runs	4 MeBT			5 MeBT			
1	7.167	52.14	2.57	7.357	80.54	1.95	
2	7.157	50.63	2.34	7.345	74.54	1.39	
3	7.145	51.57	2.48	7.333	76.82	1.60	
4	7.134	51.83	2.52	7.322	76.73	1.59	
5	7.128	51.78	2.52	7.317	76.68	1.58	
avg	7.146	**51.59**		7.335	**77.06**		
conc.			**2.49**			**1.62**	Interpolated from calibration curve
Standard Deviation		0.57			2.17		
Average of 4 & 5 MeBT				**2.05**			

100 mg/L MeBT / 1000 mg/L PG

Runs	4 MeBT			5 MeBT			
1	7.189	674.67	73.41	7.380	1065.51	69.18	
2	7.189	680.59	74.05	7.380	1070.15	69.48	
3	7.189	679.46	73.93	7.379	1068.45	69.37	
4	7.189	674.44	73.38	7.380	1063.99	69.08	
5	7.187	673.99	73.33	7.378	1065.14	69.16	
avg	7.189	**676.63**		7.379	**1066.65**		
conc.			**73.62**			**69.25**	Interpolated from calibration curve
Standard Deviation		3.13			2.56		
Average of 4 & 5 MeBT				**71.44**			

Other	
7.924	13.35
7.928	13.03
7.925	12.89
7.924	15.75
7.924	16.23

Below LOD

Appendix H

Westover ARB Soil

Sample Analysis

Appendix H

Westover ARB Soil

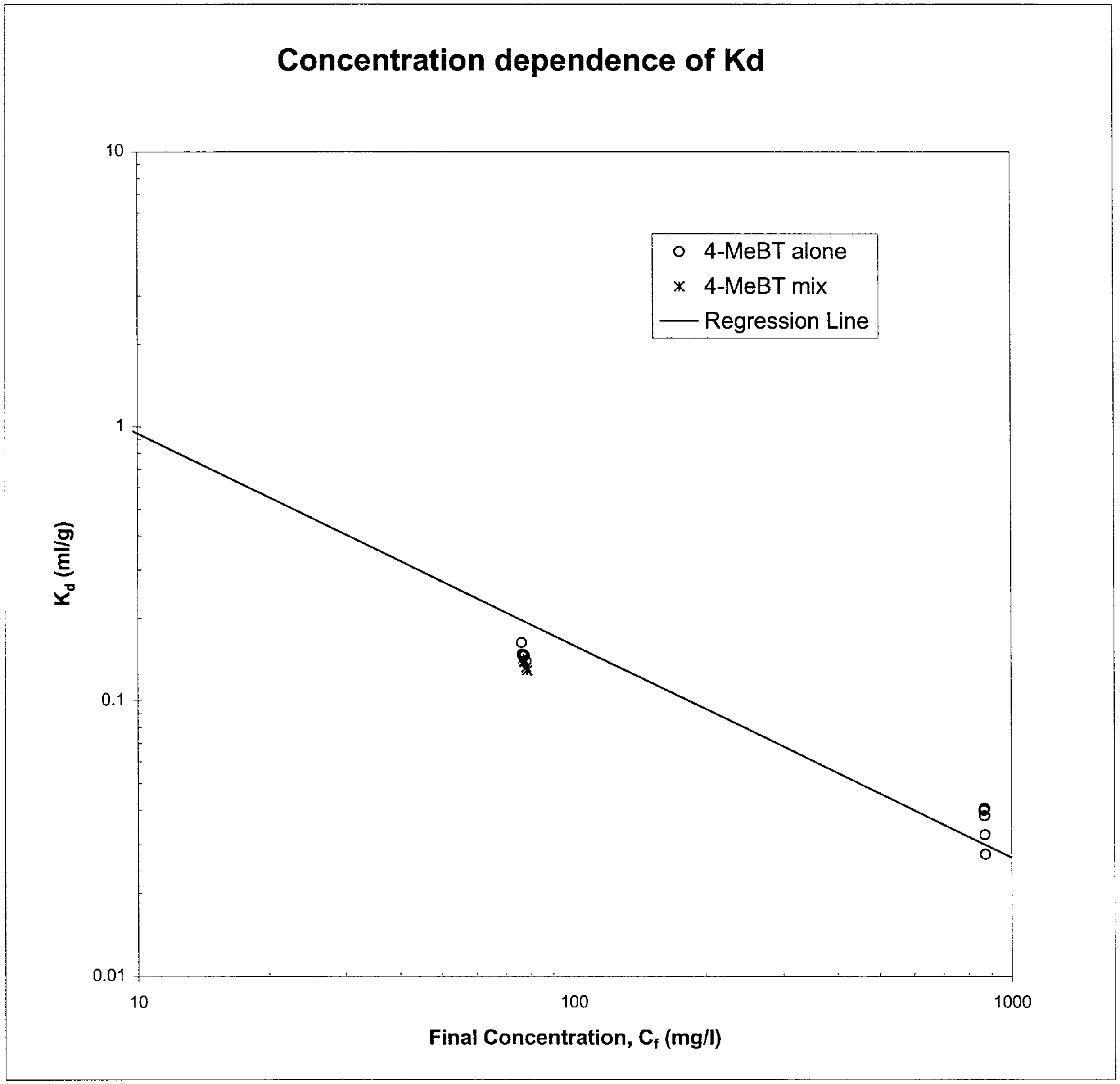
4-MeBT

4-MeBT Data
Moisture Content of soil 0.063
Outliers identified in bold

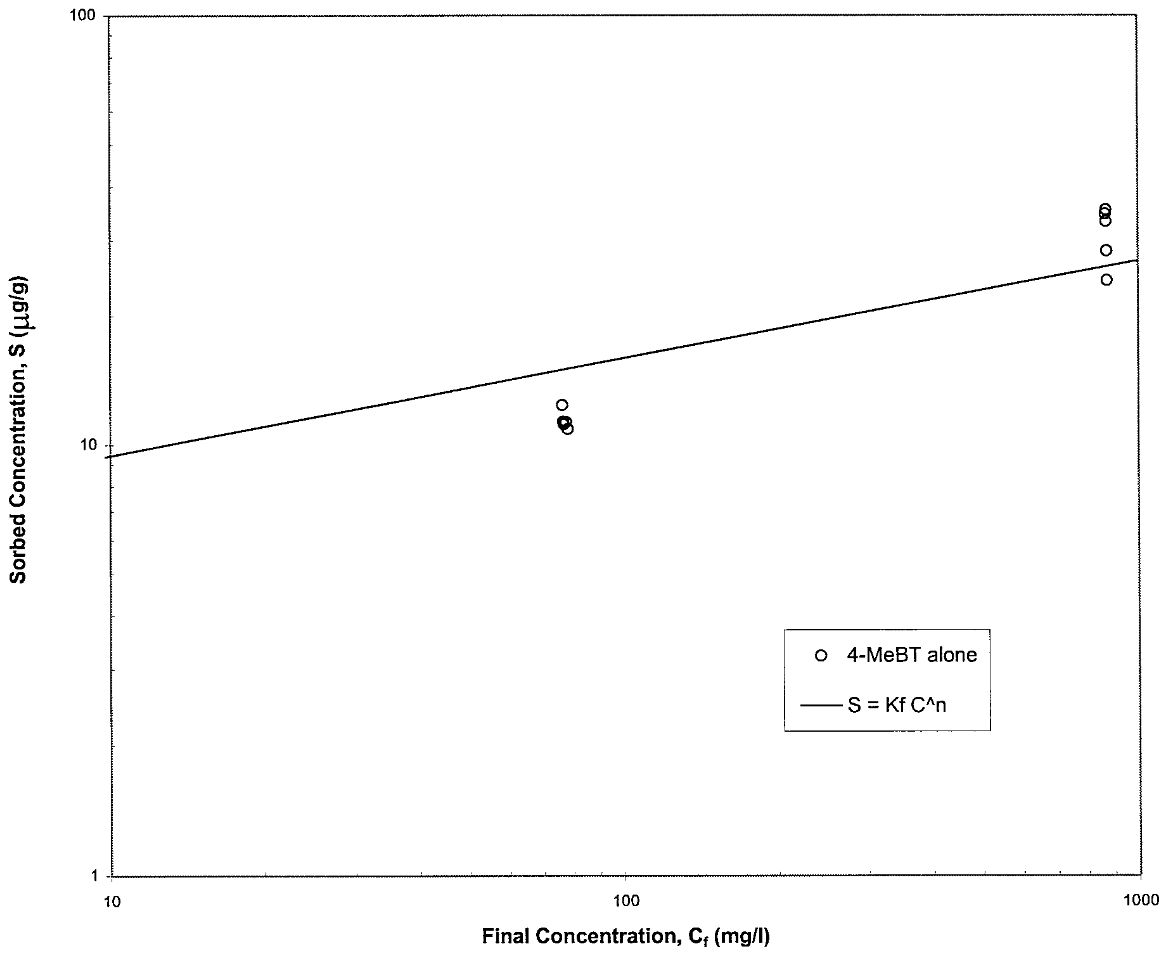
	all data	with 10 mg/L		
slope	0.4099	0.2274	n =	0.410
intercept	0.2836	0.7470	Kf =	1.921
r^2	0.9554	0.8750		

Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration **Cf** mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration **S** µg/g	1 point Sorption Coeff. **Kd** ml/g	log S	Log Cf
1000	Bottle 1	28.279	38.281	10.002	44.738	43.035	868.82	9.409	7.050	915.92	35.286	0.041	1.5476	2.93893
1000	Bottle 2	28.508	38.511	10.003	44.545	42.822	870.29	9.410	6.627	910.54	28.345	0.033	1.45247	2.93966
1000	Bottle 3	28.426	38.428	10.002	44.661	42.904	865.53	9.409	6.826	913.16	34.549	0.040	1.53844	2.93728
1000	Bottle 4	28.462	38.462	10.000	44.266	43.002	871.83	9.407	6.397	907.35	24.151	0.028	1.38294	2.94043
1000	Bottle 5	27.735	37.737	10.002	44.041	42.279	868.85	9.409	6.897	914.05	33.130	0.038	1.52023	2.93894
100	Bottle 1	27.882	37.891	10.009	44.411	42.622	76.67	9.416	7.113	91.66	11.325	0.148	1.05403	1.88463
100	Bottle 2	28.161	38.168	10.007	44.971	43.132	77.6	9.414	7.396	91.98	11.299	0.146	1.05303	1.88986
100	Bottle 3	28.052	38.056	10.004	44.577	42.767	76.89	9.411	7.114	91.67	11.169	0.145	1.04801	1.88587
100	Bottle 4	27.757	37.762	10.005	44.578	42.703	76.26	9.412	7.409	92.00	12.388	0.162	1.09299	1.8823
100	Bottle 5	27.834	37.839	10.005	44.648	42.827	78.15	9.412	7.402	91.99	10.884	0.139	1.03677	1.89293
10	Bottle 1	28.020	38.021	10.001	46.43	44.535	1.98	9.408	9.002	9.34	7.043	3.557	0.84778	0.29667
10	Bottle 2	28.234	38.240	10.006	46.643	44.808	1.53	9.413	8.996	9.34	7.465	4.879	0.87302	0.18469
10	Bottle 3	28.460	38.467	10.007	46.886	45.014	1.75	9.414	9.012	9.34	7.268	4.153	0.86141	0.24304
10	Bottle 4	28.267	38.267	10.000	46.729	44.905	1.82	9.407	9.055	9.35	7.243	3.980	0.85994	0.26007
10	Bottle 5	28.479	38.480	10.001	46.991	45.128	2.33	9.408	9.104	9.35	6.792	2.915	0.83198	0.36736
100	Mix 1	27.433	37.433	10.000	44.008	42.257	78.19	9.407	7.168	91.73	10.318	0.132		
100	Mix 2	27.847	37.855	10.008	44.443	42.674	78.51	9.415	7.181	91.74	10.091	0.129		
100	Mix 3	27.556	37.560	10.004	44.045	42.270	77.42	9.411	7.078	91.62	10.682	0.138		
100	Mix 4	27.956	37.963	10.007	44.506	42.642	77.4	9.414	7.136	91.69	10.832	0.140		
100	Mix 5	27.681	37.681	10.000	44.161	42.341	77.04	9.407	7.073	91.62	10.962	0.142		
							1				5.585	5.585		
							1000				26.872	0.027		

4-MeBT


Concentration dependence of Kd
4-MeBT alone
4-MeBT mix
Regression Line
K_d (ml/g)
10
1
0.1
0.01
10
100
1000
Final Concentration, C_f (mg/l)

