Final Summary Report

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DEVELOPMENT OF A RATIONAL MODELING APPROACH FOR THE DESIGN, AND OPTIMIZATION OF THE MULTIFILTRATION UNIT

by

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ABSTRACT

This thesis includes the development and verification of an adsorption model for analysis and optimization of the adsorption processes within the International Space Station multifiltration beds. The fixed bed adsorption model includes multicomponent equilibrium and both external and intraparticle mass transfer resistances. Single solute isotherm parameters were used in the multicomponent equilibrium description to predict the competitive adsorption interactions occurring during the adsorption process. The multicomponent equilibrium description used the Fictive Component Analysis to describe adsorption in unknown background matrices. Multicomponent isotherms were used to validate the multicomponent equilibrium description. Column studies were used to develop and validate external and intraparticle mass transfer parameter correlations for compounds of interest. The fixed bed model was verified using a shower and handwash ersatz water which served as a surrogate to the actual shower and handwash wastewater.

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LIST OF ACRONYMS

DCM	Dichloromethane
EB	Ethylbenzene
EBCT	Empty Bed Contact Time
FC	Fictive Component
FCs	Fictive Components
FCA	Fictive Component Analysis
GAC	Granular Activated Carbon
GUI	Graphical User Interface
IAST	Ideal Adsorbed Solution Theory
ISS	International Space Station
LLE	Liquid-Liquid Extraction
MFB	Multifiltration Bed
MFBs	Multifiltration Beds
MEK	Methyl Ethyl Ketone
PCE	Perchloroethylene
PGAC	Powdered Granular Activated Carbon
PSDM	Pore and Surface Diffusion Model
RAHF	Research Animal Holding Facility
RPE	Relative Percent Error
SCMT	Sodium-N-methyl-N-"coconut oil acid" taurate
SPDFR	Surface to Pore Diffusion Flux Ratio
TC	Total Carbon
1,2,4-TCB	1,2,4-Trichlorobenzene
TCE	Trichloroethylene
TIC	Total Inorganic Carbon
TOC	Total Organic Carbon
VOC	Volatile Organic Compound
VOCs	Volatile Organic Compounds

1.0 Introduction and Objectives

1.1 Multifiltration Bed Model Overview

A substantial amount of potable water is required for life support of the crew aboard the International Space Station (ISS). Water for drinking, food preparation, and personal hygiene accounts for over 90% by weight of the basic consumables (water, oxygen, and food) required for survival aboard the ISS. Life support of a four person crew would require transport of approximately 46,100 lbs of water per year to the ISS without onboard water recycling. The economic limitations of transporting water to the ISS necessitate onboard recovery and reuse of the aqueous waste streams (Carter *et al.*, 1992; Carter *et al.*, 1991).

The aqueous waste streams processed by the ISS water processor include: 1) urine distillate, 2) waste shower and handwash water, 3) humidity condensate, 4) oral hygiene and wet shave waste, and 5) a mixture of humidity condensate and evaporated urine from the Research Animal Holding Facility (RAHF). Appendix I lists the major waste streams including their identified inorganic and organic constituents and expected concentrations aboard the ISS (Carter *et al.*, 1992).

Recycling the wastewater aboard the ISS is accomplished using a series of four treatment processes. The wastewater first passes through a 0.5 micron filter to remove particulate matter. Next in the treatment process, ion exchange resins and adsorption media are combined in multifiltration beds (MFBs) for removal of ionic and organic contaminants from the wastewater. A schematic of a multifiltration bed (MFB) is shown in Figure 1-1. Table 1-1 describes the MFB components and their functions. A catalytic oxidation unit is employed following the MFBs to remove low molecular weight organic compounds not efficiently removed by the adsorption beds.

A mathematical model designed to predict the performance of the MFBs was developed. The model was verified for a surrogate prepared for the shower and handwash wastewater. Shower and handwash wastewater is expected to be the most prevalent and most concentrated waste stream aboard the ISS based on its reported flowrate, TOC concentration, and ionic contaminant concentrations (Carter *et al.*, 1992).

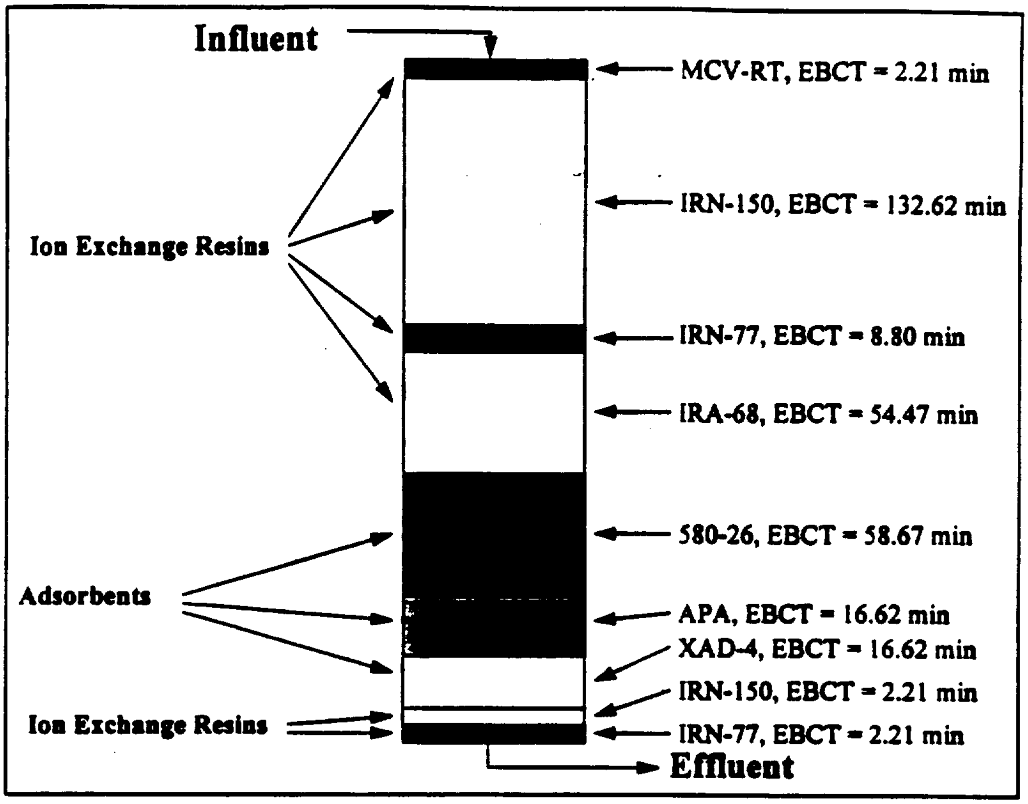

Figure 1-1. Multifiltration Bed Schematic

Consequently, it was assumed that if the performance of the ion exchange and adsorption processes could be predicted using the MFB model for this waste stream, then the model should be able to predict the performance of the MFB in treating the other wastewater streams or their mixtures.

The MFB model was developed to enable engineers to predict the impact of changing process variables on the performance of the MFBs. The model can also be used to simulate laboratory and pilot scale experiments and save the time and cost of performing them. Process variables such as the time variable influent contaminant concentrations (including number and type of contaminants), empty bed contact time (EBCT), sequence of the ion exchange resins and adsorbents (including number and type) within a multifiltration bed or multiple beds, and competitive interactions among ions and adsorbates can be evaluated with the model.

The multifiltration bed model was designed for the Microsoft Windows™ environment with a graphical user interface (GUI) in order to maximize user-friendliness. The Microsoft Windows interface was used because of its built-in file and hardware

Table 1-1. Ion exchange resins and adsorbents in the ISS multifiltration bed.

Media	Function	Media Description
MCV-RT	Disinfection	iodinated strong base anion (SBA) exchange resin
IRN-150	Removal of anions and cations	mixture of gel types strong acid cation (SAC) (IRN-77, H^+ form) and SBA (IRN-78, OH^- form)
IRN-77	Removal of cations	SAC gel exchange resin in the H^+ form
IRA-68	Removal of strong and weak acids	weak base anion (WBA) gel exchange resin in the free base form
580-26	Removal of nonpolar organics	coconut-shell based granular activated carbon
APA	Removal of nonpolar organics	bituminous-coal based activated carbon
XAD-4	Removal of nonpolar organics	polymeric adsorbent
IRN-150	Removal of anions and cations	mixture of gel types SAC (IRN-77 , H^+ form) and SBA (IRN-78, OH^- form)
IRN-77	Removal of cations	SAC gel exchange resin in the H^+ form

control features which free the engineer from concerns over printer drivers and other machine issues and allows more attention to the computational algorithms. The GUI consists of a front-end shell written in Visual Basic™ that calls FORTRAN subroutines in order to perform calculations.

1.2 Objectives

There were two overall objectives for the MFB adsorption model. The first objective was to predict the performance of the adsorption beds in series in the MFBs for removing total organic carbon (TOC) from wastestreams of unknown composition. The second objective was to predict the removal of target compounds in the MFBs in the presence of an unknown background matrix. This study includes the development and verification of the fixed bed adsorption model designed to accomplish these objectives

1.3 Adsorption Modeling Overview

The Fictive Component Analysis was developed to describe the competitive adsorption interactions in unknown background matrices making up the mixtures TOC concentrations (Crittenden *et al.*, 1986). TOC and tracer compound isotherms were performed on each of the MFB adsorbents and used to determine the fictive component parameters. Column studies were performed on each adsorbent and compared to model calculations to obtain intraparticle mass transfer correlations for the wide range of adsorbing contaminants expected in the ISS waste stream and to verify the fixed bed model. An experiment was performed using the currently reported MFB design. The adsorption model was verified by comparing the model predictions to the data for the MFB experiment.

The fixed bed model used in this study assumes both pore and surface diffusion are intraparticle transport mechanisms and plug flow is the axial transport mechanism. It is named the Pore and Surface Diffusion Model (PSDM). The complete PSDM development was presented by Friedman (1984) and Crittenden *et al.* (1986). The assumptions and mechanisms built into the model are:

- Plug-flow conditions exist in the bed (axial and radial dispersion are neglected).
- The hydraulic loading is constant.
- Single solute adsorption equilibrium is represented by the Freundlich isotherm equation.

- Ideal Adsorbed Solution Theory incorporating the Freundlich isotherm equation and the Fictive Component Analysis describes the multicomponent equilibrium.
- Local adsorption equilibrium exists between the solute adsorbed onto the adsorbent particle and the solute in the intraparticle stagnant fluid. (The rate of sorption onto the adsorbent surface is much faster than the diffusion rate.)
- A linear driving force approximation describes the liquid-phase mass transfer flux at the exterior of the adsorbent.
- Intraparticle mass flux is described by surface diffusion and/or pore diffusion.
- There are no solute-solute interactions during the diffusion process.

Figure 1-2 illustrates the adsorption and diffusion mechanisms incorporated into the PSDM. The equilibrium development and results will be explained first followed by the fixed bed model equations and kinetic description and modeling results.

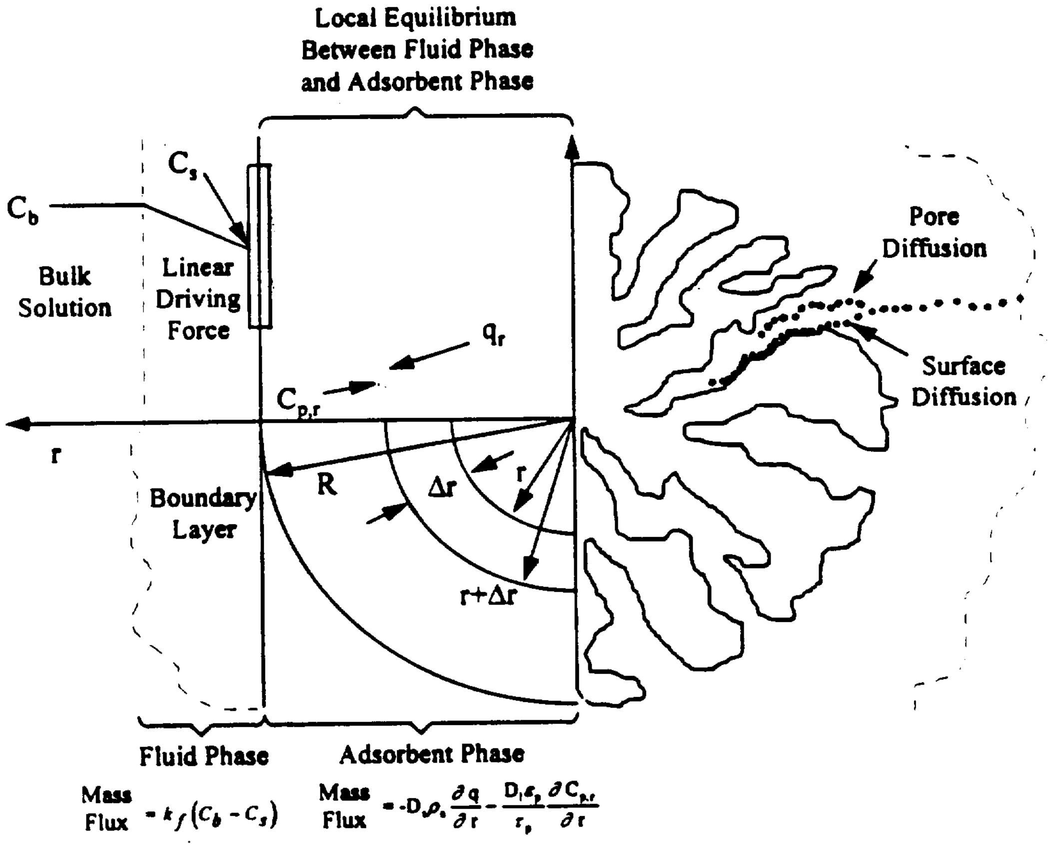

Figure 1-2. PSDM mechanisms

2.0 Experimental Materials, Methods, and Procedures

2.1 Chemicals

All chemicals used were of reagent grade or better. Dichloromethane (DCM), ethylbenzene (EB), methyl-ethyl-ketone (MEK), *m*-xylene, naphthalene, perchloroethylene (PCE), toluene, trichloroethylene (TCE), 1,2,4-trichlorobenzene (TCB), triethylamine, triethanolamine, sodium lactate, sodium acetate, lactic acid, butyric acid, and sodium butyrate were obtained from Aldrich Chemical Co. (Milwaukee, WI). Sodium bicarbonate, calcium chloride, potassium chloride, ammonium chloride, sulfuric acid, sodium chloride, sodium acetate, acetic acid, hydrochloric acid, sodium hydroxide, sodium nitrate, and potassium iodide were obtained from Fisher Scientific (Fair Lawn, NJ). NASA Whole Body Shampoo, Formula #6503.45.4, was obtained from Ecolab Inc. (Mendota Hts., MN). The major constituent of NASA Whole Body Shampoo is Sodium-N-methyl-N-"coconut oil acid" taurate (SCMT). The manufacturer reports that NASA Whole Body Shampoo is 98% pure, 24% by weight SCMT, 6.4 % by weight NaCl, SCMT's molecular weight is between 357 and 360 g/gmol, and it is monovalent.

2.2 Analytical Methods

2.2.1 Total Organic Carbon (TOC)

TOC was analyzed with a Sievers Model 800 Portable TOC Analyzer (Boulder, CO). The TOC analyzer utilizes UV-persulfate oxidation. Reagents used in the analyzer include 6 M phosphoric acid and 15% ammonium persulfate. Two membrane based conductometric CO_2 sensors measure the Total Inorganic Carbon (TIC) and Total Carbon (TC) of the sample. TOC is determined by taking the difference between the TC and the TIC of the sample. The conductivity electronics are calibrated automatically within the instrument by measuring a precision resistor prior to each conductivity measurement. The increase in conductivity is proportional to the concentration of $CO_{2(aq)}$ in the sample stream. The TIC analysis was used to measure bicarbonate concentrations. In the ersatz water, the SCMT concentration was defined by the difference between the measured TOC concentration and the TOC contributions of the individual organic constituents.

The pH was determined using an Orion (Cambridge, MA) Model 501 pH meter.

2.2.2 Volatile Organic Compounds (VOCs)

VOCs were analyzed with a Hewlett-Packard (Wilmington, DE) Model 5890 II gas chromatograph using a modified EPA Method 625 liquid-liquid extraction (LLE) and a Hewlett-Packard 5970B mass selective detector. The LLE samples were extracted using 10 ml of sample solution with 10 ml of DCM. EB and PCE were used as internal standards. The conditions for these analyses are included in Table 2-1. The extracted samples containing SCMT were centrifuged for 15 minutes at 2500 rpm to remove the SCMT from the organic phase. After centrifuging, the lower organic layer was sampled and analyzed. The detection limit for each analysis is listed in Table 2-2.

2.3 Adsorbents

The 580-26 coconut-shell based granular activated carbon (GAC) was obtained from Barneby and Sutcliffe Co. (Columbus, OH). The APA bituminous-coal based GAC was obtained from the Calgon Carbon Corporation (Pittsburgh, PA). The XAD-4 polymeric adsorbent was obtained from the Rohm and Haas Company (Philadelphia, PA). The adsorbent physical properties were determined using the procedure outlined in Appendix II. The physical properties of the adsorbents studied are included in Table 2-3.

Table 2-1. Conditions for VOC Analysis.

Initial Oven Temperature: 35°C for 3 minutes
Oven Temperature Ramp Rate: 9°C per minute
Final Oven Temperature: 135°C for one minute
Injection Port Temperature: 250°C
Detector Temperature: 280°C
Detector Mode: Electron impact mode at 70 eV
Carrier Gas: Helium @ 8.5 psi head pressure
Column Dimensions: 30m x 0.25 mm x 0.25 micron
Column Type: DB1701 (14% cyanopropylphenyl)-methylpolysiloxane capillary column (J & W Scientific, Folsom CA)

Table 2-2. Analytical Detection Limits.

Compound	Analytical Detection Limit (mg/L)
Naphthalene	0.005
TCE	0.007
TOC	0.03
Toluene	0.004
1,2,4-TCB	0.01
m-Xylene	0.004

2.3.1 Adsorbent Preparation

Representative samples of adsorbents were obtained by mixing and splitting the samples of the adsorbents as received from the manufacturer. The GACs (580-26 and APA) used in column studies were rinsed with Milli-Q water to remove the fines and dried overnight at 105°C. XAD-4 resin was rinsed with Milli-Q water to remove sodium carbonate which was added to the adsorbent to inhibit biological growth in shipping until the effluent rinse water exhibited nondetectable carbonate concentrations.

Powdered granular activated carbon (PGAC), USTM No. 200x400 sieve was used in the isotherm studies. PGAC was obtained by crushing representative samples of the virgin GAC until it all passed through a USTM No. 200 sieve. The PGAC used for isotherms was the PGAC retained on a USTM No. 400 sieve and washed using the same procedure as the GAC for the column studies.

Table 2-3. Physical properties of adsorbents studied.

