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WEST VIRGINIA COAL FLY ASH SORPTION OF BTEX

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in partial fulfillment of the requirements for the degree of

Master of Science

in

Geology

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ABSTRACT

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Sorption is a term used in the environmental field to describe how chemical contaminants in soil and groundwater adhere to solid particles such as: clay, peat and activated carbon for the purposes of remediation, fate and transport. A potential surrogate for sorption of chemical contaminants in groundwater is coal fly ash. Batch test experiments have demonstrated coal fly ash's ability to remove hydrophobic, organic petroleum contaminants including: benzene, toluene, ethylbenzene and xylenes (BTEX) in groundwater through the processes of sorption. Coal fly ash is a byproduct material of coal fired power plants that is often disposed of on-site or at landfills. A beneficial use of coal fly ash is for the sorption of BTEX in groundwater.

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Chapter 1: Introduction

More than 2000 chemical contaminants have been found in wastewater, while 750 of these chemical contaminants have been identified in drinking water. More than 600 of these drinking water contaminants are of organic origin (Singh, 1994). Petroleum hydrocarbon products are found as contaminants in soils, ground water aquifers and surface waters. This is the result of leaking underground gasoline and diesel storage tanks, surface and marine transportation spills (Krumholz et al., 1996). In 1996, underground storage tanks were reported to Congress as the leading source of groundwater contamination in the nation according to the 1996 National Water Quality Inventory Report, section 305(b) (Anzzolin and Siedlecki, 2001). In 1998, more than 85,000 underground storage tanks (USTs) were reported from hydrogeologic settings in 22 states with 57% of these USTs having had confirmed contaminant releases and 60% of these settings reported volatile organic chemicals (VOCs) and petroleum compounds as contaminants of concern (Anzzolin and Siedlecki, 2001). The BTEX organic chemicals (benzene, toluene, ethylbenzene and xylene) are very common in the petroleum and chemical industry, which makes them ubiquitous and presents great risks to public health and the environment. Benzene is a carcinogen. Toluene is currently the most produced chemical in the United States (All American Environmental Services, 2002). O-Xylene is included in the U.S. EPA’s Priority Pollutant List (Banaerjee et. al., 1997).

Some groundwater remediation strategies for treatment of organic contaminants include: chemical oxidation, coagulation, froth flotation and adsorption. Of these methods, adsorption appears to offer the best prospects for overall treatment (Singh et al., 1994).

When choosing an adsorbent to remove organic compounds, cost effectiveness, availability and adsorptive properties are the main criteria (Virargharan, 1998). The use of Permeable Reactive Barriers (PRBs) is a proven remediation technique widely used for removal of metals and non-metals in aqueous solutions. For attenuation, barrier materials should provide retardation through: adsorption, precipitation, filtration, micro-biodegradation, or any combination of these (Nhan et al., 1996). PRBs are inexpensive, low maintenance, in-situ, robust, passive remediation systems that are relatively easy to install. The PRB shape may be custom designed to provide maximum efficiency (Woodward, 2001). Adsorbents such as: activated carbon, polyurethane foam, olive shells, coconut shells, peanut hulls, montmorillonite, peat and red clay have proven effective, but are often costly. A widely available, low-cost adsorbent for organic chemicals would be high carbon coal fly ash.

High carbon coal fly ash meets all adsorbent and attenuation criteria especially when considering cost effectiveness compared to alternative sorbents. The relatively high loss on ignition content (LOI=7.9%) of high carbon coal fly ash is indicative of its sorption affinity for low molecular weight, non-polar organic compounds in aqueous solution (Nahn et al., 1996). Fly ash has a significant capacity to absorb organic compounds in aqueous solution (Nelson and Guarino, 1969; Eye and Basu, 1970; Johnson et al., 1965; Deb et al., 1966; Grupta et al., 1988, 1990; Mott and Weber, 1992; Viraraghavan and Alfara, 1994). Fly ash is an active adsorbent, which adsorbs polycyclic aromatic hydrocarbons (Rothenberg, et al.). Fly ash has been demonstrated as capable of removing O-xylene from an aqueous solution (Banerjee et al, 1995). Coal Fly ash is a by-product material of modern coal fired power plants. It is collected via cyclonic and electrostatic precipitators, from flue gas, before entering the stacks. Collected fly ash is either disposed of in landfills or lagoons on site (Banerjee, 1995). Because coal fly ash is of organic origin, it naturally has high carbon content. The amount of carbon content with in coal fly ash is generally higher than most soils, but ranges depending upon the combustion facility. Carbon content is important because it is responsible for the organic sorption behavior. In the remediation industry, activated carbon is often used to adsorb aqueous and vapor phase organic contaminants. Coal fly ash is a potential substitute for activated carbon as a low-cost PRB sorbent medium.

Chapter 2: Literature Review

At least 88 million tons of coal fly ash by-product materials are generated annually in the United States and 60 million tons annually in Europe (Querol et al., 1998). Over one billion tons of coal fly ash has been stockpiled in the United States. On average only about 25% of the coal fly ash is utilized (Nhan et al., 1996). Previous technologies involving the uses of fly ash have been as an ingredient in concrete and bricks, for the construction of roads, dams and bridges (Roy et al, 1981) (Figure1). Fly ash has been used extensively as an alkaline amendment to reduce acid mine drainage (Daniels et al, 1993; Skousen, 1998). Fly ash has also been used in the plastics industry as a low-cost, high performance substitute polymeric material filler (Quattroni, 1993). Coal fly ash is an effective chemical barrier for leachate of municipal solid waste landfills (Nhan et al., 1996).

Fly ash consists of an agglomeration of micro-spheres composed mostly of silica and aluminum, which are up to hundreds of micrometers in diameter. (Banerjee et al., 1995; Viraraghavan et al., 1998) (Figure2: Figure3). The dominant mineral compounds are amorphous silica and aluminum oxides (Tables 1: Table 2). Crystalline-like minerals include: quartz (SiO_2), hematite (Fe_2O_3), magnetite (Fe_3O_4), lime (CaO), anhydrite ($CaSO_4$), mullite ($Al_6Si_2O_{13}$) and feldspars (Querol et al., 1998). The type of coal used and degree of combustion result in variable compositions of the above end members.

There are four main classes of coal combustion products (CCPs): 1) Class F, 2) Class C,

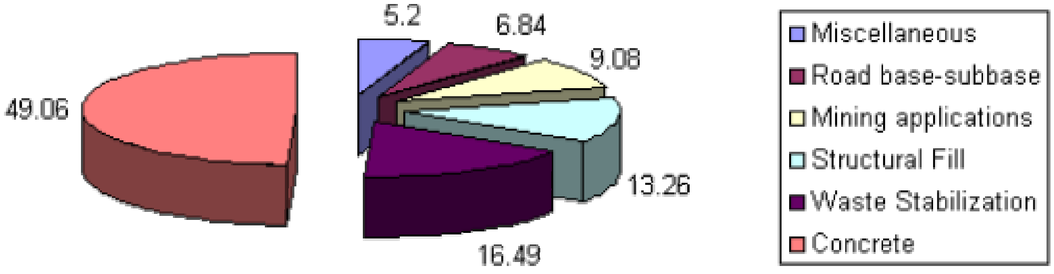

Figure 1. Percentage of Leading Coal Fly Ash Uses, 1998 (Source: American Coal Ash Association; Taken From: Kalyoncu, 1998)

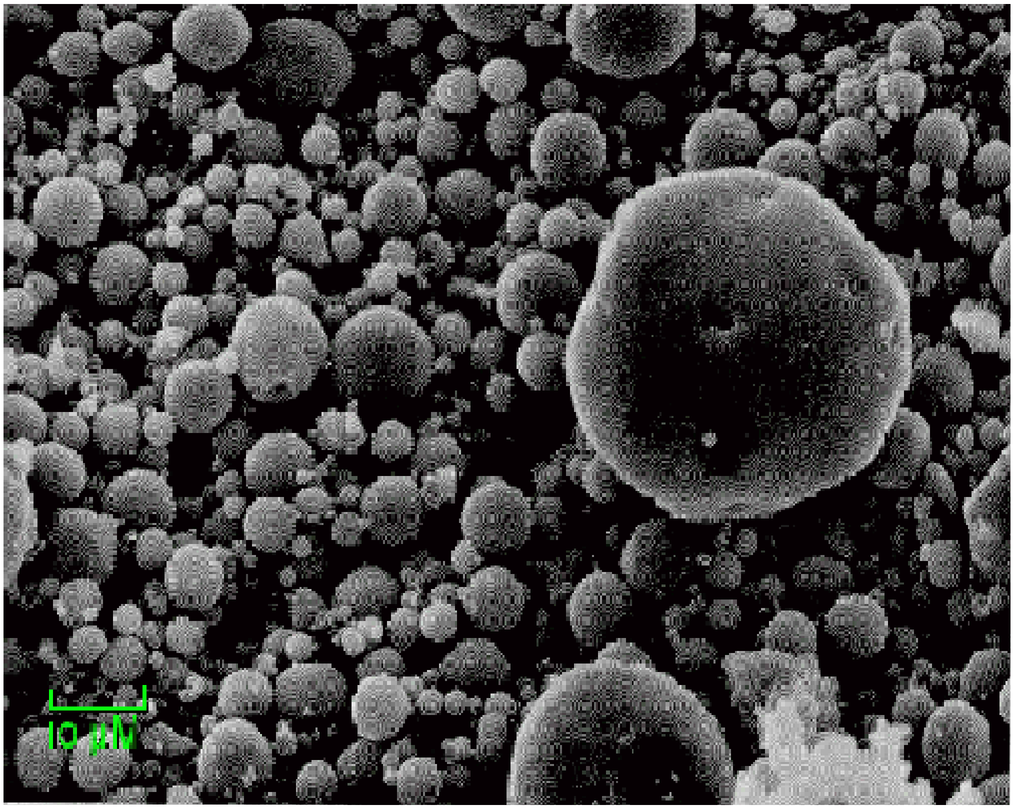

Figure 2. Microscopic Fly Ash Structure (From Western Fly Ash Company)

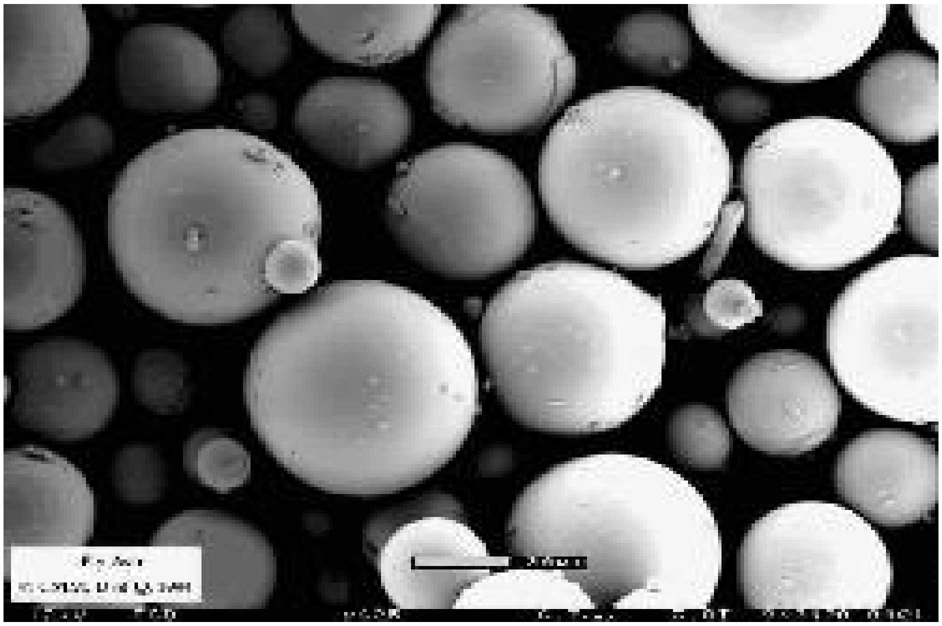

Figure 3. Microscopic Fly Ash (Courtesy of U. of Québec)

Table 1. Chemical Composition (% by weight) of ash from various coal power plants.

Coal Ash[1]	Constituent													
	MnO	K_2O	SiO_2	Al_2O_3	SO_3	Fe_2O_3	Na_2O	MgO	TiO_2	CaO	P_2O_5	C	H	N
							%							
SPC	.	.	50.7	21.8	0.53	4.5	.	4.3	0.8	11.5	.	.	.	.
WV	.	1.5	45.7	26	2.6	17.1	0.6	1.2	1.2	3.8	0.3	.	.	.
OHRD	.	.	42.3	23.2	0.9	14.7	0.7	1	1	2.8	0.5	.	.	.
A-unknown	.	2.3	62.5	24.6	0.4	1.2	0.2	0.3	0.6	0.3	.	9.2	0.2	0.3
A-Ulan	.	0.6	58	27.2	0.1	2.7	.	0.1	1	0.2	.	3.5	0.1	0.2
A-Drayton I	.	.	50.5	26.3	0.5	8	.	0.3	1.7	2	.	4.6	0.1	0.2
A-Drayton II	.	.	47.9	25.9	1	4.9	.	0.3	1.7	4.5	.	6.3	0.2	0.3
A-Grose Valley	.	0.6	53.7	30.4	0.2	1.6	.	0.1	1.1	0.4	.	5	0.1	0.2
A-Hazelwood	.	0.6	20.5	10.1	11.5	5.9	7	12	0.7	15.1	.	2.8	0.1	0.2
A-Yallourn	.	0.2	3.7	1.4	14.5	26.2	5.3	20.1	0.1	8.7	.	7.5	0.2	0.2
A-Loy Yang 0130	.	0.3	16.3	20.4	12	6.9	6.5	13.3	0.6	4.1	.	5.4	0.2	0.3
A-Loy Yang 2100	.	0.9	51.4	18.3	3.5	7.4	3.5	5.5	1.3	1.9	.	2.4	0.1	0.2
S-Escatron	0.02	0.6	19.6	5.1	23.2	2.7	0.5	0.7	0.2	44.5	0.08	.	.	.
S-Teruel	0.04	1.6	47.2	25.6	0.6	16.6	0.2	1.2	0.8	5.6	0.2	.	.	.
S-Escucha	0.03	2.3	49.5	26.7	0.4	14.3	0.3	1.1	1	2.3	0.3	.	.	.
S-La Robla	0.1	2.6	40.1	23.3	0.4	14.3	0.3	2	0.9	8.9	0.8	.	.	.
S-Compos	0.08	4.3	49.8	26.1	0.3	8.4	0.8	2.4	1	2.7	0.5	.	.	.
S-Meirama	0.05	0.8	51.9	26.4	0.2	4.8	0.4	2.3	1.5	7.5	0.4	.	.	.
S-Narcea	0.09	3.9	54.3	23	0.1	7	0.8	2.7	1.1	4.2	0.2	.	.	.
S-Pontes	0.1	1.3	46.7	31	0.8	9.4	0.3	1.9	1.2	6.7	0.2	.	.	.
S-Cercs	0.05	0.9	27.8	13.7	3.3	4.3	0.6	0.8	0.5	42.6	0.4	.	.	.
S-Dou He	0	0.6	48.7	40.7	0.4	3.5	0.2	0.5	1.3	2.8	0.4	.	.	.
S-Puerto	0.1	2.4	58.4	29.3	0.2	7.5	0.4	1	0.7	0.9	0.1	.	.	.
S-Espiel	0.1	4.1	52	34.2	0.1	6.1	0.6	1.6	0.9	2.1	0.4	.	.	.
S-Barrios	0.1	0.7	45.1	37.6	0.7	2.8	0.4	2.2	1.5	9	1.7	.	.	.
S-Sribera	0	4.2	49.6	32.3	0.4	7.7	0.7	1.7	0.9	3.2	0.1	.	.	.
Average	0.1	1.7	44.0	24.3	3.0	8.1	1.4	3.1	1.0	7.6	0.4	5.2	0.1	0.2
Maximum	0.1	4.3	62.5	40.7	23.2	26.2	7	20.1	1.7	44.5	0.5	9.2	0.2	0.3
Minimum	0	0.2	3.7	1.4	0.1	1.2	0.2	0.1	0.1	0.2	0.3	2.4	0.1	0.2

1. (A) Denotes Australian ash (modified from Low and Bately, 1988); (S) denotes Spanish ash (modified from Querol et al., 1999); (SPC) denotes Saskatchewan Power Corporation, Regina, Saskatchewan (modified from Viraraghavan and Alfaro, 1998); (OHRD) denotes Ontario Hydro Research Dept (modified from Nahn, et al., 1996); (WV) denotes average constituent percentages for West Virginia power plant fly ash produced by the electrical utility industry (Modified from Skousen, 1998).

Table 2. Typical composition of Class F and C ashes as defined by ASTM (1997).

Parameter	Class F	Class C
SiO2	54.9	39.9
Al2O3	25.8	16.7
Fe2O3	6.9	5.8
CaO	8.7	24.3
SO3	0.6	3.3
Loss on Ignition (LOI)(@750C)	2.8%	0.5%

(modified from Ziemkiewicz and Skousen, 2000)

Table 3. Comparative Surface Areas of Various Sorbents.

Coal fly ash	Surface Area	Reference
	m^{2}g^{-1}	
Karn	1.14	Mott and Webber, 1992
Trenton	2.65	Mott and Webber, 1992
Cobb	3.52	Mott and Webber, 1992
SPC	1.5-1.7	Viraraghavan and Alfaro, 1998
Montana rosebud, FBC	5.2	Rothenberg, et. al., 1991
Colorado, stoker fed	37.2	Rothenberg, et. al., 1991
Western, pulverized	5.2	Rothenberg, et. al., 1991
Typical Kaolinite clay	12	Fetter, 1993
Activated Carbon	1050-1250	CPL Carbon Link, 2000

3) Fluidized Bed Combustion, and 4) Flue Gas Desulfurization. C- and F- classes comprise the bulk of CCPs. Fly ashes are characterized as C- or F- class based on the typical constituent chemical composition (Table 2). In addition C-class fly ash typically contains greater than10% lime, whereas F-class contains less than10% lime (Ziemkiewicz and Skousen,2000).

The percent weight loss on ignition (LOI) gives a crude measure of the organic content of the soil material or fly ash. As a result of organic content, high LOI coal fly ashes tend to be more favorable for sorption of organics chemicals compared to other coal fly ashes. High LOI coal fly ash exhibits many properties similar to that of activated carbon, which is commonly used in the environmental industry for vapor and liquid phase adsorption systems. Activated carbon is a generic term generally used to describe a variety of carbonaceous adsorbents with a highly crystalline form and extensively developed internal pore structure. The finer the particle size of activated carbon, the better the access to the surface area and the faster rate of adsorption kinetics (CPL Carbon Link Corporation, 2001). The sorption capacity is directly proportional to the total exposed surface (Banerjee et al., 1995). Similarly, fly ash is characterized by its fineness, spherical particles, large surface area and its wide particle size distribution (Banerjee et al., 1995). However, activated carbon surface areas tend to be much higher than that of coal fly ash (Table 3).

The technique of steam activation, similar to coal combustion, is generally used for the activation of coal and coconut shell raw material. In the presence of steam, temperatures are raised to 800-1100°C to generate activated carbon. Coal combustion processes take place at higher temperatures of 1300-1700°C to generate steam to turn turbines. During steam activation, carbon monoxide and hydrogen gases are produced and further oxidized (burned). The resultant activated carbon exhibits a fine pore structure composed of micropores (r<1nm), mesopores (r=1-25nm) and macropores (r>25nm), which are ideal for adsorption of both liquid and vapor phase (CPL Carbon Link Corporation, 2001).

Adsorption to the surface of the granular activated carbon (GAC) is usually considered negligible because the granular surface area is so small compared to that of the micropores and submicropores (Metcalf and Eddy, 1972). The macropores are used as the entrance to the activated carbon, mesopores for the transportation and micropores for adsorption (CPL Carbon Link Corporation, 2001). Similarly Banerjee et al. speculate two modes of diffusion may be responsible for the coal fly ash adsorption process. First, is the rapid external or surface diffusion of the sorbent on to the fly ash particles via molecular diffusion. Second, is the slower internal diffusion of solute among the pores and capillaries of the carbon content present with in the fly ash.