4-MeBT isotherm



Appendix H

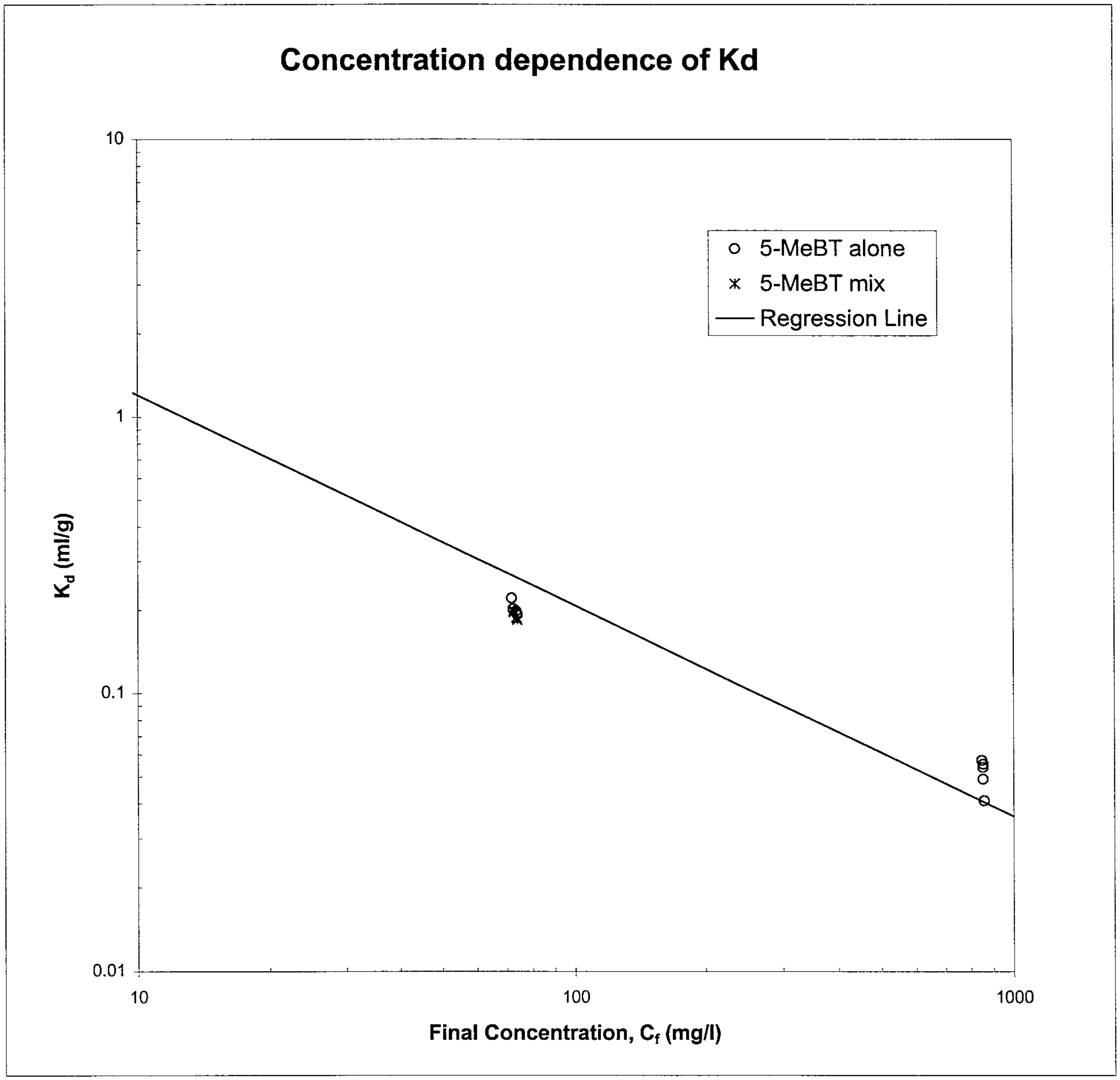
Westover ARB Soil

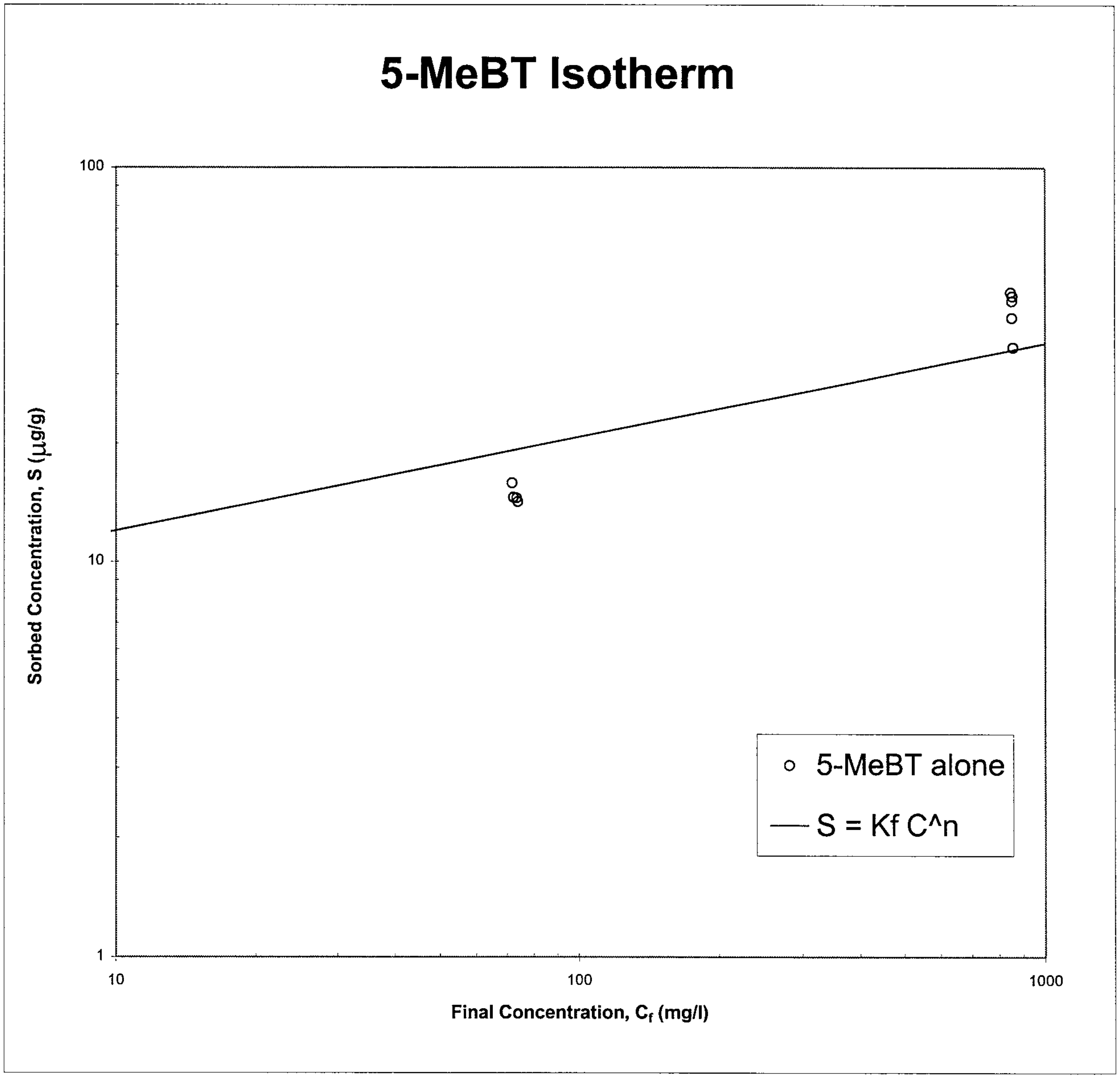
5-MeBT

5-MeBT Data
Moisture Content of soil 0.063
Outliers identified in bold

	all data	with 10 mg/L		
slope	0.4389	0.2384	n =	0.4389
intercept	0.3514	0.8405	Kf =	2.246
r^2	0.9735	0.8321		

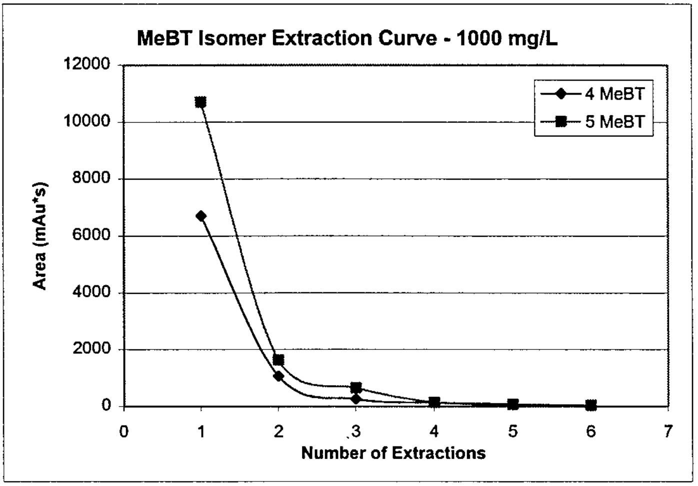
Added Concentrati		Vial Only g	Vial + soil g	Air-dried Soil g	and MeBT mix	Initial Extraction	Final Concentration Cf mg/L	Soil (dry wt) (g) M	Vol Soln (mL) Vs	Initial Concentration Ci	Sorbed Concentration S µg/g	1 point Sorption Coeff. Kd ml/g	log S	Log Cf
1000	Bottle 1	28.279	38.281	10.002	44.738	43.035	852.71	9.409	7.050	915.92	47.356	0.056	1.67537	2.930801
1000	Bottle 2	28.508	38.511	10.003	44.545	42.822	851.32	9.410	6.627	910.54	41.704	0.049	1.62017	2.930093
1000	Bottle 3	28.426	38.428	10.002	44.661	42.904	846.42	9.409	6.826	913.16	48.412	0.057	1.68496	2.927586
1000	Bottle 4	28.462	38.462	10.000	44.266	43.002	855.74	9.407	6.397	907.35	35.092	0.041	1.54521	2.932342
1000	Bottle 5	27.735	37.737	10.002	44.041	42.279	851.33	9.409	6.897	914.05	45.972	0.054	1.6625	2.930098
100	Bottle 1	27.882	37.891	10.009	44.411	42.622	72.34	9.416	7.113	91.66	14.596	0.202	1.16423	1.859379
100	Bottle 2	28.161	38.168	10.007	44.971	43.132	73.5	9.414	7.396	91.98	14.520	0.198	1.16196	1.866287
100	Bottle 3	28.052	38.056	10.004	44.577	42.767	72.38	9.411	7.114	91.67	14.578	0.201	1.1637	1.859619
100	Bottle 4	27.757	37.762	10.005	44.578	42.703	71.86	9.412	7.409	92.00	15.851	0.221	1.20006	1.856487
100	Bottle 5	27.834	37.839	10.005	44.648	42.827	73.9	9.412	7.402	91.99	14.226	0.193	1.15308	1.868644
10	Bottle 1	28.020	38.021	10.001	46.43	44.535	2.28	9.408	9.002	9.34	6.756	2.963	0.82972	0.357935
10	Bottle 2	28.234	38.240	10.006	46.643	44.808	0.14	9.413	8.996	9.34	8.795	63.733	0.94424	-0.86012
10	Bottle 3	28.460	38.467	10.007	46.886	45.014	2.25	9.414	9.012	9.34	6.789	3.017	0.83182	0.352183
10	Bottle 4	28.267	38.267	10.000	46.729	44.905	2.31	9.407	9.055	9.35	6.772	2.931	0.8307	0.363612
10	Bottle 5	28.479	38.480	10.001	46.991	45.128	1.03	9.408	9.104	9.35	8.050	7.815	0.90578	0.012837
100	Mix 1	27.433	37.433	10.000	44.008	42.257	73.6	9.407	7.168	91.73	13.815	0.188		
100	Mix 2	27.847	37.855	10.008	44.443	42.674	73.91	9.415	7.181	91.74	13.600	0.184		
100	Mix 3	27.556	37.560	10.004	44.045	42.270	72.65	9.411	7.078	91.62	14.269	0.196		
100	Mix 4	27.956	37.963	10.007	44.506	42.642	72.74	9.414	7.136	91.69	14.364	0.197		
100	Mix 5	27.681	37.681	10.000	44.161	42.341	72.47	9.407	7.073	91.62	14.398	0.199		
							1				6.927	6.927		
							1000				35.944	0.036		


Concentration dependence of Kd
10
1
0.1
0.01
K_d (ml/g)
10
100
1000
Final Concentration, C_f (mg/l)
○ 5-MeBT alone
× 5-MeBT mix
— Regression Line


5-MeBT Isotherm
100
10
1
Sorbed Concentration, S (µg/g)
10
100
1000
Final Concentration, C_f (mg/l)
○ 5-MeBT alone
— S = Kf C^n

1000 mg/L	0		8225.7		13224.4	4 MeBT	5 MeBT
Water	0.5	7.019	6699.9	7.207	10702.8	81%	81%
1 Meth	1 hr	7.026	1059.7	7.215	1626.9	13%	12%
2 Meth	6 hr	7.025	241.4	7.211	645.9	3%	5%
3 Meth	24 hr	7.018	124.8	7.205	137.5	2%	1%
4 Meth	48 hr	7.011	71.8	7.201	71.6	1%	1%
5 Meth	72 hr	7.007	21.4	7.198	33.9	0%	0%
Sum Recovered			8219.0		13218.6		
Percent MeBT Recovered			**99.92%**		**99.96%**		