Adsorbent	Particle Radius[1] (cm)	Apparent Density[2] (g/ml)	Material Density[2] (g/ml)	Bulk Density[2] (g/ml)	Particle Porosity[2]
580-26 GAC	0.042	0.651	2.033	0.361	0.679
APA GAC	0.042	0.632	1.940	0.374	0.674
XAD-4 Resin	0.060	0.443	1.035	0.326	0.572

[1] Manufacturer specification

[2] Determined experimentally in this study

XAD-4 resin was used for isotherms in the uncrushed form. The XAD-4 resin used for isotherm studies was prepared using the same procedure as outlined for the column studies.

2.4 Solution Preparation

2.4.1 Ultrapure Water

Distilled-deionized water was produced by distilling tap water and further purifying it with a Milli-Q UV Plus Water System (Millipore Corp., Bedford, MA). The Milli-Q water had a background TOC concentration <0.1 mg/L.

2.4.2 Ersatz solutions

An ersatz shower and handwash wastewater containing both ionic and nonionic species, designed to mimic the adsorption potential and ionic constituents of the actual shower and handwash wastewater, was made using the recipe listed in Table 2-4. The TOC concentration of the ersatz was equal to the average TOC concentration reported for the

Table 2-4. Organic and inorganic ersatz shower/handwash water constituents.

Ionic organic and inorganic constituents (concentration in meq/L)			
Compound	**Concentration**	**Compound**	**Concentration**
Sodium	10.86	Chloride	5.86
Triethanolamine	0.09	Butyrate	0.73
Ammonium	0.37	Acetate	0.75
Calcium	0.18	Sulfate	0.46
Potassium	0.60	SCMT	2.14
		Bicarbonate	0.67
Non-ionized organic constituents (concentration in mg/L)			
TCE	246.43	1,2,4-TCB	15.00
m-xylene	15.94	naphthalene	0.53
toluene	176.35		

actual shower and handwash wastewater (see Section 3.5.2 for the development of the ersatz shower and handwash wastewater). Large quantities of the ersatz water were needed for the kinetic experiments. Therefore, saturated solutions of the individual organic compounds were prepared. These solutions were pumped into Tedlar^{TM} bags to minimize volatilization of the organics and the ionic species were injected directly into the bags.

2.5 Isotherm Experiment Procedure

A bottle point isotherm procedure was used for all adsorption isotherms (Randtke and Snoeyink, 1983; Crittenden *et al.*, 1983). The isotherm procedure is included as Appendix III. Isotherm bottles with different dosages of adsorbent were filled with the same initial aqueous phase concentration and allowed to come to equilibrium. The equilibration time for the adsorption isotherms was 10 days.

2.6 Column Study Procedure

Pilot columns were operated using the adsorbents. The column apparatus was made of teflon, glass, and stainless steel to minimize adsorption of organics by the apparatus. The glass columns were obtained from Ace Glass Co. (Vineland, NJ). All the pumps used for the pilot columns were FMI (Oyster Bay, NJ) laboratory pumps. Sampling ports were placed at the influent and effluent of each column. The complete column set-up procedure is included as Appendix IV.

2.6.1 Beds In Series Experiment Procedure

The adsorption column studies involved using four adsorption beds in series. The MFB verification column with ersatz water involved using ion exchange columns and adsorption columns in series. For beds in series operation, the effluent from one column was the influent to the next column. Sampling was performed between the columns and at the influent and effluent of the entire beds in series apparatus. The beds in series columns were all operated in the downflow mode.

3.0 Adsorption Equilibrium Modeling

3.1 Single Solute Equilibrium

Single solute isotherms were performed to determine the single solute equilibrium of the adsorbents with various compounds. Single solute isotherms were performed for NASA Ames (Hand *et al.*, In Press) on the MFB adsorbents using a variety of chemical classes. The equilibrium solid phase loading for compound i ($q_{e,i}$) for the isotherms were calculated from the equilibrium liquid phase concentrations ($C_{e,i}$) using the following mass balance on an isotherm bottle:

$$q_{e,i} = \frac{\left(C_{o,i} - C_{e,i}\right)V}{M} \tag{3-1}$$

where $C_{o,i}$ is the initial liquid phase concentration of compound i; V is the volume of the filling solution; and M is the mass of adsorbent in the isotherm bottle. The adsorbent masses placed in the isotherm bottles were small enough such that their occupied volumes could be neglected. Several expressions have previously been developed for description of single solute adsorption equilibrium (Sontheimer *et al.*, 1988). The Freundlich equation was chosen to describe single solute equilibrium for this work:

$$q_i = K_i C_i^{1/n_i} \tag{3-2}$$

in which, K_i is the Freundlich capacity constant and $1/n_i$ is the Freundlich intensity parameter for compound i.

The single solute isotherm data was fit to determine the Freundlich isotherm parameters for the different isotherms. The logarithm (base 10) of $q_{e,i}$ was fit as a function of the logarithm (base 10) of $C_{e,i}$ using least squares regression to determine the Freundlich isotherm constants K_i and $1/n_i$ for each compound. Single solute isotherm parameters were determined experimentally for many compounds on the adsorbents.

However, experimental isotherm data is still only available for a limited number of compounds.

3.2 Ideal Adsorbed Solution Theory (IAST)

When all of the compounds present in a mixture have been identified, IAST can be used to predict the multicomponent adsorption equilibria of each compound (Radke and Prausnitz 1972; Jossens *et al.* 1978; Singer and Chen-Yu 1980; Okazaki *et al.* 1980; Fritz and Schlunder 1981). Crittenden *et al.* (1985) and Luft *et al.* (1984) demonstrated that IAST could be used to predict multicomponent equilibrium for 2, 3, and 6 component mixtures. In another study, Kuennen *et al.* (1989) used IAST to describe the multicomponent equilibria for a 14 component mixture in a fixed-bed adsorber. IAST predicts multicomponent adsorption equilibrium based on the thermodynamics of adsorption using single solute isotherm parameters for the individual compounds and their respective initial concentrations. IAST development is discussed thoroughly by Radke and Prausnitz (1972) and Crittenden *et al.* (1985). If the Freundlich isotherm equation is used to represent single solute behavior, IAST yields the following equation for the equilibrium condition of each adsorbate (Crittenden *et al.*, 1985).

$$C_{e,i} = \frac{q_{e,i}}{\sum_{j=1}^{NCOMP} q_{e,j}} \left[\frac{\sum_{j=1}^{NCOMP} n_j q_{e,j}}{n_i K_i} \right]^{n_i} \qquad for\ i = 1,\ldots,NCOMP \qquad (3\text{-}3)$$

in which, NCOMP is the number of components in the system. Equation 3-3 may be combined with the isotherm bottle mass balance equation (Equation 3-1) to eliminate the liquid phase concentration, $C_{e,i}$ in IAST calculations for bottle point isotherm equilibrium as follows:

$$C_{o,i} - \frac{m}{V} q_{e,i} - \frac{q_{e,i}}{\sum_{j=1}^{NCOMP} q_{e,j}} \left[\frac{\sum_{j=1}^{NCOMP} n_j q_{e,j}}{n_i K_i} \right]^{n_i} = F_i(q_1, \ldots, q_{NCOMP}) \quad \text{for } i = 1, \ldots, NCOMP \quad (3\text{-}4)$$

As shown in Equation 3-4, given the dosage of the adsorbent, initial concentrations, and Freundlich parameters of each adsorbate the final equilibrium state may be determined by solving Equation 3-4 simultaneously for all components in the mixture. However, IAST can only be applied in this manner when all components in a mixture have been identified. In complex mixtures, such as those wastestreams generated on the ISS, complete characterization of all chemical constituents is virtually impossible. Competitive adsorption equilibrium in unknown mixtures is described in the next section.

3.3 Fictive Component Analysis (FCA) For Unknown Mixtures

A technique known as the Fictive Component Analysis (FCA) was developed to model adsorption equilibrium in mixtures of unknown composition. The FCA uses imaginary compounds (fictive components - FCs) to represent the background compounds making up the overall TOC in unknown mixtures. Hubele and Sontheimer (1983) and Frick and Sontheimer (1983) used the FCA to predict adsorption isotherms of TOC where each FC represented a portion of the total TOC and the sum of the FC TOC concentrations equaled the TOC concentration. Crittenden *et al.* (1985) used the FCA to predict the adsorption isotherms of tracer compounds using the FCA in the presence of a multicomponent background matrix made up of similar sized organic compounds. The FCs are assigned physical properties and are used in IAST calculations to model the competitive adsorption strength of the unknown mixture. The parameters that must be assigned to the FCs for multicomponent equilibrium calculations for an isotherm bottle are: (1) molecular weight, (2) percent carbon, (3) Freundlich K, (4) Freundlich 1/n, and (5) initial concentration. The molecular weight is necessary since the IAST calculations are performed on a molar basis. The percent carbon is necessary to calculate the overall TOC at equilibrium based on the TOC contribution from each individual component at equilibrium. The Freundlich K and 1/n as well as the initial concentrations are necessary for IAST calculations on the mixture.

3.3.1 FC Parameter Determination

The physical properties of the FCs, molecular weight and percent carbon, were determined from an analysis of the actual compounds reported to be in the shower and handwash wastewater in Appendix I. The molecular weight chosen for the FCs was a weighted average based on reported concentrations of the compounds identified in the shower and handwash wastewater. SCMT was omitted from the calculations since it made up over 60% of the reported TOC in the water. The molecular weight for the FCs determined from this analysis was 111 g/gmol. The same averaging procedure was applied to the compounds in Appendix I to determine the percent carbon of the FCs. The FCs were assumed to be 50% carbon by weight based on this analysis.

The Freundlich K and 1/n and the initial concentration of each FC was determined by fitting TOC and tracer isotherm data from the mixture using IAST and the FCs. TOC isotherm data was gathered by measuring the TOC concentration at each isotherm dosage. Dilute and nondilute isotherm data were fit simultaneously to obtain a more accurate description of the mixture's competitive adsorption characteristics. Nondilute isotherms were performed directly on the unknown mixture. Dilute isotherms were performed on a sample of the same unknown mixture using Milli-Q water for dilution. Tracer isotherm data was obtained by singling one known component out of the mixture and measuring its equilibrium concentration at each isotherm dosage. The percent errors in the liquid and solid phases were minimized simultaneously when fitting the isotherm data to determine the optimum FC parameters for each adsorbent.

3.3.2 TOC Isotherm Fitting

The total TOC for the TOC isotherm fitting was made up of 6 TOC FCs and a nonadsorbing TOC fraction. The TOC isotherm prediction using the FCA is based on the solution of IAST with the FCs and calculated by summing the TOC contribution of each individual TOC FC and the nonadsorbing concentration at each dosage. The molecular weight was 111 g/gmol for five of the TOC FCs and the sixth TOC FC was assigned a molecular weight of 357 g/gmol similar to SCMT. The five TOC FCs with molecular weight of 111 g/gmol were set to be 50% carbon. The TOC FC with molecular weight of 357 g/gmol was assumed to be 60% carbon, again similar to SCMT. The TOC FCs with molecular weight of 111 g/gmol all had the same 1/n value but the TOC FC similar to SCMT had a different 1/n value. Initial guesses were entered to the nonlinear least squares fitting routine for the initial concentrations of five TOC FCs. The initial concentration of the sixth FC was based on the difference between the total initial TOC and the sum of the first five FCs and the nonadsorbing TOC. IAST was solved with the TOC FCs and the output compared with the experimental isotherm data. The objective function was calculated and new guesses for the initial concentrations of the TOC FCs were made. The objective function, f_i, was set up to minimize the error in both the liquid and solid phase TOC concentrations at each isotherm dosage using the following equation:

$$f_i = \frac{1}{2}\sum_{i=1}^{N}\left[\frac{\left|C_{e,i,data} - C_{e,i,model}\right|}{C_{e,i,data}} + \frac{\left|q_{e,i,data} - q_{e,i,model}\right|}{q_{e,i,data}}\right]^2 \quad \text{for } i = 1,\ldots..N \qquad (3\text{-}5)$$

where N is the total number of isotherm points being fit. $C_{e,i}$ and $q_{e,i}$ are the equilibrium liquid and solid phase TOC concentrations in each isotherm bottle.

The set of nonlinear equations generated using IAST were solved using a Levenberg-Marquardt algorithm with a finite-difference approximation to the Jacobian obtained from the International Math and Statistics Library (IMSL, 1989). The nonlinear least squares fitting involved in the FCA was performed using a modified Levenberg-Marquardt algorithm and a finite difference Jacobian also obtained from IMSL.

3.3.3 Tracer Isotherm Fitting

The tracer isotherms were fit using 5 tracer FCs to represent the background matrix. The tracer FCs were all assigned a molecular weight of 111 g/gmol and assumed to be 50% carbon. The tracer FCs were all assumed to have the same 1/n value. Initial guesses were entered to the nonlinear least squares fitting routine for the initial concentrations of four tracer FCs. The initial concentration of the fifth tracer FC was based on the difference between the total initial TOC and the sum of the first four tracer FCs, the tracer compound TOC, and the nonadsorbing TOC. IAST calculations were made with the tracer FCs and the tracer and the output compared with the experimental tracer data. The objective function was calculated and new guesses for the initial concentrations of the FCs were made. The minimization functions were set up to minimize the error in both the liquid and solid phase using the same form as Equation 3-5 except C_e and q_e represent the liquid and solid phase concentrations of the tracer compound in this case.

Once the tracer FCs were determined, they were used in IAST calculations with other target compounds identified in the mixture to predict equilibrium of those compounds in the isotherms. The initial concentration and Freundlich K and 1/n values of the target compound of interest were input to IAST with the tracer FC parameters determined from fitting the tracer isotherms.

3.3.4 Relationship of FCs on Different Adsorbents

Since the MFBs contain different adsorbents in series, the FCs for each adsorbent were related to one another to model the unknown mixture as it passes through the different adsorbent beds. The FC Freundlich Ks on APA and XAD-4 were correlated to the 580-26 Freundlich Ks using single solute isotherm data from NASA/Ames (Hand *et al.*, In Press). The initial concentrations of the FCs for APA and XAD-4 were kept the same as those determined from fitting isotherm data for the 580-26. The APA and XAD-4 FC 1/n values were then obtained by fitting the TOC and tracer isotherm data using the same objective function as that used for fitting the 580-26 TOC and tracer isotherms. Determination of the APA and XAD-4 FCs in this manner allows modeling of beds in series operation by simply changing the K and 1/n of the FCs making up the background matrix as the water passes from one adsorbent bed to another without a change in FC concentration.

3.4 Scope of Adsorption Equilibrium Experiments

All isotherm experiments were performed using the bottle point isotherm procedure which is described in Appendix III. Solutions were prepared and analyses were performed using the procedures described in Chapter 2.

The single solute isotherm constants determined from the NASA/Ames (Hand *et al.*, In Press) work were used in this project. Single solute isotherm experiments were performed on 580-26, APA, and XAD-4 using SCMT, trichloroethylene (TCE), toluene, m-xylene, 1,2,4-trichlorobenzene (TCB), and naphthalene

Multicomponent isotherms were performed on 580-26, APA, and XAD-4 using the shower and handwash ersatz water. One isotherm was performed on each adsorbent using the ersatz water and one isotherm was performed using a sample of the ersatz water diluted approximately 50% with Milli-Q water. The isotherms were analyzed for TOC, TCE, toluene, m-xylene, 1,2,4-TCB, naphthalene, and pH. The data for these isotherms is included in Appendix V.

3.5 Adsorption Equilibrium Modeling Results

3.5.1 Single Solute Isotherms

The single solute isotherm constants used in this project are included in Table 3-1. The Freundlich isotherm equation was able to describe the 580-26 GAC and APA GAC isotherm data. The isotherm data was linear on a $\log_{10}$-$\log_{10}$ plot with some scatter due to experimental error. The Freundlich isotherm equation did not describe the isotherm data as well for the XAD-4 resin. The XAD-4 isotherm data exhibited significant curvature when plotted on a $\log_{10}$-$\log_{10}$ plot. Therefore, individual segments of the isotherm were

Table 3-1. Single solute isotherm parameters from NASA/Ames (Hand *et al.*, In Press)

	580-26			APA			XAD-4		
Compound	K[1]	1/n	Concentration (ug/L)	K[1]	1/n	Concentration (ug/L)	K[1]	1/n	Concentration (ug/L)
TCE	45.71	0.49	20-10000	31.62	0.49	30-9400	21.25	0.55	2500-8900
toluene	61.09	0.54	20-14000	61.09	0.40	4-14000	26.09	0.58	790-14000
m-xylene	138.04	0.62	10-7500	95.50	0.48	8-10000	63.57	0.52	4-15000
1,2,4-TCB	606.74	0.49	3-8000	512.90	0.44	11-11000	289.07	0.52	14-9000
naphthalene	276.50	0.47	2-4500	181.26	0.38	12-14000	73.18	0.46	14-9900
SCMT	178.46	0.17	16000-640000	184.83	0.15	16000-480000	60.86	0.29	32000-570000

[1] K units: $(mg/g)(L/mg)^{1/n}$

fit with the Freundlich isotherm equation based on the liquid-phase concentration range desired.

3.5.2 Shower and Handwash Ersatz Water Development

Excessive costs and time requirements involved with production and delivery of actual shower and handwash wastewater from NASA to MTU for experiments necessitated the development of a surrogate mixture for use in adsorption and ion exchange experiments. The mixture served as a surrogate to the actual shower and handwash wastewater for multicomponent adsorption equilibrium and kinetic studies and will be referred to as the ersatz water.