Sorption is the transformation processes by which soluble or vapor phase molecules (sorbate) transfer to the solid phase associated with the sorption medium (sorbent). Adsorption is a two-dimensional sorption surface process, whereas absorption refers to a three dimensional integrated sorption matrix process (Schwarzenbach et al, 1993) (Figure 4). The distinction between chemical and physical adsorption is difficult to differentiate, therefore the term sorption is referred to (Metcalf and Eddy, 1972). Sorption is important because it may directly be responsible for the fate and impact of chemicals in the environment (Schwarzenbach et al, 1993). Sorption is not always a single, simple

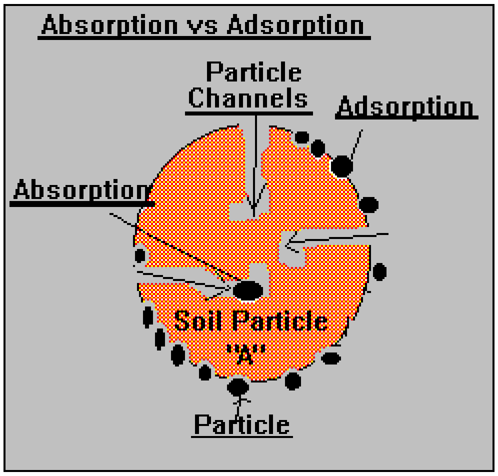

Figure 4. Schematic representation of sorption processes. (Dan Ferrante, 1996, Virginia Polytechnical Institute)

Table 4. Average carbon content and K_f values of threeMichigan fly ashes (modified from Mott and Webber, 1992).

Ash Source[1]	Carbon	Kf[1]	Kf[1]	Kf[1]
	%	CTET[2]	TCE[3]	TTCE[4]
Karn	4.69	0.348	0.658	1.37
Trenton	6.14	0.387	0.920	2.39
Cobb	6.52	1.53	1.71	4.88

[1] Freundlich Sorption Capacity. Units of Kf correspond to mg/L and mg/g for aqueous- and solid-phase concentrations respectively.

[2] Carbon Tetrachloride

[3] Trichloroethene

[4] Tetrachloroethene

process. A combination of interactions between sorbent and sorbate are involved in the sorption process (Westall, 1987; Schwarzenbach et al, 1993).

Sorption of aromatic hydrocarbons has been shown to be proportional to residual carbon content of fly ash (Low and Bately, 1988; Mott and Webber, 1992). The capacity for adsorption increases with increasing carbon content of fly ash (Banerjee et al., 1995). Penetration of neutral organic chemicals into any solid phase, natural organic matter offers a relatively non-polar environment into which hydrophobic organic chemicals tend to be attracted with out competition from surrounding water molecules (Schwarzenbach, 1993; Fetter, 1993). Adsorption of PAH (polycyclic aromatic hydrocarbons) molecules was found to increase with increasing residual carbon content of the fly ash sorbent (Low and Batley, 1988). Mott and Weber, 1992, further demonstrate this aspect in Table 4. The Cobb fly ash, because of the larger percentage of carbon present and larger surface area (Table 3), had more sorption capacity compared to the Trenton and Karn fly ashes On average, carbon content in coal-burning fly ash is currently 6 percent (Hwang, et. al., 2002).

Ultimately, greater sorption by fly ash occurs with small particle size and higher temperatures (Singh et al., 1994). Kinetics studies by Banerjee et al., 1997 and Singh et al., 1994 of batch test sorption of O-xylene and phenol onto flyash demonstrate that adsorption rate increased with increasing temperature. Sorption by fly ash is an endothermic, kinetic process whereby the rate of removal or organics is proportional to temperature (Singh et al., 1994). Singh suggested that the number of active surface centers available for sorption have increased with temperature and that increasing the temperature may also enhance the rate of intraparticle diffusion. At high temperatures, the high negative values of molar free energy (ΔG) are indicative of high sorption (Singh et al., 1994).

Some problems with the use of a high carbon ash as a sorbent, are that some coal fly ashes have potential to leach metals and non-metals inherent to the ash origin. Studies of a fly ash landfill in southern Wisconsin have shown that ground water in contact with ash has been substantially modified primarily by sulfates, calcium and magnesium inherent to the ash. However, toxic metals with in the ash are generally quite immobile in the ground water (Cherkauer, 1981). Below are several leaching case studies of coal combustion products used for remediation purposes taken from Ziemkiewicz and Skousen (2000) presented in Table 5. Also listed below in Table 6 are Pennsylvania and West Virginia leachate compliance standards for CCPs.

The Chaplin Hill mine (Table 5) demonstrated substantial decreases in metals and sulfates concentrations. The Chaplin Hill case study has demonstrated that when the application of CCPs is considered for BTEX sorption, the overall remediation benefit may certainly outweigh the minimal, low concentration side effects associated with leaching. It is important to note that metals inherent to coal fly ash are more mobile in acidic soil and groundwater environments rather than more neutral pH environments. In addition, the metals inherent to fly ash are not free metals, but rather bound as post incinerated, metal oxides, which makes these metals less available for leaching. With regard to remediation, each application is site specific and there are advantages and disadvantages to each technique.

Table 5. Summary of pre- and post-CCP application water quality at the Chaplin Hill Mine, Morgantown WV. (The data are for samples taken and analyzed by Anker Energy Corporation and reported to the state of West Virginia. All values in mg/L).

RCRA Element	TCLP Limit	EPA Drinking Water	Pre-CCB	Post-CCB
Sb	1	0.006	0.94	0.40
As	5	0.05	1.28	<0.1
Ba	100	2	<0.1	<0.1
Be	0.007	0.004	0.96	<0.1
Cd	1	0.005	<0.1	<0.1
Cr (6+)	5	0.1	0.0001	0.0001
Pb	5	0.015	0.72	<0.1
Hg	0.2	0.002	<0.0005	<0.0005
Ni	70	0.01	1.16	<0.1
Se	1	0.05	1.29	<0.1
Ag	5		<0.1	<0.1
Tl	7	0.002	2.68	1.21
Al			36	<0.1
Ca			450	750
Fe			4	<0.1
Mg			296	450
Mn			47	0.2
SO4			2022	1500

Table 6. Comparison of West Virginia and Pennsylvania standards for CCP leachate concentrations (taken from Ziemkiewicz and Skousen, 2000).

	Maximum Acceptable Leachate Concentrations (mg/L)	
State Test Method	Pennsylvania TCLP	West Virginia SPLP
Al		5.0
Sb	1	0.15
As	5	1.25
Ba	100	50
Be	0.007	
B		31.50
Cd	1	0.13
Cr	5	2.5
Cu		32.5
Fe		7.5
Pb	5	1.25
Mn		1.25
Hg	0.2	0.05
Mo		4.38
Ni	70	2.5
Se	1	1.00
Ag	5	
Tl	7	
Zn		125
SO4		2500
Cl		2500

Batch tests are the preferred method for studying most geochemical reactions associated with sorption and leaching (Zachara and Steile, Electrical Power Research Institute, 1991). Batch experiments are inexpensive and relatively easier to perform compared to other sorption/leaching experiments methods, such as column tests and can readily generate data for empirical applications. The batch reactor is the most direct way to obtain a distribution coefficient (K_d) for saturated, porous media. Batch type sorption experiments are carried out by mixing aqueous phase organic chemicals at different concentrations and temperatures with coal fly ash (Singh et al., 1994). Samples are placed on a gyrating lateral shaker or end over end tumbler. Distilled, deionized water and coal fly ash are mixed with appropriate amounts of aqueous phase organic chemicals in 40ml amber vials with septum lined screw caps leaving no head space (Banerjee et. al., 1997). The aqueous phase organic chemicals are prepared form a stock solution based on the maximum solubility of the organic chemical at ambient temperature and are further diluted to achieve desired concentrations (Banerjee et. al., 1997). Walton et. al., 1992, carried out sorption experiments at five different concentrations for each individual organic chemical. To monitor vaporization losses and adsorption to glass, blank samples containing distilled, deionized water, added BTEX compounds and no ash are prepared with the same concentrations and in the same manner as those samples with ash (Jaynes and Vance, 1996; Viraraghavan, et. al. 1997). Banerjee used three vials for each adsorption data point. Two vials containing ash were used as reps. The vials with no ash were used as the control. Aliquots were centrifuged and analyzed spectrophotmetrically using a Spectronic 20 D spectrophotmeter at wavelengths that correspond to the maximum absorbances for the organic chemicals of interest (Viraraghavan, et. al. 1997, Singh et al., 1994).

Sorption may experimentally be quantified by the use of a mass balance equation (Schwarzenbach, 1993):

$$Q = \frac{(C_f - V_f) - (C_0 - V_0)}{M} \quad (1)$$

where,

Q = sorbed concentration (mol/kg)

C_f = equilibrium concentration (mol/L)

C_o = initial concentration (mol/L)

V_f = final volume (L)

V_o = initial volume (L)

M = mass of sorbent (kg)

Data are initially plotted as constant temperature isotherms with Adsorption (mol/Kg) vs. Equilibrium concentration (mol/L): y vs. x (adsorbed vs equilibrium y vs x).

Equilibrium sorption data are often fit using either the Freundlich and Langmuir isotherms (Evangelou, 1998). The Langmuir approach suggests ion exchange mechanisms, which incorporate both organic and inorganic ion concentration charges, and total surface charge density (Schwarzenbach,1993). Through competitive ion interactions, a maximum capacity sorption plateau is achieved with the Langmuir isotherm. The Freundlich approach is most often used for nonlinear isotherms with no apparent sorption maximum ion capacity plateau. The Freundlich isotherm best describes the interactions between hydrophobic sorbate and hydrophobic sorbent with no apparent sorption maximum (Evangelou, 1998). The Freundlich adsorption isotherm is used to describe macroscopic data and no proof with regard to reaction mechanism should be inferred (Sparks, 1995). The use of an adsorption isotherm does not allow one to differentiate between adsorption and precipitation (Sparks, 1995). Sparks describes the Freundlich Equation as:

$$Q_e = K_f (C_e)^{1/n} \tag{2}$$

where,

Q_e = amount of adsorption(mol/kg)

C_e = equilibrium concentration of the adsorptive(mol/L)

1/n = Freundlich fitting parameter

K_f = Freundlich constant (L/kg)

The linear form of the Freundlich adsorption isotherm is:

$$\log Q_e = \log K_f + \frac{1}{n} \log C_e \tag{3}$$

If 1/n = 1, then $K_f = K_d$, the ratio of the substance's equilibrium concentration in the sorbed phase to that of the solution phase (Table 7):

$$K_d = \frac{Q_e}{C_e} \tag{4}$$

Table 7. BTEX Sorption Coefficients

	Sorbate				
Sorbent	Benzene	Toluene	Ethylbenzene	Total Xylenes	Total BTEX
			L kg^{-1}		
Soil[1]	0.32				
Organo-clays[2]	98.64	231.64	528.73	581.31	378.91

[1] Schwarzenbach, 1993

[2] Jaynes & Vance, 1996

Table 8. Organic matter normalized sorption coefficients

	Sorbate				
Sorbent	Benzene	Toluene	Ethylbenzene	Total Xylenes	Total BTEX
			L kg^{-1}		
Soil[1]	17				
Organo-clays[2]	2.5	2.83	3.18	3.22	

[1] Schwarzenbach, 1993

[2] Jaynes & Vance, 1996

Table 9. Physical Characteristics of BTEX.

	water solubility[1] (25°C)	density[1] (25/4°C)	Log K_{ow}[1]	formula weight[2]
	mg/l	g/cm^3		g/mol
benzene	1,780	0.874	2.13	78.11
toluene	535	0.862	2.16	92.14
ethyl benzene	152	0.867	3.13	106.17
o-xylene	175	0.88	3.13	106.17
m-xylene	130	0.868	3.13	106.17
p-xylene	196			
total xylenes	167	0.857	3.18	106.17

[1] Modified from USEPA, Modeling Subsurface Transport of Petroleum Hydrocarbons, Effective Solubility calculation(2001). An online training course of EPA Region 9 and ERD, Athens, GA.

[2] Modified from Sax and Lewis, Hawley's Condensed Chemical Dictionary 11th ed., (1997).

Partitioning of a solute onto a mineral or organic content of the soil is almost exclusively a function of the organic carbon fraction of the soil (f_{om}) if it constitutes at least 1% (Fetter, 1993). As a result, a partition coefficient (K_{om}; Table 8) with respect to carbon fraction of soil matter is expressed as:

$$K_{OM} = \frac{K_d}{f_{om}} \tag{5}$$

The octanol/water partition coefficient (K_{ow}; Table 9) is used by researchers to simulate hydrophobic sorption by soil organic matter. It is a measure of hydrophobicity. The K_{ow} represents the ratio of organic contaminant in octanol (C_o) to that of water (C_w) (Evangelou, 1998).

$$K_{ow} = \frac{C_o}{C_w} \tag{6}$$

The BTEX class of aromatic, petroleum, hydrocarbon chemicals consist of: benzene, toluene, ethylbenzene and 3 xylene isomers (Figure 5: Table 9). Benzene, the simplest aromatic hydrocarbon, is a carcinogen, highly toxic and flammable. It is colorless to light yellow, mobile, non-polar liquid (Sax and Lewis, 1987). Benzene has a water solubility of 1,780mg/L at 25 degrees C (USEPA, 2001), density of 0.87378 at 25/4 degrees C (Kirchnerova and Cave, 1976), and an octanol/water partition coefficient, log K_{ow}, of 2.13 (DeKock and Lord, 1987; Hansch and Fujita, 1964),

Toluene is a colorless liquid with a benzene-like odor, flammable and toxic(Sax and Lewis, 1987). Toluene has a water solubility of 535mg/L at 25 degrees C (Benerjee et al., 1984) density of 0.86233 at 25/4 degrees C (Huntress and Mulliken, 1941) and an

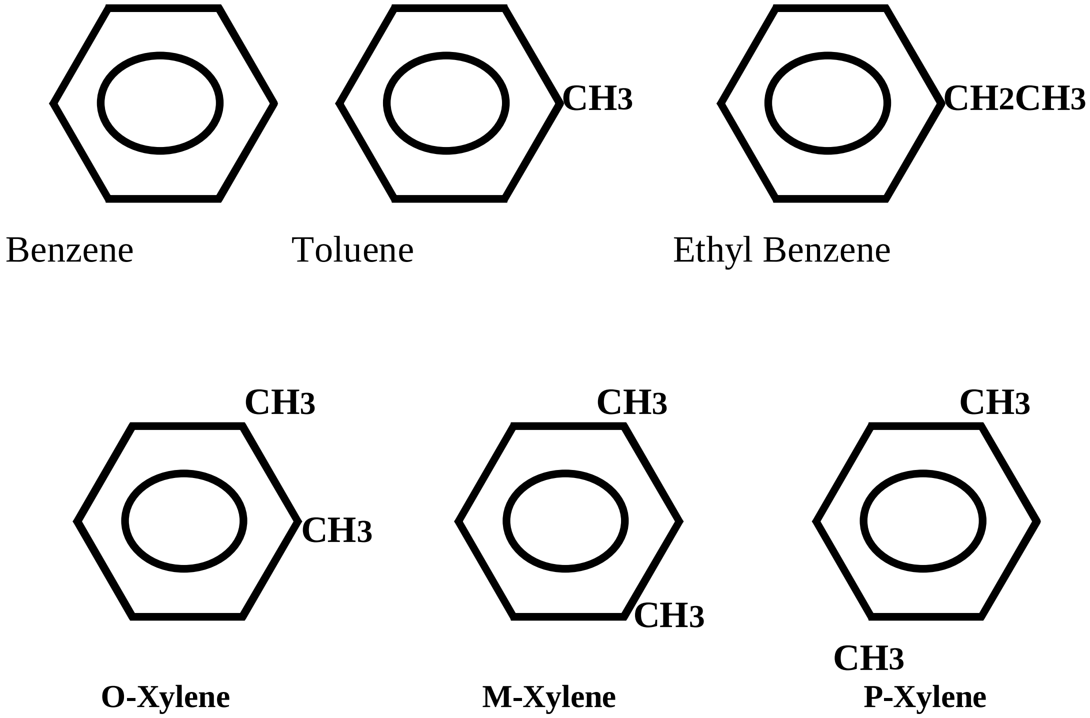

Figure 5. BTEX Molecular Organic Structures (taken from Sax and Lewis, Hawley's Condensed Chemical Dictionary. 11th ed., 1987).

octanol/water coefficient, K_{ow}, of 2.61 (Sangster, 1989).

Ethylbenzene is a flammable, colorless, toxic liquid with an aromatic odor (Sax and Lewis, 1987). Methylbenzene has a water solubility of 152mg/L at 25 degrees C (Miller et al., 1985), a density of 0.867 at 25 degrees C (Hunterss and Mulliken, 1941), and an octanol/water coefficient, log K_{ow}, of 3.13 (Wasik et al., 1981, 1983; Yalkowsky et al., 1983).

O-Xylene (1,2 dimethylbenzene) is also a clear, colorless liquid with an aromatic odor that is moderately flammable (Sax and Lewis, 1987). O-Xylene has a water solubility of 175mg/L at 25 degrees C(Andrews and Keefer, 1949), density of 0.8802 at 20 degrees C (Weast, 1986), octanol/water partition coefficient, log K_{ow}, of 3.13(Tewari et al., 1982, Wasik et al., 1981, 1983).

M-Xylene (1,3-dimethylbenzene) is a clear, colorless watery liquid with a sweet aromatic odor that is moderately flammable (Sax and Lewis, 1987). M-Xylene has a water solubility of 130mg/L at 25 degrees C (Andrews and Keefer, 1949), density of 0.8684 at 25 degrees C (Hawley, 1981) and octanol/water partition coefficient, log K_{ow}, of 3.13 (Wasik et al., 1981, 1983).

P-Xylene (1,4-dimethylbenzene) is also a colorless, watery liquid, with a sweet aromatic odor that is highly flammable (Sax and Lewis, 1987). P-Xylene has a water solubility of 196mg/L at 25 degrees C (Andrews and Keefer, 1949), density of 0.85665 at 25 degrees C (Kirchnerova and Cave, 1976) and octanol/water partition coefficient of 3.18 (Tewari et al., 1982; Wasik et al., 1981, 1983).

Chapter 3: Materials and Methods

3.1 Chemical Composition:

The constituent XRF chemical composition was determined through a Phillips 1480 XRF Wavelength Spectrometer courtesy of Dr. John Renton and Harry(Duke)Brown in the West Virginia University Department of Geology and Geography.

3.2 Classification:

Coal fly ash samples were analyzed in terms of chemical composition using XRF analysis and further classified as C or F class using the ASTM classification for coal fly ash.

3.3 Percent Carbon:

The percent carbon was determined with a LECO CNS-2000 courtesy of Dr. John Sencindiver and Brian Cooley from the College of Agriculture and Forestry and Consumer Sciences, division of Plant and Soil Sciences.

3.4 Batch Test:

After the method of Banerjee et al. (1995) and Mott et al. (1992), the fly ashes were mixed with Benzene, Toluene, Ethyl benzene, and Xylene samples separately at varying temperatures and concentrations of BTEX.

3.5 Sample Preparation:

Day 1: A total of 15, 40ml amber glass vials with Teflon-lined screw caps were used for each batch test experiment. Experimentally, 3, 4 and 5 gram masses of ash were taken, placed in 10 out of 15 of the amber vials. The vials with out flyash were used as a control. Two sets vials with fly ash yielded replicates. Subsequently all amber vials were filled with distilled, deionized water to the appropriate volume via pipet and 10ml volumetric cylinder. All pipets and volumetric cylinders were calibrated daily to deliver distilled deionized water.

All 15 vials were then vortexed and placed at the corresponding isotherm temperature for a period of 12hrs.

The BTEX stock solution was prepared by adding distilled, deionized water and individual BTEX organic chemicals into a seperatory funnel, shaken vigorously and let stand overnite. Aqueous phase BTEX stock solutions were based on the maximum solubities of each individual species (Table 9).

Day 2: The aqueous phase organic stock solution was withdrawn from the bottom of the seperatory funnel into a tallform beaker covered with a watch glass. Aqueous phase BTEX solute stock solutions were immediately pipetted into the corresponding amber vials to appropriate diluted concentrations, sealed immediately, leaving no head space. Benzene and Toluene concentrations ranged from 400mg/L to 0mg/l. Ethyl Benzene and Xylenes concentrations ranged from 100mg/L to 0mg/L. Amber vial sample lids were further sealed with paraffin wrap to maintain seal and prevent breakage. All pipets were calibrated daily to deliver appropriate amounts of BTEX solution.

All samples were further vortex and subsequently placed on either an end over end tumbler or a lateral shaker, and allowed to equilibrate at constant temperature for a period of 12hrs.