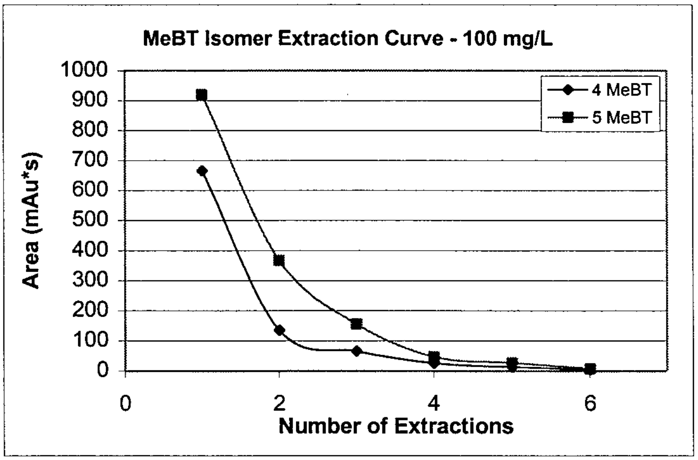
Empty	27.735	Refilled	Difference
w/ Soil only	37.737		
Soil Weight (air-dried)	10.002		
w/ Soil and MeBT mix	44.041		
After Initial Extraction	42.279		1.762
of water/MeBT		44.221	
1 Meth	42.355	44.395	1.866
2 Meth	42.113	44.249	2.282
3 Meth	42.343	44.340	1.906
4 Meth	42.813	44.199	1.527
5 Meth	42.746		1.453



100 mg/L	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.056	665.2	7.241	920.6	72%	60%
1 Meth	1 hr	7.041	134.7	7.226	367.5	15%	24%
2 Meth	6 hr	7.04	65.1	7.224	155.4	7%	10%
3 Meth	24 hr	7.037	25.5	7.224	45.9	3%	3%
4 Meth	48 hr	7.035	12.2	7.222	26.7	1%	2%
5 Meth	72 hr	7.031	4.2	7.216	7.8	0%	1%
Sum Recovered			906.9		1523.9		
Percent MeBT Recovered			**98.79%**		**99.15%**		

No additional spikes

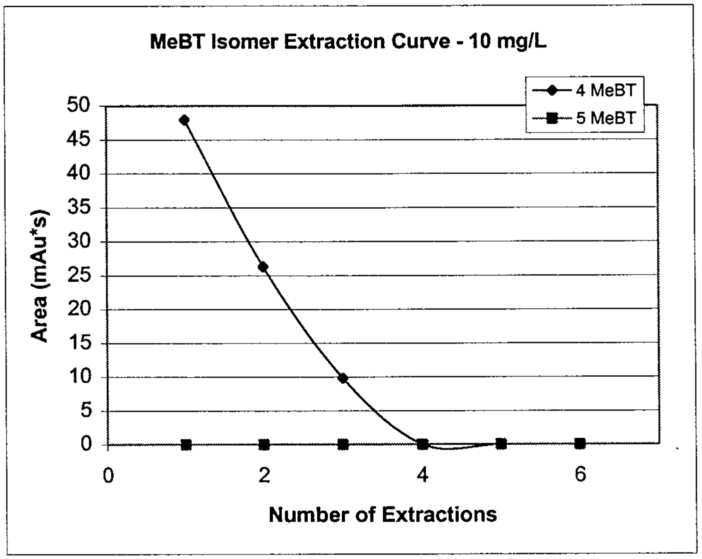
Empty	27.834	Refilled	Difference
w/ Soil only	37.839		
Soil Weight (air-dried)	10.005		
w/ Soil and MeBT mix	44.648		
After Initial Extraction	42.827		1.821
of water/MeBT		44.722	
1 Meth	42.864	44.608	1.858
2 Meth	42.620	45.006	1.988
3 Meth	42.955	44.638	2.051
4 Meth	42.994	44.875	1.644
5 Meth	43.181		1.694



10 mg/L	0		119.9		201.1	4 MeBT	5 MeBT
Water	0.5	7.139	47.9	7.35	0.0	40%	0%
1 Meth	1 hr	7.140	26.3	7.35	0.0	22%	0%
2 Meth	6 hr	7.164	9.8	7.35	0	8%	0%
3 Meth	24 hr	7.135	0	7.35	0	0%	0%
4 Meth	48 hr	7.135	0	7.35	0	0%	0%
5 Meth	72 hr	7.135	0	7.35	0	0%	0%
Sum Recovered			84		0		
Percent MeBT Recovered			**70.06%**		**0.00%**		

No additional spike

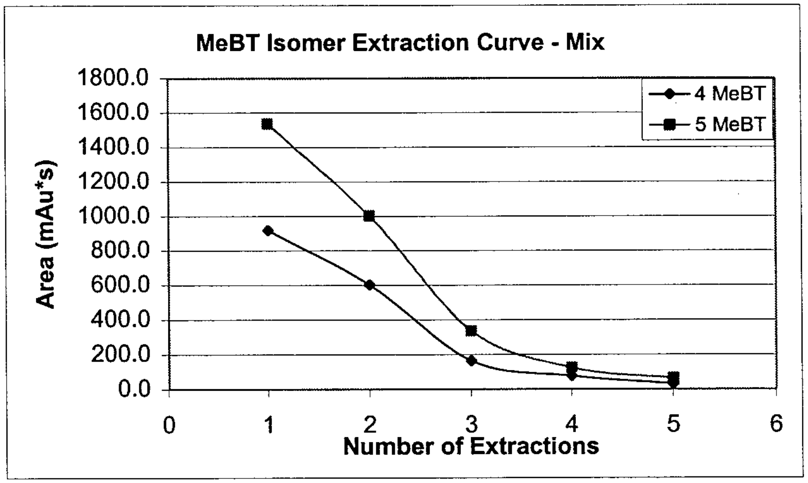
		Refilled	Difference
Empty	28.479		
w/ Soil only	38.480		
Soil Weight (air-dried)	10.001		
w/ Soil and MeBT mix	46.991		
After Initial Extraction	45.128		1.863
of water/MeBT		45.880	
1 Meth	44.257	46.084	1.623
2 Meth	44.646	45.896	1.438
3 Meth	44.177	46.293	1.719
4 Meth	44.555		1.738


MeBT Isomer Extraction Curve - 10 mg/L

Mix	0		918.0		1537.0	4 MeBT	5 MeBT
Water	0.5	7.278	602.4	7.478	1002.3	66%	65%
1 Meth	1 hr	7.269	164.7	7.468	336.1	18%	22%
2 Meth	6 hr	7.256	76.6	7.455	124.1	8%	8%
3 Meth	24 hr	7.252	31.1	7.451	63.6	3%	4%
4 Meth	48 hr					0%	0%
5 Meth	72 hr					0%	0%
Sum Recovered			874.8		1526.1		
Percent MeBT Recovered			**95.29%**		**99.29%**		

No additional spike

		Refilled	Difference
Empty	27.681		
w/ Soil only	37.681		
Soil Weight (air-dried)	10.000		
w/ Soil and MeBT mix	44.161		
After Initial Extraction	42.341		1.820
of water/MeBT		44.483	
1 Meth	42.861	44.530	1.622
2 Meth	42.609	44.216	1.921
3 Meth	42.510	44.453	1.706
4 Meth	42.642		1.811


MeBT Isomer Extraction Curve - Mix

0 mg/L	0		**4.8**		**20.5**	4 MeBT	5 MeBT
Water	0.5		0.0		0.0	0%	0%
1 Meth	1 hr		0.0		0.0	0%	0%
2 Meth	6 hr		0.0		0.0	0%	0%
3 Meth	24 hr					0%	0%
4 Meth	48 hr					0%	0%
5 Meth	72 hr					0%	0%
Sum Recovered			0		0		
Percent MeBT Recovered			**0.00%**		**0.00%**		

No additional spike - Zero result after background subtraction

	Refilled	Difference
Empty		
w/ Soil only		
Soil Weight (air-dried)		
w/ Soil and MeBT mix		
After Initial Extraction of water/MeBT		0.000
1 Meth		0.000
2 Meth		0.000
3 Meth		0.000
4 Meth		0.000

1000 mg/L

Runs	4 MeBT			5 MeBT			
1	7.432	7160.7	868.82	7.631	11368.7	852.71	
2	7.422	7172.6	870.29	7.621	11351.1	851.32	
3	7.409	7134.0	865.53	7.608	11289.4	846.42	
4	7.427	7185.1	871.83	7.631	11406.9	855.74	
5	7.386	7160.9	868.85	7.584	11351.3	851.33	
avg	7.415	**7162.66**		7.615	**11353.48**		
conc.			**869.064**			**851.50**	Interpolated from calib
Standard Deviation		18.91			42.43		
	Average of 4 & 5 MeBT			**0.00**			

100 mg/L

Runs	4 MeBT			5 MeBT			
1	7.467	704.57	76.67	7.667	1113.88	72.34	
2	7.441	713.08	77.60	7.640	1131.53	73.50	
3	7.414	706.54	76.89	7.606	1114.38	72.38	
4	7.389	700.78	76.26	7.587	1106.49	71.86	
5	7.367	718.06	78.15	7.564	1137.67	73.90	
avg	7.416	**708.61**		7.613	**1120.79**		
conc.			**77.114**			**72.80**	Interpolated from calib
Standard Deviation		6.91			13.17		
	Average of 4 & 5 MeBT			**0.00**			

10 mg/L

Runs	4 MeBT			5 MeBT			
1	7.147	48.21	1.98	7.343	21.73	0.03	
2	7.142	45.21	1.53	7.350	20.67	0.01	
3	7.143	46.66	1.75	7.335	20.51	0.00	
4	7.145	47.14	1.82	7.335	27.43	0.14	
5	7.146	50.53	2.33	7.337	23.47	0.06	
avg	7.145	**47.55**		7.340	**22.76**		
conc.			**1.882**			**0.05**	Interpolated from calib
Standard Deviation		1.98			2.86		
	Average of 4 & 5 MeBT			**0.00**			

100 mg/L MeBT / 1000 mg/L PG

Runs	4 MeBT			5 MeBT			
1	7.189	718.48	78.19	7.379	1133.13	73.60	
2	7.189	721.39	78.51	7.380	1137.91	73.91	
3	7.190	711.39	77.42	7.381	1118.58	72.65	
4	7.187	711.25	77.40	7.379	1119.97	72.74	
5	7.190	707.88	77.04	7.38	1115.83	72.47	
avg	7.189	**714.08**		7.380	**1125.08**		
conc.			**77.712**			**73.07**	Interpolated from calib
Standard Deviation		5.62			9.79		
	Average of 4 & 5 MeBT			**0.00**			

Below LOD

Appendix I

Achieved Kow Values

Calculations

1000 mg/	Untreated		Treated		DIA		Westover	
	4	5	4	5	4	5	4	5
erage Kd	0.860	0.825	0.350	0.512	0.044	0.075	0.036	0.051
foc	0.030	0.030	0.030	0.030	0.008	0.008	0.005	0.005
Koc	28.680	27.507	11.667	17.053	5.450	9.425	7.200	10.280
Kom	16.636	15.955	6.767	9.892	3.161	5.467	4.176	5.963
log Kow	**1.16**	**1.12**	**0.40**	**0.72**	**-0.23**	**0.23**	**0.00**	**0.30**
log Kow	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17
ifference	1.01	1.05	1.77	1.45	2.40	1.94	2.17	1.87

100 mg/L	Untreated		Treated		DIA		Westover	
	4	5	4	5	4	5	4	5
erage Kd	1.203	330.260	0.706	44.523	0.160	0.255	0.148	0.203
foc	0.030	0.030	0.030	0.030	0.008	0.008	0.005	0.005
Koc	40.107	11008.67	23.547	1484.10	20.050	31.875	29.600	40.600
Kom	23.264	6385.538	13.658	860.847	11.630	18.489	17.169	23.550
log Kow	**1.44**	**6.13**	**0.99**	**4.45**	**0.86**	**1.24**	**1.18**	**1.45**
log Kow	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17
ifference	0.73	-3.96	1.18	-2.28	1.31	0.93	0.99	0.72

10 mg/L	Untreated		Treated		DIA		Westover	
	4	5	4	5	4	5	4	5
erage Kd	32.850	55.203	0.521	400.000	2.844	5.021	3.897	16.092
foc	0.030	0.030	0.030	0.030	0.008	0.008	0.005	0.005
Koc	1095.0	1840.1	17.4	13333	355.5	627.6	779.4	3218.4
Kom	635.2	1067.3	10.1	7734.0	206.2	364.0	452.1	1866.8
log Kow	**4.20**	**4.63**	**0.74**	**6.29**	**3.26**	**3.73**	**3.91**	**5.10**
log Kow	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17
ifference	-2.03	-2.46	1.43	-4.12	-1.09	-1.56	-1.74	-2.93

100 Mix	Untreated		Treated		DIA		Westover	
	4	5	4	5	4	5	4	5
erage Kd	1.219	1.735	0.547	2.325	0.208	0.291	0.136	0.193
foc	0.030	0.030	0.030	0.030	0.008	0.008	0.005	0.005
Koc	40.6	57.8	18.2	77.5	26.0	36.4	27.2	38.6
Kom	23.6	33.5	10.6	45.0	15.1	21.1	15.8	22.4
log Kow	**1.45**	**1.74**	**0.78**	**1.99**	**1.07**	**1.35**	**1.11**	**1.40**
log Kow	2.17	2.17	2.17	2.17	2.17	2.17	2.17	2.17
ifference	0.72	0.43	1.39	0.18	1.10	0.82	1.06	0.77