A TOC isotherm was performed on 580-26 with a sample of the actual shower and handwash wastewater to determine its TOC adsorption capacity. The results indicated that the shower and handwash wastewater was multicomponent since the isotherm showed a significant degree of curvature plotted on a log-log basis. The isotherm results also indicated that the water had a nonadsorbable TOC fraction as the TOC isotherm became nearly vertical at high adsorbent dosages signifying that little or no additional TOC was being removed as higher and higher dosages of adsorbent were added. The results of this isotherm were fit with IAST using different initial concentrations of six compounds with single solute isotherm data available such that the total TOC concentration was 320 mg/L, the same as the initial concentration of the actual shower and handwash wastewater isotherm. However, the initial TOC concentration reported to be in the actual shower and handwash wastewater was 704 mg/L based on the waste stream characterization studies included in Appendix I. Therefore, the initial TOC concentration of the ersatz mixture was increased to 704 mg/L by increasing the concentration of all the constituents on a molar basis. Major ionic species reported to be present in the actual shower and handwash wastewater were also added to the ersatz water to approximately the ionic strength reported in Appendix I. The recipe for the ersatz water was included in Table 2-3. A TOC isotherm was performed on the ersatz water with 580-26 to verify that the ersatz water TOC isotherm capacity was similar to that of the actual shower and handwash wastewater. The results of the ersatz TOC isotherm are compared to the results of the actual water TOC isotherm in Figure 3-1. Results of the

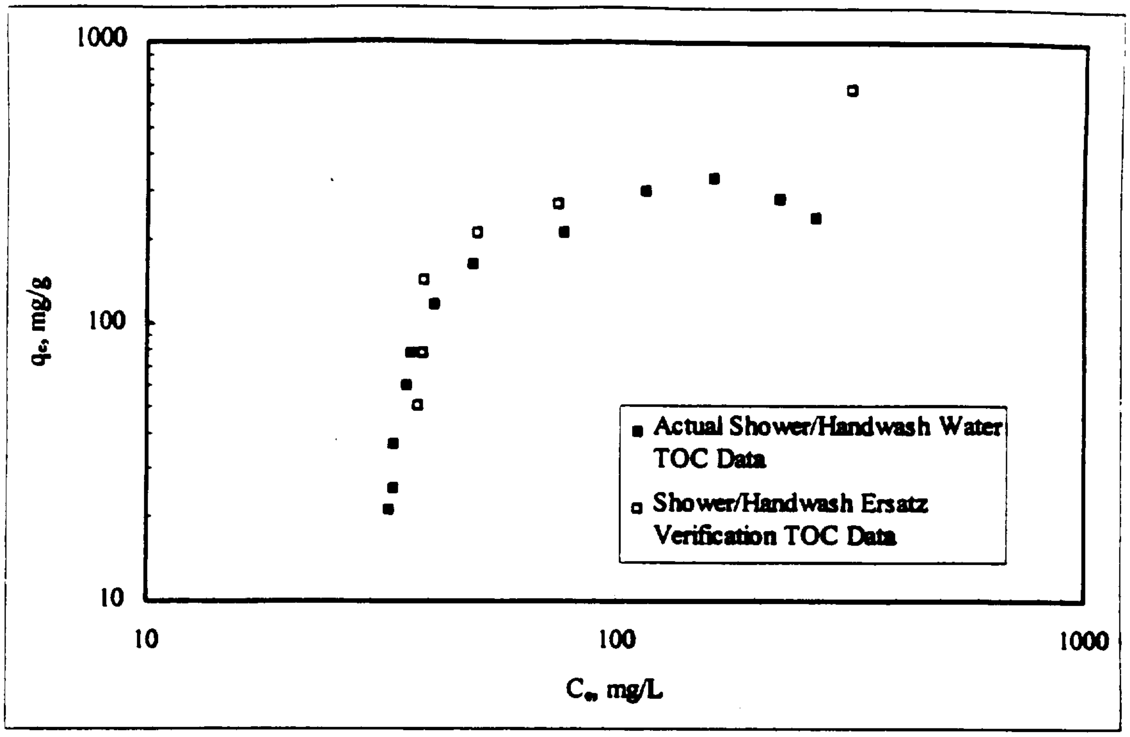

Figure 3-1. Comparison of the actual shower and handwash wastewater TOC isotherm on 580-26 to the ersatz water TOC isotherm on 580-26.

TOC isotherms indicated that the adsorption strength of the ersatz water was similar to that of the actual shower and handwash wastewater. Once verified in this manner as being a suitable surrogate for the actual water, the ersatz water was treated as an unknown mixture for modeling purposes.

3.5.3 TOC FC Results For 580-26

The TOC FCs for 580-26 were determined by fitting the dilute and nondilute TOC isotherm data obtained from the isotherms performed with the ersatz water and 580-26. The complete chemical makeup of the ersatz water used for the 580-26 ersatz isotherms is included in Table 3-2. Notice that several of the concentrations in this list are less than those in the actual ersatz recipe (Table 2-3). This is because the ersatz water had to be made up in mass quantities for column experiments. Saturated solutions of the organic compounds were used for making the ersatz water. The low solubilities of many of the compounds made it physically impossible to achieve the desired concentrations using saturated solutions to make the ersatz water. Therefore, the concentrations were made as

Table 3-2. Analyses of ersatz water used for isotherms

Compound	Initial concentration, mg/L 580-26	APA	XAD-4
TCE	145.70	153.07	154.19
toluene	86.83	85.52	85.58
m-xylene	24.86	21.63	20.30
1,2,4-TCB	1.63	1.47	2.26
naphthalene	0.333	0.279	0.36
TOC	574.3	573.4	582.0
pH	9.0	9.3	9.2

close as possible to the target levels and the water still served as a complex unknown mixture with TOC adsorption capacity similar to the actual shower and handwash wastewater. The TOC isotherm results from the ersatz water on 580-26 were fit using the FCA to determine the TOC FC parameters for the system using the fitting procedure outlined in Section 3.3.2. The TOC FC parameters determined from fitting the isotherm data are included in Table 3-3. Note that the dilute and nondilute TOC isotherms were fit simultaneously to determine the FCs. FC 1 was assigned the properties of SCMT since it was known that SCMT makes up the majority of the TOC in the shower and handwash wastewater. FCs 2 through 6 were truly FCs since they have no correspondence whatsoever to actual compounds present in the ersatz water. The K values of FCs 2 through 6 were chosen at equally spaced intervals to cover a wide range of adsorption potentials. The FCA was used to determine the initial concentrations of the FCs by fitting the TOC isotherm data.

Table 3-3. TOC FCs determined from fitting ersatz TOC isotherms

Component	Molecular Weight	Percent Carbon	580-26 GAC K	 1/n	 C_o, mg/L	APA GAC K	 1/n	 C_o, mg/L	XAD-4 Resin K	 1/n	 C_o, mg/L
TOC FC 1	357	60	200	0.15	661.76	170	0.22	676.09	85	0.26	661.76
TOC FC 2	111	50	199	0.30	57.77	169	0.28	59.02	84	0.33	57.77
TOC FC 3	111	50	230	0.30	60.28	195	0.28	61.59	95	0.33	60.28
TOC FC 4	111	50	266	0.30	65.69	224	0.28	67.11	107	0.33	65.69
TOC FC 5	111	50	307	0.30	83.25	256	0.28	85.06	118	0.33	83.25
TOC FC 6	111	50	355	0.30	0.89	291	0.28	0.91	131	0.33	0.89

* All K units: $(mg/g)(L/mg)^{1/n}$

The results of the TOC FCA fit of the 580-26 ersatz nondilute TOC isotherm are compared to the data in Figure 3-2. Included in these plots are the TOC isotherm data (solid squares) and the FCA fit (hollow squares linked with solid line). The hollow squares correspond to the same isotherm dosages as the points shown in the experimental data. The results plotted in Figure 3-2 illustrate that the TOC capacity based on the FCs in IAST calculations is close to the TOC capacity observed in the experimental isotherm. It was very difficult to get good TOC isotherm data in the low dosage (high equilibrium concentration) region for all of the ersatz isotherms. The results of the dilute isotherm fit are shown in Figure 3-3 and were described quite well using the TOC FCs. This indicates that the FCs are able to account for initial concentration changes due to dilution in the ersatz water. Table 3-4 contains a comparison of the relative percent error (RPE) in the liquid and solid phase concentrations for the dilute and nondilute TOC isotherms on 580-26 based on the fit results. RPE is defined as:

$$RPE = \frac{100}{N}\sum\left[\frac{\left|X_{experimental} - X_{model}\right|}{X_{experimental}}\right] \tag{3-6}$$

where X is C_e if the RPE in the liquid phase is being determined and q_e if RPE in the solid phase is being determined.

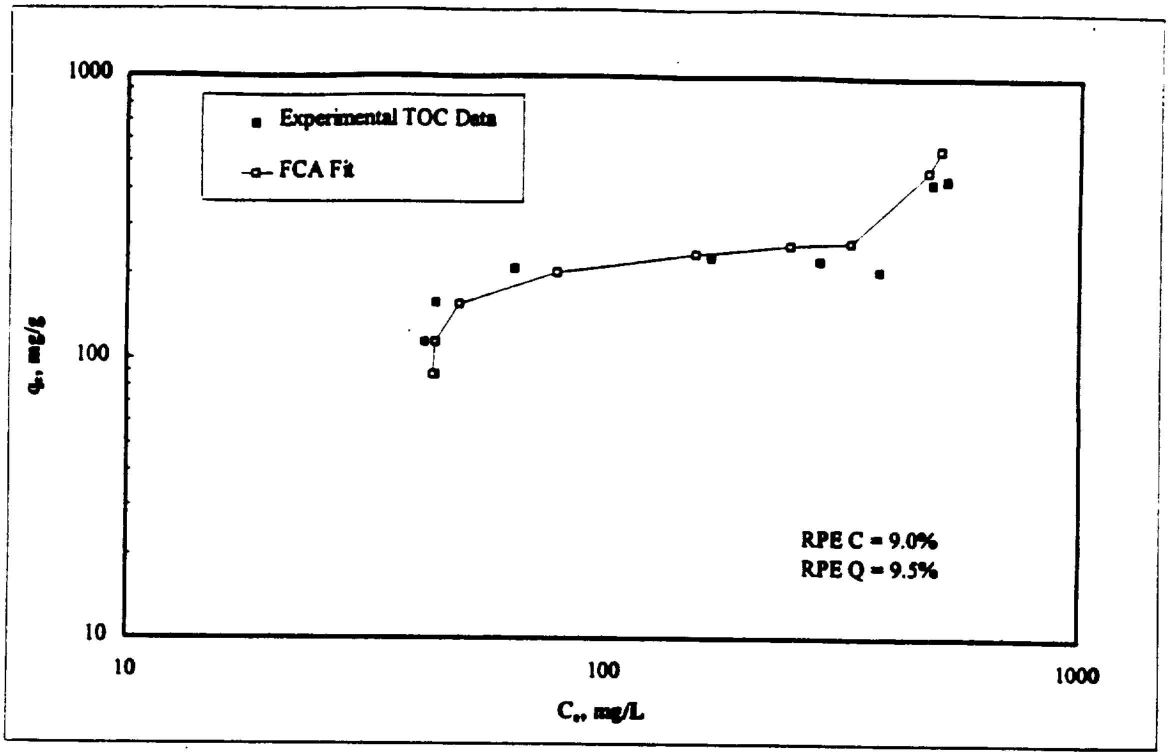

Figure 3-2. FCA fit of ersatz water TOC isotherm on 580-26. Fit simultaneously with dilute TOC isotherm.

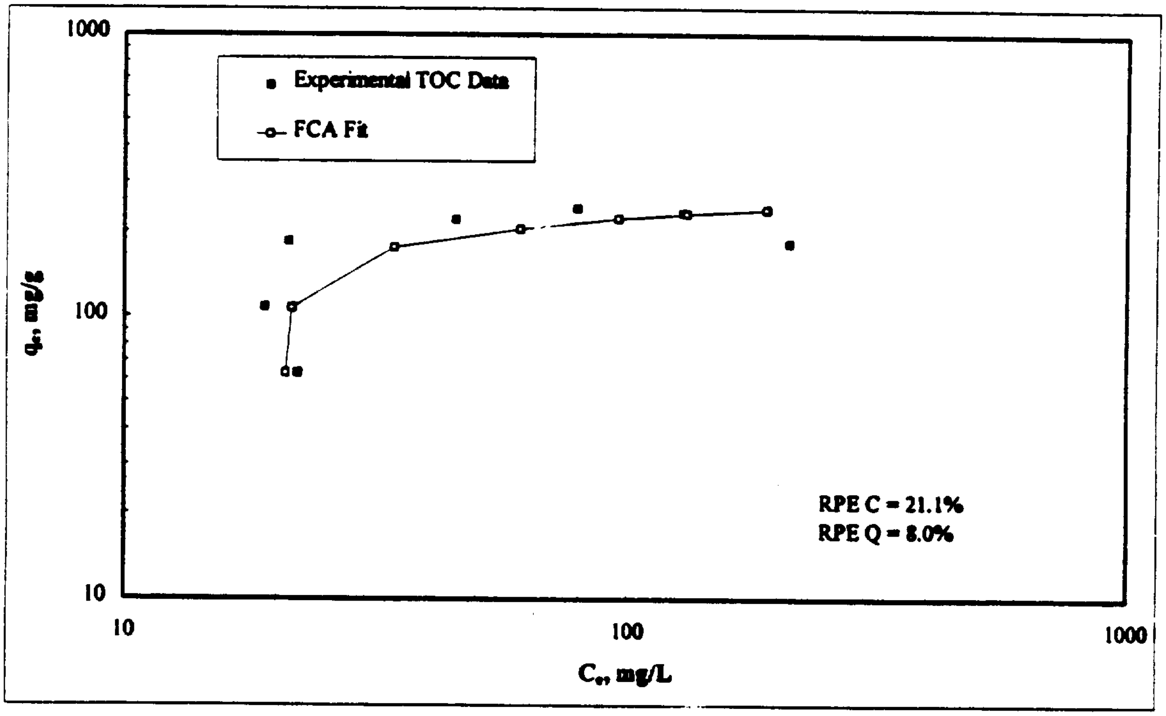

Figure 3-3. FCA fit of dilute ersatz water TOC isotherm on 580-26. Fit simultaneously with nondilute TOC isotherm.

Table 3-4. RPE of ersatz isotherm fits and predictions for 580-26

Compound	**Fit/Prediction**	**Nondilute ersatz isotherm**			**Dilute ersatz isotherm**		
		Relative % Error		**# of Data Points**	**Relative % Error**		**# of Data Points**
		C	**q**		**C**	**q**	
TOC	Fit	9.0	9.5	9	21.1	8	7
TCE	Fit	25.9	15.0	11	40	8.4	13
Toluene	Prediction	88.4	16.3	13	149.8	25.5	15
m-Xylene	Prediction	35.7	33.6	11	99.3	24.2	13
1,2,4-TCB	Prediction	68.6	11.4	8	140.1	25.5	5
Naphthalene	Prediction	336.6	44.6	8	305.6	59.3	5
SCMT	Prediction	611.0	70.6	7	255.2	83.7	5

3.5.4 TOC FC results for APA

The TOC FCs for APA were determined using the approach explained in Section 3.3.4 based on the results of the 580-26 TOC isotherm fitting. The initial concentrations of the TOC FCs were kept the same as those determined for 580-26. The FC Freundlich Ks were determined based on correlation to the TOC FCs determined for the 580-26. The correlation used to determine the K values is included as Figure 3-4. The 1/n values of the APA TOC FCs were used as the fitting parameters to fit the TOC isotherm data with the FCA

It was desired to keep the initial concentrations of the TOC FCs exactly the same for the APA as the 580-26. However, the initial TOC concentration of the ersatz water used for the APA ersatz isotherm was slightly different than that used for the 580-26 ersatz isotherm. The results of chemical analyses on the ersatz water used for the APA ersatz isotherms are included in Table 3-2. The nonadsorbing concentration was also different for the APA and 580-26 ersatz TOC isotherms. Therefore, the FC concentrations were scaled based on their TOC concentrations to the ratio of the adsorbing TOC from each of the isotherms. Since the Ks and C_0s of the APA FCs were fixed in this manner, the 1/n values were used to fit the isotherm data. The 1/n value used for FC 1 was different than that used for FC 2 through FC 6 for the same reason discussed for the 580-26 ersatz TOC FCs. The parameters for the APA TOC FCs determined from fitting the 1/n values are included in Table 3-3. The results of the TOC isotherm fits for the nondilute and dilute TOC isotherms are included in Figures 3-5 and 3-6 respectively. The results of the fits look similar to the results achieved for the 580-26 TOC isotherms. The RPE in C and q for the APA TOC isotherm fits are shown in Table 3-5. The RPEs of the isotherm fits were close to those achieved for the 580-26 TOC isotherm fits. This indicates that the fitting procedure used to accommodate beds in series using equal TOC FC C_0s is capable of fitting the equilibrium TOC isotherm for APA based on 580-26.

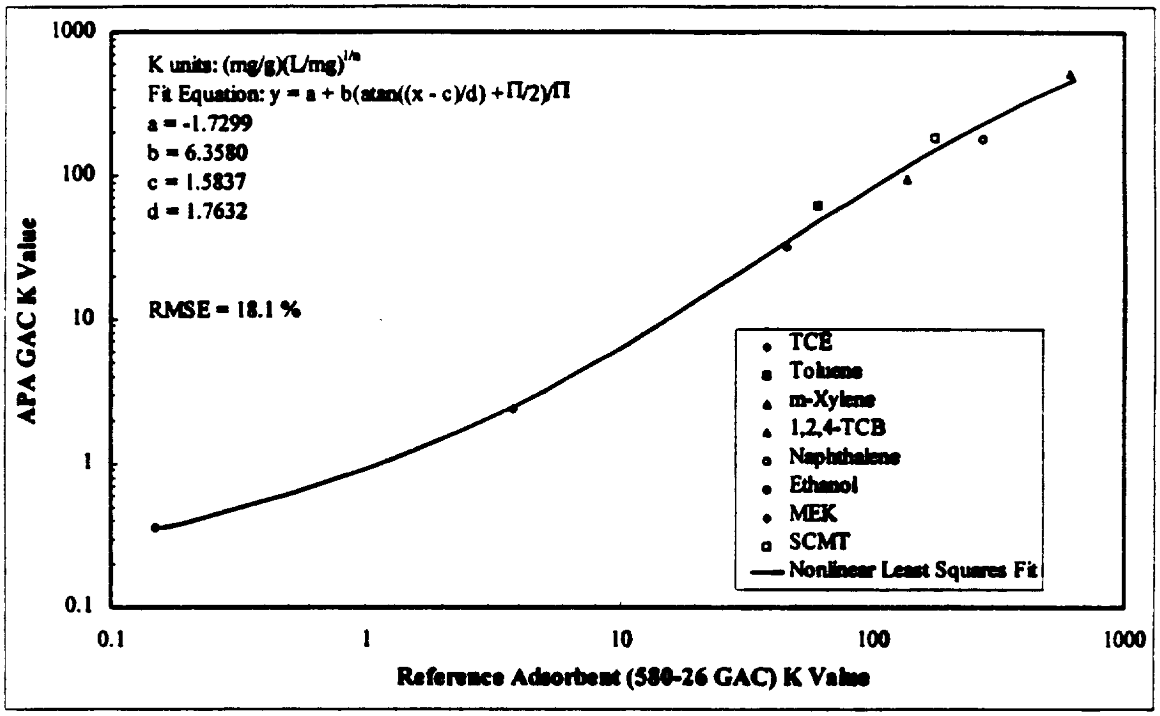

Figure 3-4. Freundlich K correlation for APA GAC referenced to 580-26 GAC.