Day 3: All samples were centrifuged for ½ hour at 2500rpm. Solid coal fly ash settled to the bottom of the 40ml amber vials and aloquits of aqueous phase BTEX were extracted from the top of each vial. Subsequently, all samples were analyzed via UV spectroscopy at corresponding wavelength values of maximum absorbance for each BTEX sample (Table 10)

3.6 UV Analytical Procedure:

The Spectronic 20®, Genesys 5, single wavelength Spectrophotmeter (UV Spec 20), courtesy of Dr. Sven Verlinden in the WVU college of Agriculture, Forestry and Consumer Science, Division of Plant and Soil Science, was turned on at least ½ hr. before any samples were run to allow the machine to warm up. Viraraghavan et. al. 1998 and Singh and Rawat, 1994 also analyzed fly ash sorption of organic chemicals using UV Spec 20.

Quartz cuvettes were initially rinsed with ethanol followed by distilled, deionized water. A new, dedicated, disposable pipette tip was used each time to withdraw aliquots from the amber sample vials into the quartz cuvette. The cuvette was then rinsed once with sample. Then the cuvette was refilled with sample aliquot, wiped clean outside with a disposable Kimwipe® and placed in the UV spectrophotometer chamber where

Table 10. Max UV Absorbance Peaks for BTEX

Substance	**Formula**	**Max UV Absorbance Peaks**
Benzene	C_6H_6	254*+♦
Toluene	C_7H_8	261*+♦
EthylBenzene	C_8H_{10}	270♦
Xylenes	C_8H_{10}	264*+♦

*Source:Colby College Dept.of Chemistry
www.colby.edu/chemistry/cmp/mole.cgi
+Source:Applied Analytics, Inc.
www.a-a-inc.com/BTX?BTX1.htm
¨ Sadtler UV Indexes (1960,1961,1963,1966)

maximum absorbance was recorded. First, a zero value absorbance baseline was established with sample containing only distilled, deionized water. The UV analytical device was then calibrated from strongest concentration to weakest concentration with the 5 control samples which had no ash added.

The 10 samples (2 reps) which had ash added were analyzed via UV spectrophotometry ranging from strongest concentration to weakest concentration. Between trials, all cuvettes were rinsed and prepared in the same manner as the zero absorbance value.

Lastly, the UV Spec 20 analytical device was recalibrated with blank sample from weakest concentration to strongest concentration. The average of initial and final absorbance values of blank samples were used as calibration standard curves for each batch test experiment.

Appendix II contains UV calibration curves for analytical work performed for this thesis.

3.7 Glassware cleaning and Preparation:

All glassware used during the batch test experiments were rinsed with distilled, deionized water, followed by ethanol. All glassware were then soaked overnite with Liquinox soap, rinsed with tap water, followed by distilled, deionized water and set inverted to dry on drying racks.

3.8 Particle Size Distribution:

The particle size analysis was determined using the most widely accepted pipet extraction method (Indorante et. al., 1990).

Masses of 10 grams of ash were placed in a tared 500ml Fleaker. One Fleaker contained no ash and was used as a blank control. Organic matter in the samples was digested with 30% hydrogen peroxide and heated on a hotplate to approximately 60°C prior to the particle size analysis.

A volume of 10ml of 10%Na-Hexametaphosphate dispersion solution was then added to each Fleaker and the volume was brought to 150ml with distilled, deionized water. The blank control was used as the correction factor for Na-hexametaphosphate. All Fleakers were stoppered and shaken overnite at a minimum of 120 oscillations per minute. Stoppers were next removed and fleakers were brought to an exact volume of 400ml with distilled deionized water at room temperature. Then, samples were shaken vigorously to ensure no particle adherence to the bottom of the Fleaker. Fleaker stoppers were left ajar and arranged for pipetting based on Stokes Law for corresponding temperatures for pipeting of fractions <2 micrometers at 5cm depth. Aliquots were withdrawn and dispensed into a tared beaker, oven dried, cooled in a desicator and masses taken. Mass of Na-hexametaphosphate was subtracted and percent clay size particles determined. Soils remaining in the Fleaker were wet sieved through a tared, 270 mesh size sieve. Sand fractions remaining were oven dried prior to mass taken as determined by the Soil Survey Staff (1984).

%sand = 100 x (total sand weight/total soil weight)

%clay = (clay weight) x (400/pipet volume)(100/total soil weight)

%silt = 100 – (%sand + %clay).

3.9 Surface Area:

The surface areas of the three fly ash samples were determined by Multipoint BET Quantachrome® Autosorb gas sorption system analysis courtesy of Bob Romanofski and Don Floyd, DOE, National Energy Technology Laboratories (NETL), Morgantown, WV.

3.10 Experimental Focus:

The focus of these batch test experiments was to test a broad range of BTEX sorption with respect to coal fly ash. An assumption was made that if sorption occurred at higher concentrations, then it would certainly be reliable at more dilute concentrations of BTEX. When chemicals are released into the environment, the actual solubilities are far lower than the published solubilities. This is because most chemicals, like petroleum hydrocarbon fuel exist as a mixture and their concentrations depend on the abundance of the individual chemical in the mixture, otherwise know as the effective solubility. Benzene has a published solubility in water of 1780mg/L. Typical fuel mixture concentrations of Benzene at equilibrium in the aqueous phase are 20-40mg/L (U.S.EPA, 2001). The sorption isotherm line is inclusive of low concentrations when it is traced to zero X and Y axis values of the sorption isotherms. In addition, the single wavelength UV Spec 20 analytical device used in these experiments was more reliable for organic chemicals at higher concentrations resulting in a stronger peak.

3.11 Freundlich Model Rationale:

The Freundlich model approach was used to fit isotherms where it applies. The Freundlich isotherm best describes the interactions between hydrophobic sorbate and hydrophobic sorbent (Evangelou, 1998). The most significant sorption attributes of these batch test experiments were assumed to be the interactions of hydrophobic properties associated with the BTEXs and the high carbon content nature of coal fly ash. The Langmuir approach was abandoned because organic and inorganic ion concentration charges and total surface charge density were not assumed significant interactions with respect to coal fly ash sorption of BTEX. The Freundlich equilibrium sorption model was possible to fit in some cases where Log [Eqm] v. Log [Ads] fit a straight line with at least three valid data points. The Freundlich sorption isotherm model is acquired by empirically fitting experimental data. The Freundlich isotherm is fit by taking the Log of the X and Y axis of the sorption isotherm. The purpose of fitting a Freundlich isotherm is to linearize sorption isotherms so that the K_f and 1/n terms may be extracted over a significant range. The distribution coefficient, K_f value, is the y-intercept of the linearized Log (Eqm) v. Log (Ads) plot of the empirical sorption data. 1/n is the empirical linearization constant obtained from the slope of the Freundlich plot (Evangelou, 1998). In some cases, whereby $1/n = 1$, the linear isotherm is a special case and the K_f is equal to the slope of the line. A disadvantage of the Freundlich isotherm is that it cannot predict an adsorption maximum (Sparks, 1995). The linear isotherm equation should not be extrapolated beyond the limits of the experimental data (Fetter,1999). Statistical analysis presented in Table 13 and Table 14 were performed using the GLM Procedure, with all factors as class variables and Mean Separations using Duncan’s Multiple Range Test. (SAS Inst., Cary, NC; version 8.01). Full model analyses were performed with all possible interactions. Non- Significant parameters were removed based on Type III Sum of Squares. The best model was chosen based on minimizing Mean Square Error.

3.12 Statistical Analysis

Statistical analysis presented in Table 13 and Table 14 were performed using the GLM Procedure, with all factors as class variables and Mean Separations using Duncan's Multiple Range Test. (SAS Inst., Cary, NC; version 8.01). Full model analyses were performed with all possible interactions. Non- Significant parameters were removed based on Type III Sum of Squares. The best model was chosen based on minimizing Mean Square Error.

Chapter 4: Results

4.1 Ash Characterization

As discussed in Chapter 2, the dominant matrix components of coal fly ash are amorphous micro-spheres predominantly composed of silica and aluminum oxides. The average of 26 coal fly ashes sampled from three continents (Table 1) contained over 60% silica and aluminum oxides. In this study, XRF analysis from Table 11 demonstrates that both the Alb-D and Alb-L contained more than the average of the 26 samples, with over 80% w/w silica and aluminum oxides. The MEA-L ash contained over 50% w/w silica and aluminum oxides, which was more similar to the average of the 26 fly ashes sampled. According to the XRF analysis, Table 11, the MEA-L ash had greater than 10% CaO, while the Alb-D and Alb-L coal fly ashes contained less that 10% CaO. On average, the 26 fly ash samples from Table 1, contained less than 10% CaO. The differences in CaO composition among the ashes are the result of combustion type influences. The MEA power plant is a modern Fluidized Bed Combustion (FBC) facility, which requires the addition of lime (CaO) to aid in the reduction of sulfur emissions, by precipitating sulfur as gypsum (CaSO4) (Ziemkiewicz and Skousen, 2000). The Albright Power Station is a pulverized coal combustion facility. As a result, Alb-D and Alb-L ashes would be considered Class F, while the MEA-L ash would be considered Class C or FBC type ash, based on the XRF analysis and in accordance with the typical composition of Class F and C ashes defined by ASTM (1997; Table 11).

From Table 12, it can be determined that the Alb-D had 26.94% carbon, which is 86.34%

Table 11. XRF Chemical Composition % by weight

	Constituent											
Coal Ash	MnO	K_2O	SiO_2	Al_2O_3	SO_2	SO_3	Fe_2O_3	Na_2O	MgO	TiO_2	CaO	P_2O_5
	% (w/w)											
Alb-D[1]	0.04	1.6	56.14	31.87	0.76	-	2.61	0.18	0.65	2.74	3	0.41
Alb-L[2]	0.02	2.35	54.52	30.22	0.08	-	7.55	0.47	0.83	1.69	1.97	0.3
MEA-L[3]	0.04	1.62	37.19	16.11	7.08	-	6.1	0.68	1.59	1.1	28.27	0.24
Average	0.033	1.86	49.28	26.07	2.64	-	5.42	0.44	1.02	1.84	11.08	0.32
Maximum	0.04	2.35	56.14	31.87	7.08	0	7.55	0.68	1.59	2.74	28.27	0.41
Minimum	0.02	1.6	37.19	16.11	0.08	0	2.61	0.18	0.65	1.1	1.97	0.24

[1] Albright Dark fly ash, Albright Power Station, Albright, WV

[2] Albright Light fly ash, Albright Power Station, Albright, WV

[3] Morgantown Energy Assoc. Light fly ash, Morgantown Energy Assoc. Power Station, Morgantown, WV

Table 12. Coal Flyash Physical Characteristics

Coal Ash	Surface Area	Sand	Silt	Clay	Carbon
	m^2 g^{-1}	%			
Alb-D[1]	27.09	67.77	27.66	6.58	26.94
Alb-L[2]	3.42	83.70	13.91	2.39	3.68
MEA-L[3]	13.53	46.77	52.80	0.43	2.36

[1] Albright Dark fly ash, Albright Power Station, Albright, WV

[2] Albright Light fly ash, Albright Power Station, Albright, WV

[3] Morgantown Energy Associates Light fly ash, Morgantown Energy Associates Power Station, Morgantown, WV

more carbon content than the Alb-L and 91.24% more carbon content than the MEA-L. The carbon content of the Alb-D was well above the 2002 average of 6% carbon for coal-burning fly ash (Hwang, et. al., 2002). While the carbon content of the Alb-L and MEA-L coal fly ashes fell below average at 3.68% and 2.36% respectively.

Other important sorption attributes are surface area and particle size distribution. As discussed in Chapter 2, the coal fly ashes with greater percentage of clay size particles and larger surface areas have potential to sorb more BTEX. Table 12 list surface area measurements on the three coal fly ashes in this study, which were 3.42, 13.53 and 27.09 m^2/g for Alb-L, MEA-L and Alb-D respectively and the results of particle size analysis performed in the soils testing laboratory at the WVU college of Agriculture and Forestry and Consumer Sciences, Soil Science Division. From Table 12, the percent clay size particles are 0.43, 2.39 and 6.58 for MEA-L, Alb-L and Alb-D respectively. Table 13 demonstrates that on average the Alb-D ash had a greater percentage of benzene sorption than either the Alb-L or MEA-L ashes. However, the differences between percent benzene sorption of Alb-L and Alb-D were not as great as one would expect with respect to variability in surface area and particle size between the two ashes. As discussed in Chapter 2, surface areas for activated carbon, on the order of 1,050 to 1,250 m^2/g, are substantially higher than that of coal fly ash as a result of greater surface areas found in the micropores of the activated carbon particles. Surface areas for seven coal fly ashes in Table 3, ranged from 1.14 to 37.5 m^2/g. Both coal fly ash and activated carbon sorption rely on high surface areas for greater access for adsorption.

Table 13. Effects of temperature and ash source on average (standard deviation) percent benzene sorption.

Temperature	Alb-Dark	Alb-Light	MEA	avg
	----------------------------------	-%-	----------------------------------	
25°C	41.9 (0.31)	45.3 (1.73)	6.1 (0.17)	31.1[a]
45°C	67.2 (0.01)	46.7 (2.18)	-14.0	33.8[a]
avg.	54.6[a]	46.8[b]	-3.9[c]	32.5

4.2 Effect of Carbon on Benzene Sorption

The overall model for the effect of ash type and temperature on percent benzene sorption was significant (Pr>F < 0.0001; $R^2 = 0.99$) with significant effects due to ash type (Pr>F <0.001) and ash type * temperature interaction (Pr>F=0.0002). The temperature effect was not significant (Pr>F = 0.1807). The Albright-Dark ash had the highest average percent sorption and the MEA ash had the lowest (Table 13). There was no significant effect of temperature on percent benzene sorption to the Albright-Light ash. Increasing temperature increased percent sorption to the Albright-Dark ash, but decreased percent sorption to the MEA ash (Table 13). The relationship between percent sorption and percent carbon was not linear, which suggests there may be differences in the quality of the carbon on each ash and/or differences in mineral matrix, which may influence analyte sorption.

The best fit isotherms among two trials for benzene sorption to three different coal ashes is demonstrated in Figure 6. The Alb-D-45°C, Alb-L-5°C and Alb-L-45°C are Case I isotherms whereby at higher and higher concentrations it becomes more difficult to sorb additional molecules (Schwarzenbach, 1993). Alb-D-25°C and Alb-L-25°C are Case II isotherms whereby the attractiveness of the solid for the sorbate remains constant for all levels of the sorbed state (Schwarzenbach, 1993). MEA-L-5°C, MEA-L-25°C and MEA-

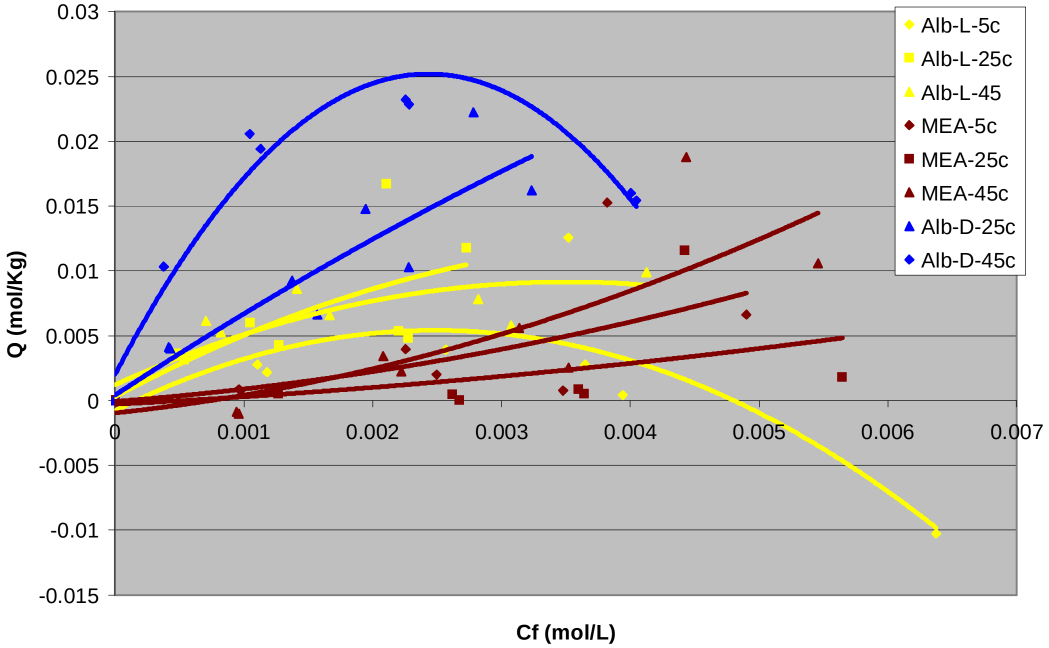

Figure 4.1
Eqm vs Ads
Benzene sorption to three different coal fly ashes
Alb-Dark, Alb-Light and MEA-Light

Figure 6. Benzene sorption onto three different coal fly ashes: Alb-dark, Ald-light, and MEA-light

L-45°C are Class III isotherms in which previously sorbed molecules modify the surface which favors further sorption (Schwarzenbach, 1993).

In general, at higher concentrations of benzene, analytes tend to reach a sorption peak and begin to desorb except in the Case III isotherms typical of the MEA-L ash. This desorption effect may be attributed to overloading of sorbate at higher concentrations, which results in the analyte acting as a solvent for other UV-active components of the ash.

For benzene sorption to coal fly ashes (Figure 6), the Albright dark ash at 25°C is the only ash for which the Freundlich model reasonably fits with an R^2 value of 0.8421. The calculated Freundlich parameters are $K_f = 0.8943$ and $1/n = 0.7295$. The R^2 values for the Alb-L and MEA-L ash sorption of benzene are less than 0.5 at 25°C.

4.3 Effects of analyte and temperature on two low carbon ashes

The analyte*temperature and analyte*ash interactions are the main effects which influence BTEX sorption, and are compared below in Table 14. From Table 14, the overall model is significant ($Pr>F <0.0001$; $R^2=0.99$)

4.3.1 Temperature effects

For the analyte*temperature interaction, there is a general trend of increase in sorption with increase in temperature. Maximum percent sorption occurred at 25°C for benzene and toluene, and 45°C for xylenes and ethyl benzene (Table 14).

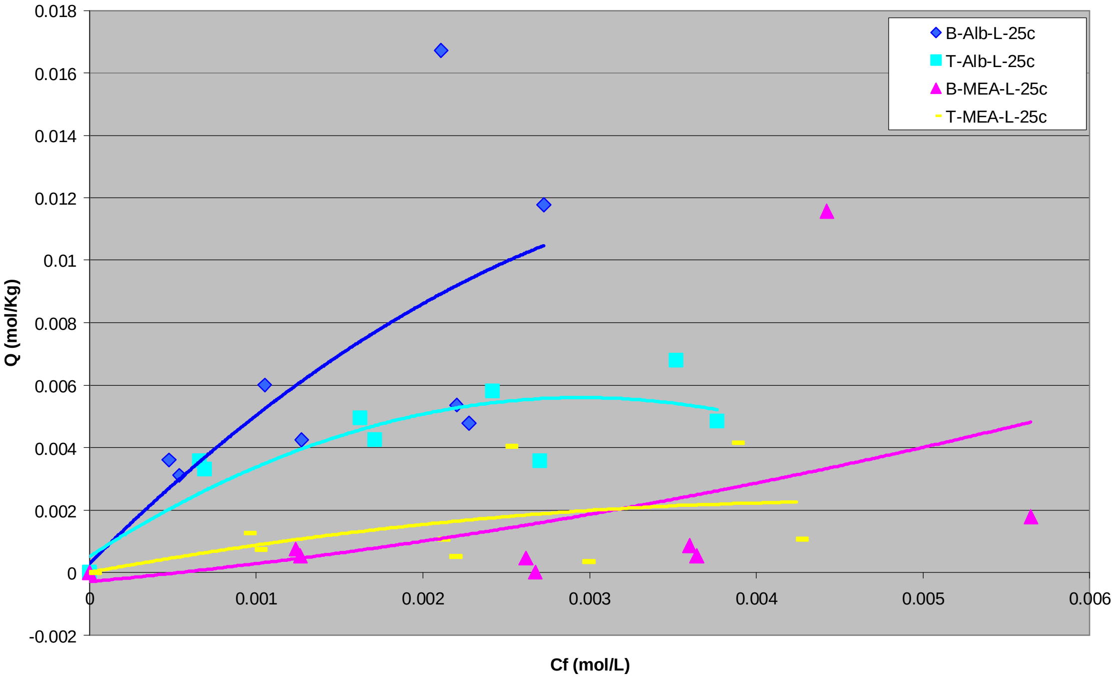

Figure 4.2
Eqm vs Ads -- Albright Light, MEA-L
Benzene & Toluene at 25C

Figure 7. Equilibrium concentration vs adsorbed concentration of benzene and toluene on ashes Alb-L and MEA-L at 25°C.