Back-calculated log Kow values
Differences < or = 1.00 (acceptable)
Differences < 0 (not good)

Appendix J

Statistical Analysis

Calculations

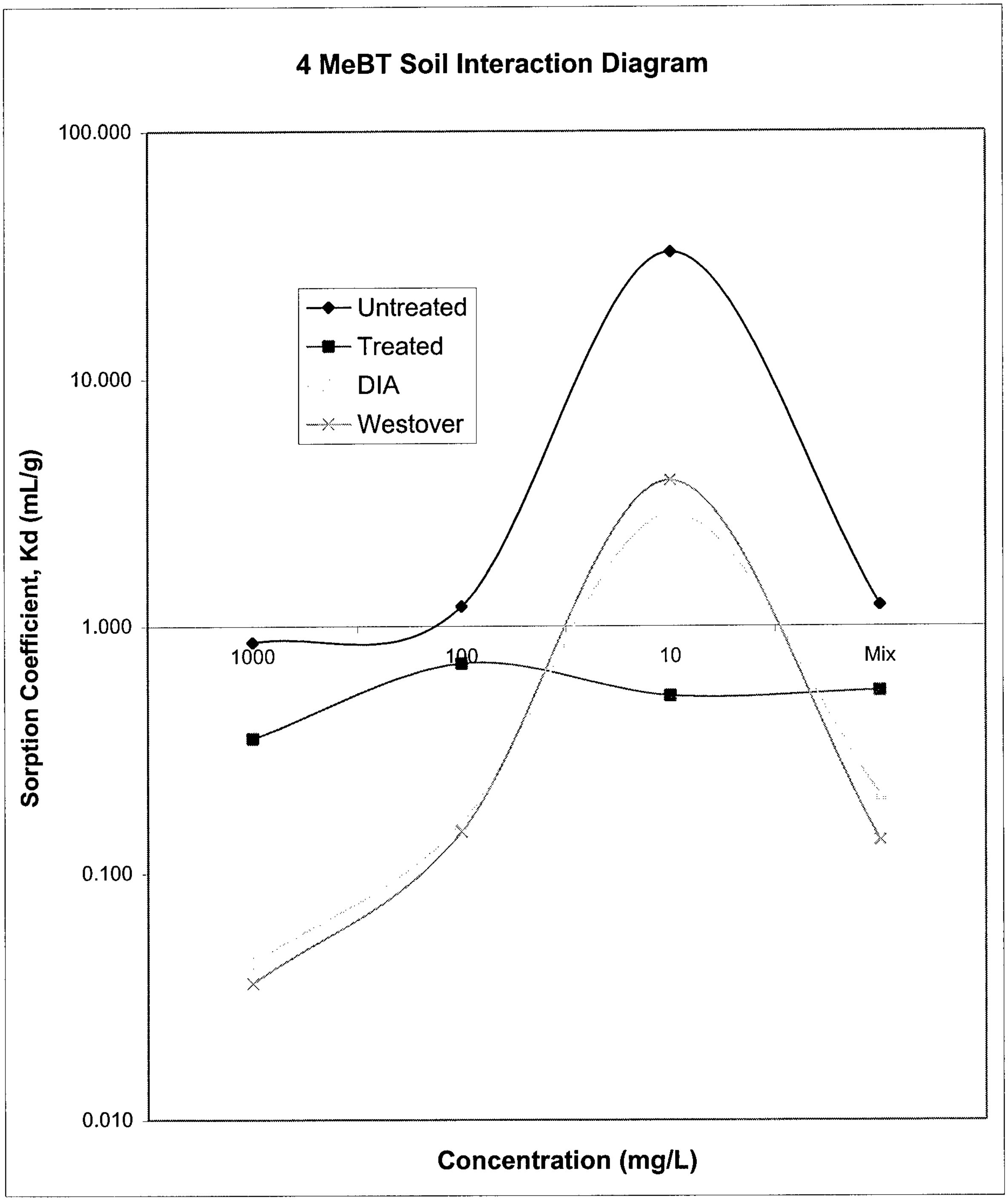
Appendix J

Statistical Analysis

4-MeBT

4 MeBT

	1000	100	10	Mix
Untreate	0.860	1.203	32.849	1.219
Treated	0.350	0.706	0.521	0.547
DIA	0.044	0.160	2.844	0.208
Westove	0.036	0.148	3.897	0.136



```
CASE        SOIL      CONC    OBSERVE       YHAT      RESID
   1           1         1      0.817     0.8604    -0.0434
   2           1         1      0.907     0.8604     0.0466
   3           1         1       0.83     0.8604    -0.0304
   4           1         1      0.841     0.8604    -0.0194
   5           1         1      0.907     0.8604     0.0466
   6           1         2      1.169     1.2032    -0.0342
   7           1         2       1.14     1.2032    -0.0632
   8           1         2      1.085     1.2032    -0.1182
   9           1         2      1.445     1.2032     0.2418
  10           1         2      1.177     1.2032    -0.0262
  11           1         3      32.68     32.849     -0.169
  12           1         3     32.029     32.849      -0.82
  13           1         3     32.317     32.849     -0.532
  14           1         3     34.877     32.849      2.028
  15           1         3     32.342     32.849     -0.507
  16           1         4      1.128     1.2188    -0.0908
  17           1         4      1.281     1.2188     0.0622
  18           1         4      1.204     1.2188    -0.0148
  19           1         4      1.223     1.2188     0.0042
  20           1         4      1.258     1.2188     0.0392
  21           2         1       0.35       0.35       -0.0
  22           2         1      0.343       0.35     -0.007
  23           2         1      0.365       0.35      0.015
  24           2         1      0.359       0.35      0.009
  25           2         1      0.333       0.35     -0.017
  26           2         2       0.71     0.7064     0.0036
  27           2         2      0.718     0.7064     0.0116
  28           2         2      0.676     0.7064    -0.0304
  29           2         2      0.707     0.7064     0.0006
  30           2         2      0.721     0.7064     0.0146
  31           2         3       0.56     0.5212     0.0388
  32           2         3      0.494     0.5212    -0.0272
  33           2         3      0.506     0.5212    -0.0152
  34           2         3      0.562     0.5212     0.0408
  35           2         3      0.484     0.5212    -0.0372
  36           2         4      0.538      0.547     -0.009
  37           2         4       0.54      0.547     -0.007
  38           2         4      0.572      0.547      0.025
  39           2         4      0.536      0.547     -0.011
  40           2         4      0.549      0.547      0.002
  41           3         1      0.027     0.0436    -0.0166
  42           3         1      0.046     0.0436     0.0024
  43           3         1      0.051     0.0436     0.0074
  44           3         1      0.041     0.0436    -0.0026
  45           3         1      0.053     0.0436     0.0094
  46           3         2      0.142     0.1604    -0.0184
  47           3         2      0.161     0.1604     0.0006
  48           3         2       0.15     0.1604    -0.0104
  49           3         2      0.171     0.1604     0.0106
  50           3         2      0.178     0.1604     0.0176
  51           3         3      2.738     2.8442    -0.1062
  52           3         3      3.055     2.8442     0.2108
  53           3         3      2.834     2.8442    -0.0102
  54           3         3      2.814     2.8442    -0.0302
  55           3         3       2.78     2.8442    -0.0642
  56           3         4      0.208     0.2078     0.0002
  57           3         4      0.197     0.2078    -0.0108
  58           3         4      0.203     0.2078    -0.0048
  59           3         4      0.215     0.2078     0.0072
  60           3         4      0.216     0.2078     0.0082
```

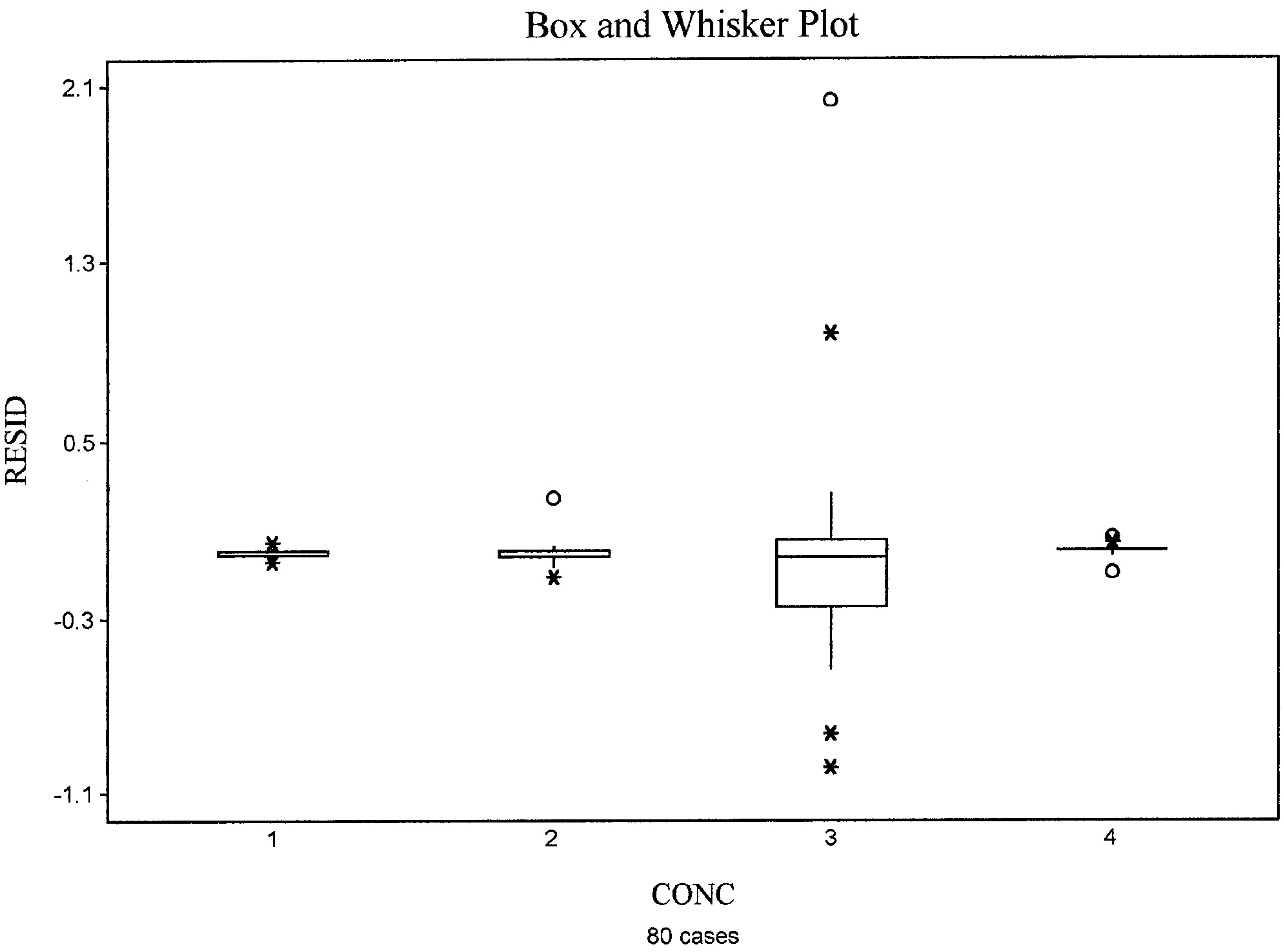
```
CASE      SOIL      CONC   OBSERVE      YHAT     RESID
  61         4         1     0.041     0.036     0.005
  62         4         1     0.033     0.036    -0.003
  63         4         1      0.04     0.036     0.004
  64         4         1     0.028     0.036    -0.008
  65         4         1     0.038     0.036     0.002
  66         4         2     0.148     0.148       0.0
  67         4         2     0.146     0.148    -0.002
  68         4         2     0.145     0.148    -0.003
  69         4         2     0.162     0.148     0.014
  70         4         2     0.139     0.148    -0.009
  71         4         3     3.557    3.8968   -0.3398
  72         4         3     4.879    3.8968    0.9822
  73         4         3     4.153    3.8968    0.2562
  74         4         3      3.98    3.8968    0.0832
  75         4         3     2.915    3.8968   -0.9818
  76         4         4     0.132    0.1362   -0.0042
  77         4         4     0.129    0.1362   -0.0072
  78         4         4     0.138    0.1362    0.0018
  79         4         4      0.14    0.1362    0.0038
  80         4         4     0.142    0.1362    0.0058
```

```
STUDENT EDITION OF STATISTIX                              4MEBT, 03/02/99, 9:50

ANALYSIS OF VARIANCE TABLE FOR OBSERVE

SOURCE         DF       SS          MS           F          P
-------------  ----  ----------  ----------  ---------  ---------
SOIL (A)          3    1019.49     339.830    2846.19    0.0000
CONC (B)          3    1371.45     457.149    3828.79    0.0000
A*B               9    2492.13     276.903    2319.16    0.0000
RESIDUAL         64    7.64147     0.11940
-------------  ----  ----------
TOTAL            79    4890.71
```

```
STUDENT EDITION OF STATISTIX                         4MEBT, 03/02/99, 10:23

GRAND MEAN    2.8581    SE    0.0386


MEANS OF OBSERVE FOR SOIL

   SOIL          MEAN       SS (MEAN)
 ---------   ----------   -----------
     1         9.0328        3787.3
     2         0.5312        0.3277
     3         0.8140        27.612
     4         1.0542        56.022

OBSERVATIONS PER CELL                 20
STD ERROR OF AN AVERAGE           0.0773
STD ERROR (DIFF OF 2 AVE'S)       0.1093
ERROR TERM USED: RESIDUAL, 64 DF


MEANS OF OBSERVE FOR CONC

   CONC          MEAN       SS (MEAN)
 ---------   ----------   -----------
     1         0.3225        2.2585
     2         0.5545        3.9029
     3         10.028        3509.4
     4         0.5274        3.6831

OBSERVATIONS PER CELL                 20
STD ERROR OF AN AVERAGE           0.0773
STD ERROR (DIFF OF 2 AVE'S)       0.1093
ERROR TERM USED: RESIDUAL, 64 DF


MEANS OF OBSERVE FOR SOIL*CONC

   SOIL        CONC          MEAN       SS (MEAN)
 ---------   ---------   ----------   -----------
     1           1          0.8604      7.53E-03
     1           2          1.2032        0.0783
     1           3          32.849        5.3538
     1           4          1.2188        0.0139
     2           1          0.3500      6.44E-04
     2           2          0.7064      1.29E-03
     2           3          0.5212      5.52E-03
     2           4          0.5470      8.80E-04
     3           1          0.0436      4.31E-04
     3           2          0.1604      8.69E-04
     3           3          2.8442        0.0609
     3           4          0.2078      2.59E-04
     4           1          0.0360      1.18E-04
     4           2          0.1480      2.90E-04
     4           3          3.8968        2.1167
     4           4          0.1362      1.21E-04

OBSERVATIONS PER CELL                  5
STD ERROR OF AN AVERAGE           0.1545
STD ERROR (DIFF OF 2 AVE'S)       0.2185
ERROR TERM USED: RESIDUAL, 64 DF
```

```
STUDENT EDITION OF STATISTIX                            4MEBT, 03/02/99, 10:28

TUKEY (HSD) COMPARISON OF MEANS OF OBSERVE BY SOIL

                          HOMOGENEOUS
   SOIL        MEAN       GROUPS
---------    ----------   -----------
     1         9.0328      I
     4         1.0543     .. I
     3         0.8140     .. I I
     2         0.5312     .... I

THERE ARE 3 GROUPS IN WHICH THE MEANS ARE
NOT SIGNIFICANTLY DIFFERENT FROM ONE ANOTHER.

CRITICAL Q VALUE                   3.731    REJECTION LEVEL    0.050
CRITICAL VALUE FOR COMPARISON     0.2883
STANDARD ERROR FOR COMPARISON     0.1093

ERROR TERM USED: RESIDUAL, 64 DF
```

```
STUDENT EDITION OF STATISTIX                                4MEBT, 03/02/99, 10:28

TUKEY (HSD) COMPARISON OF MEANS OF OBSERVE BY CONC

                          HOMOGENEOUS
   CONC         MEAN      GROUPS
---------    ----------   -----------
     3        10.028       I
     2        0.5545      .. I
     4        0.5274      .. I
     1        0.3225      .. I

THERE ARE 2 GROUPS IN WHICH THE MEANS ARE
NOT SIGNIFICANTLY DIFFERENT FROM ONE ANOTHER.

CRITICAL Q VALUE                     3.731    REJECTION LEVEL    0.050
CRITICAL VALUE FOR COMPARISON       0.2883
STANDARD ERROR FOR COMPARISON       0.1093

ERROR TERM USED: RESIDUAL, 64 DF
```