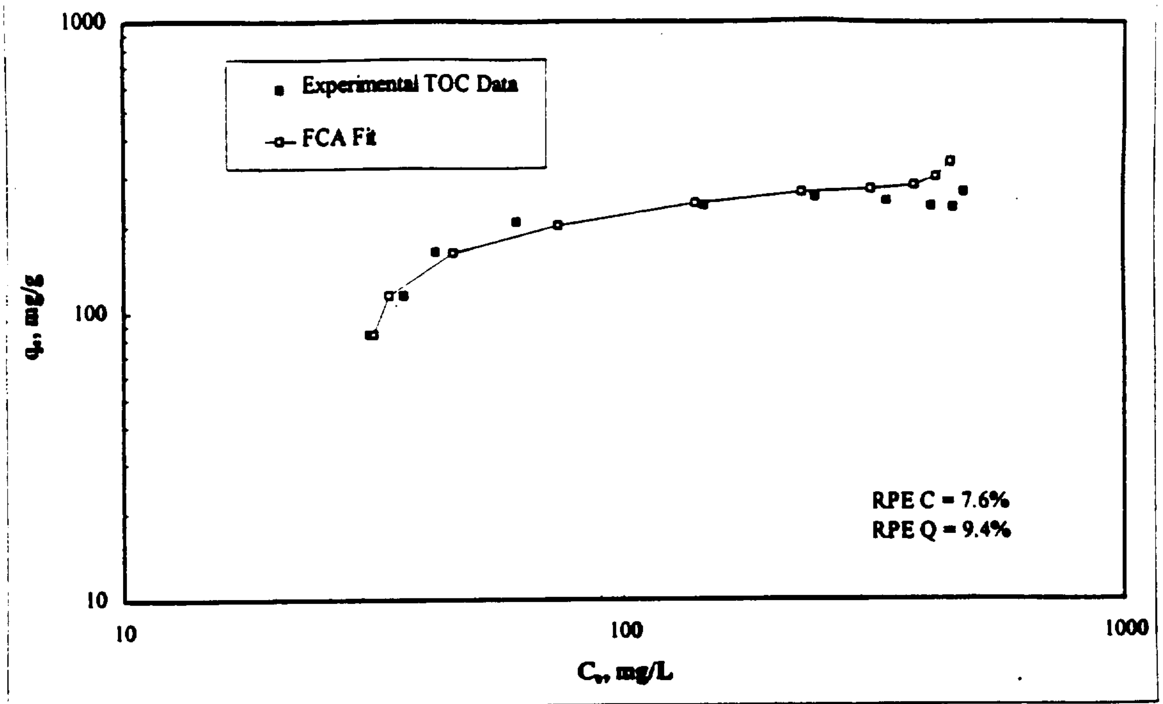

Figure 3-5. FCA fit of ersatz water TOC isotherm on APA. Fit simultaneously with dilute TOC isotherm.

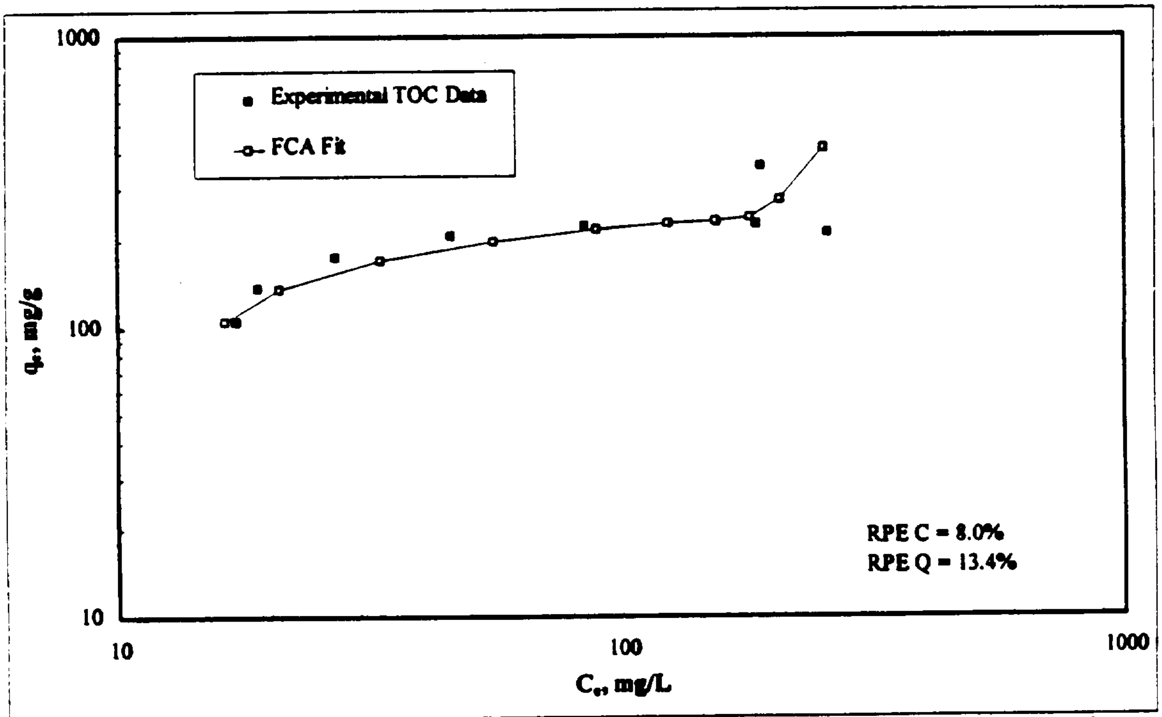

Figure 3-6. FCA fit of dilute ersatz water TOC isotherm on APA. Fit simultaneously with nondilute TOC isotherm.

Table 3-5. RPE of ersatz isotherm fits and predictions for APA

Compound	Fit/Prediction	Nondilute ersatz isotherm			Dilute ersatz isotherm		
		Relative % Error		# of Data Points	Relative % Error		# of Data Points
		C	q		C	q	
TOC	Fit	7.6	9.4	10	8	13.4	10
TCE	Fit	17.7	16.3	8	23.2	9.7	9
Toluene	Prediction	24.1	11.1	11	26.8	12.7	13
m-Xylene	Prediction	109.5	5.2	12	110.3	17.7	15
1,2,4-TCB	Prediction	73.8	20.9	9	106.1	31.1	5
Naphthalene	Prediction	479.1	72.4	8	265.6	90.5	4
SCMT	Prediction	380.5	60.3	9	137.6	81.7	7

3.5.5 TOC FC results for XAD-4 resin

XAD-4 ersatz water TOC isotherms were fit using the same methods as were used for the APA ersatz isotherm fitting. The chemical makeup of the ersatz water used for the XAD-4 isotherms is presented in Table 3-2. The ersatz TOC concentration and the nonadsorbing concentration were again different from that used in the 580-26 ersatz isotherm so the same scaling procedure was used as that for the APA ersatz FC C_0s. The XAD-4 TOC FC Freundlich K values were determined from correlation included as Figure 3-7. The TOC FC 1/ns were then used to fit the TOC isotherm data. The TOC FC properties are included in Table 3-3. The results of the fits are compared to the data for the nondilute and dilute isotherms in Figures 3-8 and 3-9 respectively. The RPEs of the XAD-4 ersatz TOC isotherm fits are included in Table 3-6. The results of these fits were much better than those for the 580-26 and APA based on the RPEs in both the solid and liquid phase concentrations.

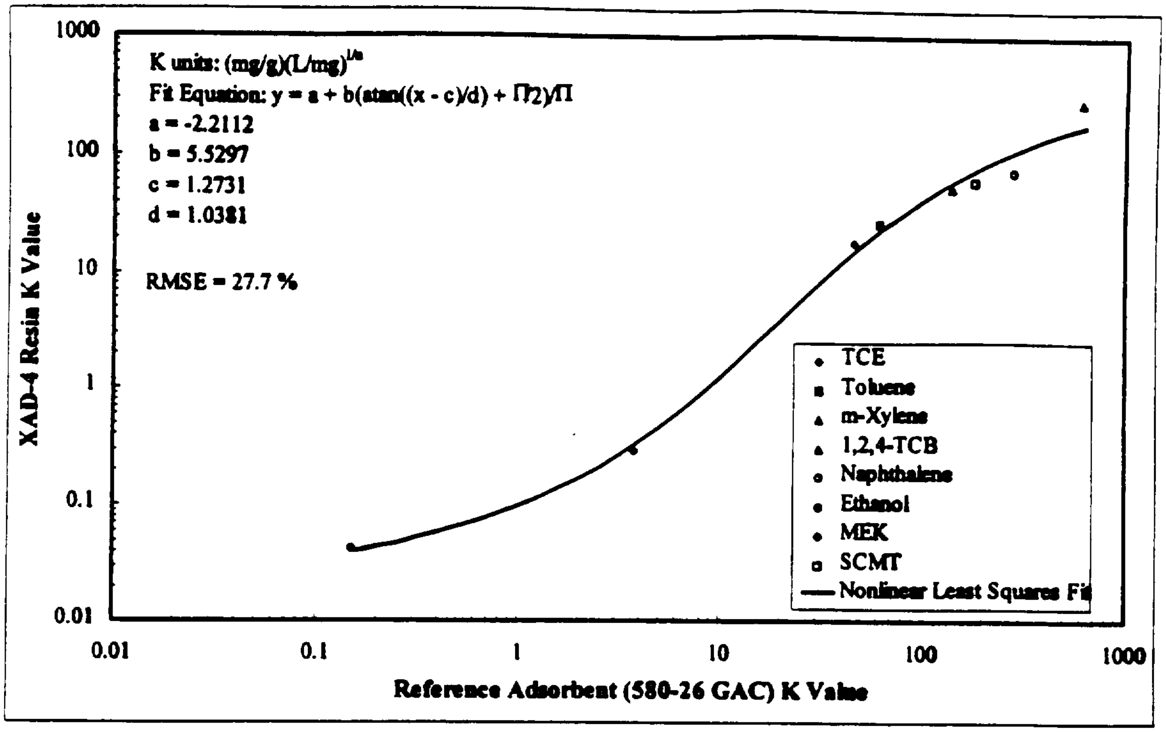

Figure 3-7. Freundlich K correlation for XAD-4 resin referenced to 580-26 GAC.

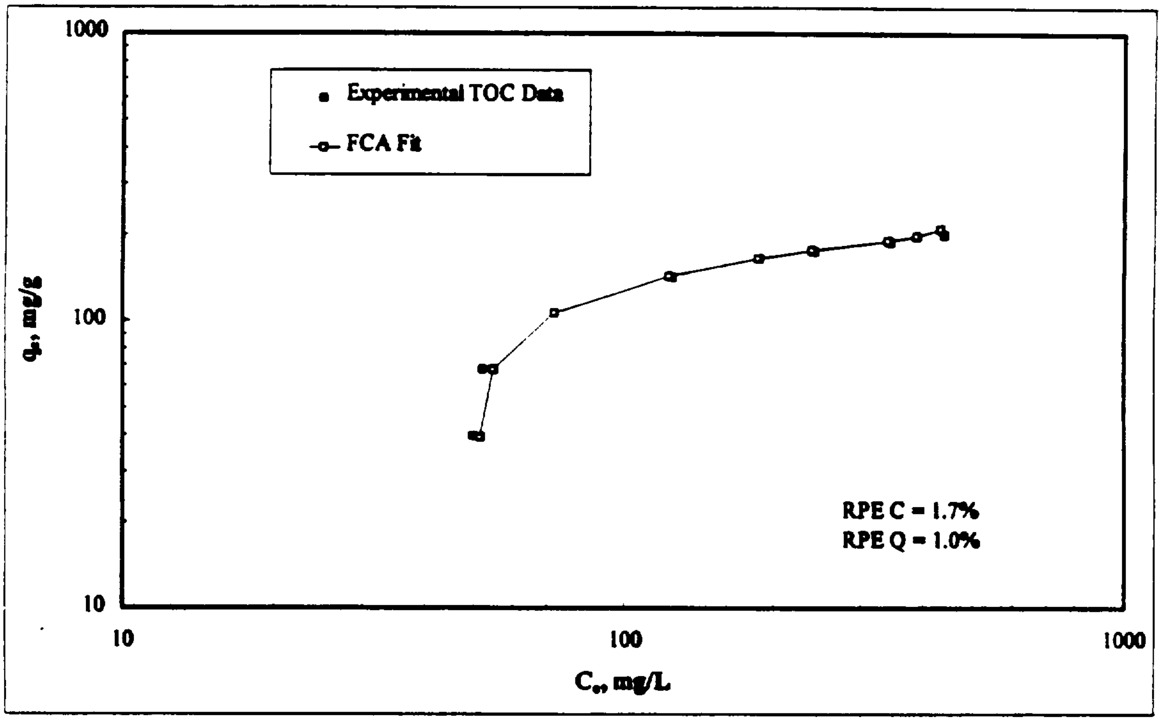

Figure 3-8. FCA fit of ersatz water TOC isotherm on XAD-4. Fit simultaneously with dilute TOC isotherm.

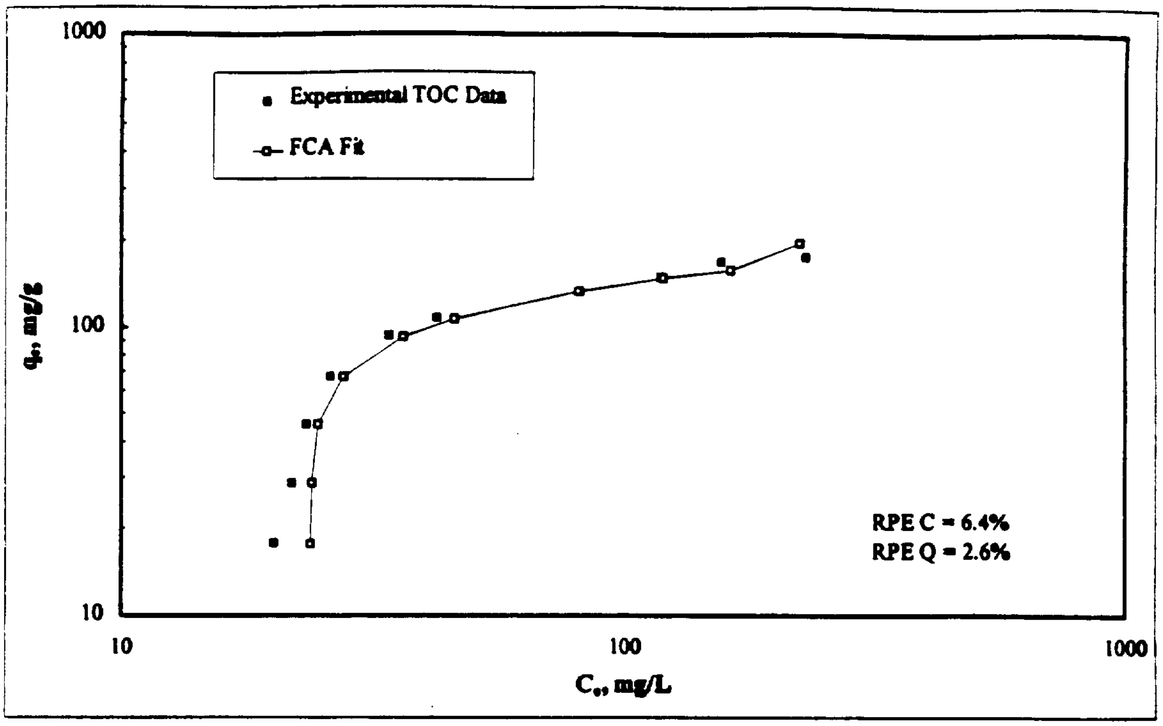

Figure 3-9. FCA fit of dilute ersatz water TOC isotherm on XAD-4. Fit simultaneously with nondilute TOC isotherm.

Table 3-6. RPE of ersatz isotherm fits and predictions for XAD-4

Compound	Fit/Prediction	Nondilute ersatz isotherm Relative % Error C	Nondilute ersatz isotherm Relative % Error q	Nondilute ersatz isotherm # of Data Points	Dilute ersatz isotherm Relative % Error C	Dilute ersatz isotherm Relative % Error q	Dilute ersatz isotherm # of Data Points
TOC	Fit	1.7	1.0	9	6.4	2.6	10
TCE	Fit	5.1	4.7	11	4.4	2.8	11
Toluene	Prediction	19.7	6.1	11	18.4	4.7	12
m-Xylene	Prediction	11.6	16.3	13	11.4	13.2	15
1,2,4-TCB	Prediction	10.5	9.5	9	14.1	12.8	7
Naphthalene	Prediction	63.3	47.4	8	56.2	62.3	6
SCMT	Prediction	93.8	65.6	9	236	61.2	12

3.5.6 Tracer FC Results For 580-26

The 580-26 dilute and nondilute ersatz tracer isotherms were fit simultaneously to determine the tracer FCs for the ersatz water on 580-26. The same isotherm was used to obtain the tracer isotherm data and the TOC isotherm data. TCE was simply singled out of the dilute and nondilute ersatz isotherms as the tracer compound for fitting purposes since it is weakly adsorbed.

Tracer FC K values were chosen at equally spaced intervals to cover the broad spectrum of adsorption potentials observed for the wastewaters aboard the ISS. Tracer isotherm fitting revealed that the same 1/n value could be used for each FC to fit the tracer isotherm data. The tracer FC parameters determined from fitting the isotherm data are included in Table 3-7. The tracer isotherm fits and data are compared for the nondilute and dilute ersatz isotherms on 580-26 in Figures 3-10 and 3-11 respectively. Included in these plots are the data (solid squares), FCA fit (hollow squares linked with solid line), and the single solute isotherm (dashed line). The hollow squares correspond to the same dosages as the points shown in the experimental data. The single solute isotherm is included to illustrate how well the FCA predicts the reduction in capacity from the single solute level due to the competitive adsorption. Note that the scales of the isotherm plots vary based on the concentration range observed in the experiments. The fits follow the data more closely at the low dosages (high liquid phase concentrations). This is a trend that will follow in other tracer isotherm fits and predictions in this report. This can be explained by looking at the mass balance on an isotherm bottle (Equation 3-1). As the mass of adsorbent in the bottle increases and nearly all of the adsorbate is on the surface of the adsorbent, a small error in the solid phase concentration can cause a large error in the liquid phase concentration. However, Figures 3-10 and 3-11 indicate that using the fitted tracer FCs in equilibrium calculations adequately describes the TCE equilibrium capacity in the ersatz water on 580-26.