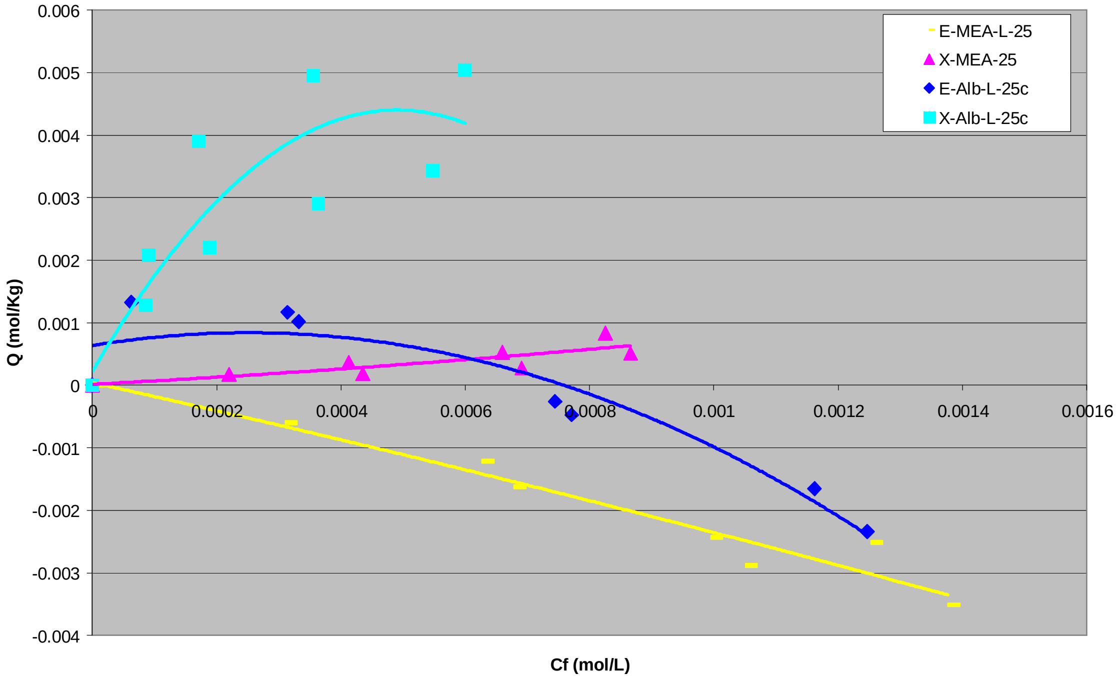

Figure 4.3
Eqm vs Ads -- Albright Light, MEA-L
Ethylbenzene & Xylenes

Figure 8. Equilibrium concentration vs adsorbed concentration of ethylbenzene and xylene on ashes Alb-L and MEA-L at 25°C.

Table 14. The SAS System, GLM Procedure: Duncan's Multiple Range Test for Percent Sorption

Ash	Analyte	Temperature°C	Mean
Albright Light			51.6[a]
MEA			-3.8[b]
	Xylenes		41.6[a]
	Ethylbenzene		16.7[b]
	Benzene		19.4[b]
	Toluene		18.0[b]
		5	20.0[b]
		25	26.3[a]
		45	25.5[a]
Albright Light	Xylene		73.6
Albright Light	Ethylbenzene		66.2
Albright Light	Benzene		38.3
Albright Light	Toluene		28.4
MEA	Xylene		9.5
MEA	Ethylbenzene		-32.7
MEA	Benzene		0.56
MEA	Toluene		7.6
	Xylenes	5	41.0
	Xylenes	25	36.5
	Xylenes	45	47.1
	Ethylbenzene	5	8.7
	Ethylbenzene	25	20.2
	Ethylbenzene	45	21.3
	Benzene	5	15.4
	Benzene	25	25.7
	Benzene	45	17.1
	Toluene	5	14.9
	Toluene	25	22.8
	Toluene	45	16.4

4.3.2 Analyte effects

For the analyte*ash interaction, the percent sorption onto the MEA-L ash is low for all analytes as demonstrated in Table 14, Figure 7 and Figure 8. The Albright light ash demonstrates much greater percent sorption compared to MEA-L in a preferred order (Xylenes>Ethylbenzene>Benzene>Toluene). Ethylbenzene is 66.2% sorbed to Alb-L and desorbed by –32.7% from MEA-L In the case of ethylbenzene sorption to MEA-L, more sorbate was found at the end of the batch test experiment than at the beginning. The increase in ethylbenzene at the end of the experiment may be attributed to an analyte solvent leaching effect of ethylbenzene inherent to the MEA-L ash or other chemical species inherent to the MEA-L ash which have broad overlap interferences of the same UV analytical absorbance wavelength peak.

The individual BTEX sorbate chemical species also proved to have a significant effect on the sorption process. Benzene is favorable to sorption compared to toluene, and xylenes are favorable to sorption compared to ethylbenzene. Therefore, the effect of sorption may be related to the solubility of the chemical species. Benzene (1780 mg/L) is more soluble than toluene (535 mg/L), and total xylenes (167 mg/L) are more soluble that ethylbenzene (152 mg/L). The low sorption effect of xylenes may be attributed to differences in solubility and interferences of the xylene isomers. Therefore, it would be recommended that individual xylene isomers be tested separately in future experiments.

The Albright light ash sorption of toluene at 45°C and sorption of xylenes at 5°C, 25°C and 45°C are isotherms which significantly fit the Freundlich model by taking the log of equilibrium (Cf) versus the log of sorption (Q) with R^2 values close to one. The calculated Freundlich parameters for the Albright light ash sorption of toluene at 45°C are K_f =0.1095 and 1/n = 1.1645, with an R^2 value of 0.8541. The calculated Freundlich parameters for Albright light ash sorption of xylenes are: K_f =5.0119 and 1/n = 0.4449 with an R^2 value of 0.9697 at 5°C, K_f =4.3102 and 1/n = 0.4929 with an R^2 value of .9085 at 25°C and K_f =3.8851 and 1/n = 0.4640 with an R^2 value of 0.9692 at 45°C.

When a sorption isotherm is not straight or cannot be fit to the Freundlich isotherm model it does not mean that sorption did not occur. In fact in almost all cases, except batch tests with ethylbenzene, there was a reduction in benzene, toluene and xylenes attributed to percent sorption as demonstrated in Table 14.

Chapter 5: Conclusion and Discussion

The temperatures at with the batch tests took place were varied to compare results for optimum sorption. The statistical analysis presented in Table 13 and Table 14 demonstrate a significant difference between benzene and toluene, and between ethylbenzene and xylenes with respect to mean percent sorption for the effect of temperature. In general when considering sorption potential and temperature, it is true that sorption increased with increasing temperature. However, in some cases, such as ethyl benzene sorption onto MEA-L ash, the effect was opposite (Figure 8). In fact, there was a gain in the maximum UV analytical absorbance wavelength peak for average ethylbenzene sorbance to the MEA-L ash as temperature increased from 5°C to 45°C. The MEA-L ash is non-ideal for ethylbenzene sorption and poor for toluene and xylenes sorption. There are no significant sorption increases of BTEX by the MEA-L ash when considering temperature.

The types of ash used in these batch test experiments prove to have significant effects with respect to mean percent sorption (Figures 7: Figure 8: Tables 13: Table14). The sorption effect has been attributed to the greater percentage of carbon content inherent to the ash (Low and Bately, 1988; Mott and Webber, 1992; Banerjee et al., 1995). As discussed in Chapter 2, sorption capacity increases with increasing carbon content of the coal fly ash (Banerjee et al., 1995). However, during these experiments the relationship between percent carbon and percent sorption was not linear. The non-linear effect may be attributed to variation in carbon quality as a raw coal product combined with variable combustion procedures. Also, the complex mineral properties of coal, demonstrated in the XRF analysis in Table 11, may interfere with or modify the sorptive properties of carbon content of the coal fly ash product. Additional work, perhaps with a scanning electron microscope, would be necessary to evaluate the carbon quality in relation to its structure in the context of soption potential.

Both coal fly ash and activated carbon offer a relatively non-polar, natural, solid, organic substrate for the adherence and penetration of neutral, hydrophobic, organic chemicals. However, coal fly ash offers less of this non-polar, natural, solid organic substrate because it inherently contains less carbon, less surface area of carbon material and mineral components inherent to coal as compared to activated carbon. Freundlich models do not fit well to the MEA-L batch test trials with BTEX. Therefore, the MEA-L ash is non-ideal for sorption of BTEX, but because of the higher ratio of calcium oxide compared to other ashes observed in this study, it may be more suitable for remedial applications which require the addition of lime.

The Alb-D and Alb-L ashes tend to show more sorption potential for BTEX versus the MEA-L ash. Greater sorption is mostly attributed to the higher percent carbon content, higher temperatures and larger percentage of clay size particles and surface area. These observations are consistent with Sign's 1994 study. Based on previous studies by Banerjee, Schwarzenbach, Low and Bately and Mott and Webber, discussed in Chapter 2, one would expect the Alb-D ash to have a greater percent sorption of BTEX versus the Alb-L ash because it contains 86.34% more carbon content, a greater percentage of clay size particles and larger surface area compared to the Alb-L ash as presented in Table 12.

Instead the results of the batch test experiments in this study indicate that the percent sorption of benzene between the two ashes is not much different as presented in Table 13. Future experiments would be recommended at lower BTEX concentrations more typical of fuel mixture concentrations found in groundwater which may be less likely to desorb and with an analytical device that is more discrete to detect BTEX analytes with out interference or overlap of absorbance peaks.

In conclusion, coal fly ash is not only a waste byproduct of the coal combustion process, but is a highly available, low maintenance and more cost effective for consideration of sorption in the aqueous setting even though it sorbs less BTEX as compare to activated carbon.

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Appendix I. Batch Test Experimental Data

Trial 30-Flayash Batch test with Benzene

1-Aug-01

Albright--Light

5.0g 5C

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption

{(Cf - Ci) * V} / m = Q

tumbler

UV curve

y = 0.0007x + 0.0076

Abs=0.0007[conc(mg/L)]+.0076

m	**yintercept**
7.00E-04	7.60E-03

Rep2&3 AvgC6H6 persent in ash(mg/l): 12.71

sample	**Concentration-mg/L** **initialCi**	 **final-Cf**	**Concentration mol/L** **initial-Ci**	 **final-Cf**	**adsorption** **Q(mol/Kg)**	**Actual** **negative** **Log EQ**	 **negative** **Log ADS**	**%Reduct** **Conc** **init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	397.71	397.71							
D002	312.00	312.00							
D003	239.14	239.14							
D004	113.43	113.43							
D005	0.00	0.00							
Rep2 **ash**									
D101	397.71	497.86	5.09E-03	6.37E-03	-1.28E-02	2.20		-25.18	44.76
D102	312.00	307.86	3.99E-03	3.94E-03	5.30E-04	2.40	3.28	1.33	7.42
D103	239.14	200.71	3.06E-03	2.57E-03	4.92E-03	2.59	2.31	16.07	0.00
D104	113.43	92.14	1.45E-03	1.18E-03	2.73E-03	2.93	2.56	18.77	6.20
D105	0.00	0.00							0.00
Rep3 **ash**									
D201	397.71	275.00	5.09E-03	3.52E-03	1.57E-02	2.45	1.80	30.85	
D202	312.00	285.00	3.99E-03	3.65E-03	3.46E-03	2.44	2.46	8.65	
D203	239.14	200.71	3.06E-03	2.57E-03	4.92E-03	2.59	2.31	16.07	
D204	113.43	86.43	1.45E-03	1.11E-03	3.46E-03	2.96	2.46	23.80	
D205	0.00	0.00							

Trial 27-Flayash Batch test with Benzene

25-Jul-01

Albright--Light

25C 5.0g

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption

{(Cf - Ci) * V} / m = Q

tumbler

UV curve

y = 0.0009x - 0.0032

Abs=0.0009[conc(mg/L)]-.0032

m	**yintercept**
9.00E-04	-3.20E-03

Rep2&3 AvgC6H6 persent in ash(mg/l): 37.44

sample	**Concentration-mg/L** **initialCi**	 **final-Cf**	**Concentration mol/L** **initial-Ci**	 **final-Cf**	**adsorption** **Q(mol/Kg)**	**Actual** **negative** **Log EQ**	 **negative** **Log ADS**	**%Reduct** **Conc** **init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	445.78	445.78							
D002	305.22	305.22							
D003	191.33	191.33							
D004	98.56	98.56							
D005	0.00	0.00							
Rep2 **ash**									
D101	445.78	223.89	4.20E-03	2.11E-03	2.79E-02	2.68	1.55	49.78	22.65
D102	305.22	233.89	2.87E-03	2.20E-03	8.96E-03	2.66	2.05	23.37	3.22
D103	191.33	111.67	1.80E-03	1.05E-03	1.00E-02	2.98	2.00	41.64	17.28
D104	98.56	50.56	9.28E-04	4.76E-04	6.03E-03	3.32	2.22	48.70	11.65
D105	0.00	0.00							0.00
Rep3 **ash**									
D201	445.78	289.44	4.20E-03	2.73E-03	1.96E-02	2.56	1.71	35.07	
D202	305.22	241.67	2.87E-03	2.28E-03	7.98E-03	2.64	2.10	20.82	
D203	191.33	135.00	1.80E-03	1.27E-03	7.07E-03	2.90	2.15	29.44	
D204	98.56	57.22	9.28E-04	5.39E-04	5.19E-03	3.27	2.28	41.94	
D205	0.00	0.00							

Trial 38-Flayash Batch test with Benzene

10-Aug-01 Albright Light
45C

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.001x - 0.0008
Abs=0.001[conc(mg/L)]-.0008

m	**yintercept**
1.00E-03	-8.00E-04

Rep2&3 AvgC6H6 persent in ash(mg/l) 54.60

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	418.80	418.80							
D002	296.80	296.80							
D003	194.30	194.30							
D004	115.30	115.30							
D005	0.00	0.00							
Rep2 ash									
D101	418.80	322.20	5.36E-03	4.12E-03	1.65E-02	2.38	1.78	23.07	0.00
D102	296.80	220.20	3.80E-03	2.82E-03	1.31E-02	2.55	1.88	25.81	8.33
D103	194.30	110.20	2.49E-03	1.41E-03	1.44E-02	2.85	1.84	43.28	15.36
D104	115.30	55.20	1.48E-03	7.07E-04	1.03E-02	3.15	1.99	52.12	14.02
D105	0.00	0.00							0.00
Rep3 ash									
D201	418.80	322.20	5.36E-03	4.12E-03	1.65E-02	2.38	1.78	23.07	
D202	296.80	240.20	3.80E-03	3.08E-03	9.66E-03	2.51	2.01	19.07	
D203	194.30	130.20	2.49E-03	1.67E-03	1.09E-02	2.78	1.96	32.99	
D204	115.30	64.20	1.48E-03	8.22E-04	8.72E-03	3.09	2.06	44.32	
D205	0.00	0.00							

Trial 5-Flayash Batch test with Benzene

4/20/01 Albright dark
254nm 25C

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0013x - 0.006
Abs=0.0013[conc(mg/L)]+.006

m	**yintercept**
1.30E-03	6.00E-03

Rep2&3 AvgC6H6 persent in ash(mg/l) 33.46

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Cf v. Ci init v final**	**% Error Cf Reps 2&3**
no ash									
D001	347.69	347.69							
D002	238.46	238.46							
D003	161.54	161.54							
D004	56.92	56.92							
D005	0.00	0.00							
Rep2 ash									
D101	347.69	217.31	4.45E-03	2.78E-03	2.23E-02	2.56	1.65	37.50	14.00
D102	238.46	151.92	3.05E-03	1.94E-03	1.48E-02	2.71	1.83	36.29	14.69
D103	161.54	122.69	2.07E-03	1.57E-03	6.63E-03	2.80	2.18	24.05	12.54
D104	56.92	33.46	7.29E-04	4.28E-04	4.00E-03	3.37	2.40	41.22	2.30
D105	0.00	0.00							0.00
Rep3 ash									
D201	347.69	252.69	4.45E-03	3.24E-03	1.62E-02	2.49	1.79	27.32	
D202	238.46	178.08	3.05E-03	2.28E-03	1.03E-02	2.64	1.99	25.32	
D203	161.54	107.31	2.07E-03	1.37E-03	9.26E-03	2.86	2.03	33.57	
D204	56.92	32.69	7.29E-04	4.19E-04	4.14E-03	3.38	2.38	42.57	
D205	0.00	0.00							

Trial 12-Flayash Batch test with Benzene

6/19/01 Albright dark 45C
254nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0009x - 0.0011
Abs=0.0009[conc(mg/L)]-.0011

m	yintercept
9.00E-04	1.10E-03

Rep2&3 AvgC6H6 persent in ash(mg/l) 4.89

sample	Concentration-mg/L initialCi	final-Cf	Concentration mol/L initial-Ci	final-Cf	adsorption Q(mol/Kg)	Actual negative Log EQ	negative Log ADS	%Reduct Conc init v final	% Error Amoung Reps 2&3
no ash									
D001	406.56	406.56							
D002	312.11	312.11							
D003	202.11	202.11							
D004	89.89	89.89							
D005	0.00	0.00							
Rep2 ash									
D101	406.56	316.11	5.20E-03	4.05E-03	1.54E-02	2.39	1.81	22.25	1.05
D102	312.11	178.33	4.00E-03	2.28E-03	2.28E-02	2.64	1.64	42.86	1.25
D103	202.11	81.67	2.59E-03	1.05E-03	2.06E-02	2.98	1.69	59.59	7.55
D104	89.89	29.44	1.15E-03	3.77E-04	1.03E-02	3.42	1.99	67.24	0.00
D105	0.00	0.00							
Rep3 ash									
D201	406.56	312.78	5.20E-03	4.00E-03	1.60E-02	2.40	1.80	23.07	
D202	312.11	176.11	4.00E-03	2.25E-03	2.32E-02	2.65	1.63	43.57	
D203	202.11	88.33	2.59E-03	1.13E-03	1.94E-02	2.95	1.71	56.29	
D204	89.89	29.44	1.15E-03	3.77E-04	1.03E-02	3.42	1.99	67.24	
D205	0.00	0.00							

Trial 42-Flayash Batch test with Benzene

29-Aug-01 MEA, Light
5.0g 5C
254nm
tumbler

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0009x - 0.0012
Abs=0.0009[conc(mg/L)]-.0012

m	yintercept
9.00E-04	-1.20E-03

Rep2&3 AvgC6H6 persent in ash(mg/l) 10.78

sample	Concentration-mg/L initialCi	final-Cf	Concentration mol/L initial-Ci	final-Cf	adsorption Q(mol/Kg)	Actual negative Log EQ	negative Log ADS	%Reduct Conc init v final	% Error Amoung Reps 2&3 Cf
no ash									
D001	447.44	447.44							
D002	279.11	279.11							
D003	214.67	214.67							
D004	83.56	83.56							
D005	0.00	0.00							
Rep2 ash									
D101	447.44	298.33	5.73E-03	3.82E-03	1.91E-02	2.42	1.72	33.33	22.06
D102	279.11	271.67	3.57E-03	3.48E-03	9.53E-04	2.46	3.02	2.67	0.00
D103	214.67	176.11	2.75E-03	2.25E-03	4.94E-03	2.65	2.31	17.96	9.69
D104	83.56	75.00	1.07E-03	9.60E-04	1.10E-03	3.02	2.96	10.24	1.46
D105	0.00	0.00							0.00
Rep3 ash									
D201	447.44	382.78	5.73E-03	4.90E-03	8.28E-03	2.31	2.08	14.45	
D202	279.11	271.67	3.57E-03	3.48E-03	9.53E-04	2.46	3.02	2.67	
D203	214.67	195.00	2.75E-03	2.50E-03	2.52E-03	2.60	2.60	9.16	
D204	83.56	76.11	1.07E-03	9.74E-04	9.53E-04	3.01	3.02	8.91	
D205	0.00	0.00							