Box and Whisker Plot
2.1
1.3
0.5
-0.3
-1.1
RESID
1
2
3
4
CONC
80 cases

```
STUDENT EDITION OF STATISTIX                          4MEBT, 03/02/99, 10:04

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                              SAMPLE
   SOIL           MEAN         SIZE       S.D.         S.E.
----------     ----------     ------   ---------    ---------
     3           0.0436         5        0.0104     4.64E-03
     4           0.0360         5      5.43E-03     2.43E-03
DIFFERENCE    7.60E-03

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION               T        DF        P      95% CI FOR DIFFERENCE
-----------------     ------   ------   ------   ---------------------
EQUAL VARIANCES        1.45       8     0.1850     (-4.48E-03, 0.0197)
UNEQUAL VARIANCES      1.45      6.0    0.1969     (-5.20E-03, 0.0204)

                            F      NUM DF   DEN DF      P
TESTS FOR EQUALITY       -------   ------   ------   ------
      OF VARIANCES         3.65       4        4     0.1187

CASES INCLUDED 10     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                               4MEBT, 03/02/99, 10:06

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                              SAMPLE
    SOIL           MEAN        SIZE        S.D.          S.E.
 ----------     ----------   -------   ----------    ----------
      3           0.1604        5        0.0147      6.59E-03
      4           0.1480        5      8.51E-03      3.81E-03
 DIFFERENCE       0.0124

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                 T        DF         P       95% CI FOR DIFFERENCE
-----------------      ------    ------    ------    ----------------------
EQUAL VARIANCES          1.63        8     0.1420     (-5.16E-03, 0.0300)
UNEQUAL VARIANCES        1.63       6.4    0.1514     (-5.95E-03, 0.0307)

                            F       NUM DF     DEN DF       P
TESTS FOR EQUALITY      -------    -------    -------    -------
      OF VARIANCES        3.00        4          4        0.1564

CASES INCLUDED 10     MISSING CASES 0
```

Test 1 for 4-MeBT looks at the clayey vs. sandy soil comparison.

$t_{star} = 1.637$ From Statistix

$t_{025} < t_{star} < t_{975}$

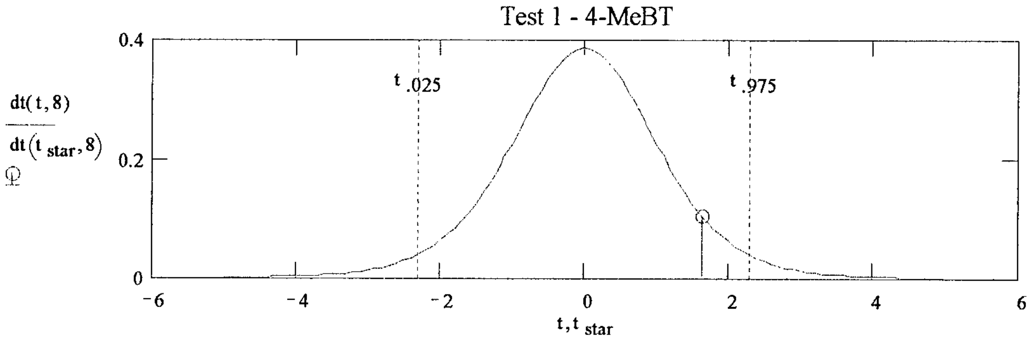
Table A.5, Devore, 8 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Not Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                               4MEBT, 03/02/99, 10:09

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                              SAMPLE
   SOIL           MEAN         SIZE        S.D.          S.E.
----------     ----------   ------    ---------     ---------
     1           0.8604        5        0.0434        0.0194
     4           0.0360        5      5.43E-03      2.43E-03
DIFFERENCE       0.8244

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                  T        DF         P       95% CI FOR DIFFERENCE
-----------------        ------    ------    ------    ---------------------
EQUAL VARIANCES           42.17       8      0.0000      (0.7793, 0.8695)
UNEQUAL VARIANCES         42.17      4.1     0.0000      (0.7708, 0.8780)

                             F      NUM DF    DEN DF       P
TESTS FOR EQUALITY        -------   ------    ------    ------
      OF VARIANCES         63.79       4         4      0.0007

CASES INCLUDED 10    MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                           4MEBT, 03/02/99, 10:10

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                                SAMPLE
   SOIL            MEAN          SIZE        S.D.         S.E.
 ----------     ----------     ------     ---------    ---------
     1            1.2032          5         0.1399       0.0626
     4            0.1480          5       8.51E-03     3.81E-03
DIFFERENCE        1.0552

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION              T         DF        P        95% CI FOR DIFFERENCE
-----------------    ------    ------    ------    ---------------------
EQUAL VARIANCES      16.83       8       0.0000       (0.9107, 1.1997)
UNEQUAL VARIANCES    16.83        4.0    0.0001       (0.8817, 1.2287)

                        F       NUM DF    DEN DF       P
TESTS FOR EQUALITY   -------    ------    ------    ------
      OF VARIANCES   269.96        4         4      0.0000

CASES INCLUDED 10    MISSING CASES 0
```

Test 2 for 4-MeBT looks at the higher f_{oc} vs. low f_{oc} soil comparison.

$t_{star} = 42.495$ From Statistix

$t_{025} < t_{star} < t_{975}$

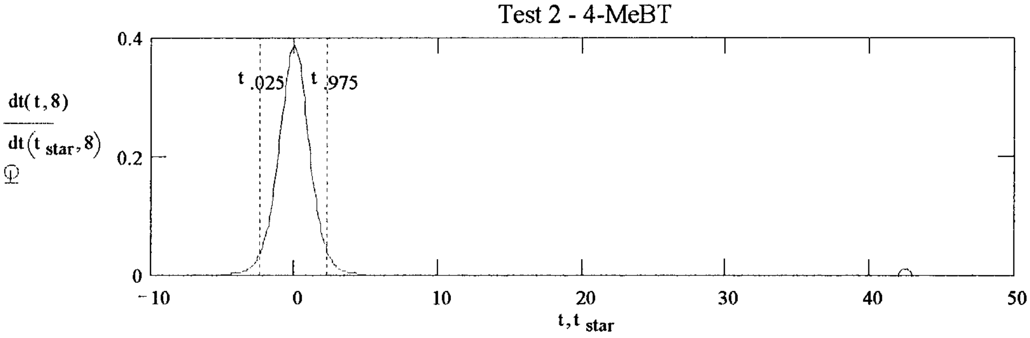
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306$ $t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                            4MEBT, 03/02/99, 10:12

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                          SAMPLE
   SOIL          MEAN      SIZE       S.D.        S.E.
----------    ----------  ------   ---------   ---------
     1          0.8604      5       0.0434      0.0194
     2          0.3500      5       0.0127     5.67E-03
DIFFERENCE      0.5104

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION               T        DF        P       95% CI FOR DIFFERENCE
-----------------    ------    ------    ------    ---------------------
EQUAL VARIANCES       25.25       8      0.0000       (0.4638, 0.5570)
UNEQUAL VARIANCES     25.25      4.7     0.0000       (0.4574, 0.5634)

                           F      NUM DF    DEN DF       P
TESTS FOR EQUALITY     -------   ------    ------    ------
      OF VARIANCES      11.69       4         4      0.0177

CASES INCLUDED 10     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                                4MEBT, 03/02/99, 10:14

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                                    SAMPLE
   SOIL             MEAN             SIZE        S.D.          S.E.
----------       ----------        ------     ---------     ---------
    1              1.2032             5         0.1399        0.0626
    2              0.7064             5         0.0179      8.02E-03
DIFFERENCE         0.4968

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                  T         DF         P       95% CI FOR DIFFERENCE
-----------------        ------     ------     ------    ---------------------
EQUAL VARIANCES           7.88        8       0.0000        (0.3513, 0.6423)
UNEQUAL VARIANCES         7.88       4.1      0.0012        (0.3238, 0.6698)

                             F       NUM DF    DEN DF        P
TESTS FOR EQUALITY        -------    ------    ------     ------
      OF VARIANCES        60.92        4         4        0.0008

CASES INCLUDED 10     MISSING CASES 0
```

Test 3 for 4-MeBT looks at an acclimated vs. unacclimated soil comparison.