Since the other compounds making up the ersatz water were known, the tracer

Table 3-7. Tracer FCs determined from fitting ersatz tracer isotherms

	Molecular	Percent	580-26 GAC			APA GAC			XAD-4 Resin		
Component	Weight	Carbon	K	1/n	C_o, mg/L	K	1/n	C_o, mg/L	K	1/n	C_o, mg/L
Tracer FC 1	111	50	63	0.35	221.72	50	0.44	226.18	24	0.59	225.48
Tracer FC 2	111	50	97	0.35	19.11	80	0.44	19.5	41	0.59	19.44
Tracer FC 3	111	50	150	0.35	14.71	127	0.44	15.01	65	0.59	14.96
Tracer FC 4	111	50	231	0.35	40.67	196	0.44	41.49	95	0.59	41.36
Tracer FC 5	111	50	355	0.35	668.17	291	0.44	681.62	131	0.59	679.53

* All K units: $(mg/g)(L/mg)^{1/n}$

FCs were used in IAST calculations to determine if the tracer FCs could predict equilibrium for compounds in the mixture other than the tracer. The RPEs of the predictions for each known compound in the 580-26 ersatz dilute and nondilute isotherms are shown in Table 3-4. The results for the prediction of toluene equilibrium in the presence of the tracer FCs for the nondilute and dilute ersatz isotherms are shown in Figures 3-12 and 3-13. The toluene predictions agree quite well with the data at the low dosages but stray farther from the data at the high dosages. This may be explained due to mass balance as indicated earlier. The predictions of *m*-xylene in the presence of the nondilute and dilute ersatz isotherms are included in Figures 3-14 and 3-15. The equilibrium calculations for *m*-xylene predicted a higher capacity than was achieved in the isotherm experiments at low dosages. However, relative to the single solute equilibrium, the reduction in capacity due to competitive adsorption was predicted reasonably well. The predictions for 1,2,4-TCB are shown in Figures 3-16 and 3-17. The FCs overpredict the reduction in capacity for 1,2,4-TCB at all isotherm points. This is likely since a weakly adsorbing compound was used for fitting for the FC parameters, and the strongly adsorbing compounds are already accounted for by the FCs. However, the capacity reduction predicted for the 1,2,4-TCB was larger than the experimental capacity reduction so the model prediction is conservative with respect to equilibrium capacity calculations. The predictions for naphthalene in the ersatz isotherm are included as Figures 3-18 and 3-19. The reduction in capacity for naphthalene is greatly overpredicted by the tracer FCs. This is probably due to the same reasons as the 1,2,4-TCB capacity overprediction. The predictions for SCMT in the ersatz isotherms are included in Figures 3-20 and 3-21. The reduction in capacity for SCMT is greatly overpredicted by the tracer FCs. This may be explained due to the high concentration of SCMT in the mixture. Crittenden *et al.* (1985) reported that a predicted component must be a small part of the adsorption strength of the mixture, because its adsorption potential is already accounted for by the FC parameters. If this condition is not met, the prediction would yield a lower capacity than that of the isotherm. SCMT makes up over half of the total TOC in the ersatz water. Therefore, it would be expected that the tracer FCs would overpredict the capacity reduction for SCMT.

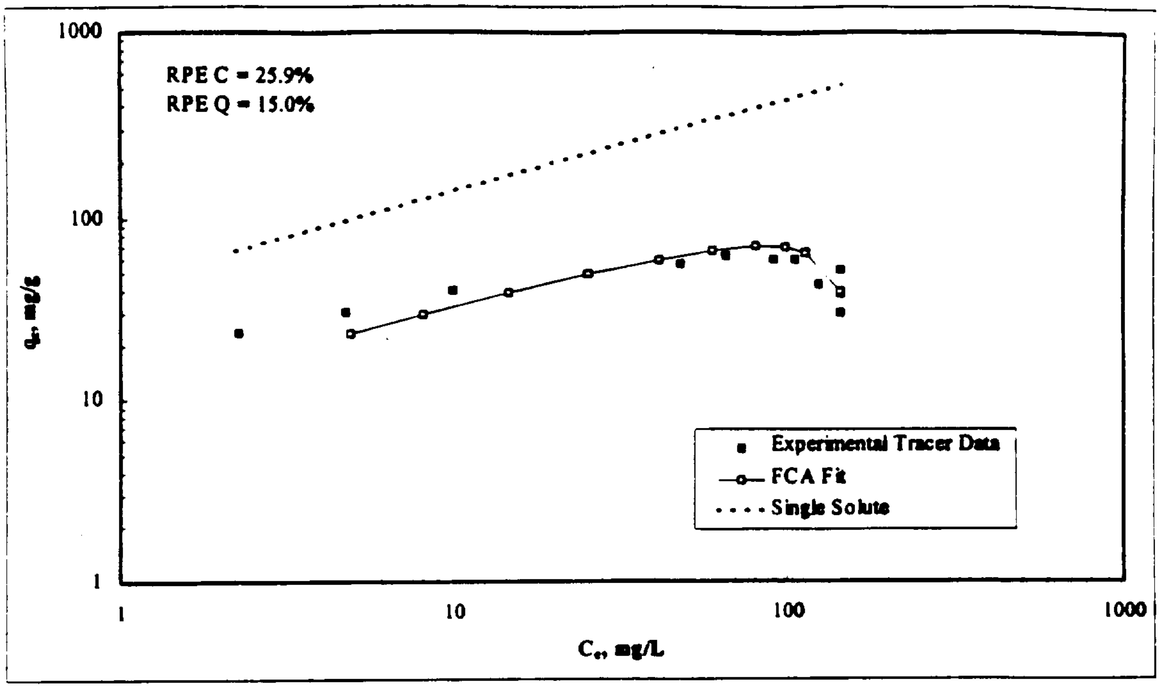

Figure 3-10. FCA fit of ersatz water tracer (TCE) isotherm on 580-26. Fit simultaneously with dilute tracer isotherm.

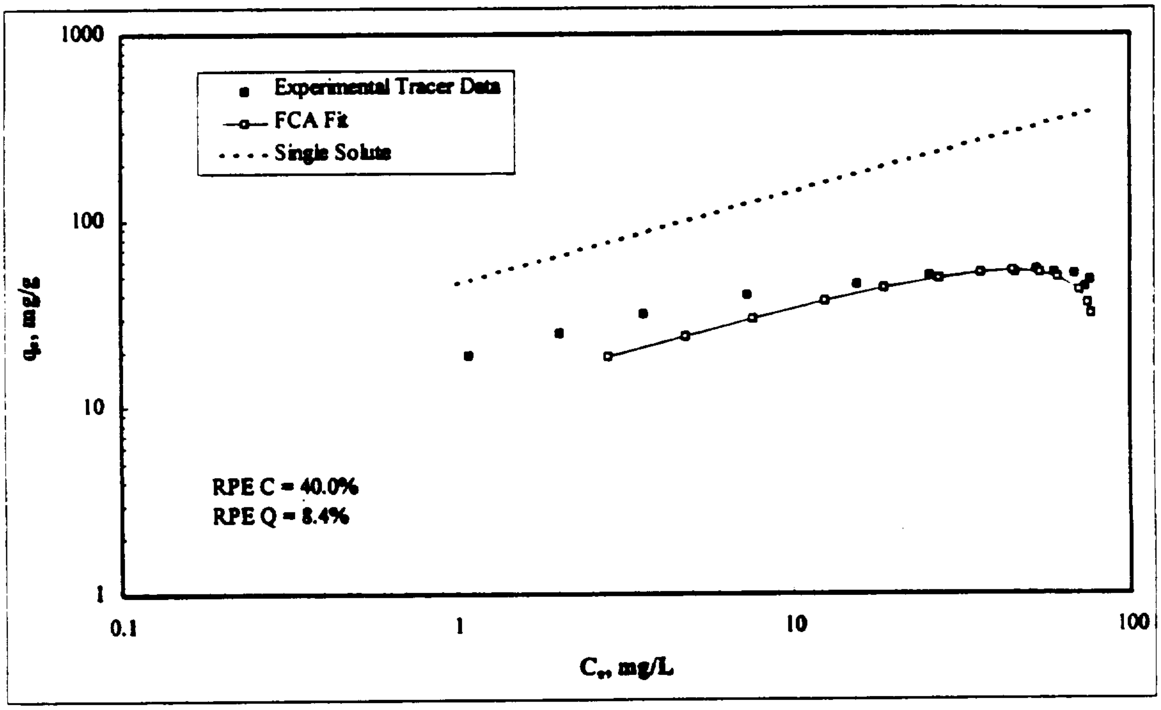

Figure 3-11. FCA fit of dilute ersatz water tracer (TCE) isotherm on 580-26. Fit simultaneously with nondilute tracer isotherm.

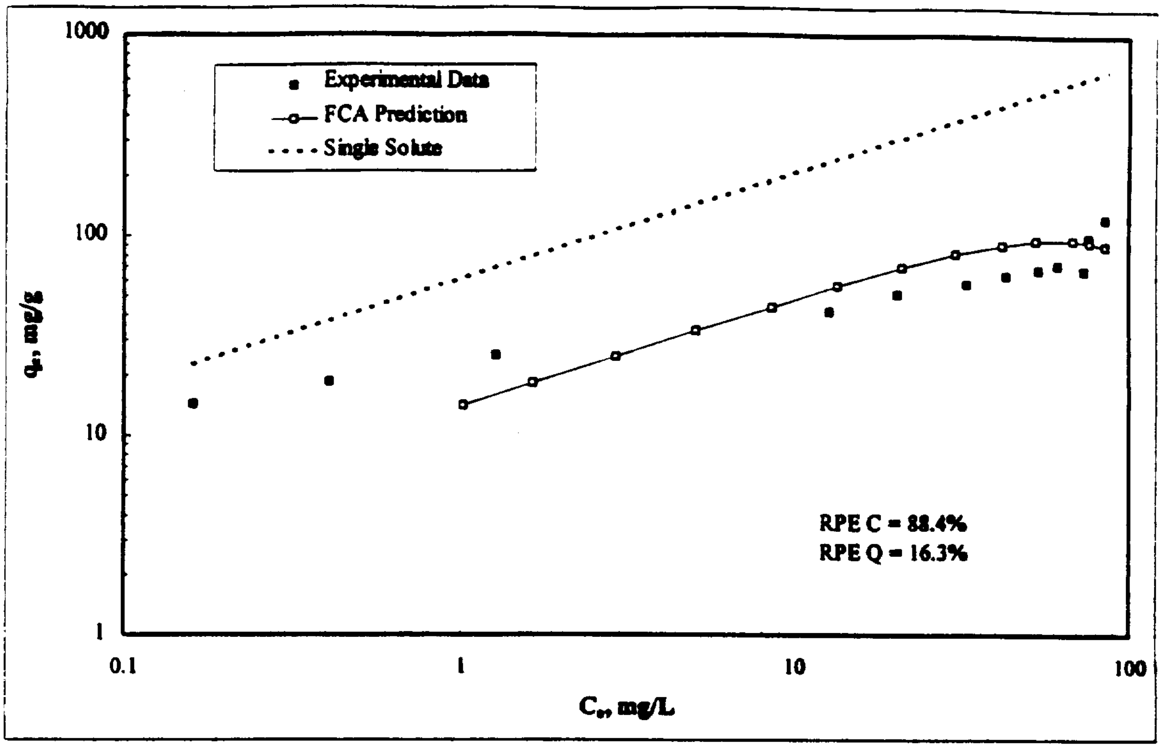

Figure 3-12. FCA prediction of toluene isotherm in ersatz water on 580-26.

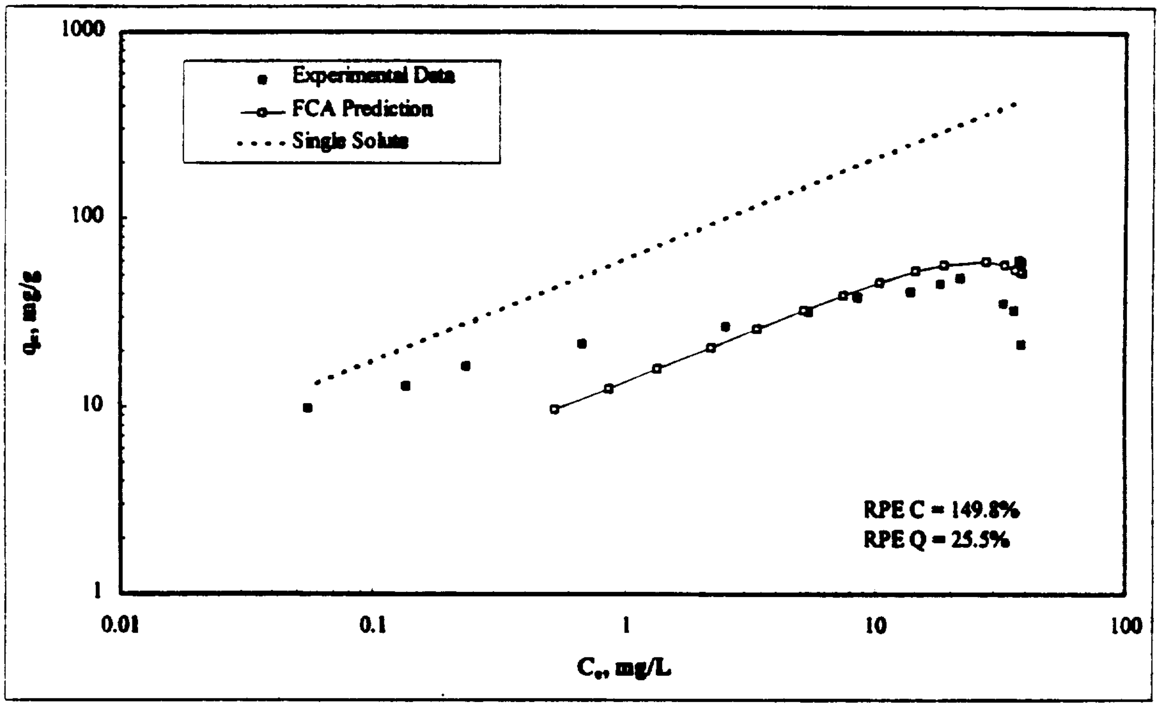

Figure 3-13. FCA prediction of toluene isotherm in dilute ersatz water on 580-26.

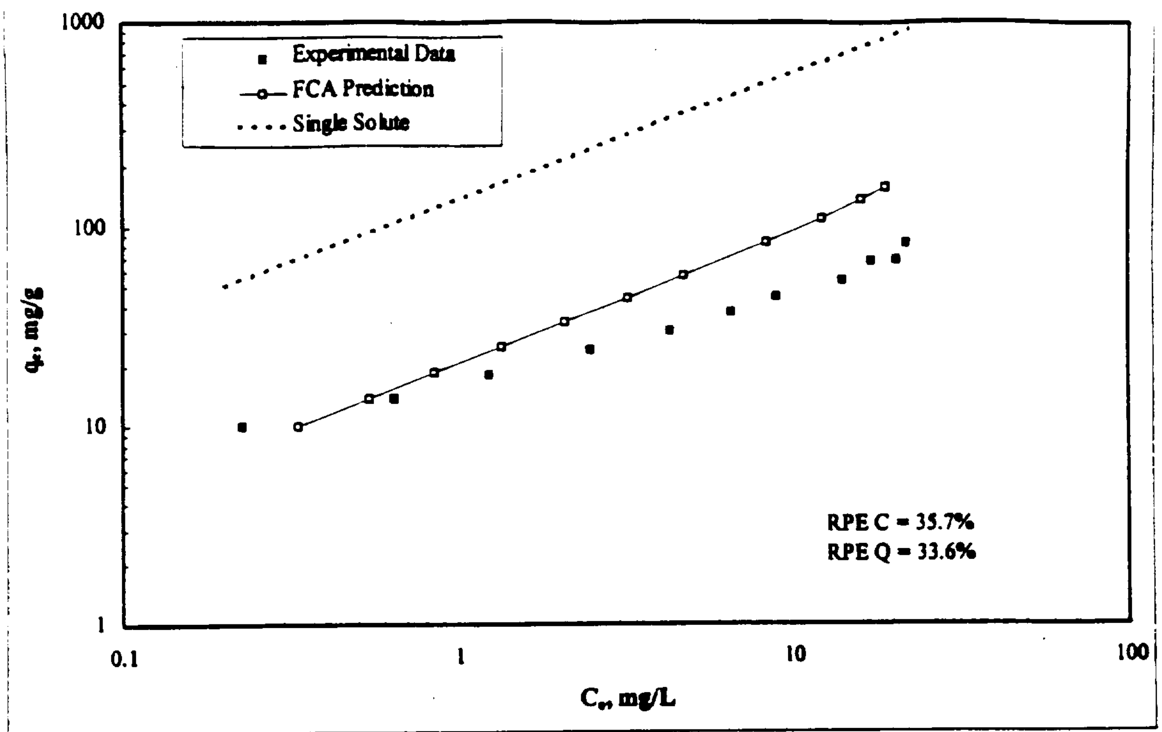

Figure 3-14. FCA prediction of m-xylene isotherm in ersatz water on 580-26.

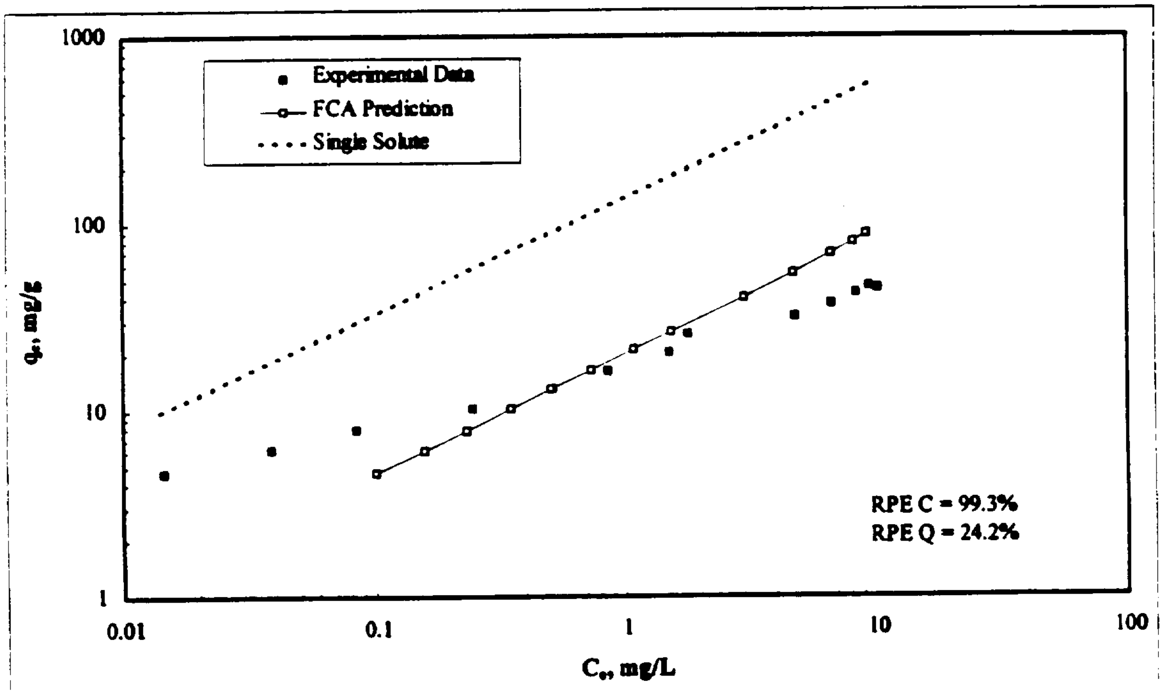

Figure 3-15. FCA prediction of m-xylene isotherm in dilute ersatz water on 580-26.