Trial 46-Flayash Batch test with Benzene

30-Aug-01
MEA, Light
5.0g
25C
tumbler

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0009x - 0.0012
Abs=0.0009[conc(mg/L)]-.0012

m	**yintercept**
9.00E-04	-1.20E-03

Rep2&3 AvgC6H6 persent in ash(mg/l) 9.11

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error Amoung Reps 2&3 Cf**
no ash									
D001	458.56	458.56							
D002	289.67	289.67							
D003	209.11	209.11							
D004	104.11	104.11							
D005	0.00	0.00							
Rep2 ash									
D101	458.56	441.11	5.87E-03	5.65E-03	2.23E-03	2.25	2.65	3.80	21.66
D102	289.67	284.44	3.71E-03	3.64E-03	6.69E-04	2.44	3.17	1.80	1.17
D103	209.11	208.89	2.68E-03	2.67E-03	2.84E-05	2.57	4.55	0.11	2.13
D104	104.11	98.89	1.33E-03	1.27E-03	6.69E-04	2.90	3.17	5.02	2.25
D105	0.00	0.00							0.00
Rep3 ash									
D201	458.56	345.56	5.87E-03	4.42E-03	1.45E-02	2.35	1.84	24.64	
D202	289.67	281.11	3.71E-03	3.60E-03	1.10E-03	2.44	2.96	2.95	
D203	209.11	204.44	2.68E-03	2.62E-03	5.97E-04	2.58	3.22	2.23	
D204	104.11	96.67	1.33E-03	1.24E-03	9.53E-04	2.91	3.02	7.15	
D205	0.00	0.00							

Trial 50-Flayash Batch test with Benzene

31-Aug-01
MEA, Light
5.0g
45C
tumbler

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0008x - 0.0007
Abs=0.0008[conc(mg/L)]-.0007

m	**yintercept**
8.00E-04	-7.00E-04

Rep2&3 AvgC6H6 persent in ash(mg/l) 9.63

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	529.63	529.63							
D002	299.63	299.63							
D003	195.88	195.88							
D004	65.25	65.25							
D005	0.00	0.00							
Rep2 ash									
D101	529.63	426.25	6.78E-03	5.46E-03	1.32E-02	2.26	1.88	19.52	18.77
D102	299.63	275.00	3.84E-03	3.52E-03	3.15E-03	2.45	2.50	8.22	10.91
D103	195.88	173.75	2.51E-03	2.22E-03	2.83E-03	2.65	2.55	11.30	6.47
D104	65.25	73.75	8.35E-04	9.44E-04	-1.09E-03	3.02		-13.03	1.67
D105	0.00	0.00							0.00
Rep3 ash									
D201	529.63	346.25	6.78E-03	4.43E-03	2.35E-02	2.35	1.63	34.62	
D202	299.63	245.00	3.84E-03	3.14E-03	6.99E-03	2.50	2.16	18.23	
D203	195.88	162.50	2.51E-03	2.08E-03	4.27E-03	2.68	2.37	17.04	
D204	65.25	75.00	8.35E-04	9.60E-04	-1.25E-03	3.02		-14.94	
D205	0.00	0.00							

Trial 31-Flayash Batch test with Toluene

8/1/01
Albright, Light
5.0g

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q
5C
261nm

UV curve
y = 0.0019x + 0.0113
Abs=0.0019[conc(mg/L)]+.0113

m	**yintercept**
1.90E-03	1.13E-02

Rep2&3 AvgC7H8 persent in ash(mg/l) 2.74

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	403.79	403.79							
D002	296.42	296.42							
D003	210.89	210.89							
D004	105.37	105.37							
D005	0.00	0.00							
Rep2									
ash									
D101	403.79	356.58	4.38E-03	3.87E-03	6.83E-03	2.41	2.17	11.69	4.43
D102	296.42	267.63	3.22E-03	2.90E-03	4.17E-03	2.54	2.38	9.71	4.72
D103	210.89	170.26	2.29E-03	1.85E-03	5.88E-03	2.73	2.23	19.27	7.73
D104	105.37	69.21	1.14E-03	7.51E-04	5.23E-03	3.12	2.28	34.32	3.04
D105	0.00	0.00							0.00
Rep3									
ash									
D201	403.79	340.79	4.38E-03	3.70E-03	9.12E-03	2.43	2.04	15.60	
D202	296.42	255.00	3.22E-03	2.77E-03	5.99E-03	2.56	2.22	13.97	
D203	210.89	157.11	2.29E-03	1.71E-03	7.78E-03	2.77	2.11	25.51	
D204	105.37	67.11	1.14E-03	7.28E-04	5.54E-03	3.14	2.26	36.31	
D205	0.00	0.00							

Trial 28-Flayash Batch test with Toluene

25-Jul-01
Albright, Light
5.0g
25C
261nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.002x + 0.0053
Abs=0.002[conc(mg/L)]+.0053

m	**yintercept**
2.00E-03	5.30E-03

Rep2&3 AvgC7H8 persent in ash(mg/l) 5.10

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	402.60	402.60							
D002	289.85	289.85							
D003	206.85	206.85							
D004	101.85	101.85							
D005	0.00	0.00							
Rep2									
ash									
D101	402.60	324.25	4.37E-03	3.52E-03	1.13E-02	2.45	1.95	19.461	6.488825
D102	289.85	248.75	3.15E-03	2.70E-03	5.95E-03	2.57	2.23	14.17975	10.45226
D103	206.85	157.75	2.24E-03	1.71E-03	7.11E-03	2.77	2.15	23.73701	5.071315
D104	101.85	60.75	1.11E-03	6.59E-04	5.95E-03	3.18	2.23	40.35346	4.705882
D105	0.00	0.00							0
Rep3									
ash									
D201	402.60	346.75	4.37E-03	3.76E-03	8.08E-03	2.42	2.09	13.87233	
D202	289.85	222.75	3.15E-03	2.42E-03	9.71E-03	2.62	2.01	23.14991	
D203	206.85	149.75	2.24E-03	1.63E-03	8.26E-03	2.79	2.08	27.60454	
D204	101.85	63.75	1.11E-03	6.92E-04	5.51E-03	3.16	2.26	37.40795	
D205	0.00	0.00							

Trial 39-Flayash Batch test with Toluene

10-Aug-01
Albright, Light
5.0g
45C
261nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.002x + 0.006
Abs=0.002[conc(mg/L)]+.006

m	**yintercept**
2.00E-03	6.00E-03

Rep2&3 AvgC7H8 persent in ash(mg/l) 9.50

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	407.00	407.00							
D002	300.25	300.25							
D003	213.25	213.25							
D004	79.50	79.50							
D005	0.00	0.00							
Rep2 ash									
D101	407.00	322.50	4.42E-03	3.50E-03	1.22E-02	2.46	1.91	20.76	8.37
D102	300.25	256.50	3.26E-03	2.78E-03	6.33E-03	2.56	2.20	14.57	8.58
D103	213.25	159.50	2.31E-03	1.73E-03	7.78E-03	2.76	2.11	25.21	3.33
D104	79.50	65.00	8.63E-04	7.05E-04	2.10E-03	3.15	2.68	18.24	5.11
D105	0.00	0.00							0.00
Rep3 ash									
D201	407.00	295.50	4.42E-03	3.21E-03	1.61E-02	2.49	1.79	27.40	
D202	300.25	234.50	3.26E-03	2.55E-03	9.51E-03	2.59	2.02	21.90	
D203	213.25	165.00	2.31E-03	1.79E-03	6.98E-03	2.75	2.16	22.63	
D204	79.50	68.50	8.63E-04	7.43E-04	1.59E-03	3.13	2.80	13.84	
D205	0.00	0.00							

Trial 43-Flayash Batch test with Toluene

29-Aug-01
MEA ash--Light
5.0g
5C
261nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0017x + 0.0054
Abs=0.0017[conc(mg/L)]+.0054

m	**yintercept**
1.70E-03	5.40E-03

Rep2&3 AvgC7H8 persent in ash(mg/l) 0.65

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	382.41	382.41							
D002	332.12	332.12							
D003	187.71	187.71							
D004	102.12	102.12							
D005	0.00	0.00							
Rep2 ash									
D101	382.41	423.24	4.15E-03	4.59E-03	-5.91E-03	2.34		-10.68	6.62
D102	332.12	285.00	3.60E-03	3.09E-03	6.82E-03	2.51	2.17	14.19	9.91
D103	187.71	215.00	2.04E-03	2.33E-03	-3.95E-03	2.63		-14.54	12.87
D104	102.12	111.47	1.11E-03	1.21E-03	-1.35E-03	2.92		-9.16	6.86
D105	0.00	0.00							0.00
Rep3 ash									
D201	382.41	453.24	4.15E-03	4.92E-03	-1.02E-02	2.31		-18.52	
D202	332.12	256.76	3.60E-03	2.79E-03	1.09E-02	2.55	1.96	22.69	
D203	187.71	246.76	2.04E-03	2.68E-03	-8.55E-03	2.57		-31.46	
D204	102.12	103.82	1.11E-03	1.13E-03	-2.47E-04	2.95		-1.67	
D205	0.00	0.00							

Trial 47-Flayash Batch test with Toluene

30-Aug-01
MEA ash--Light
5.0g
25C
261nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.002x + 0.0018
Abs=0.002[conc(mg/L)]+.0018

m	**yintercept**
2.00E-03	1.80E-03

Rep2&3
AvgC7H8
persent in
ash(mg/l)
3.35

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual**		**%Reduct Conc**	**% Error** Amoung
						negative	**negative**	**init v final**	Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	403.10	403.10							
D002	276.85	276.85							
D003	205.10	205.10							
D004	100.35	100.35							
D005	0.00	0.00							
Rep2									
ash									
D101	403.10	355.25	4.37E-03	3.86E-03	6.92E-03	2.41	2.16	11.87	9.09
D102	276.85	230.25	3.00E-03	2.50E-03	6.74E-03	2.60	2.17	16.83	15.58
D103	205.10	199.25	2.23E-03	2.16E-03	8.47E-04	2.67	3.07	2.85	3.26
D104	100.35	91.75	1.09E-03	9.96E-04	1.24E-03	3.00	2.91	8.57	6.54
D105	0.00	0.00							0.00
Rep3									
ash									
D201	403.10	390.75	4.37E-03	4.24E-03	1.79E-03	2.37	2.75	3.06	
D202	276.85	272.75	3.00E-03	2.96E-03	5.93E-04	2.53	3.23	1.48	
D203	205.10	192.75	2.23E-03	2.09E-03	1.79E-03	2.68	2.75	6.02	
D204	100.35	85.75	1.09E-03	9.31E-04	2.11E-03	3.03	2.68	14.55	
D205	0.00	0.00							

Trial 51-Flayash Batch test with Toluene

30-Aug-01
MEA ash--Light
5.0g
45C
261nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0021x - 0.0081
Abs=0.0021[conc(mg/L)]-.0081

m	**yintercept**
2.10E-03	-8.10E-03

Rep2&3
AvgC7H8
persent in
ash(mg/l)
8.14

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual**		**%Reduct Conc**	**% Error** Amoung
						negative	**negative**	**init v final**	Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	412.90	412.90							
D002	292.43	292.43							
D003	195.52	195.52							
D004	102.90	102.90							
D005	0.00	0.00							
Rep2									
ash									
D101	412.90	374.76	4.48E-03	4.07E-03	5.52E-03	2.39	2.26	9.24	0.89
D102	292.43	266.67	3.17E-03	2.89E-03	3.73E-03	2.54	2.43	8.81	1.93
D103	195.52	193.33	2.12E-03	2.10E-03	3.17E-04	2.68	3.50	1.12	0.73
D104	102.90	93.33	1.12E-03	1.01E-03	1.39E-03	2.99	2.86	9.30	16.33
D105	0.00	0.00							0.00
Rep3									
ash									
D201	412.90	371.43	4.48E-03	4.03E-03	6.00E-03	2.39	2.22	10.04	
D202	292.43	271.90	3.17E-03	2.95E-03	2.97E-03	2.53	2.53	7.02	
D203	195.52	194.76	2.12E-03	2.11E-03	1.10E-04	2.67	3.96	0.39	
D204	102.90	78.10	1.12E-03	8.48E-04	3.59E-03	3.07	2.44	24.11	
D205	0.00	0.00							

Trial 37-Flayash Batch test with Et-Benzene

9-Aug-01
Albright Light
5.0g
5C
270nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0023x - 0.0012
Abs=0.0023[conc(mg/L)]-.0012

m	**yintercept**
2.30E-03	-1.20E-03

Rep2&3 AvgC8H10 persent in ash(mg/l) 7.91

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual negative**	**negative**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	99.22	99.22							
D002	72.70	72.70							
D003	49.22	49.22							
D004	24.22	24.22							
D005	0.00	0.00							
Rep2 ash									
D101	99.22	110.00	9.35E-04	1.04E-03	-8.12E-04	2.98		-10.87	2.37
D102	72.70	75.65	6.85E-04	7.13E-04	-2.23E-04	3.15		-4.07	5.75
D103	49.22	34.35	4.64E-04	3.24E-04	1.12E-03	3.49	2.95	30.21	2.53
D104	24.22	10.87	2.28E-04	1.02E-04	1.01E-03	3.99	3.00	55.12	4.00
D105	0.00	0.00							0.00
Rep3 ash									
D201	99.22	107.39	9.35E-04	1.01E-03	-6.16E-04	3.00		-8.24	
D202	72.70	71.30	6.85E-04	6.72E-04	1.05E-04	3.17	3.98	1.91	
D203	49.22	33.48	4.64E-04	3.15E-04	1.19E-03	3.50	2.93	31.98	
D204	24.22	10.43	2.28E-04	9.83E-05	1.04E-03	4.01	2.98	56.91	
D205	0.00	0.00							

Trial 34-Flayash Batch test with Et-Benzene

3-Aug-01
Albright Light
5.0g
25C
270nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0021x - 0.0029
Abs=0.0021[conc(mg/L)]-.0029

m	**yintercept**
2.10E-03	-2.90E-03

Rep2&3 AvgC8H10 persent in ash(mg/l) 9.48

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual negative**	**negative**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	101.38	101.38							
D002	75.67	75.67							
D003	48.76	48.76							
D004	24.24	24.24							
D005	0.00	0.00							
Rep2 ash									
D101	101.38	123.33	9.55E-04	1.16E-03	-1.65E-03	2.93		-21.65	6.83
D102	75.67	81.90	7.13E-04	7.71E-04	-4.70E-04	3.11		-8.24	3.49
D103	48.76	33.33	4.59E-04	3.14E-04	1.16E-03	3.50	2.93	31.64	5.41
D104	24.24	6.67	2.28E-04	6.28E-05	1.32E-03	4.20	2.88	72.50	0.00
D105	0.00	0.00							0.00
Rep3 ash									
D201	101.38	132.38	9.55E-04	1.25E-03	-2.34E-03	2.90		-30.58	
D202	75.67	79.05	7.13E-04	7.45E-04	-2.55E-04	3.13		-4.47	
D203	48.76	35.24	4.59E-04	3.32E-04	1.02E-03	3.48	2.99	27.73	
D204	24.24	6.67	2.28E-04	6.28E-05	1.32E-03	4.20	2.88	72.50	
D205	0.00	0.00							

Trial 40-Flayash Batch test with Et-Benzene

16-Aug-01
Albright Light
5.0g
45C
270nm

UV curve
y = 0.0021x - 0.0018
Abs=0.0021[conc(mg/L)]-.0018

m	yintercept
2.10E-03	-1.80E-03

Rep2&3 AvgC8H10 persent in ash(mg/l)
13.71

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	Concentration-mg/L		Concentration mol/L		adsorption	Actual		%Reduct Conc	% Error Amoung
	initialCi	final-Cf	initial-Ci	final-Cf	Q(mol/Kg)	negative Log EQ	negative Log ADS	init v final	Reps 2&3
no ash									
D001	102.05	102.05							
D002	75.86	75.86							
D003	50.14	50.14							
D004	24.67	24.67							
D005	0.00	0.00							
Rep2 ash									
D101	102.05	112.38	9.61E-04	1.06E-03	-7.79E-04	2.98		-10.13	3.67
D102	75.86	76.19	7.14E-04	7.18E-04	-2.51E-05	3.14		-0.44	11.88
D103	50.14	34.76	4.72E-04	3.27E-04	1.16E-03	3.48	2.94	30.67	8.22
D104	24.67	6.67	2.32E-04	6.28E-05	1.36E-03	4.20	2.87	72.97	17.65
D105	0.00	0.00							0.00
Rep3 ash									
D201	102.05	116.67	9.61E-04	1.10E-03	-1.10E-03	2.96		-14.33	
D202	75.86	67.14	7.14E-04	6.32E-04	6.57E-04	3.20	3.18	11.49	
D203	50.14	31.90	4.72E-04	3.01E-04	1.37E-03	3.52	2.86	36.37	
D204	24.67	8.10	2.32E-04	7.62E-05	1.25E-03	4.12	2.90	67.18	
D205	0.00	0.00							

Trial 44-Flayash Batch test with Et-Benzene

6-Sep-01
Morgantown,MEA--Light
5.0g
5C
270nm

UV curve
y = 0.0024x - 0.0033
Abs=0.0024[conc(mg/L)]-.0033

m	yintercept
2.40E-03	-3.30E-03

Rep2&3 AvgC8H10 persent in ash(mg/l)
4.08

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	Concentration-mg/L		Concentration mol/L		adsorption	Actual		%Reduct Conc	% Error Amoung
	initialCi	final-Cf	initial-Ci	final-Cf	Q(mol/Kg)	negative Log EQ	negative Log ADS	init v final	Reps 2&3
no ash									
D001	98.46	98.46							
D002	76.38	76.38							
D003	48.67	48.67							
D004	22.83	22.83							
D005	0.00	0.00							
Rep2 ash									
D101	98.46	125.21	9.27E-04	1.18E-03	-2.02E-03	2.93		-27.17	4.33
D102	76.38	102.29	7.19E-04	9.63E-04	-1.95E-03	3.02		-33.93	6.52
D103	48.67	64.79	4.58E-04	6.10E-04	-1.22E-03	3.21		-33.13	3.22
D104	22.83	32.29	2.15E-04	3.04E-04	-7.13E-04	3.52		-41.42	3.87
D105	0.00	0.00							0.00
Rep3 ash									
D201	98.46	119.79	9.27E-04	1.13E-03	-1.61E-03	2.95		-21.67	
D202	76.38	95.63	7.19E-04	9.01E-04	-1.45E-03	3.05		-25.20	
D203	48.67	62.71	4.58E-04	5.91E-04	-1.06E-03	3.23		-28.85	
D204	22.83	31.04	2.15E-04	2.92E-04	-6.19E-04	3.53		-35.95	
D205	0.00	0.00							

Trial 48-Flayash Batch test with Et-Benzene

7-Sep-01
Morgantown,MEA--Light
5.0g
25C
270nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0022x + 0.0006
Abs=0.0022[conc(mg/L)]+.0006

m	**yintercept**
2.20E-03	6.00E-04

Rep2&3 AvgC8H10 persent in ash(mg/l)
3.14

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	99.50	99.50							
D002	73.36	73.36							
D003	50.41	50.41							
D004	24.95	24.95							
D005	0.00	0.00							
Rep2 ash									
D101	99.50	146.14	9.37E-04	1.38E-03	-3.51E-03	2.86		-46.87	9.02
D102	73.36	105.68	6.91E-04	9.95E-04	-2.44E-03	3.00		-44.05	5.30
D103	50.41	72.05	4.75E-04	6.79E-04	-1.63E-03	3.17		-42.92	7.57
D104	24.95	32.95	2.35E-04	3.10E-04	-6.03E-04	3.51		-32.06	0.00
D105	0.00	0.00							0.00
Rep3 ash									
D201	99.50	132.95	9.37E-04	1.25E-03	-2.52E-03	2.90		-33.62	
D202	73.36	111.59	6.91E-04	1.05E-03	-2.88E-03	2.98		-52.11	
D203	50.41	66.59	4.75E-04	6.27E-04	-1.22E-03	3.20		-32.10	
D204	24.95	32.95	2.35E-04	3.10E-04	-6.03E-04	3.51		-32.06	
D205	0.00	0.00							

Trial 52-Flayash Batch test with Et-Benzene

12-Sep-01
Morgantown,MEA--Light
5.0g
45C
270nm

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0024x - 0.0028
Abs=0.0024[conc(mg/L)]-.0028

m	**yintercept**
2.40E-03	-2.80E-03

Rep2&3 AvgC8H10 persent in ash(mg/l)
4.08

sample	**Concentration-mg/L initialCi**	**final-Cf**	**Concentration mol/L initial-Ci**	**final-Cf**	**adsorption Q(mol/Kg)**	**Actual negative Log EQ**	**negative Log ADS**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	99.29	99.29							
D002	77.42	77.42							
D003	43.46	43.46							
D004	26.17	26.17							
D005	0.00	0.00							
Rep2 ash									
D101	99.29	156.25	9.35E-04	1.47E-03	-4.29E-03	2.83		-57.36	11.73
D102	77.42	111.25	7.29E-04	1.05E-03	-2.55E-03	2.98		-43.70	3.96
D103	43.46	72.08	4.09E-04	6.79E-04	-2.16E-03	3.17		-65.87	0.00
D104	26.17	34.17	2.46E-04	3.22E-04	-6.03E-04	3.49		-30.57	4.88
D105	0.00	0.00							0.00
Rep3 ash									
D201	99.29	137.92	9.35E-04	1.30E-03	-2.91E-03	2.89		-38.90	
D202	77.42	115.83	7.29E-04	1.09E-03	-2.89E-03	2.96		-49.62	
D203	43.46	72.08	4.09E-04	6.79E-04	-2.16E-03	3.17		-65.87	
D204	26.17	32.50	2.46E-04	3.06E-04	-4.77E-04	3.51		-24.20	
D205	0.00	0.00							