$t_{star} = 26.309$ From Statisitx

$t_{025} < t_{star} < t_{975}$

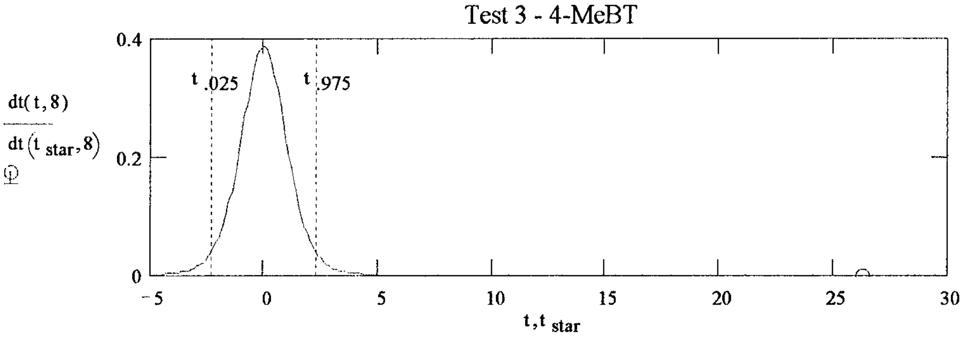
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                        4MEBT, 03/02/99, 10:16

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                                SAMPLE
   CONC            MEAN          SIZE       S.D.         S.E.
____________    ____________    ______    __________   __________

     2            1.2032          5       0.1399        0.0626
     4            1.2188          5       0.0589        0.0264
DIFFERENCE       -0.0156

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                 T        DF         P      95% CI FOR DIFFERENCE
_________________       ______    ______    ______   _____________________

EQUAL VARIANCES          -0.23       8      0.8240     (-0.1721, 0.1409)
UNEQUAL VARIANCES        -0.23     5.4      0.8267     (-0.1865, 0.1553)

                             F      NUM DF    DEN DF       P
TESTS FOR EQUALITY       _______    ______    ______    ______
      OF VARIANCES        5.64         4         4      0.0613

CASES INCLUDED 10    MISSING CASES 0
```

Test 4 for 4-MeBT looks at a PG additive vs. no PG added concentration mix comparison.

$t_{star} = -0.249$

$t_{025} < t_{star} < t_{975}$

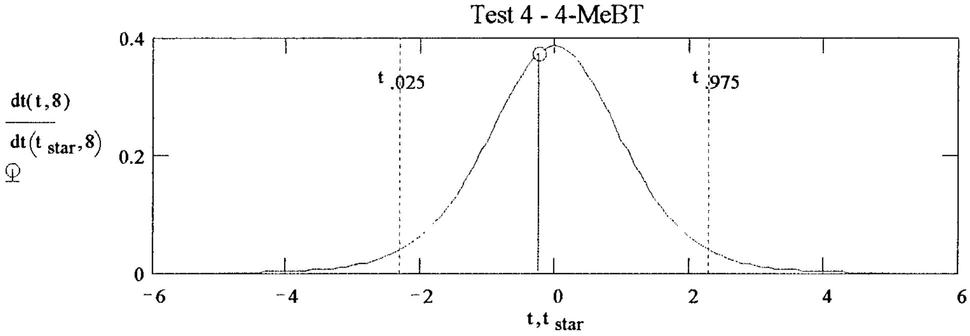
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Not Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                        4MEBT, 03/02/99, 10:17

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                           SAMPLE
   CONC           MEAN      SIZE       S.D.         S.E.
 ----------    ----------  ------   ----------   ----------
     2           0.4334      10       0.2882       0.0911
     4           0.3774      10       0.1791       0.0566
DIFFERENCE       0.0560

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T        DF         P       95% CI FOR DIFFERENCE
-----------------      ------    ------    ------    ---------------------
EQUAL VARIANCES         0.52      18       0.6081      (-0.1694, 0.2814)
UNEQUAL VARIANCES       0.52      15.1     0.6093      (-0.1726, 0.2846)

                           F      NUM DF    DEN DF       P
TESTS FOR EQUALITY      -------   ------    ------    ------
      OF VARIANCES        2.59      9         9       0.0864

CASES INCLUDED 20     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                              4MEBT, 03/02/99, 10:19

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                              SAMPLE
   CONC            MEAN        SIZE       S.D.        S.E.
 ----------     ----------   ------   ---------   ---------
      2            0.1604        5      0.0147     6.59E-03
      4            0.2078        5    8.04E-03     3.60E-03
 DIFFERENCE       -0.0474

 NULL HYPOTHESIS: DIFFERENCE =  0
 ALTERNATIVE HYP: DIFFERENCE <> 0

 ASSUMPTION               T        DF        P       95% CI FOR DIFFERENCE
 -----------------     ------   ------   ------   ---------------------
 EQUAL VARIANCES        -6.31       8    0.0002     (-0.0647, -0.0301)
 UNEQUAL VARIANCES      -6.31     6.2    0.0007     (-0.0656, -0.0292)

                           F      NUM DF   DEN DF      P
 TESTS FOR EQUALITY     -------   ------   ------   ------
       OF VARIANCES       3.36       4        4     0.1338

 CASES INCLUDED 10     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                                4MEBT, 03/02/99, 10:20

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                                 SAMPLE
   CONC            MEAN           SIZE       S.D.         S.E.
-------------   ------------   ---------   ----------   ----------
     2            0.1480           5       8.51E-03     3.81E-03
     4            0.1362           5       5.50E-03     2.46E-03
DIFFERENCE        0.0118

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                 T          DF          P       95% CI FOR DIFFERENCE
--------------------    -------    -------    -------    ---------------------------
EQUAL VARIANCES          2.60         8       0.0314       (1.35E-03, 0.0223)
UNEQUAL VARIANCES        2.60        6.8      0.0360       (1.03E-03, 0.0226)

                            F        NUM DF     DEN DF        P
TESTS FOR EQUALITY      ---------   -------    -------    -------
       OF VARIANCES       2.40         4          4        0.2086

CASES INCLUDED 10     MISSING CASES 0
```

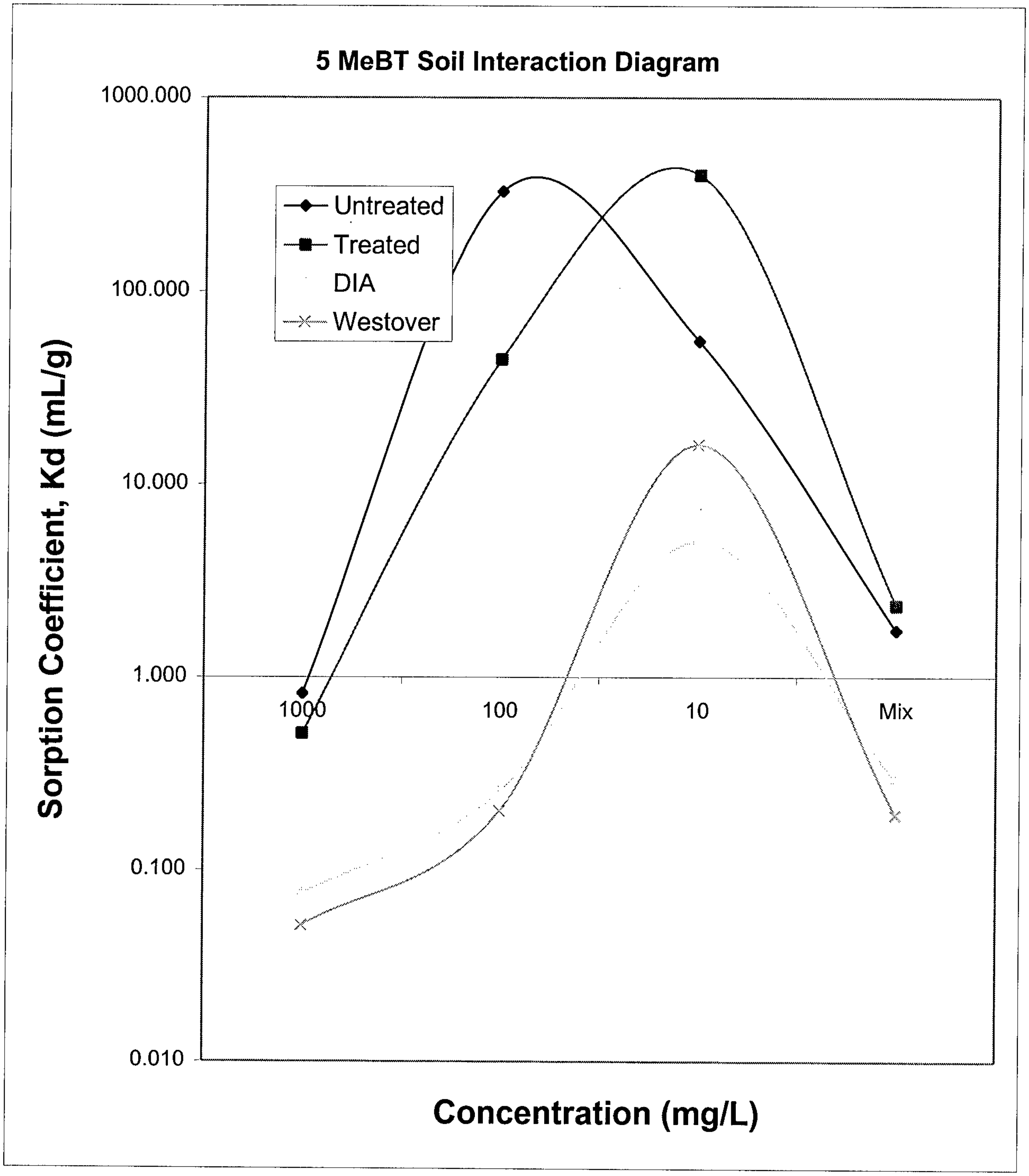
Appendix J

Statistical Analysis

5-MeBT

5 MeBT

	1000	100	10	Mix
Untreate	0.825	330.000	55.200	1.735
Treated	0.512	44.500	400	2.325
DIA	0.075	0.255	5.021	0.291
Westove	0.051	0.203	16.092	0.193



```
CASE     SOIL     CONC   OBSERVE      YHAT      RESID
   1        1        1     0.788     0.8252   -0.0372
   2        1        1     0.871     0.8252    0.0458
   3        1        1     0.799     0.8252   -0.0262
   4        1        1     0.805     0.8252   -0.0202
   5        1        1     0.863     0.8252    0.0378
   6        1        2     1.617   330.2648 -328.6478
   7        1        2     1.574   330.2648 -328.6908
   8        1        2     1.493   330.2648 -328.7718
   9        1        2      1645   330.2648 1314.7352
  10        1        2      1.64   330.2648 -328.6248
  11        1        3    52.221    55.2028   -2.9818
  12        1        3    54.016    55.2028   -1.1868
  13        1        3     51.98    55.2028   -3.2228
  14        1        3    60.419    55.2028    5.2162
  15        1        3    57.378    55.2028    2.1752
  16        1        4      1.63     1.7348   -0.1048
  17        1        4     1.781     1.7348    0.0462
  18        1        4     1.735     1.7348    0.0002
  19        1        4     1.716     1.7348   -0.0188
  20        1        4     1.812     1.7348    0.0772
  21        2        1      0.52     0.5116    0.0084
  22        2        1     0.498     0.5116   -0.0136
  23        2        1     0.533     0.5116    0.0214
  24        2        1     0.515     0.5116    0.0034
  25        2        1     0.492     0.5116   -0.0196
  26        2        2     3.211     44.523   -41.312
  27        2        2   188.557     44.523   144.034
  28        2        2    24.383     44.523    -20.14
  29        2        2     3.223     44.523     -41.3
  30        2        2     3.241     44.523   -41.282
  31        2        3     1.874  40346.361 -40344.48
  32        2        3     1.934  40346.361 -40344.42
  33        2        3      5756  40346.361 -34590.36
  34        2        3       232  40346.361 -40114.36
  35        2        3    195740  40346.361 155393.63
  36        2        4     2.387     2.3252    0.0618
  37        2        4     2.367     2.3252    0.0418
  38        2        4     2.245     2.3252   -0.0802
  39        2        4     2.309     2.3252   -0.0162
  40        2        4     2.318     2.3252   -0.0072
  41        3        1     0.049     0.0754   -0.0264
  42        3        1     0.072     0.0754   -0.0034
  43        3        1     0.087     0.0754    0.0116
  44        3        1     0.077     0.0754    0.0016
  45        3        1     0.092     0.0754    0.0166
  46        3        2     0.249      0.255    -0.006
  47        3        2     0.269      0.255     0.014
  48        3        2     0.232      0.255    -0.023
  49        3        2     0.258      0.255     0.003
  50        3        2     0.267      0.255     0.012
  51        3        3     3.969     5.0206   -1.0516
  52        3        3     5.904     5.0206    0.8834
  53        3        3     5.007     5.0206   -0.0136
  54        3        3     5.122     5.0206    0.1014
  55        3        3     5.101     5.0206    0.0804
  56        3        4     0.288     0.2906   -0.0026
  57        3        4     0.282     0.2906   -0.0086
  58        3        4     0.289     0.2906   -0.0016
  59        3        4     0.297     0.2906    0.0064
  60        3        4     0.297     0.2906    0.0064
```

```
CASE       SOIL       CONC   OBSERVE       YHAT      RESID
  61          4          1     0.056     0.0514     0.0046
  62          4          1     0.049     0.0514    -0.0024
  63          4          1     0.057     0.0514     0.0056
  64          4          1     0.041     0.0514    -0.0104
  65          4          1     0.054     0.0514     0.0026
  66          4          2     0.202      0.203     -0.001
  67          4          2     0.198      0.203     -0.005
  68          4          2     0.201      0.203     -0.002
  69          4          2     0.221      0.203      0.018
  70          4          2     0.193      0.203      -0.01
  71          4          3     2.963    16.0918   -13.1288
  72          4          3    63.733    16.0918    47.6412
  73          4          3     3.017    16.0918   -13.0748
  74          4          3     2.931    16.0918   -13.1608
  75          4          3     7.815    16.0918    -8.2768
  76          4          4     0.188     0.1928    -0.0048
  77          4          4     0.184     0.1928    -0.0088
  78          4          4     0.196     0.1928     0.0032
  79          4          4     0.197     0.1928     0.0042
  80          4          4     0.199     0.1928     0.0062
```