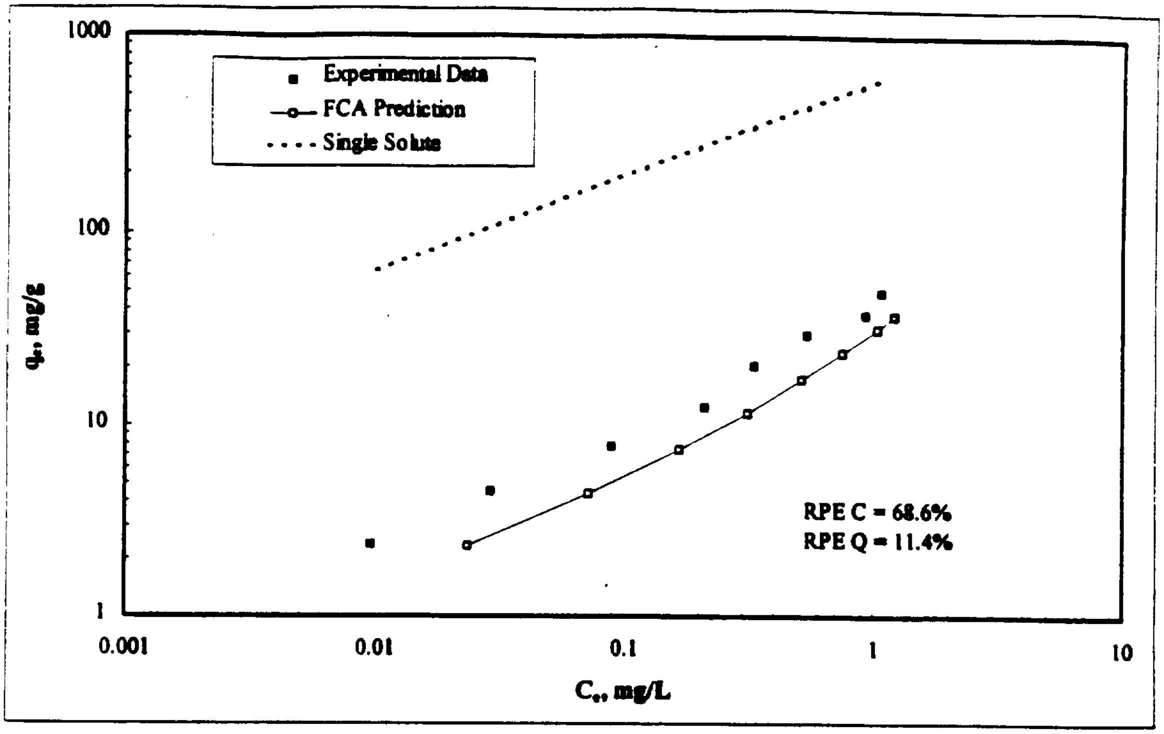

Figure 3-16. FCA prediction of 1,2,4-TCB isotherm in ersatz water on 580-26.

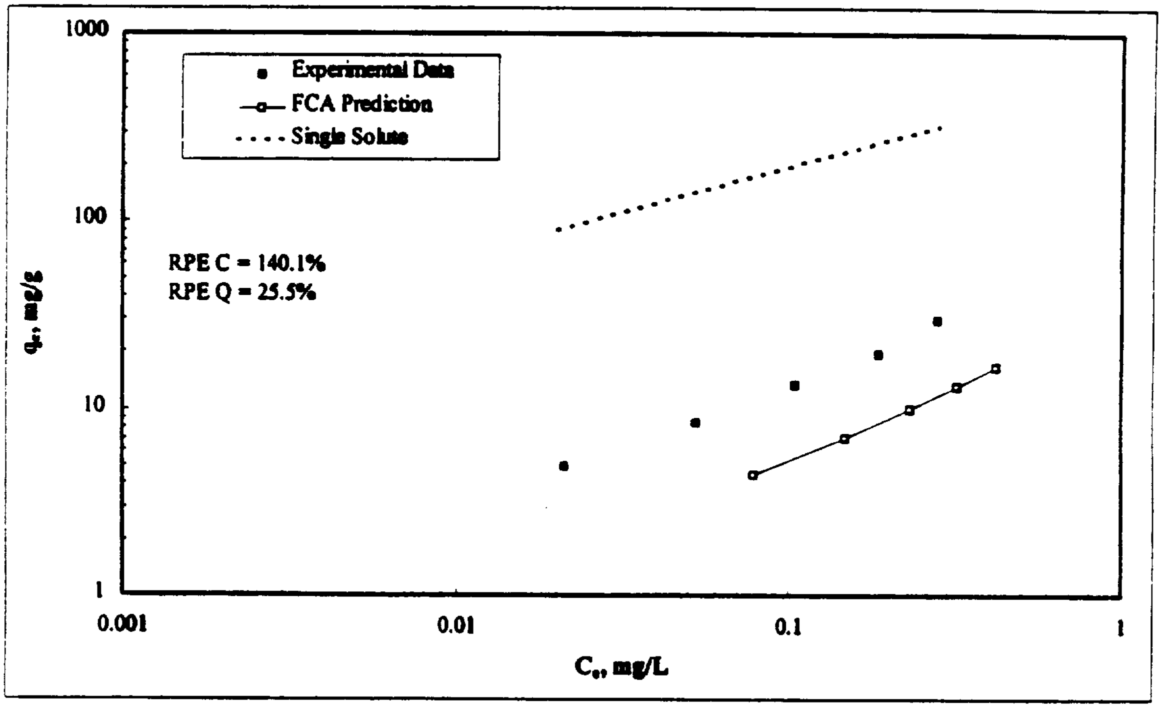

Figure 3-17. FCA prediction of 1,2,4-TCB isotherm in dilute ersatz water on 580-26.

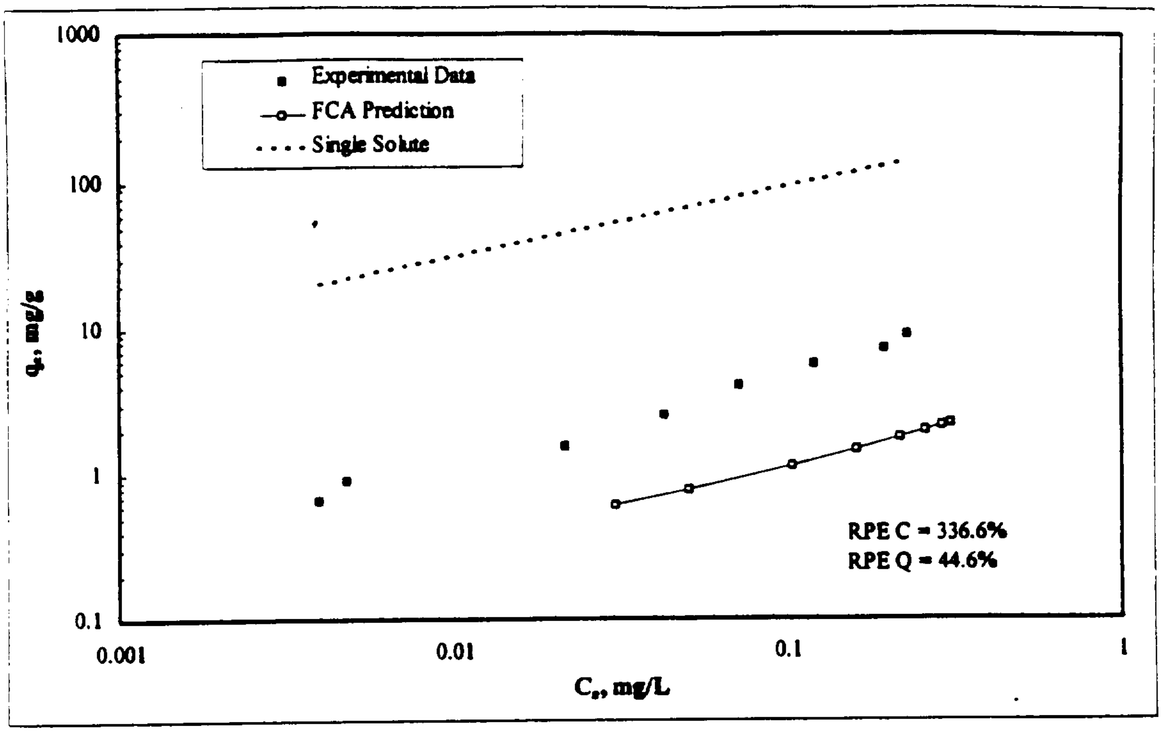

Figure 3-18. FCA prediction of naphthalene isotherm in ersatz water on 580-26.

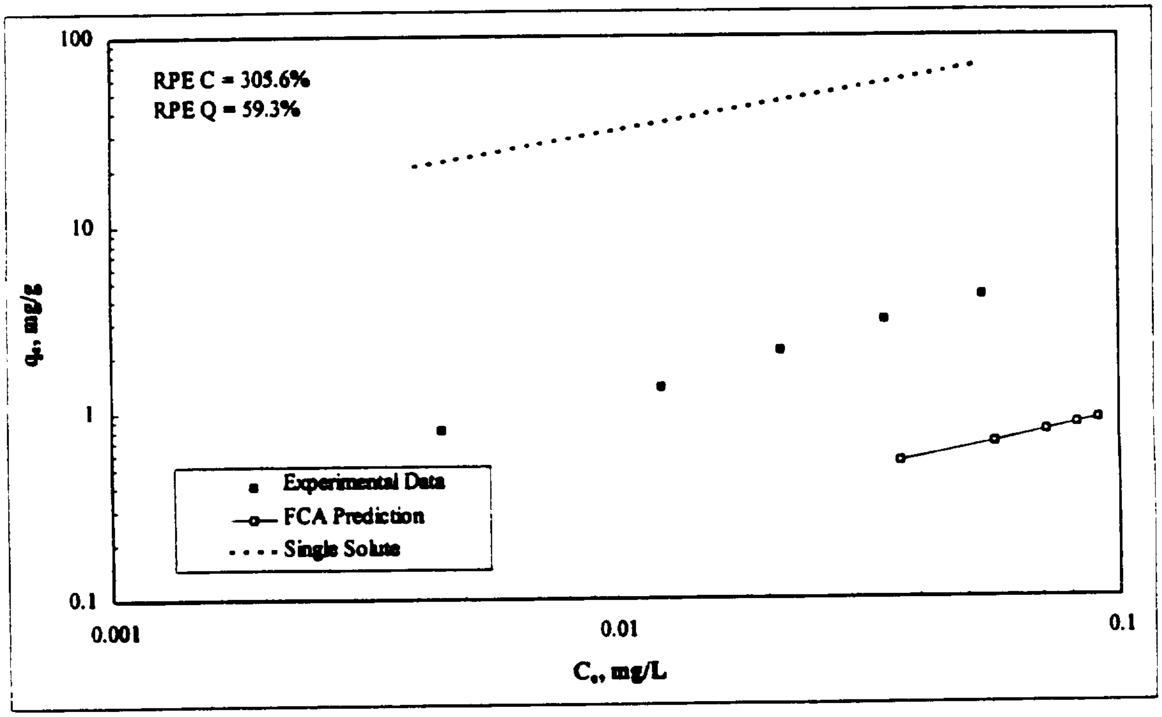

Figure 3-19. FCA prediction of naphthalene isotherm in dilute ersatz water on 580-26.

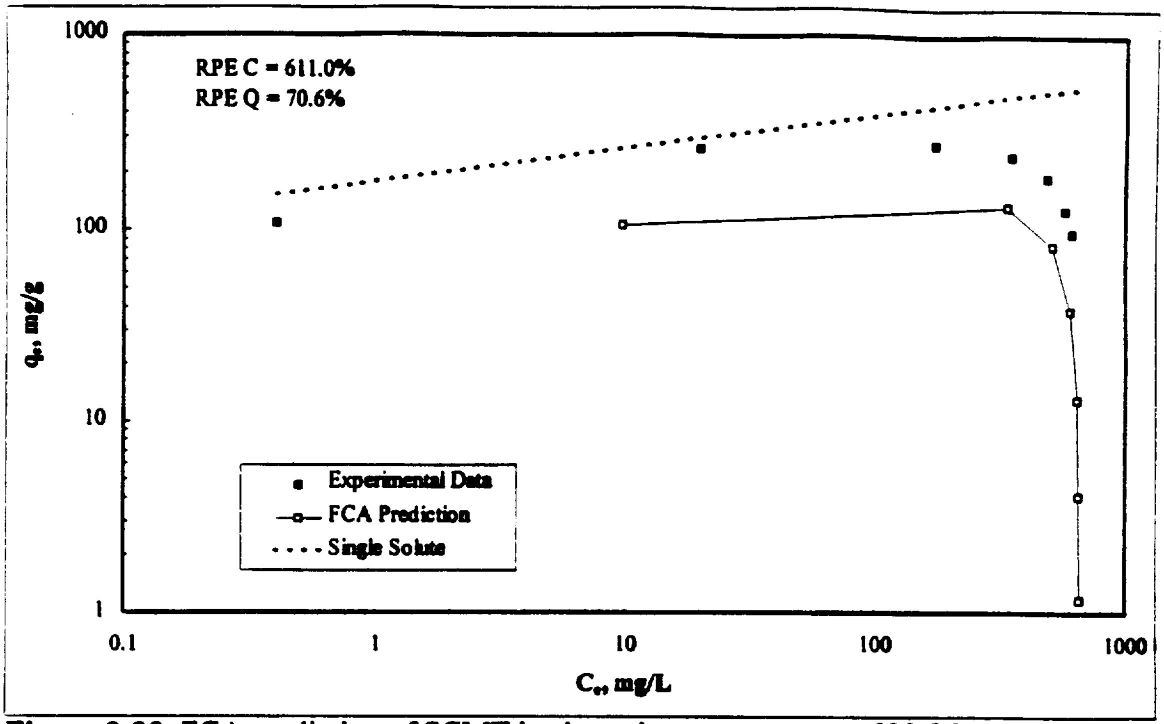

Figure 3-20. FCA prediction of SCMT isotherm in ersatz water on 580-26.

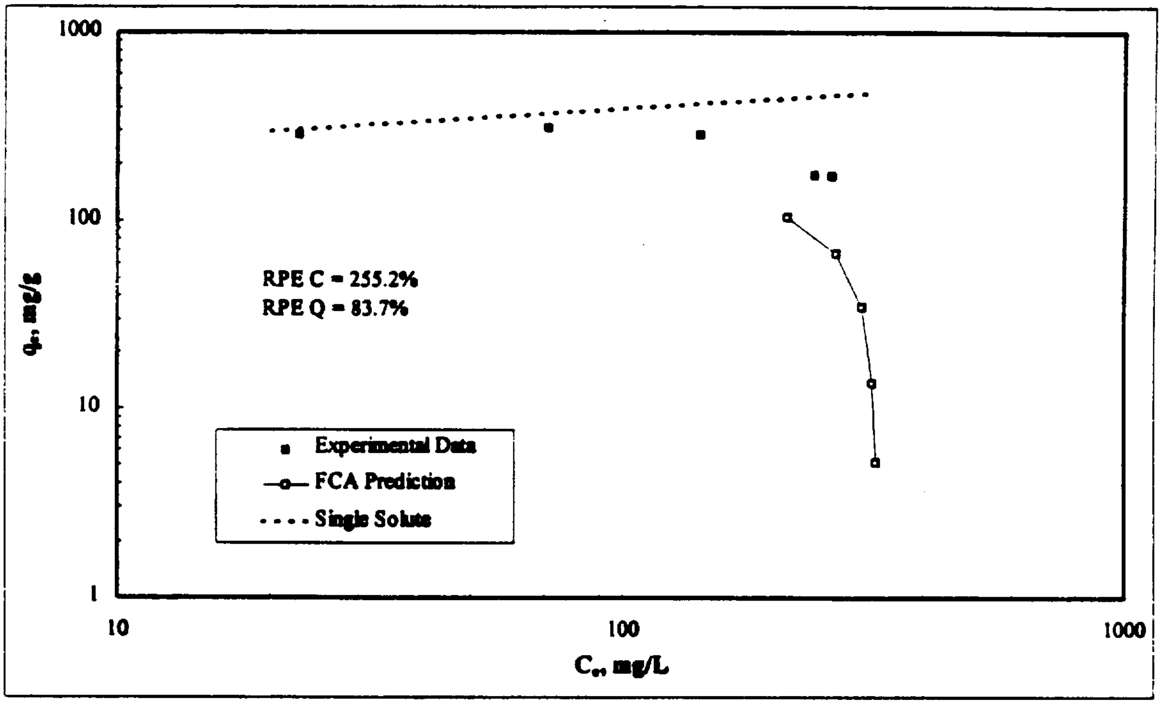

Figure 3-21. FCA prediction of SCMT isotherm in dilute ersatz water on 580-26.

3.5.7 Tracer FC Results For APA

The tracer FCs for APA were determined relative to the 580-26 tracer FCs in similar fashion as the TOC FCs. The tracer FC Freundlich K values were determined based on the 580-26 tracer FC Freundlich K values using the correlation in Figure 3-4. The initial concentrations of the APA tracer FCs were kept nearly equal to the initial concentrations determined for the 580-26 tracer FCs to facilitate beds in series modeling. The APA tracer FC initial concentrations were scaled to account for differences in initial TOC, tracer, and nonadsorbing concentrations between the 580-26 and APA ersatz isotherms on a TOC concentration basis. The tracer (TCE) isotherms (dilute and nondilute) on APA in the ersatz water were fit simultaneously to determine the 1/n value to be used for the FCs. The APA ersatz tracer FC parameters are included in Table 3-7. The nondilute and dilute tracer isotherm fits are shown in Figures 3-22 and 3-23 respectively. The results of the fit indicate that the tracer FCs determined for the APA can describe the reduction in capacity for TCE in the ersatz water. The RPEs for each fit and prediction for the APA ersatz isotherm are included in Table 3-5. Once the tracer FC parameters were identified for the APA by fitting the tracer isotherms, the isotherms of the other compounds in the ersatz water were predicted to test if the tracer FCs could predict the reduction in capacity for compounds in the ersatz other than the tracer. The results for toluene in Figures 3-24 and 3-25 illustrate that the tracer FCs can predict the equilibrium for toluene quite well. The error in the liquid phase concentration at high dosages is due to the mass balance as discussed previously. The results for *m*-xylene are shown in Figures 3-26 and 3-27. The tracer FCs predict the reduction in capacity well at the low dosages but the error in liquid phase concentrations at high dosages also becomes large in this case due to the mass balance. For example, at the highest isotherm dosage predicted, a 0.3% error in solid phase concentration causes a 596.8% error in the liquid phase concentration. The results for 1,2,4-TCB are shown in Figures 3-28 and 3-29. The results are similar to those obtained for the 580-26. The reduction in capacity due to the ersatz is overpredicted by the tracer FCs in IAST calculations. Figures 3-30 and 3-31 display the results for naphthalene and illustrate the same phenomenon. These results are found due to the same reasons explained for the 580-26 1,2,4-TCB and naphthalene isotherm predictions. Figures 3-32 and 3-33 contain the results of the SCMT prediction in the ersatz water. The results are also similar to those found for the SCMT prediction on 580-26 as the capacity for SCMT is underpredicted by the model. This may be explained due to the same reasons as it was for the 580-26 as the large amount of TOC attributable to SCMT was already accounted for by the FCs.