Trial 32-Flayash Batch test with Xylenes

26-Jul-01
Albright Light
5.0g
5C
264nm

UV curve
y = 0.0022x - 0.0011
Abs=0.0022[conc(mg/L)]-.00011
m yintercept
2.20E-03 -1.10E-03

Rep2&3
AvgC8H10
persent in
ash(mg/l)
9.59

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	Concentration-mg/L initialCi	final-Cf	Concentration mol/L initial-Ci	final-Cf	adsorption Q(mol/Kg)	Actual negative Log EQ	negative Log ADS	%Reduct Conc init v final	% Error Amoung Reps 2&3
no ash									
D001	102.77	102.77							
D002	75.50	75.50							
D003	50.73	50.73							
D004	25.27	25.27							
D005	0.00	0.00							
Rep2 ash									
D101	102.77	50.45	9.68E-04	4.75E-04	6.57E-03	3.32	2.18	50.91	3.48
D102	75.50	29.09	7.11E-04	2.74E-04	5.83E-03	3.56	2.23	61.47	9.86
D103	50.73	17.73	4.78E-04	1.67E-04	4.14E-03	3.78	2.38	65.05	0.00
D104x	25.27	6.36	2.38E-04	5.99E-05	2.37E-03	4.22	2.62	74.82	21.43
D105	0.00	0.00							0.00
Rep3 ash									
D201	102.77	52.27	9.68E-04	4.92E-04	6.34E-03	3.31	2.20	49.14	
D202	75.50	32.27	7.11E-04	3.04E-04	5.43E-03	3.52	2.27	57.25	
D203	50.73	17.73	4.78E-04	1.67E-04	4.14E-03	3.78	2.38	65.05	
D204	25.27	5.00	2.38E-04	4.71E-05	2.55E-03	4.33	2.59	80.22	
D205	0.00	0.00							

Trial 29-Flayash Batch test with Xylenes

26-Jul-01
Albright Light
25C
264nm

UV curve
y = 0.0022x - 0.0003
Abs=0.0022[conc(mg/L)]-.0003
m yintercept
2.20E-03 -3.00E-04

Rep2&3
AvgC6H6
persent in
ash(mg/l)
6.95

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	Concentration-mg/L initialCi	final-Cf	Concentration mol/L initial-Ci	final-Cf	adsorption Q(mol/Kg)	Actual negative Log EQ	negative Log ADS	%Reduct Conc init v final	% Error Amoung Reps 2&3
no ash									
D001	103.77	103.77							
D002	77.18	77.18							
D003	49.23	49.23							
D004	26.05	26.05							
D005	0.00	0.00							
Rep2 ash									
D101	103.77	63.64	9.77E-04	5.99E-04	5.04E-03	3.22	2.30	38.68	8.57
D102	77.18	37.73	7.27E-04	3.55E-04	4.95E-03	3.45	2.30	51.12	2.35
D103	49.23	18.18	4.64E-04	1.71E-04	3.90E-03	3.77	2.41	63.07	9.09
D104x	26.05	9.55	2.45E-04	8.99E-05	2.07E-03	4.05	2.68	63.35	4.76
D105	0.00	0.00							0.00
Rep3 ash									
D201	103.77	58.18	9.77E-04	5.48E-04	5.73E-03	3.26	2.24	43.93	
D202	77.18	38.64	7.27E-04	3.64E-04	4.84E-03	3.44	2.32	49.94	
D203	49.23	20.00	4.64E-04	1.88E-04	3.67E-03	3.72	2.44	59.37	
D204	26.05	9.09	2.45E-04	8.56E-05	2.13E-03	4.07	2.67	65.10	
D205	0.00	0.00							

Trial 41-Flayash Batch test with Xylenes

16-Aug-01
Albright Light
45C
264nm

UV curve
y = 0.0022x - 0.001
Abs=0.0022[conc(mg/L)]-.001
m **yintercept**
2.20E-03 -1.00E-03

Rep2&3
AvgC8H10
persent in
ash(mg/l)
8.64

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual negative**	**negative**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	100.00	100.00							
D002	75.23	75.23							
D003	47.27	47.27							
D004	25.00	25.00							
D005	0.00	0.00							
Rep2 ash									
D101	100.00	49.09	9.42E-04	4.62E-04	6.39E-03	3.34	2.19	50.91	9.26
D102	75.23	26.82	7.09E-04	2.53E-04	6.08E-03	3.60	2.22	64.35	4.84
D103	47.27	14.09	4.45E-04	1.33E-04	4.17E-03	3.88	2.38	70.19	3.23
D104x	25.00	5.00	2.35E-04	4.71E-05	2.51E-03	4.33	2.60	80.00	8.33
D105	0.00	0.00							0.00
Rep3 ash									
D201	100.00	44.55	9.42E-04	4.20E-04	6.96E-03	3.38	2.16	55.45	
D202	75.23	28.18	7.09E-04	2.65E-04	5.91E-03	3.58	2.23	62.54	
D203	47.27	13.64	4.45E-04	1.28E-04	4.22E-03	3.89	2.37	71.15	
D204	25.00	5.45	2.35E-04	5.14E-05	2.45E-03	4.29	2.61	78.18	
D205	0.00	0.00							

Trial 45-Flayash Batch test with Xylenes

26-Jul-01
Morgantown, MEA--Light
5.0g
5C
264nm

UV curve
y = 0.0022x - 0.0019
Abs=0.0022[conc(mg/L)]-.00019
m **yintercept**
2.20E-03 -1.90E-03

Rep2&3
AvgC8H10
persent in
ash(mg/l)
3.59

{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

sample	**Concentration-mg/L**		**Concentration mol/L**		**adsorption**	**Actual negative**	**negative**	**%Reduct Conc init v final**	**% Error** Amoung Reps 2&3
	initialCi	**final-Cf**	**initial-Ci**	**final-Cf**	**Q(mol/Kg)**	**Log EQ**	**Log ADS**		
no ash									
D001	100.64	100.64							
D002	75.86	75.86							
D003	49.95	49.95							
D004	24.05	24.05							
D005	0.00	0.00							
Rep2 ash									
D101	100.64	96.36	9.48E-04	9.08E-04	5.37E-04	3.04	3.27	4.25	7.08
D102	75.86	71.36	7.15E-04	6.72E-04	5.65E-04	3.17	3.25	5.93	1.91
D103	49.95	47.27	4.71E-04	4.45E-04	3.37E-04	3.35	3.47	5.37	5.77
D104	24.05	23.18	2.26E-04	2.18E-04	1.08E-04	3.66	3.96	3.59	1.96
D105	0.00	0.00							0.00
Rep3 ash									
D201	100.64	89.55	9.48E-04	8.43E-04	1.39E-03	3.07	2.86	11.02	
D202	75.86	70.00	7.15E-04	6.59E-04	7.36E-04	3.18	3.13	7.73	
D203	49.95	44.55	4.71E-04	4.20E-04	6.79E-04	3.38	3.17	10.83	
D204	24.05	22.73	2.26E-04	2.14E-04	1.66E-04	3.67	3.78	5.48	
D205	0.00	0.00							

Trial 49-Flayash Batch test with Xylenes

7-Sep-01
Morgantown, MEA--Light
5.0g 25C
264nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

UV curve
y = 0.0021x + 0.0008
Abs=0.0021[conc(mg/L)]+.0008

m	**yintercept**
2.10E-03	8.00E-04

Rep2&3 AvgC8H10 persent in ash(mg/l) 2.95

sample	**Concentration-mg/L** **initialCi**	**final-Cf**	**Concentration mol/L** **initial-Ci**	**final-Cf**	**adsorption** **Q(mol/Kg)**	**Actual** **negative** **Log EQ**	**negative** **Log ADS**	**%Reduct** **Conc** **init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	98.67	98.67							
D002	77.00	77.00							
D003	48.67	48.67							
D004	25.57	25.57							
D005	0.00	0.00							
Rep2 ash									
D101	98.67	91.90	9.29E-04	8.66E-04	8.49E-04	3.06	3.07	6.85	4.66
D102	77.00	73.33	7.25E-04	6.91E-04	4.60E-04	3.16	3.34	4.76	4.55
D103	48.67	46.19	4.58E-04	4.35E-04	3.11E-04	3.36	3.51	5.09	5.15
D104	25.57	23.33	2.41E-04	2.20E-04	2.81E-04	3.66	3.55	8.75	0.00
D105	0.00	0.00							0.00
Rep3 ash									
D201	98.67	87.62	9.29E-04	8.25E-04	1.39E-03	3.08	2.86	11.20	
D202	77.00	70.00	7.25E-04	6.59E-04	8.79E-04	3.18	3.06	9.09	
D203	48.67	43.81	4.58E-04	4.13E-04	6.10E-04	3.38	3.21	9.98	
D204	25.57	23.33	2.41E-04	2.20E-04	2.81E-04	3.66	3.55	8.75	
D205	0.00	0.00							

Trial 53-Flayash Batch test with Xylenes

13-Sep-01
Morgantown, MEA--Light
5.0g 45C
264nm
{(Cf*Vf) - (Ci*Vi)} / m = Q = Sorption
{(Cf - Ci) * V} / m = Q

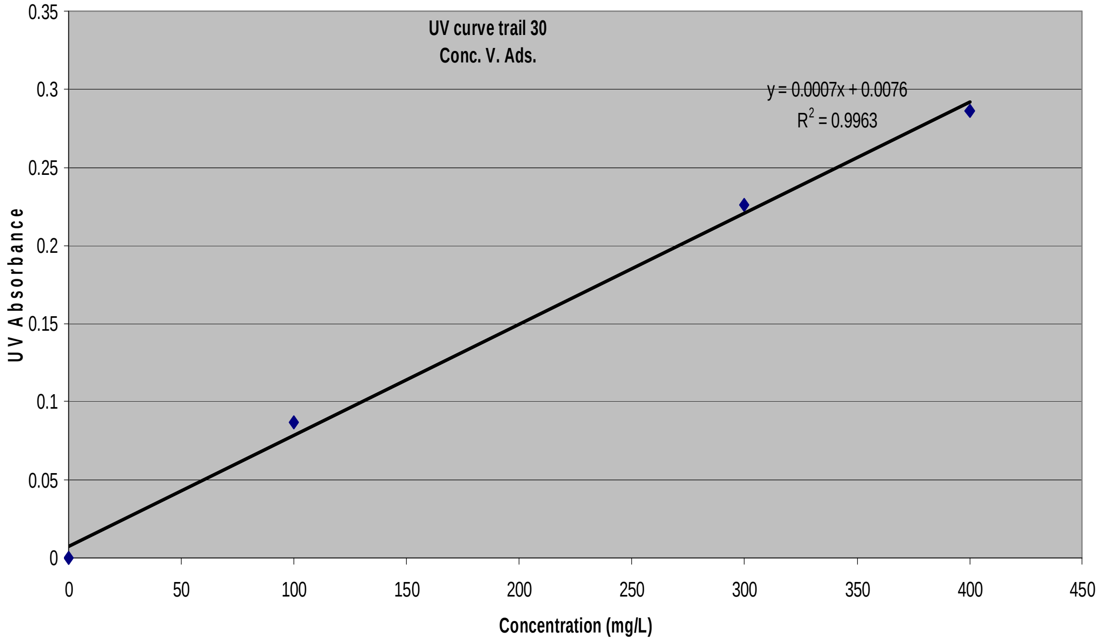
UV curve
y = 0.0022x + 0.0004
Abs=0.0022[conc(mg/L)]+.0004

m	**yintercept**
2.20E-03	4.00E-04

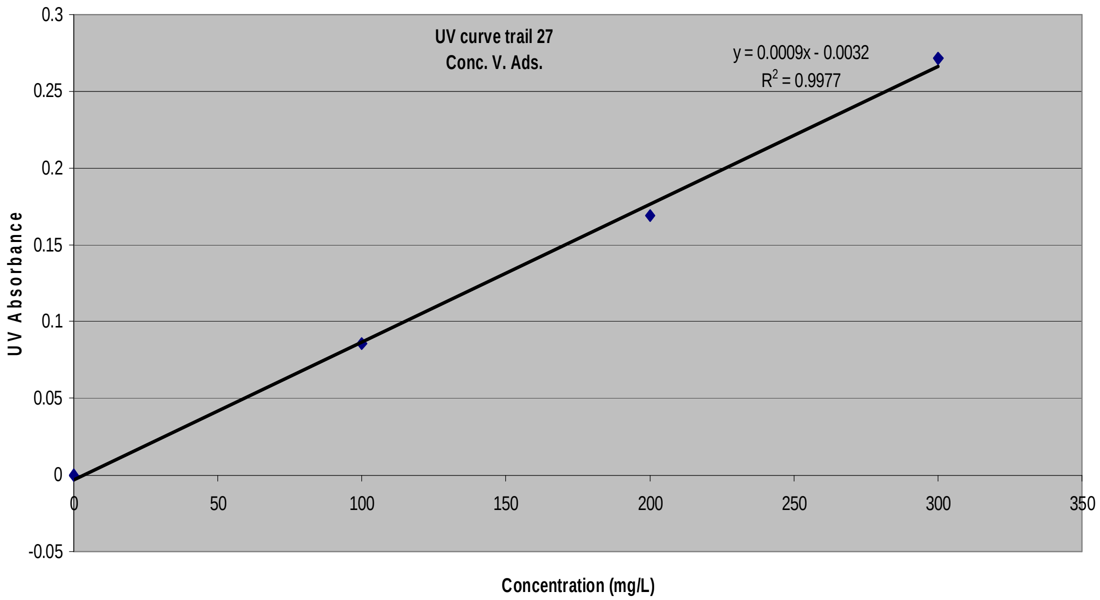
Rep2&3 AvgC8H10 persent in ash(mg/l) 5.27

sample	**Concentration-mg/L** **initialCi**	**final-Cf**	**Concentration mol/L** **initial-Ci**	**final-Cf**	**adsorption** **Q(mol/Kg)**	**Actual** **negative** **Log EQ**	**negative** **Log ADS**	**%Reduct** **Conc** **init v final**	**% Error** Amoung Reps 2&3
no ash									
D001	102.77	102.77							
D002	67.55	67.55							
D003	51.86	51.86							
D004	25.73	25.73							
D005	0.00	0.00							
Rep2 ash									
D101	102.77	94.55	9.68E-04	8.91E-04	1.03E-03	3.05	2.99	8.01	0.48
D102	67.55	65.00	6.36E-04	6.12E-04	3.20E-04	3.21	3.50	3.77	5.30
D103	51.86	45.00	4.88E-04	4.24E-04	8.62E-04	3.37	3.06	13.23	2.94
D104	25.73	20.00	2.42E-04	1.88E-04	7.19E-04	3.72	3.14	22.26	15.38
D105	0.00	0.00							0.00
Rep3 ash									
D201	102.77	95.00	9.68E-04	8.95E-04	9.76E-04	3.05	3.01	7.56	
D202	67.55	68.64	6.36E-04	6.46E-04	-1.37E-04	3.19		-1.62	
D203	51.86	46.36	4.88E-04	4.37E-04	6.91E-04	3.36	3.16	10.60	
D204	25.73	23.64	2.42E-04	2.23E-04	2.63E-04	3.65	3.58	8.13	
D205	0.00	0.00							

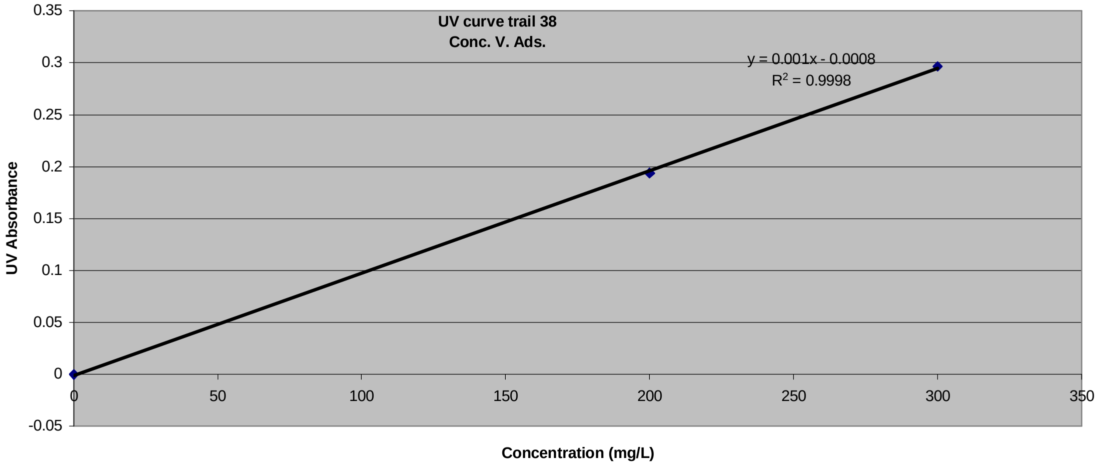
Appendix II. UV Analytical Curves



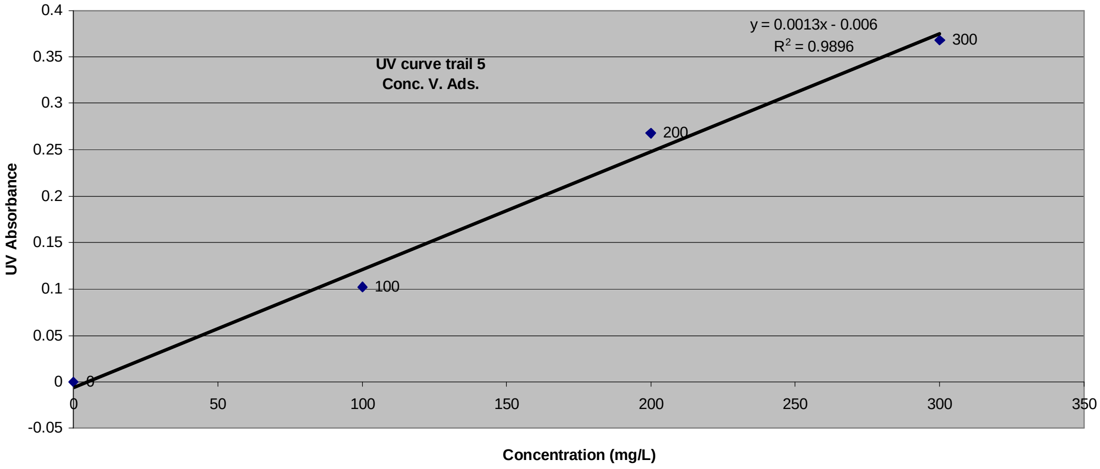
UV Curve Trial 30		Wavelength=254nm
Conc. ppm	Abs.	Max absorbance
400	0.286	
300	0.226	
100	0.087	
0	0	



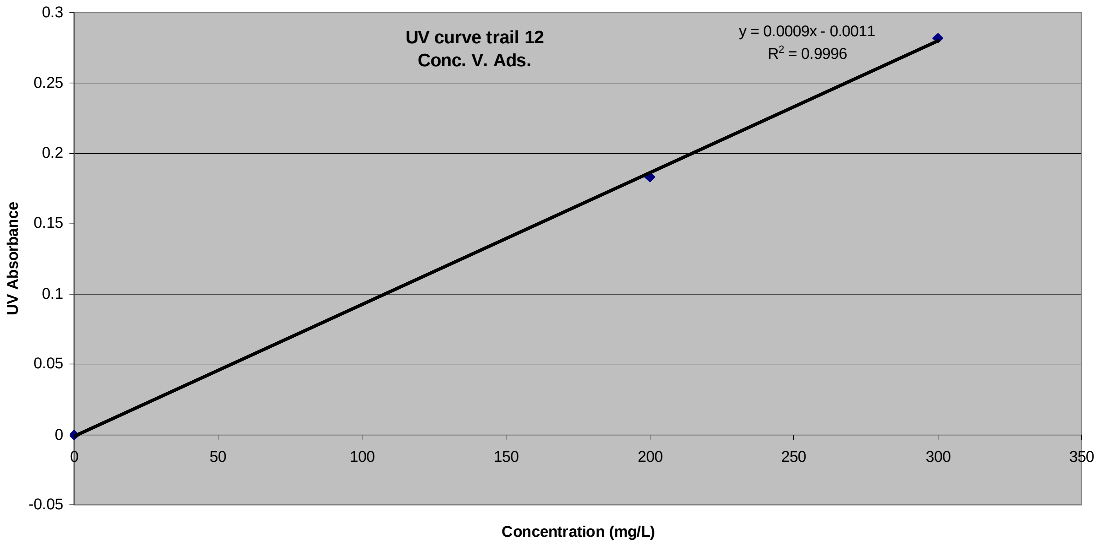
UV Curve Conc. ppm	Trial 27 Abs.	Wavelength=254nm Max absorbance
300	0.2715	
200	0.169	
100	0.0855	
0	0	