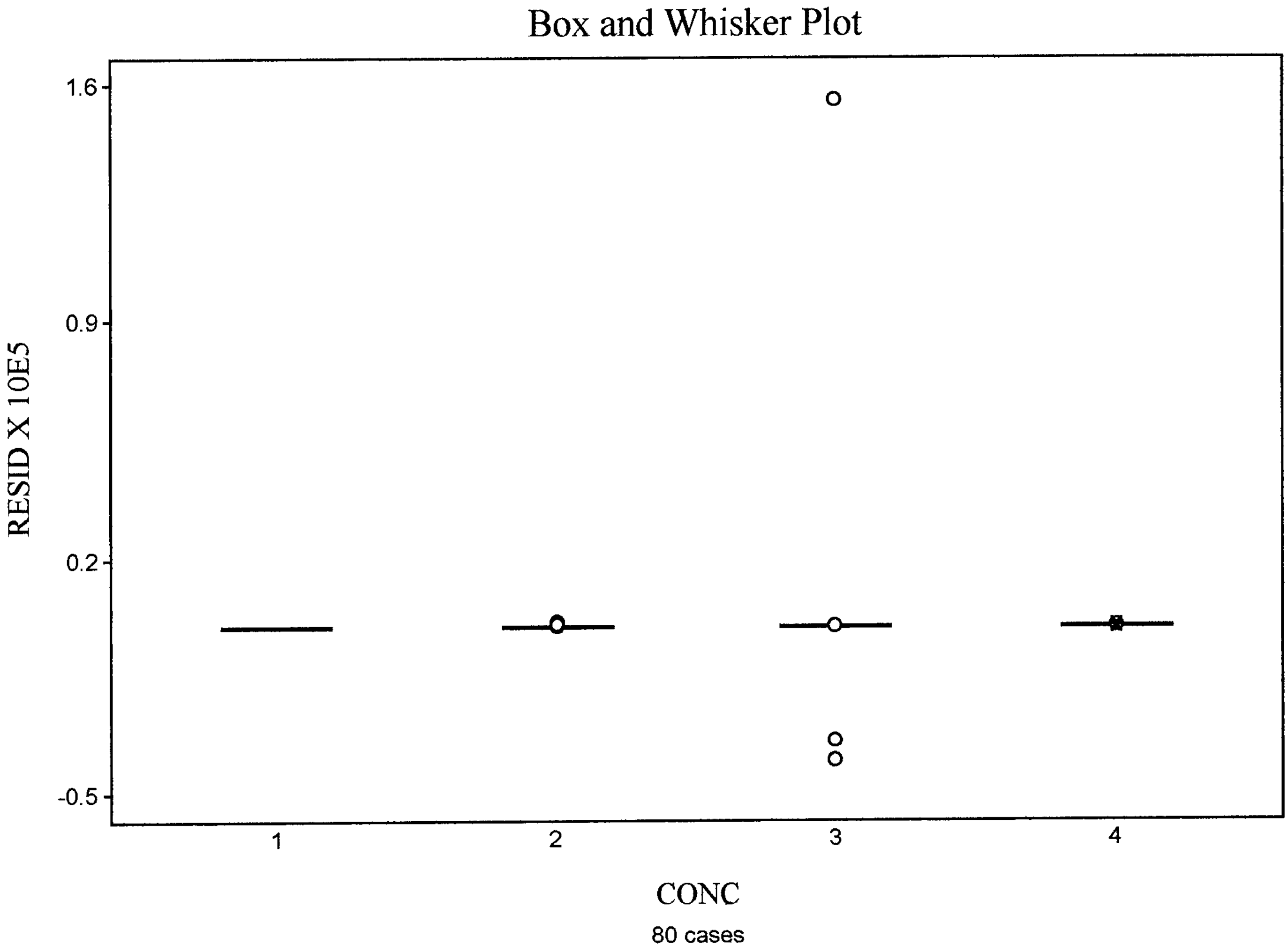
```
STUDENT EDITION OF STATISTIX                              5MEBT, 03/02/99, 10:50

ANALYSIS OF VARIANCE TABLE FOR OBSERVE

SOURCE          DF       SS           MS           F        P
------------   ----  ----------   ----------   -------  ------
SOIL  (A)         3  1.519E+09    5.065E+08       1.07  0.3676
CONC  (B)         3  1.522E+09    5.075E+08       1.08  0.3667
A*B               9  4.578E+09    5.086E+08       1.08  0.3916
RESIDUAL         64  3.021E+10    4.720E+08
------------   ----  ----------
TOTAL            79  3.783E+10
```

```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 10:51

GRAND MEAN     2550.2     SE     2429.1


MEANS OF OBSERVE FOR SOIL

   SOIL          MEAN        SS (MEAN)
 ---------    ---------    -----------
     1         97.007       2.53E+06
     2          10098       3.63E+10
     3         1.4104         88.929
     4         4.1348         3807.9

OBSERVATIONS PER CELL                    20
STD ERROR OF AN AVERAGE              4858.2
STD ERROR (DIFF OF 2 AVE'S)          6870.5
ERROR TERM USED: RESIDUAL, 64 DF


MEANS OF OBSERVE FOR CONC

   CONC          MEAN        SS (MEAN)
 ---------    ---------    -----------
     1         0.3659         2.0858
     2         93.811       2.57E+06
     3          10106       3.63E+10
     4         1.1359         16.918

OBSERVATIONS PER CELL                    20
STD ERROR OF AN AVERAGE              4858.2
STD ERROR (DIFF OF 2 AVE'S)          6870.5
ERROR TERM USED: RESIDUAL, 64 DF


MEANS OF OBSERVE FOR SOIL*CONC

   SOIL         CONC          MEAN        SS (MEAN)
 ---------    ---------    ---------    -----------
     1            1         0.8252        6.00E-03
     1            2         330.26        2.16E+06
     1            3         55.203          52.626
     1            4         1.7348          0.0194
     2            1         0.5116        1.11E-03
     2            2         44.523           26268
     2            3          40346        3.02E+10
     2            4         2.3252          0.0123
     3            1         0.0754        1.12E-03
     3            2         0.2550        9.14E-04
     3            3         5.0206          1.9032
     3            4         0.2906        1.65E-04
     4            1         0.0514        1.73E-04
     4            2         0.2030        4.54E-04
     4            3         16.092          2854.7
     4            4         0.1928        1.67E-04

OBSERVATIONS PER CELL                     5
STD ERROR OF AN AVERAGE              9716.3
STD ERROR (DIFF OF 2 AVE'S)           13741
ERROR TERM USED: RESIDUAL, 64 DF
```

```
GRAND MEAN     31.771     SE     27.556


MEANS OF OBSERVE FOR SOIL

    SOIL           MEAN         SS (MEAN)
 ----------     ----------     ----------
     1            110.94        2.52E+06
     2            15.787           32470
     3            0.2070          0.1353
     4            0.1491          0.0726

OBSERVATIONS PER CELL                   15
STD ERROR OF AN AVERAGE             55.113
STD ERROR (DIFF OF 2 AVE'S)         77.941
ERROR TERM USED: RESIDUAL, 48 DF


MEANS OF OBSERVE FOR CONC

    CONC           MEAN         SS (MEAN)
 ----------     ----------     ----------
     1            0.3659          2.0858
     2            93.811        2.57E+06
     4            1.1359          16.918

OBSERVATIONS PER CELL                   20
STD ERROR OF AN AVERAGE             47.729
STD ERROR (DIFF OF 2 AVE'S)         67.499
ERROR TERM USED: RESIDUAL, 48 DF


MEANS OF OBSERVE FOR SOIL*CONC

    SOIL           CONC            MEAN         SS (MEAN)
 ----------     ----------     ----------     ----------
     1              1            0.8252        6.00E-03
     1              2            330.26        2.16E+06
     1              4            1.7348          0.0194
     2              1            0.5116        1.11E-03
     2              2            44.523           26268
     2              4            2.3252          0.0123
     3              1            0.0754        1.12E-03
     3              2            0.2550        9.14E-04
     3              4            0.2906        1.65E-04
     4              1            0.0514        1.73E-04
     4              2            0.2030        4.54E-04
     4              4            0.1928        1.67E-04

OBSERVATIONS PER CELL                    5
STD ERROR OF AN AVERAGE             95.458
STD ERROR (DIFF OF 2 AVE'S)         135.00
ERROR TERM USED: RESIDUAL, 48 DF
```

```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 10:55

BONFERRONI COMPARISON OF MEANS OF OBSERVE BY SOIL

                        HOMOGENEOUS
  SOIL         MEAN     GROUPS
---------    ---------  -----------
    2          10098     I
    1         97.007     I
    4         4.1347     I
    3         1.4104     I

THERE ARE NO SIGNIFICANT PAIRWISE DIFFERENCES AMONG THE MEANS.

CRITICAL T VALUE                     2.723    REJECTION LEVEL    0.050
CRITICAL VALUE FOR COMPARISON        18707
STANDARD ERROR FOR COMPARISON       6870.5

ERROR TERM USED: RESIDUAL, 64 DF
```

```
STUDENT EDITION OF STATISTIX                             5MEBT, 03/02/99, 10:55

BONFERRONI COMPARISON OF MEANS OF OBSERVE BY CONC

                       HOMOGENEOUS
   CONC       MEAN     GROUPS
---------  ----------  ------------
     3         10106    I
     2        93.811    I
     4        1.1359    I
     1        0.3659    I

THERE ARE NO SIGNIFICANT PAIRWISE DIFFERENCES AMONG THE MEANS.

CRITICAL T VALUE                   2.723    REJECTION LEVEL    0.050
CRITICAL VALUE FOR COMPARISON      18707
STANDARD ERROR FOR COMPARISON     6870.5

ERROR TERM USED: RESIDUAL, 64 DF
```


Box and Whisker Plot
1.6
0.9
0.2
-0.5
RESID X 10E5
1
2
3
4
CONC
80 cases

```
STUDENT EDITION OF STATISTIX                               5MEBT, 03/02/99, 10:59

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                                SAMPLE
    SOIL            MEAN         SIZE        S.D.          S.E.
 ----------      ----------    ------    ----------    ----------
     3            0.0754          5         0.0167      7.49E-03
     4            0.0514          5       6.58E-03      2.94E-03
 DIFFERENCE       0.0240

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                  T        DF        P      95% CI FOR DIFFERENCE
-----------------        ------    ------    ------   ---------------------
EQUAL VARIANCES           2.98        8      0.0175    (5.45E-03, 0.0426)
UNEQUAL VARIANCES         2.98       5.2     0.0292    (3.56E-03, 0.0444)

                             F       NUM DF    DEN DF       P
TESTS FOR EQUALITY        -------    ------    ------    ------
      OF VARIANCES          6.47        4         4      0.0489

CASES INCLUDED 10     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                              5MEBT, 03/02/99, 11:00

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                                SAMPLE
   SOIL           MEAN           SIZE        S.D.         S.E.
 ----------    ----------      ------     ---------    ---------
     3           0.2550           5         0.0151      6.76E-03
     4           0.2030           5         0.0107      4.76E-03
DIFFERENCE       0.0520

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                  T        DF         P       95% CI FOR DIFFERENCE
-----------------        ------    ------    ------    ---------------------
EQUAL VARIANCES           6.29       8      0.0002       (0.0329, 0.0711)
UNEQUAL VARIANCES         6.29      7.2     0.0004       (0.0325, 0.0715)

                            F       NUM DF    DEN DF       P
TESTS FOR EQUALITY       -------    ------    ------    ------
      OF VARIANCES         2.01        4         4      0.2573

CASES INCLUDED 10     MISSING CASES 0
```

Test 1 for 5-MeBT looks at the clayey vs. sandy soil comparison.