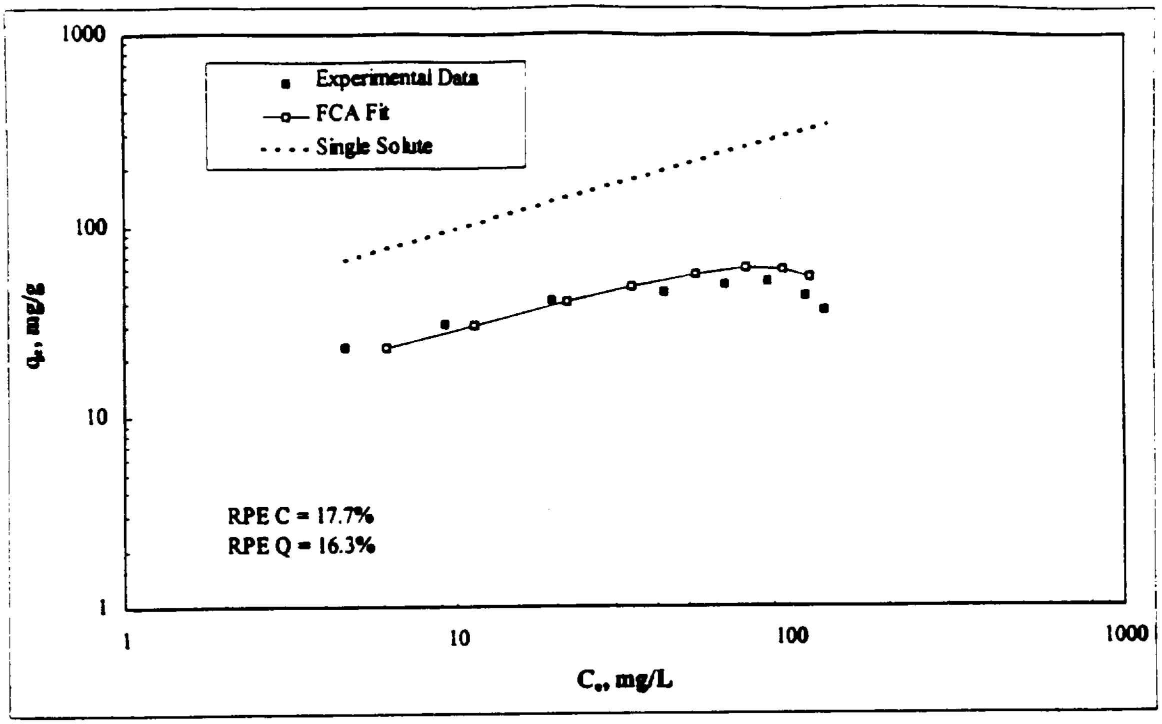

Figure 3-22. FCA fit of ersatz water tracer (TCE) isotherm on APA. Fit simultaneously with dilute tracer isotherm.

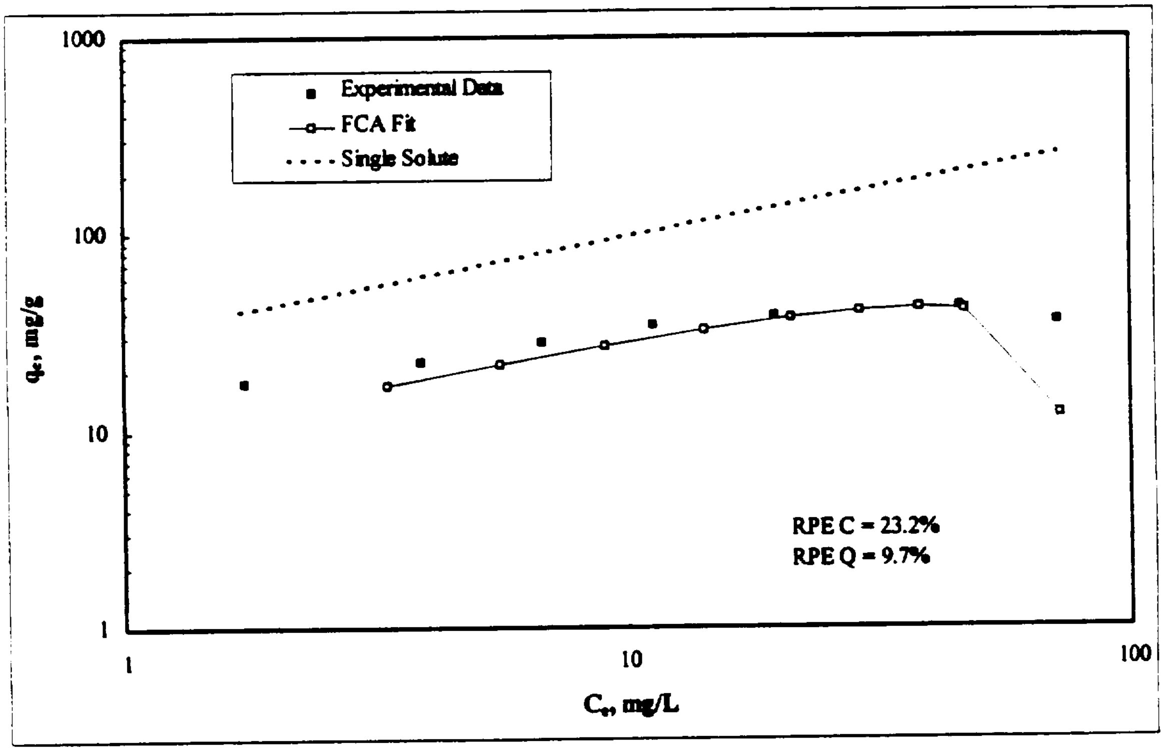

Figure 3-23. FCA fit of dilute ersatz water tracer (TCE) isotherm on APA. Fit simultaneously with nondilute tracer isotherm.

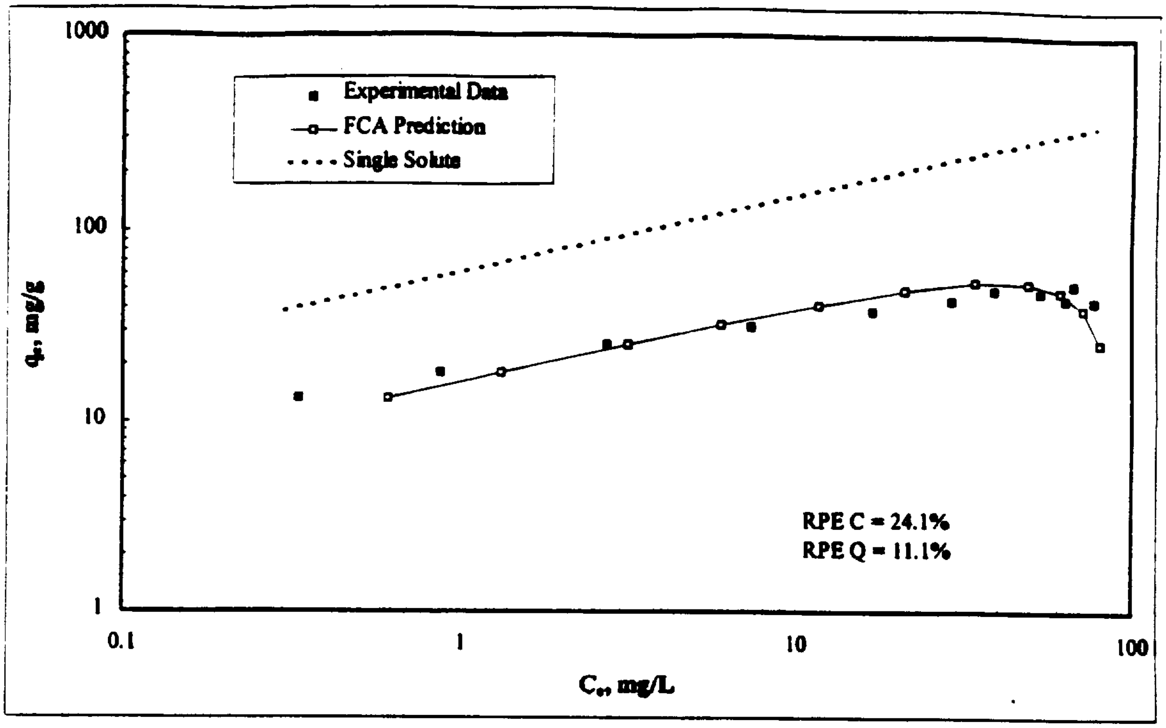

Figure 3-24. FCA prediction of toluene isotherm in ersatz water on APA.

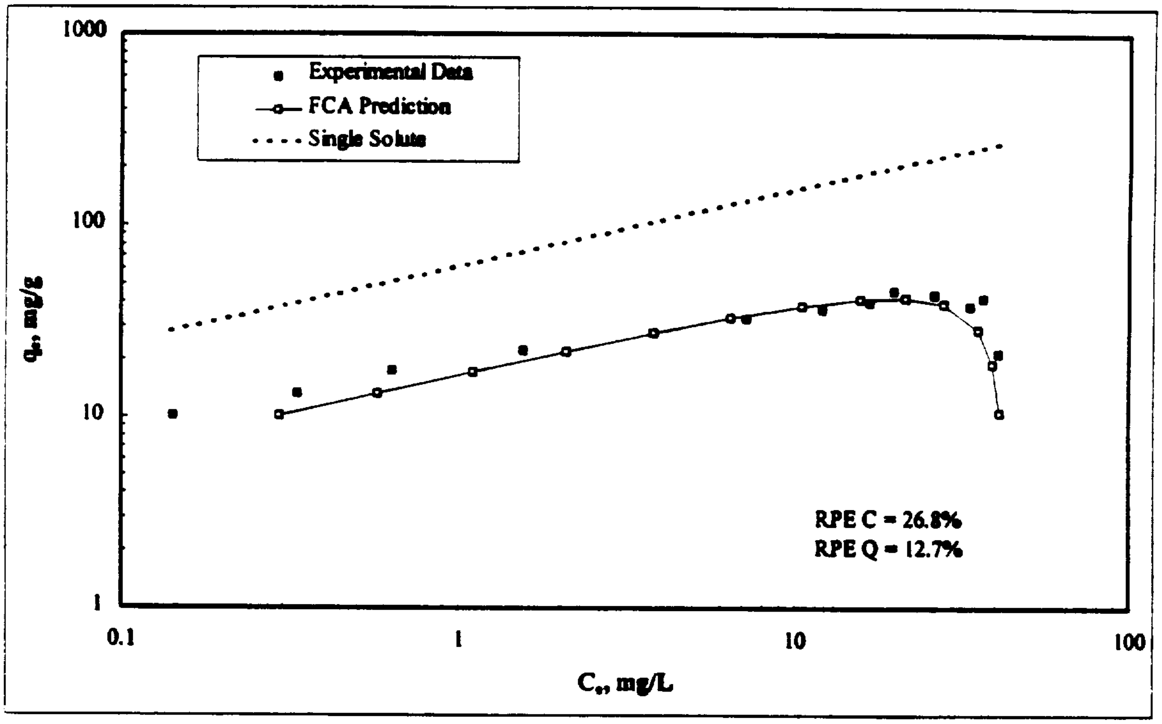

Figure 3-25. FCA prediction of toluene isotherm in dilute ersatz water on APA.

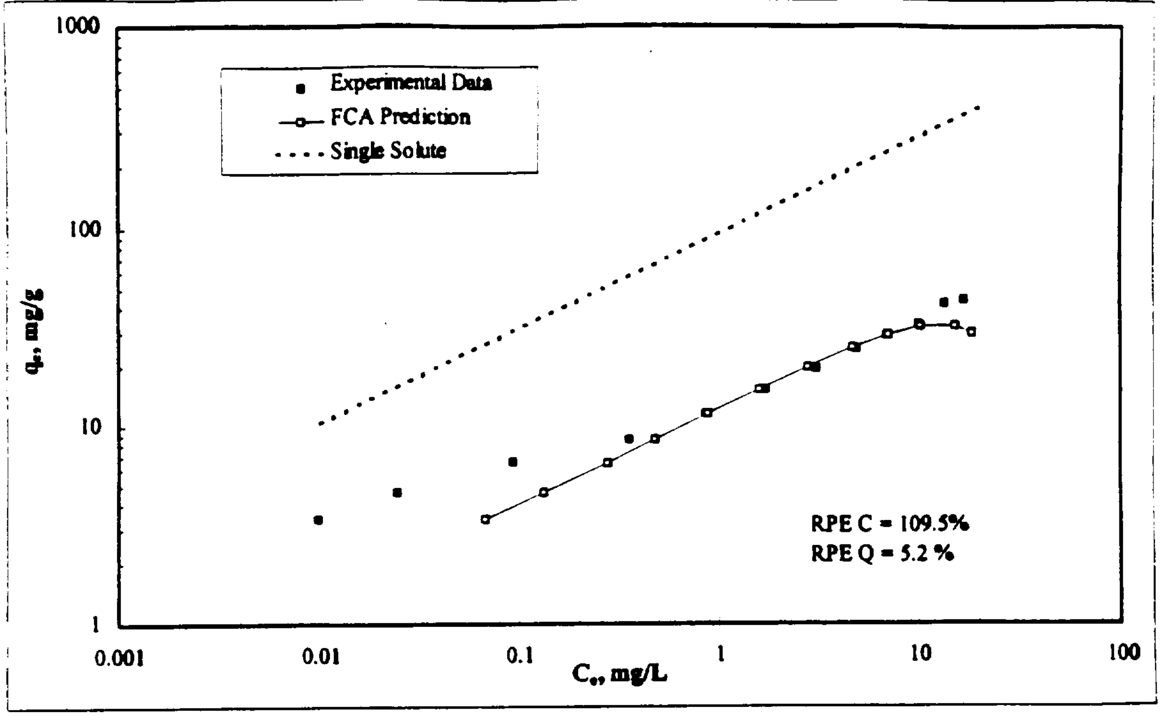

Figure 3-26. FCA prediction of m-xylene isotherm in ersatz water on APA.

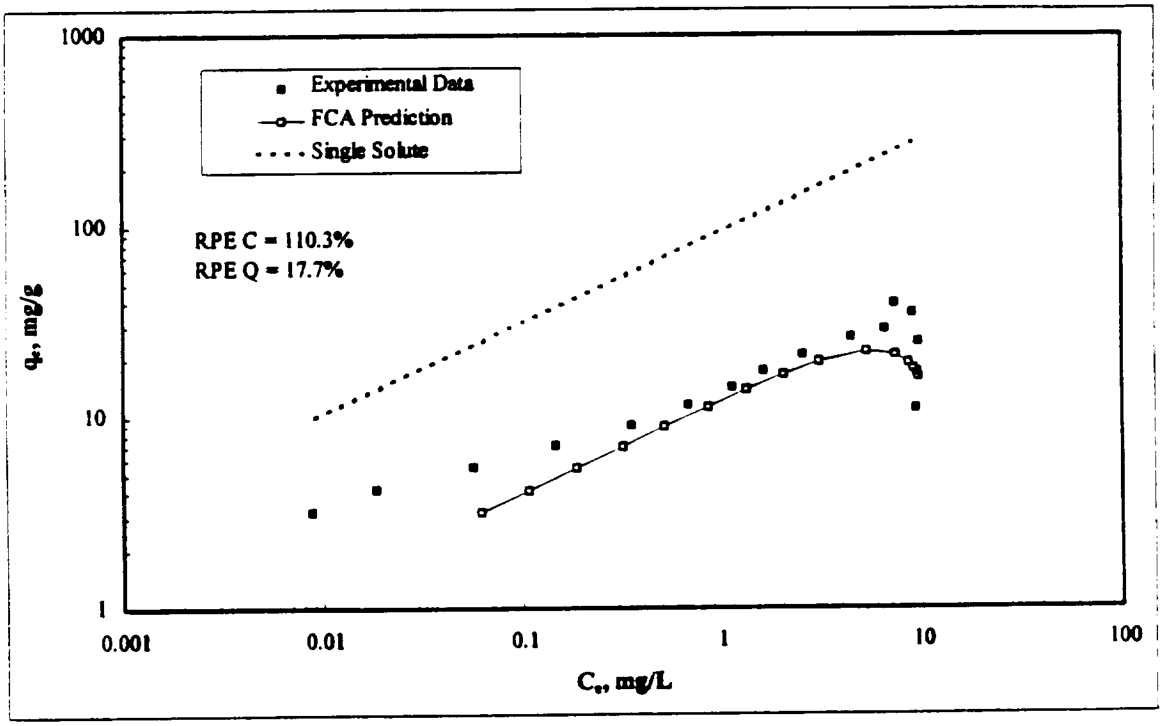

Figure 3-27. FCA prediction of m-xylene isotherm in dilute ersatz water on APA.

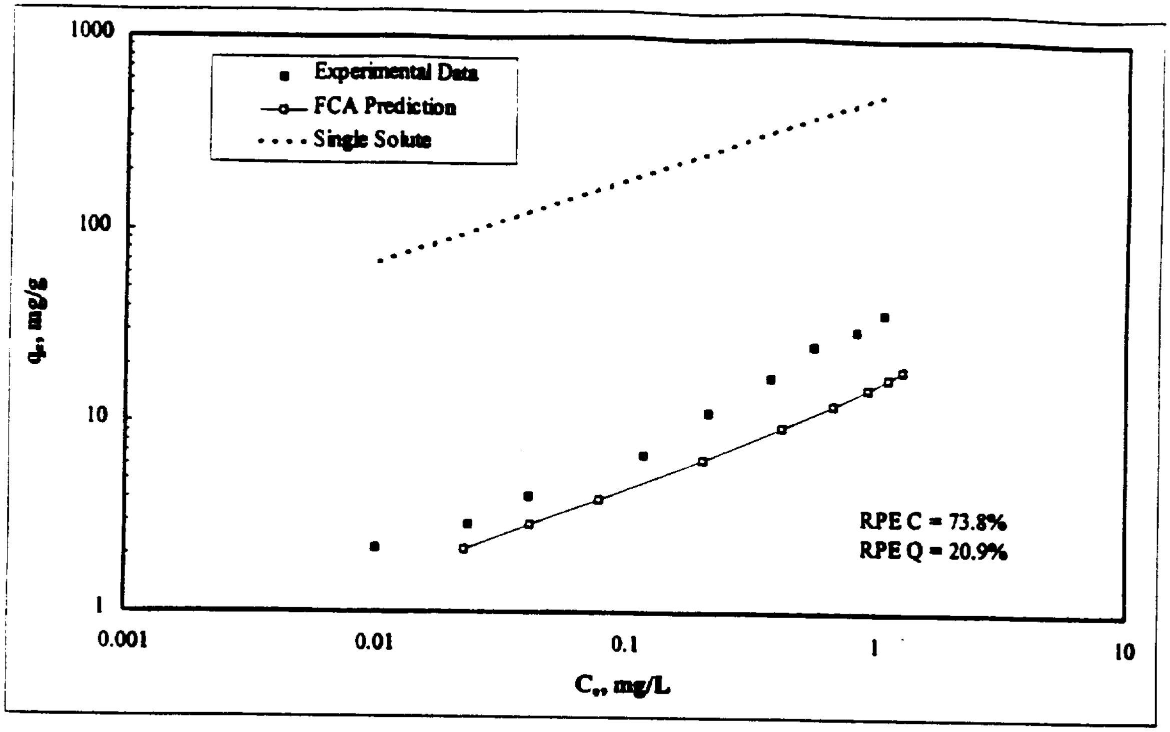

Figure 3-28. FCA prediction of 1,2,4-TCB isotherm in ersatz water on APA.