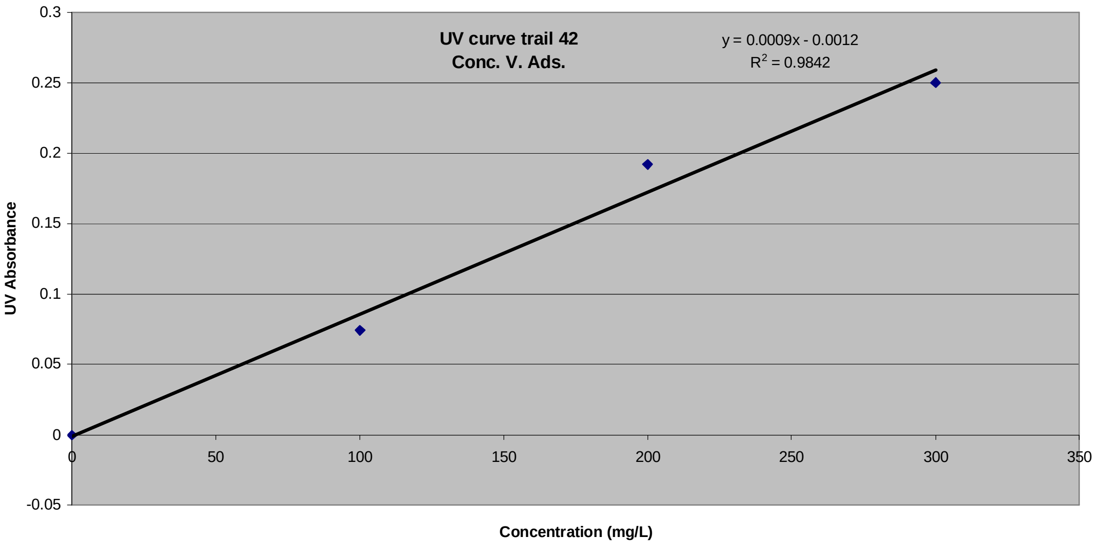
UV Curve Conc. ppm	Trial 38 Abs.	Wavelength=254nm Max absorbance
300	0.296	
200	0.1935	
0	0	



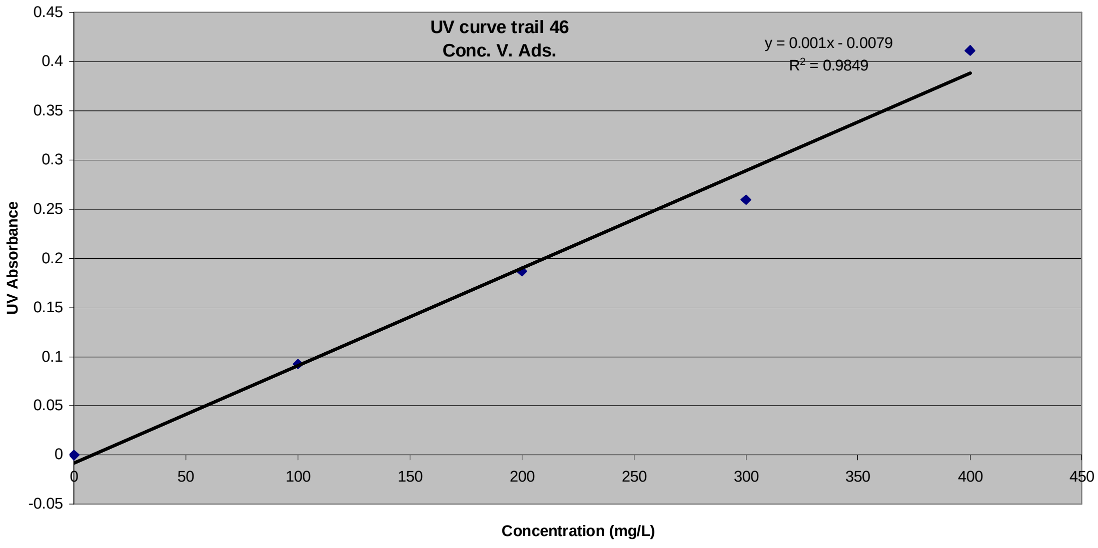
UV Curve Conc. ppm	**Trial 5 Abs.**	**Wavelength=254nm Max absorbance**
300	0.368	
200	0.268	
100	0.102	
0	0	



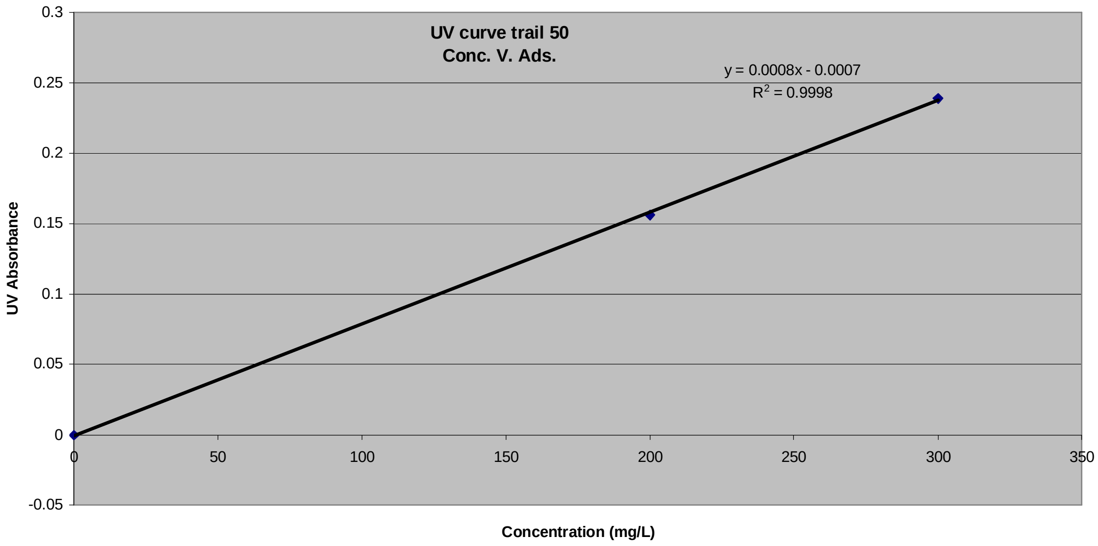
UV Curve Conc. ppm	Trial 12 Abs.	Wavelength=254nm Max absorbance
300	0.282	
200	0.183	
	0.082	
0	0	



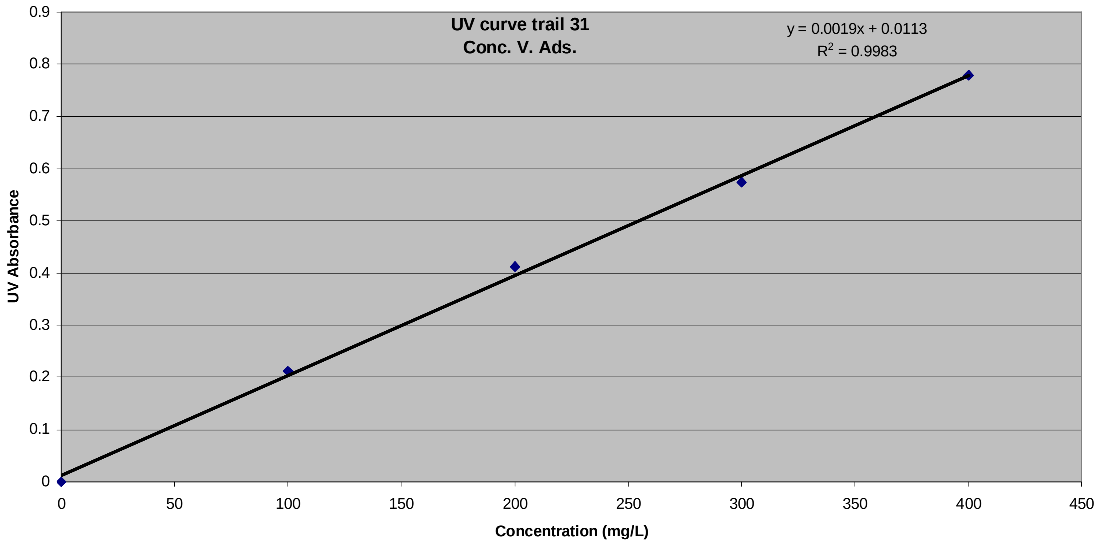
UV Curve Conc. ppm	**Trial 42 Abs.**	**Wavelength=254nm Max absorbance**
300	0.25	
200	0.192	
100	0.074	
0	0	



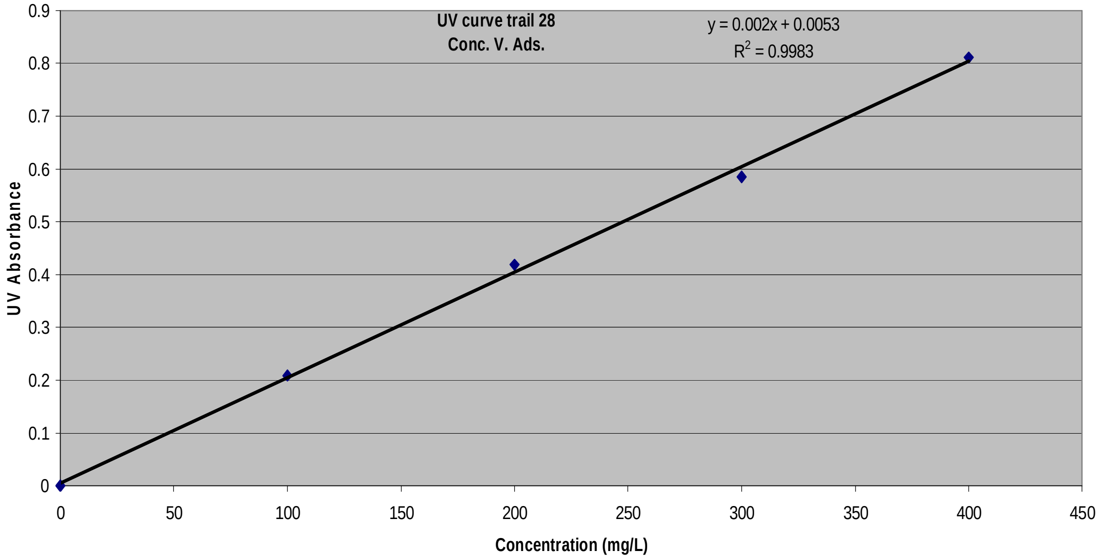
UV Curve Conc. ppm	**Trial 46 Abs.**	**Wavelength=254nm Max absorbance**
400	0.4115	
300	0.2595	
200	0.187	
100	0.0925	
0	0	



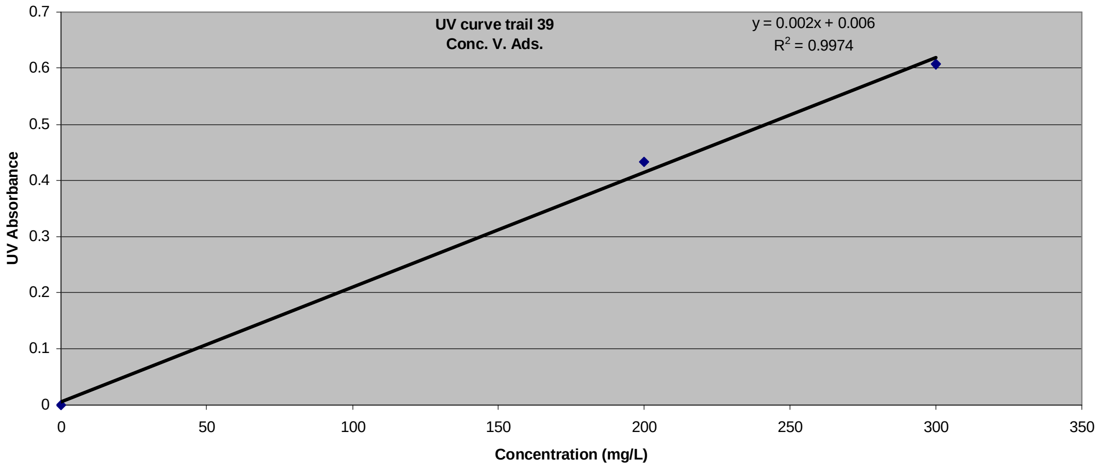
UV Curve Conc. ppm	**Trial 50 Abs.**	**Wavelength=254nm Max absorbance**
300	0.239	
200	0.156	
0	0	



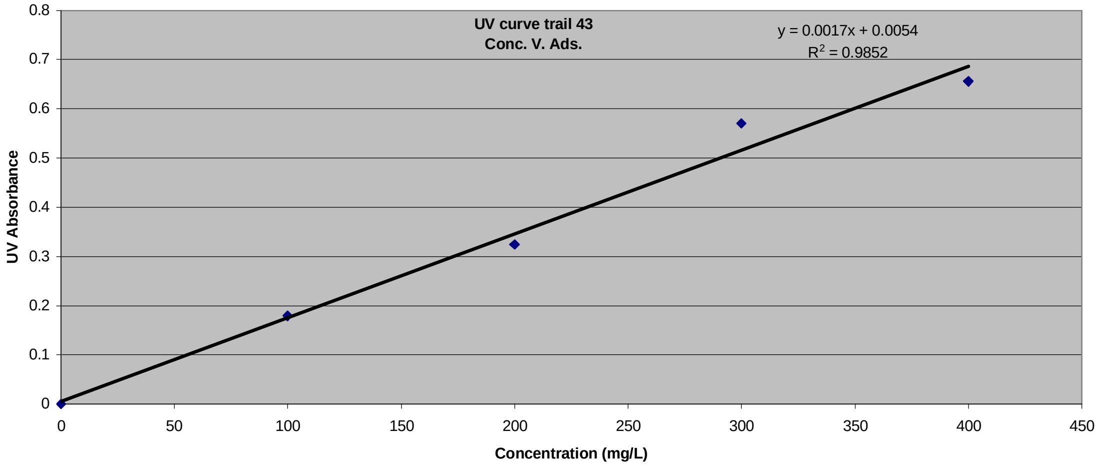
UV Curve Conc. ppm	Trial 31 Abs.	Wavelength=261nm Max absorbance
400	0.7785	
300	0.5745	
200	0.412	
100	0.2115	
0	0	



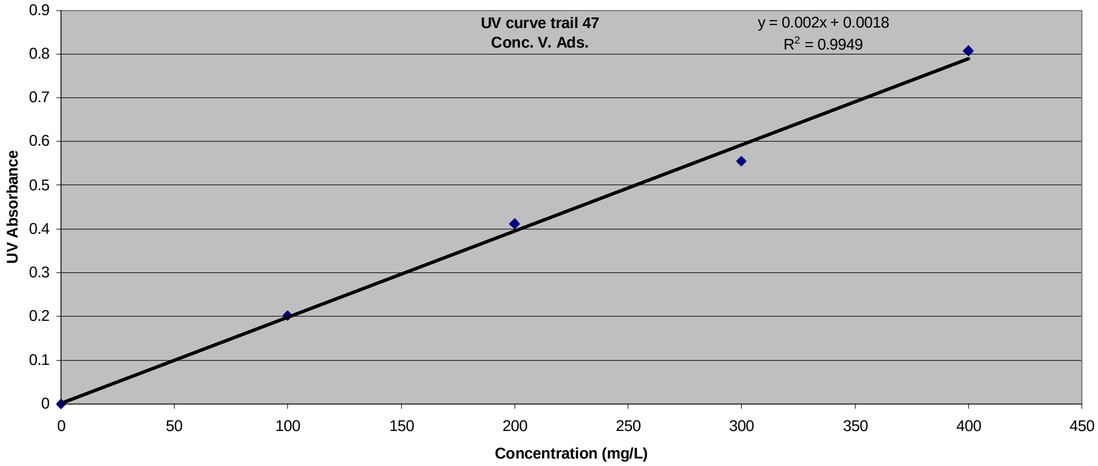
UV Curve Conc. ppm	Trial 28 Abs.	Wavelength=261nm Max absorbance
400	0.8105	
300	0.585	
200	0.419	
100	0.209	
0	0	



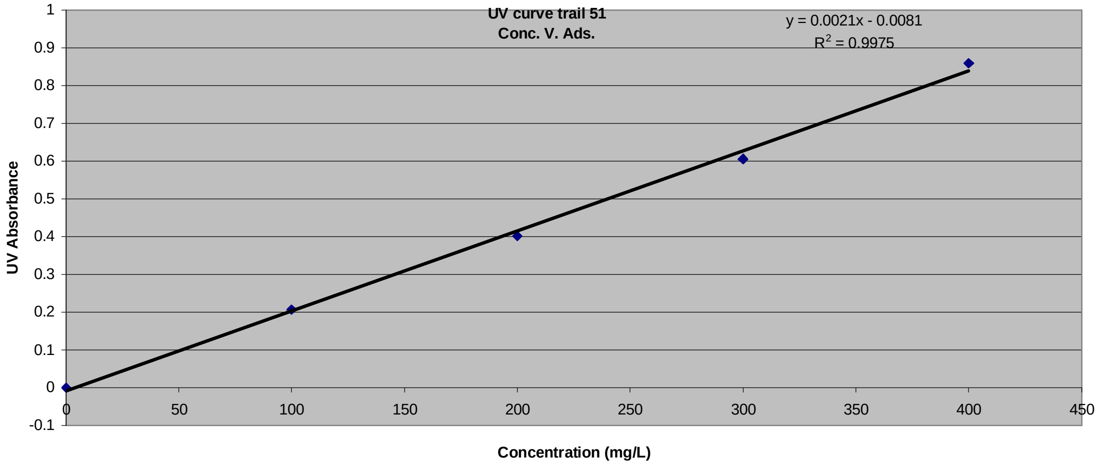
UV Curve Conc. ppm	Trial 39 Abs.	Wavelength=261nm Max absorbance
300	0.6065	
200	0.4325	
0	0	



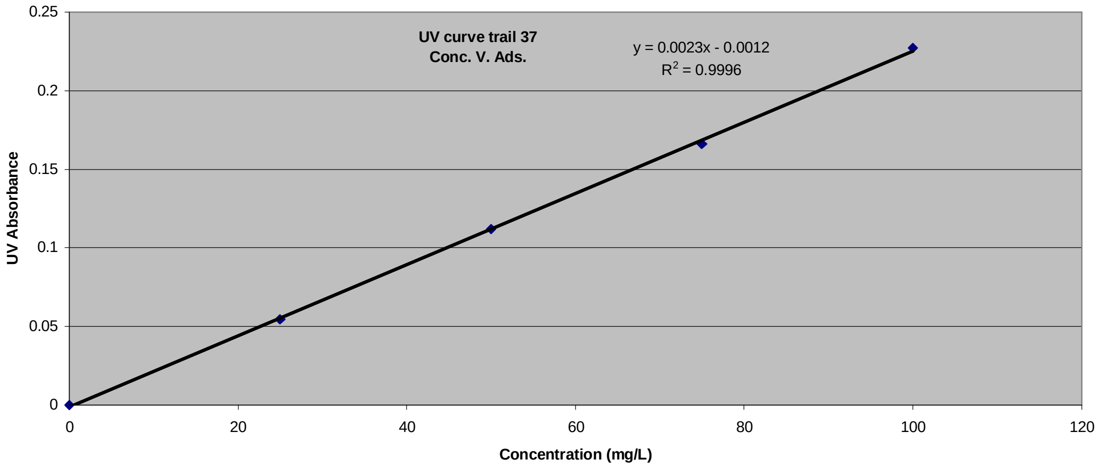
UV Curve Conc. ppm	Trial 43 Abs.	Wavelength=261nm Max absorbance
400	0.6555	
300	0.57	
200	0.3245	
100	0.179	
0	0	