$t_{star} := 2.98$ From Statistix

$t_{025} < t_{star} < t_{975}$

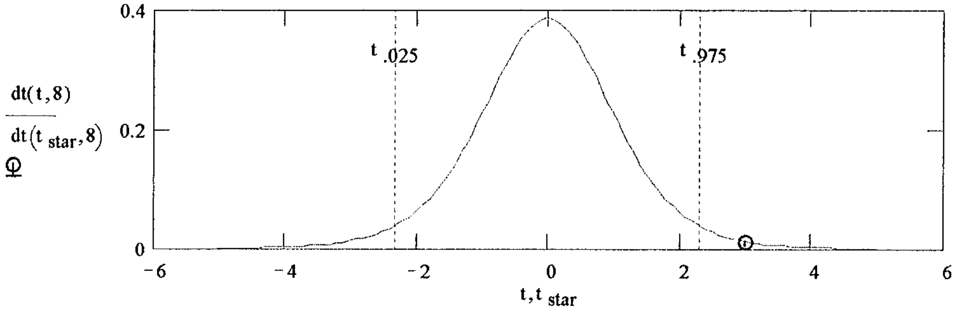
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                              5MEBT, 03/02/99, 11:01

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                                SAMPLE
   SOIL              MEAN        SIZE        S.D.         S.E.
----------       ----------    ------    ---------    ---------
     1             0.8252        5         0.0387       0.0173
     4             0.0514        5       6.58E-03     2.94E-03
DIFFERENCE         0.7738

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                 T         DF         P      95% CI FOR DIFFERENCE
-----------------      ------     ------     ------    ---------------------
EQUAL VARIANCES         44.03        8       0.0000      (0.7333, 0.8143)
UNEQUAL VARIANCES       44.03        4.2     0.0000      (0.7260, 0.8216)

                            F        NUM DF     DEN DF       P
TESTS FOR EQUALITY     -------     ------     ------     ------
      OF VARIANCES      34.67        4          4        0.0023

CASES INCLUDED 10    MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 11:02

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                            SAMPLE
   SOIL          MEAN        SIZE       S.D.        S.E.
 ---------     ---------   ------   ---------   ---------
     1          330.26        5       734.96      328.68
     4          0.2030        5       0.0107    4.76E-03
 DIFFERENCE     330.06

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T        DF       P      95% CI FOR DIFFERENCE
-----------------      ------   ------   ------   ---------------------
EQUAL VARIANCES         1.00       8     0.3447     (-427.88, 1088.0)
UNEQUAL VARIANCES       1.00      4.0    0.3721     (-582.51, 1242.6)

                            F        NUM DF     DEN DF       P
TESTS FOR EQUALITY       -------    -------    -------    ------
      OF VARIANCES4759164802.24        4          4        0.0000

CASES INCLUDED 10     MISSING CASES 0
```

Test 2 for 5-MeBT looks at the higher f_{oc} vs. low f_{oc} soil comparison.

$t_{star} = 44.658$ From Statistix

$t_{.025} < t_{star} < t_{.975}$

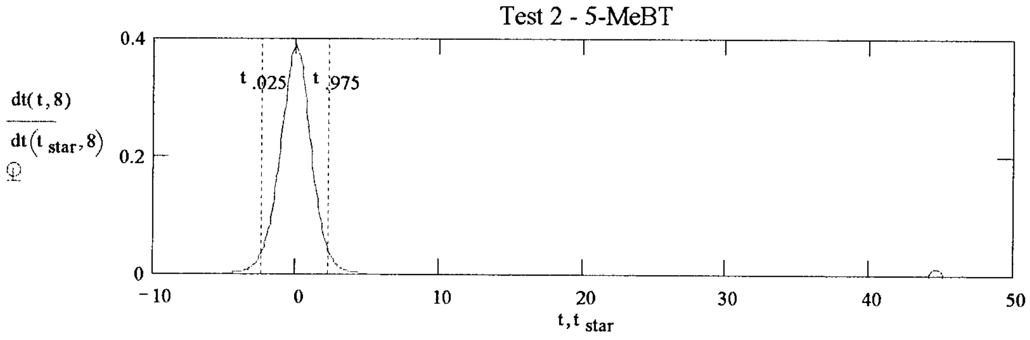
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306$ $t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 11:03

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                          SAMPLE
   SOIL          MEAN      SIZE       S.D.        S.E.
-------------  ---------  ------  ----------  ----------
     1          0.8252      5       0.0387      0.0173
     2          0.5116      5       0.0167    7.45E-03
DIFFERENCE      0.3136

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T       DF        P      95% CI FOR DIFFERENCE
-----------------     ------   ------   ------   ---------------------
EQUAL VARIANCES        16.63      8     0.0000     (0.2701, 0.3571)
UNEQUAL VARIANCES      16.63     5.4    0.0000     (0.2662, 0.3610)

                           F     NUM DF   DEN DF      P
TESTS FOR EQUALITY     -------   ------   ------   ------
      OF VARIANCES       5.41      4         4     0.0654

CASES INCLUDED 10    MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 11:04

TWO-SAMPLE T TESTS FOR OBSERVE BY SOIL

                               SAMPLE
   SOIL          MEAN           SIZE        S.D.          S.E.
 ----------    ----------    ---------   ----------    ----------
     1          330.26           5         734.96        328.68
     2          44.523           5         81.037        36.241
 DIFFERENCE     285.74

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T         DF        P      95% CI FOR DIFFERENCE
-----------------      ------    ------    ------    ---------------------
EQUAL VARIANCES         0.86       8      0.4127      (-476.80, 1048.3)
UNEQUAL VARIANCES       0.86      4.1     0.4352      (-623.83, 1195.3)

                          F       NUM DF    DEN DF       P
TESTS FOR EQUALITY     -------    ------    ------    ------
      OF VARIANCES      82.25        4         4      0.0004

CASES INCLUDED 10     MISSING CASES 0
```

Test 3 for 5-MeBT looks at an acclimated vs. unacclimated soil comparison.

$t_{star} = 18.098$

$t_{025} < t_{star} < t_{975}$

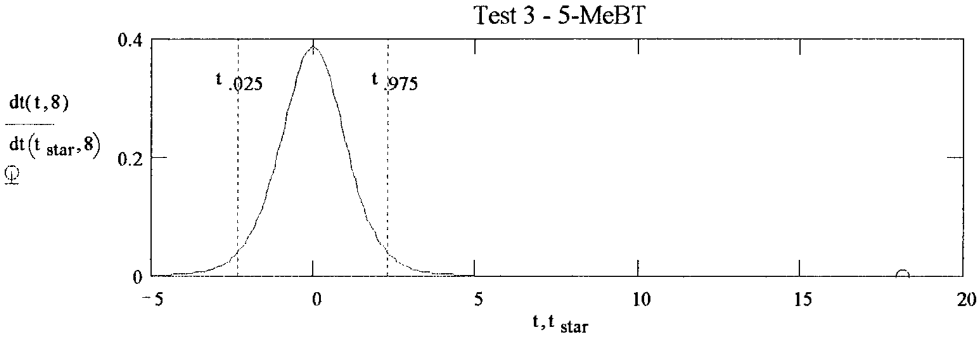
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 11:06

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                                SAMPLE
    CONC           MEAN          SIZE       S.D.        S.E.
 ----------     ----------     ------   ---------   ---------
     2           330.26          5       734.96      328.68
     4           1.7348          5       0.0697      0.0312
DIFFERENCE       328.53

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION              T       DF        P      95% CI FOR DIFFERENCE
-----------------   ------   ------   ------   ----------------------
EQUAL VARIANCES      1.00       8     0.3468     (-429.42, 1086.5)
UNEQUAL VARIANCES    1.00      4.0    0.3741     (-584.04, 1241.1)

                          F       NUM DF    DEN DF       P
TESTS FOR EQUALITY     -------   -------   -------   ------
      OF VARIANCES111197728.36       4         4     0.0000

CASES INCLUDED 10     MISSING CASES 0
```

Test 4 for 5-MeBT looks at a PG additive vs. no PG added concentration mix comparison.

$t_{star} = -5.009$

$t_{025} < t_{star} < t_{975}$

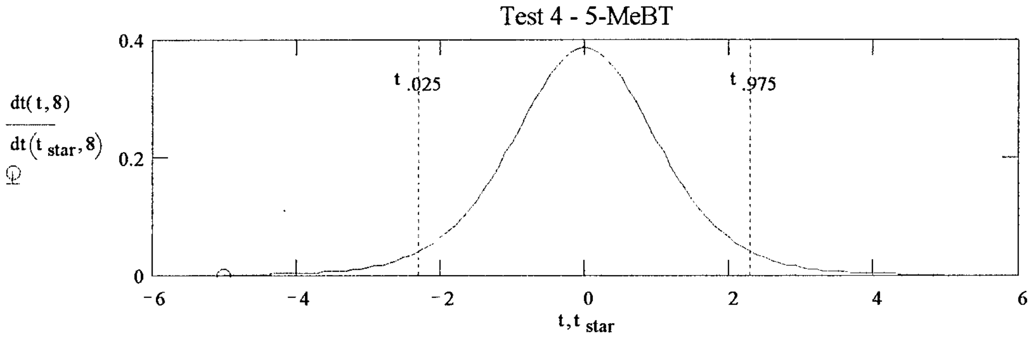
Table A.5, devour, 22 degree of freedom

$t_{.025} := -2.306 \quad t_{.975} := 2.306$

Do Reject H_o

ORGIN≡0

$t := -5, -4.9 .. 5$



```
STUDENT EDITION OF STATISTIX                          5MEBT, 03/02/99, 11:08

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                                SAMPLE
   CONC           MEAN           SIZE       S.D.        S.E.
------------   ------------   -------   ---------   ---------
     2           44.523           5       81.037      36.241
     4           2.3252           5       0.0555      0.0248
DIFFERENCE       42.198

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T        DF         P      95% CI FOR DIFFERENCE
---------------------   -------   -------   -------   --------------------------
EQUAL VARIANCES          1.16       8      0.2778     (-41.374, 125.77)
UNEQUAL VARIANCES        1.16      4.0     0.3090     (-58.423, 142.82)

                              F        NUM DF    DEN DF       P
TESTS FOR EQUALITY        ---------   -------   -------   -------
     OF VARIANCES2133388.64          4         4      0.0000

CASES INCLUDED 10    MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                                5MEBT, 03/02/99, 11:09

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                                SAMPLE
    CONC           MEAN          SIZE        S.D.          S.E.
 ------------  ------------  ---------  ------------  ------------
       2          0.2550          5        0.0151       6.76E-03
       4          0.2906          5      6.43E-03       2.87E-03
 DIFFERENCE      -0.0356

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION                T        DF         P       95% CI FOR DIFFERENCE
----------------------  -------  -------  -------  ---------------------------
EQUAL VARIANCES          -4.85      8      0.0013     (-0.0525, -0.0187)
UNEQUAL VARIANCES        -4.85      5.4    0.0038     (-0.0541, -0.0171)

                             F      NUM DF   DEN DF        P
TESTS FOR EQUALITY        -------  -------  -------   -------
      OF VARIANCES          5.53       4        4      0.0631

CASES INCLUDED 10     MISSING CASES 0
```

```
STUDENT EDITION OF STATISTIX                            5MEBT, 03/02/99, 11:11

TWO-SAMPLE T TESTS FOR OBSERVE BY CONC

                            SAMPLE
   CONC          MEAN        SIZE       S.D.        S.E.
 ----------   ----------   ------   ---------   ---------
     2          0.2030       5        0.0107     4.76E-03
     4          0.1928       5      6.46E-03     2.89E-03
 DIFFERENCE     0.0102

NULL HYPOTHESIS: DIFFERENCE =  0
ALTERNATIVE HYP: DIFFERENCE <> 0

ASSUMPTION               T       DF        P      95% CI FOR DIFFERENCE
-----------------      ------   ------   ------   ----------------------
EQUAL VARIANCES         1.83      8      0.1045    (-2.65E-03, 0.0230)
UNEQUAL VARIANCES       1.83      6.6    0.1125    (-3.14E-03, 0.0235)

                          F      NUM DF   DEN DF      P
TESTS FOR EQUALITY     ------   ------   ------   ------
      OF VARIANCES      2.72      4        4      0.1778

CASES INCLUDED 10     MISSING CASES 0
```

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Vita

First Lieutenant David L. Kellner was born in Buffalo, New York on February 11, 1968. After high school graduation he obtained an Associate Degree of Applied Science in Accounting in 1989. He then joined the United States Air Force in November 1989 as a Nondestructive Inspection Specialist in the 28th Maintenance Squadron at Ellsworth AFB, South Dakota after a 3 month technical school at Chanute AFB, IL. He was married on April 21, 1990 to Nancy Sunick. While at Ellsworth AFB, he attended the South Dakota School of Mines and Technology and obtained his Bachelor of Science in Civil Engineering in only 4 and ½ years. Upon his graduation from Officers Training School (OTS) 22 September 1995 at Maxwell AFB, Alabama; he was assigned to the 437th Civil Engineer Squadron, Charleston AFB, South Carolina from 28 September 95 to 13 August 1997. While at Charleston AFB, he served as a Project Officer (32E1G), Section Commander (C36P1), and Readiness Flight Commander (32E3B). He was selected to study for his Masters of Science in Engineering and Environmental Management (GEEM) at the Air Force Institute of Technology from August 1997 to March 1999. Upon completion of the GEEM program, he will be assigned to the 7th Civil Engineer Squadron, Dyess AFB, Texas.

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13. ABSTRACT *(Maximum 200 words)*

The air transportation industry requires deicing/anti-icing (ADAF) fluids to maintain flight operations in cold weather conditions. Additives to the ADAF aid in the performance of these agents. Approximately 52M liters of concentrated aircraft deicing fluid are used in North America per year in an attempt to correct this safety problem. Among the additives to ADAF are corrosion inhibitors/ flame retardants, wetting agents, and thickening agents. Some of these agents are known to be toxic to microorganisms. Identification of the transport processes of these agents in the environment is a necessary first step to understanding how to remediate ADAF. Methyl-Benzotriazole (MeBT) is a corrosion inhibitor/flame retardant toxic additive in ADAF. This study investigates the sorption characteristics of MeBT in various soils. Three soil types were used to evaluate the sorption characteristics of MeBT at 1000 mg/L, 100 mg/L, and a mixture of MeBT and propylene glycol (PG). A High Pressure Liquid Chromatograph (HPLC) was used to conduct the recovery experimentation after the samples had reached equilibrium. Resulting sorption coefficients revealed that MeBT did not sorb well to any of the soils types used. The organic carbon content affects the sorption coefficient by slightly raising the sorbed amount of MeBT.

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