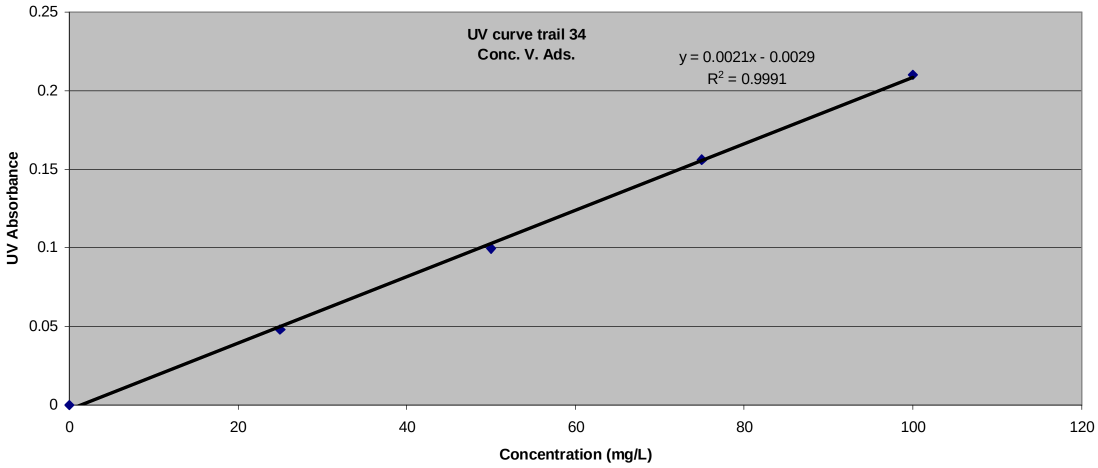
UV Curve Conc. ppm	**Trial 47 Abs.**	**Wavelength=261nm Max absorbance**
400	0.808	
300	0.5555	
200	0.412	
100	0.2025	
0	0	



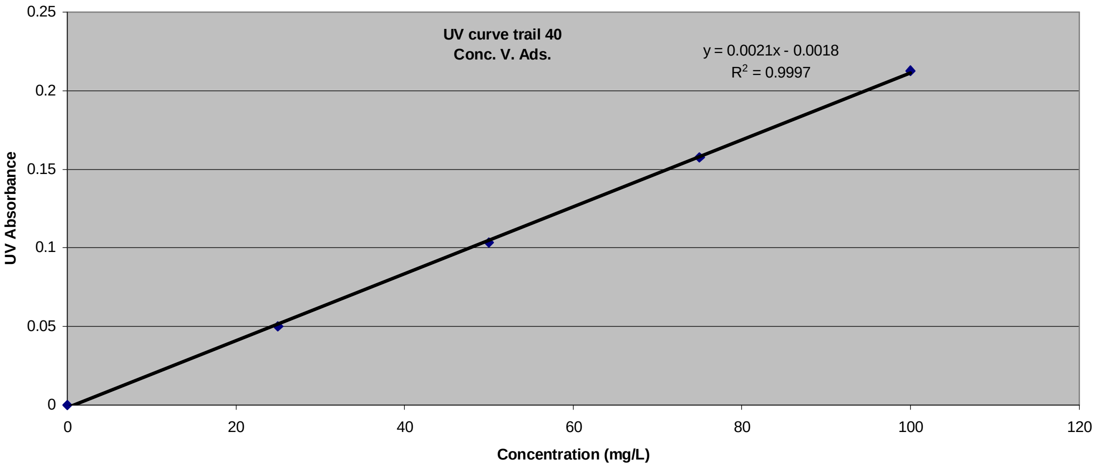
UV Curve Conc. ppm	**Trial 51 Abs.**	**Wavelength=261nm Max absorbance**
400	0.859	
300	0.606	
200	0.4025	
100	0.208	
0	0	



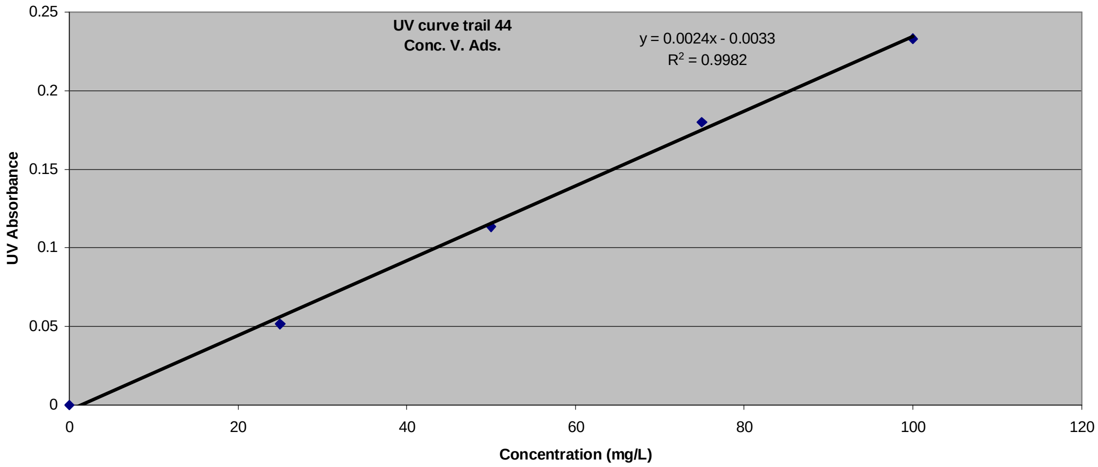
UV Curve Conc. ppm	Trial 37 Abs.	Wavelength=270nm Max absorbance
100	0.227	
75	0.166	
50	0.112	
25	0.0545	
0	0	



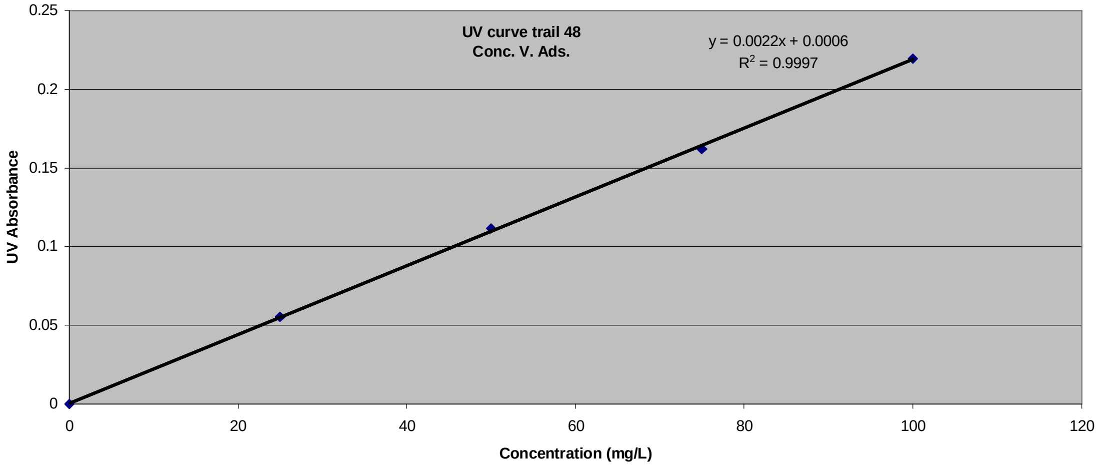
UV Curve Conc. ppm	Trial 34 Abs.	Wavelength=270nm Max absorbance
100	0.21	
75	0.156	
50	0.0995	
25	0.048	
0	0	



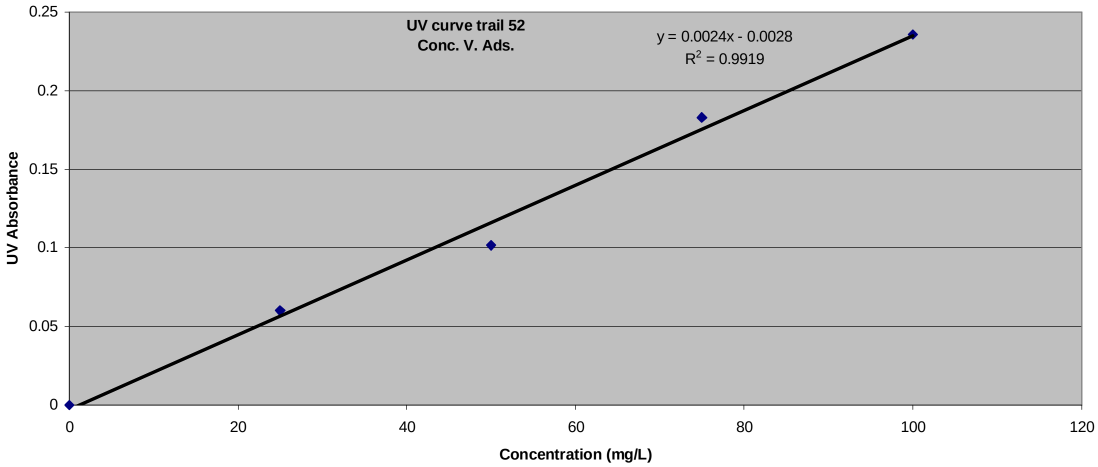
UV Curve Conc. ppm	Trial 40 Abs.	Wavelength=270nm Max absorbance
100	0.2125	
75	0.1575	
50	0.1035	
25	0.05	
0	0	



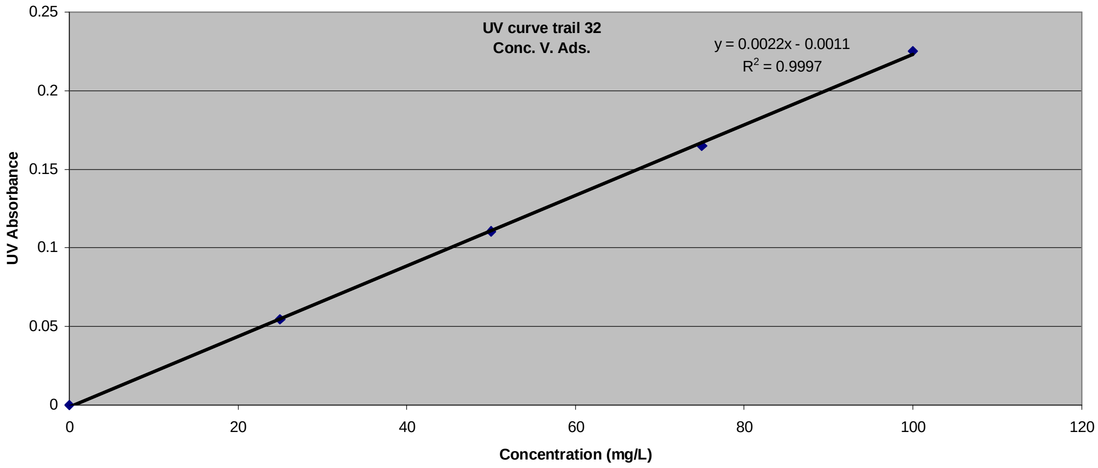
UV Curve Conc. ppm	Trial 44 Abs.	Wavelength=270nm Max absorbance
100	0.233	
75	0.18	
50	0.1135	
25	0.0515	
0	0	



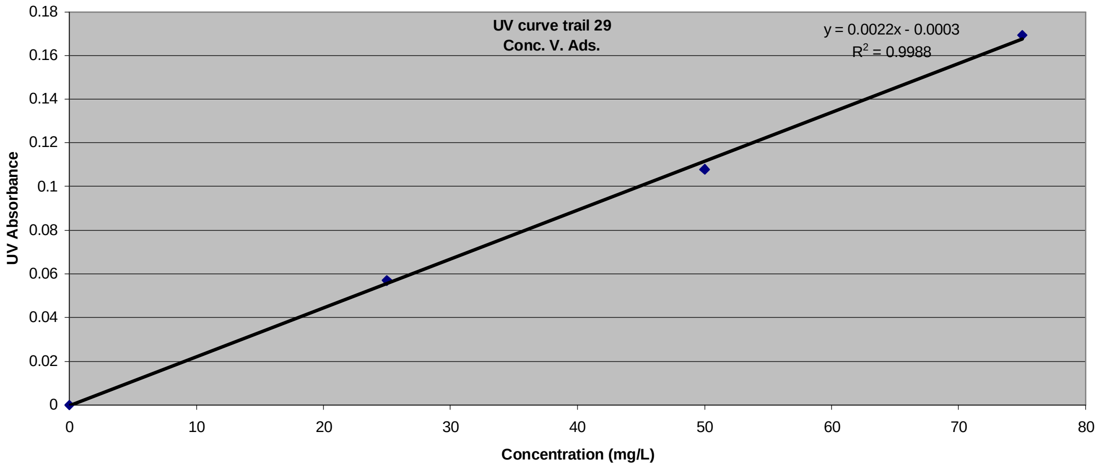
UV Curve	**Trial 48**	**Wavelength=270nm**
Conc. ppm	**Abs.**	**Max absorbance**
100	0.2195	
75	0.162	
50	0.1115	
25	0.0555	
0	0	



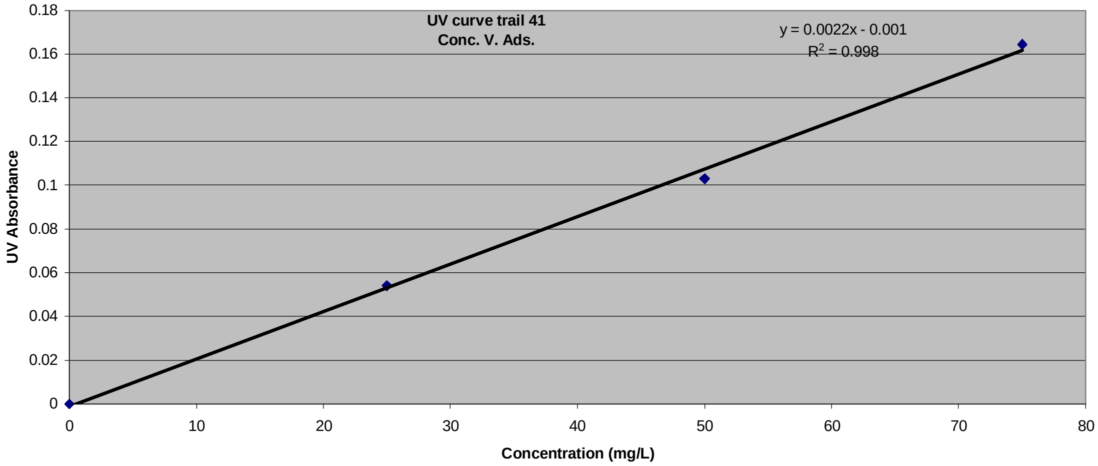
UV Curve Conc. ppm	Trial 52 Abs.	Wavelength=270nm Max absorbance
100	0.2355	
75	0.183	
50	0.1015	
25	0.06	
0	0	



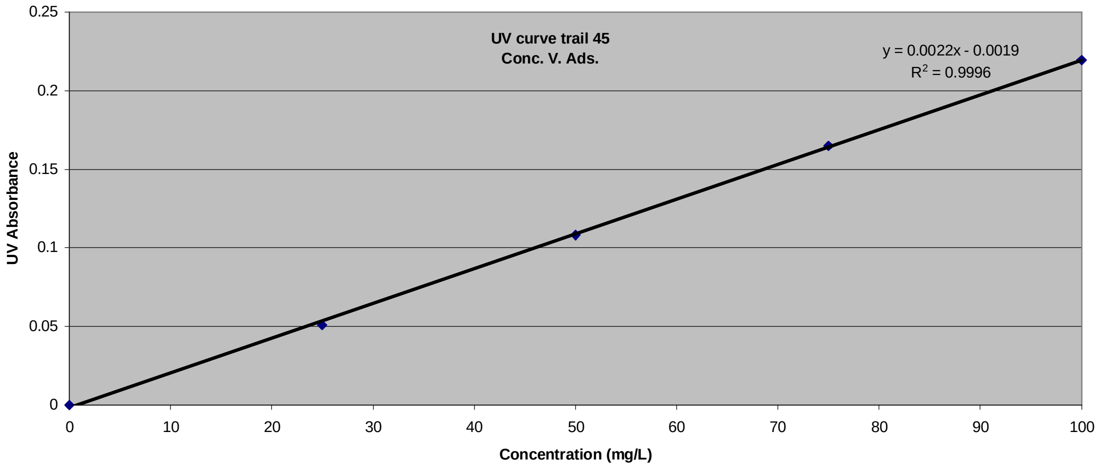
UV Curve Conc. ppm	Trial 32 Abs.	Wavelength=264nm Max absorbance
100	0.225	
75	0.165	
50	0.1105	
25	0.0545	
0	0	



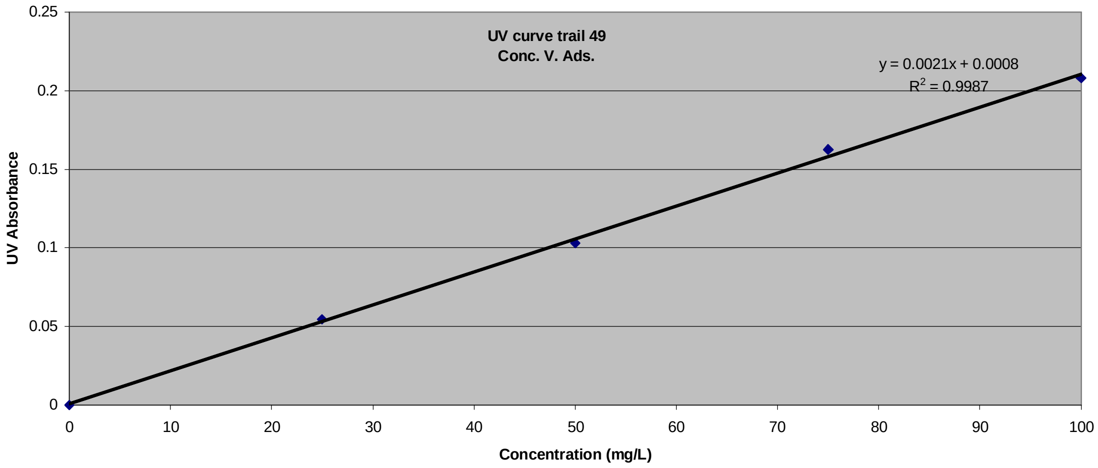
UV Curve Conc. ppm	Trial 29 Abs.	Wavelength=264nm Max absorbance
75	0.1695	
50	0.108	
25	0.057	
0	0	



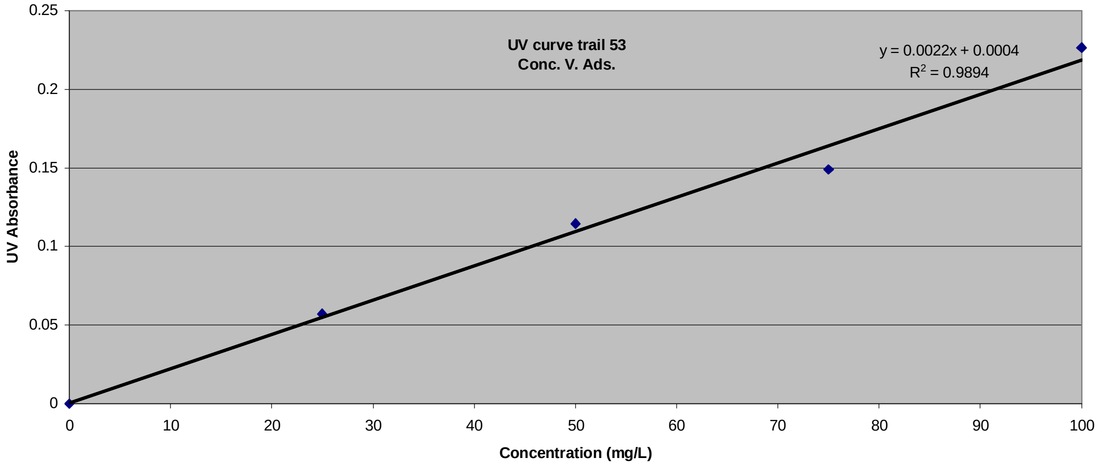
UV Curve Conc. ppm	Trial 41 Abs.	Wavelength=264nm Max absorbance
75	0.1645	
50	0.103	
25	0.054	
0	0	



UV Curve Conc. ppm	Trial 45 Abs.	Wavelength=264nm Max absorbance
100	0.2195	
75	0.165	
50	0.108	
25	0.051	
0	0	



UV Curve Conc. ppm	Trial 49 Abs.	Wavelength=264nm Max absorbance
100	0.208	
75	0.1625	
50	0.103	
25	0.0545	
0	0	



UV Curve Conc. ppm	**Trial 53 Abs.**	**Wavelength=264nm Max absorbance**
100	0.2265	
75	0.149	
50	0.1145	
25	0.057	
0	0	