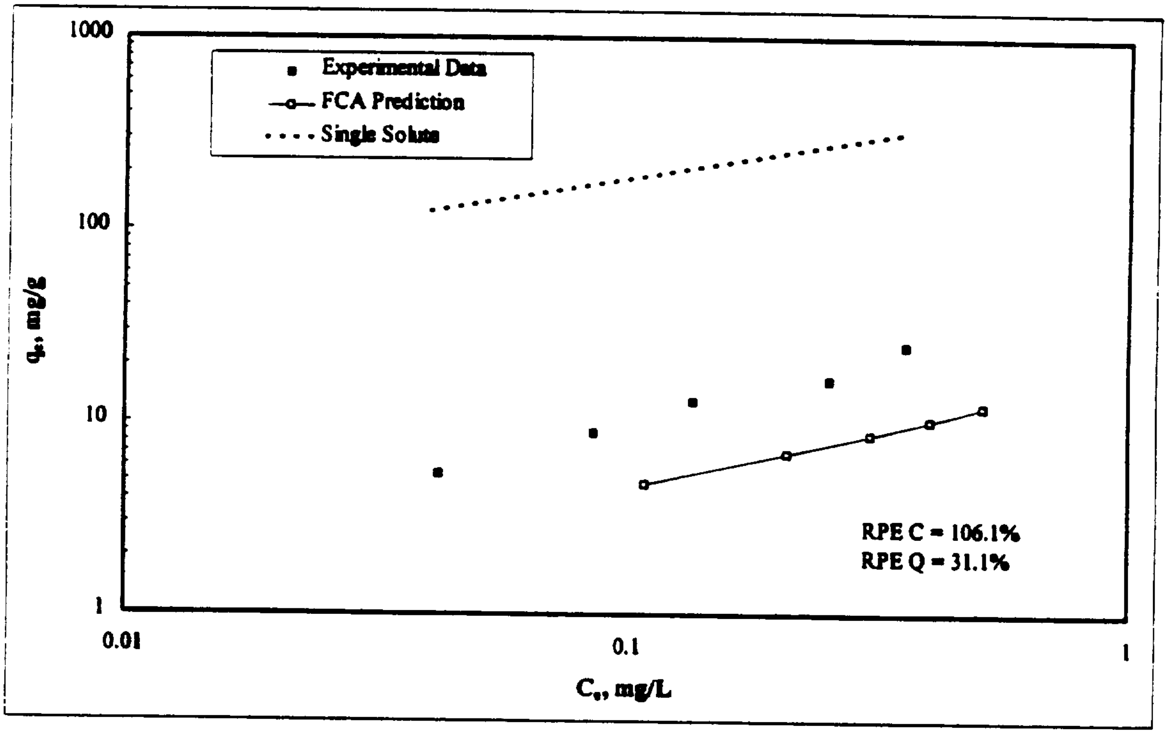

Figure 3-29. FCA prediction of 1,2,4-TCB isotherm in dilute ersatz water on APA.

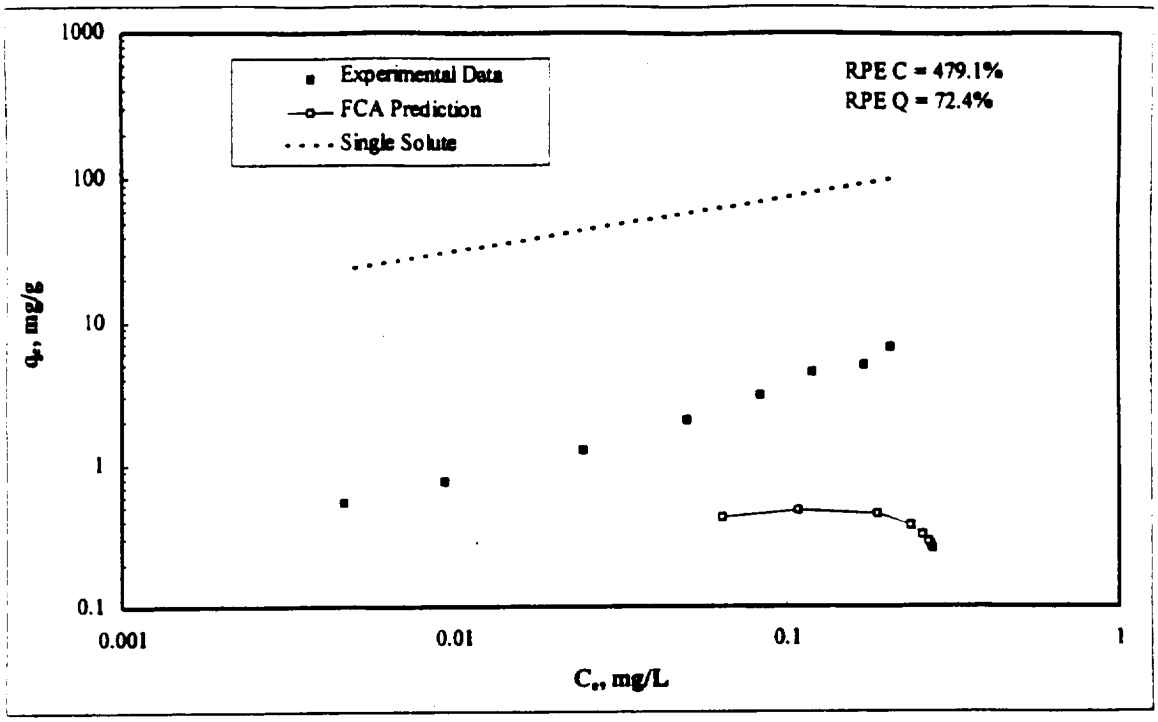

Figure 3-30. FCA prediction of naphthalene isotherm in ersatz water on APA.

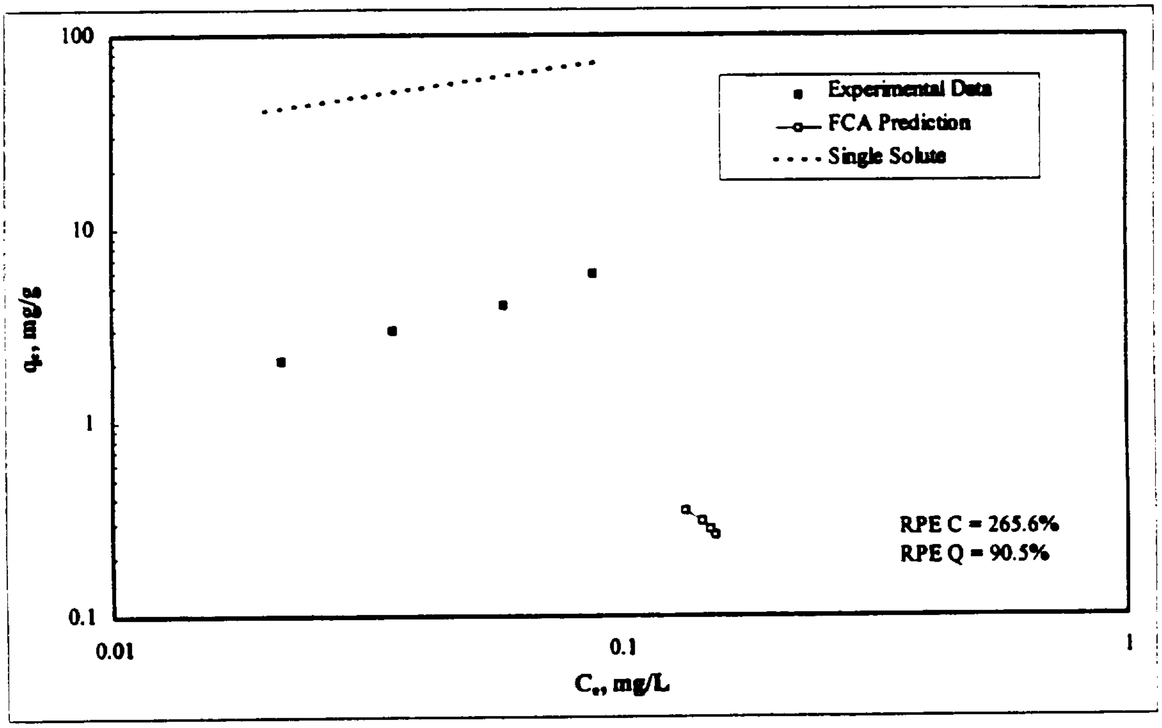

Figure 3-31. FCA prediction of naphthalene isotherm in dilute ersatz water on APA.

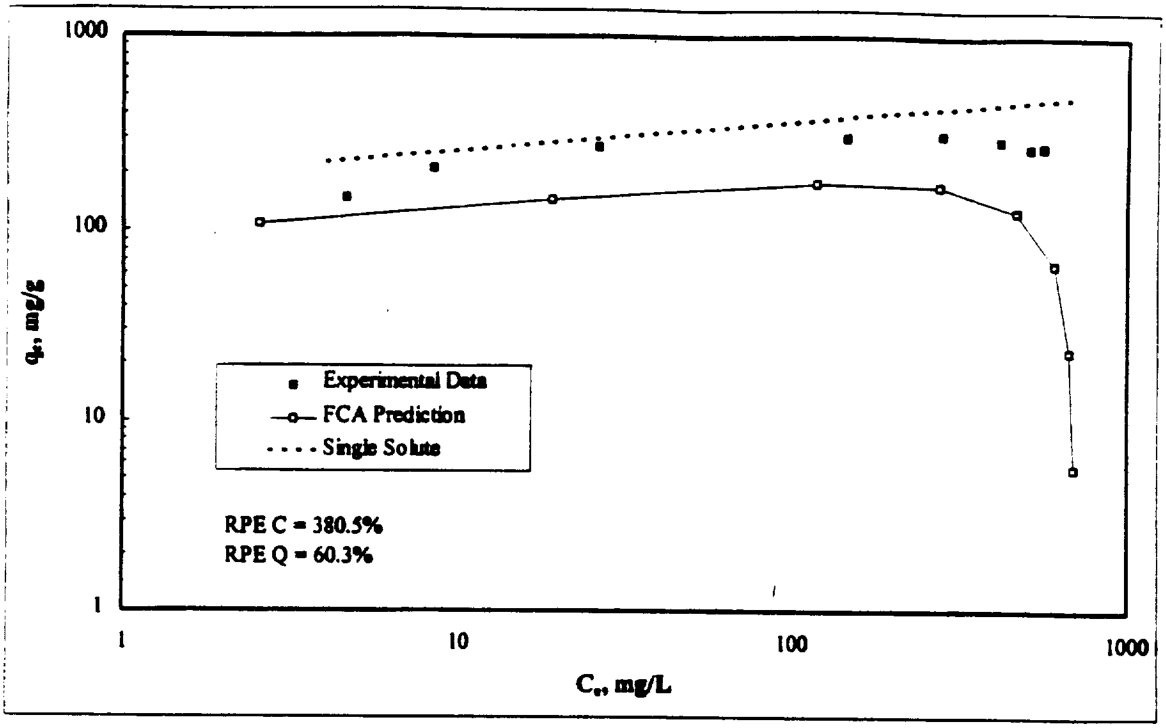

Figure 3-32. FCA prediction of SCMT isotherm in ersatz water on APA.

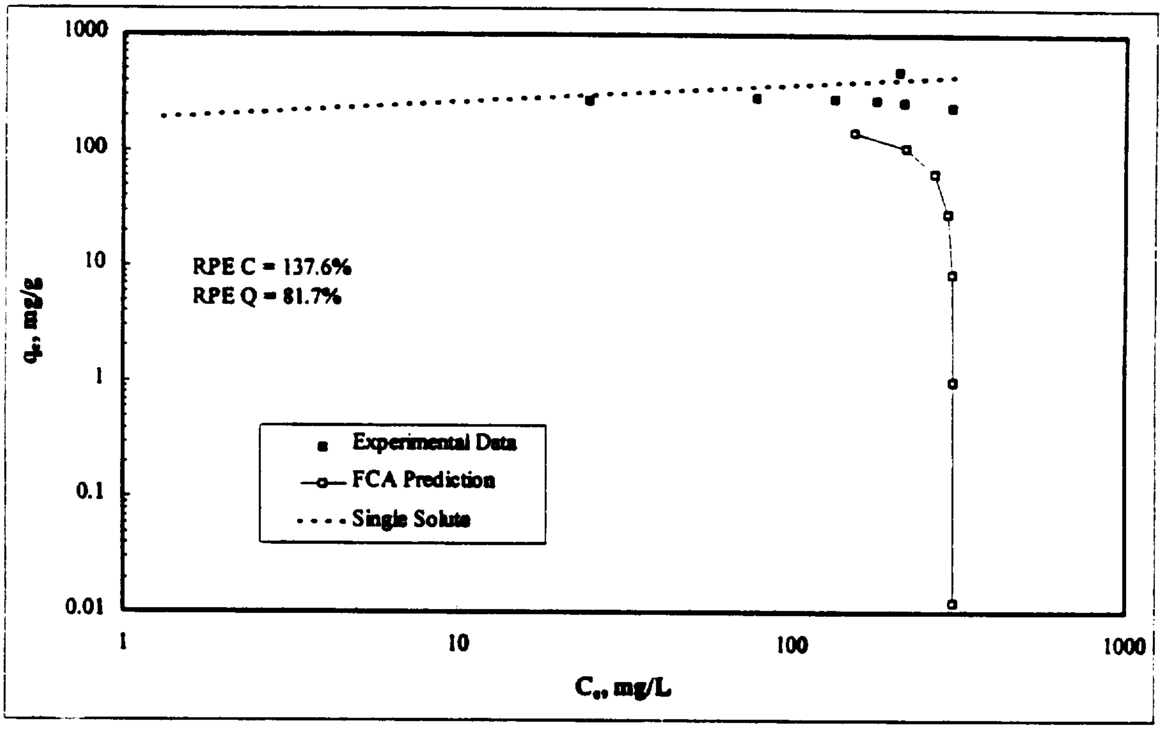

Figure 3-33. FCA prediction of dilute SCMT isotherm in ersatz water on APA.

3.5.8 Tracer FC Results For XAD-4 Resin

The tracer FCs were determined for the XAD-4 resin following the same procedure used to determine the APA tracer FCs. The XAD-4 tracer FCs determined from the fitting procedure are included in Table 3-7. The results of the fit for the nondilute and dilute tracer isotherm are shown in Figures 3-34 and 3-35. The fit of the XAD-4 tracer data is excellent with a RPE in both the liquid and solid phase for both isotherms ranging from 2.8-5.1%. The RPEs of the fits and predictions are included in Table 3-6.

Once the XAD-4 tracer FCs were determined, the isotherms for the other ersatz water constituents were predicted. The results for the toluene isotherms, Figures 3-36 and 3-37, show that the FCs accurately predict the equilibrium for toluene in the ersatz isotherms. The predictions for *m*-xylene, Figures 3-38 and 3-39, are also very close to the isotherm data except for a few of the lowest isotherm dosages where the reduction in capacity is slightly overpredicted by the tracer FCs. The results for the prediction of 1,2,4-TCB are included in Figures 3-40 and 3-41. The tracer FCs also accurately predicted the equilibrium of 1,2,4-TCB in the ersatz water on XAD-4. However, the predictions for naphthalene shown in Figures 3-42 and 3-43 are similar to the other adsorbents as the capacity reduction is significantly overpredicted by the tracer FCs. The results for SCMT shown in Figures 3-44 and 3-45 are also similar to the results obtained for the 580-26 and APA GACs for the reasons explained previously.

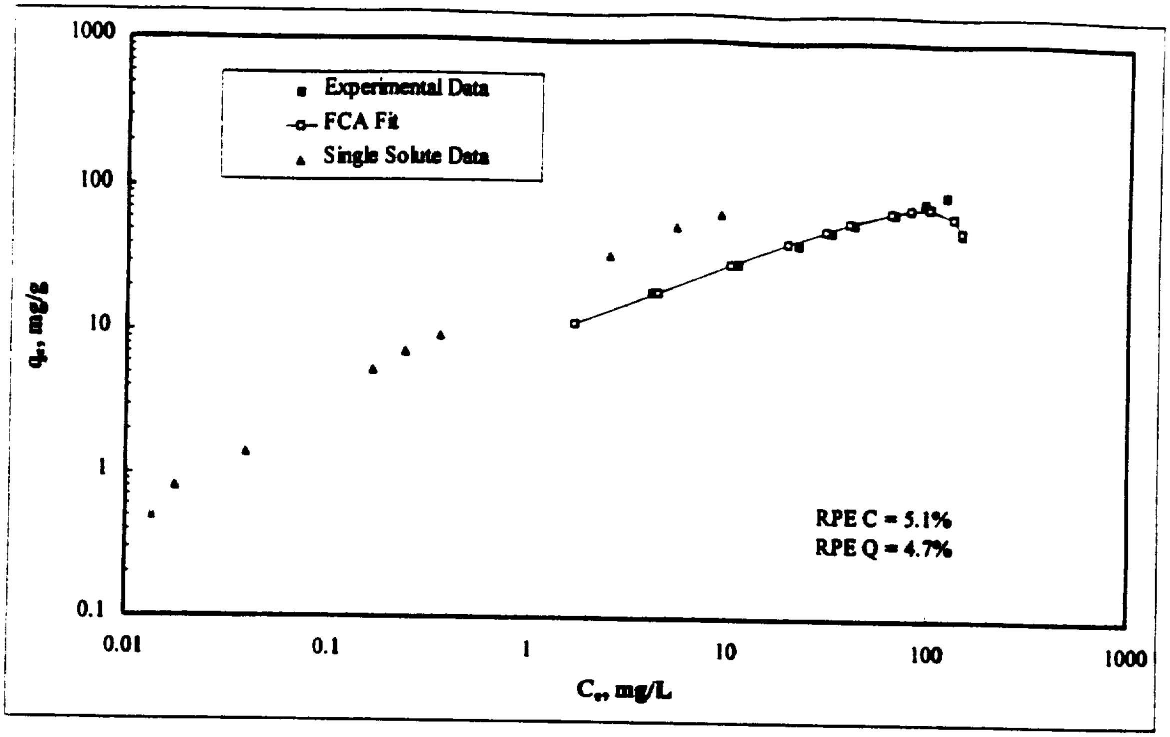

Figure 3-34. FCA fit of ersatz water tracer (TCE) isotherm on XAD-4. Fit simultaneously with dilute tracer isotherm.

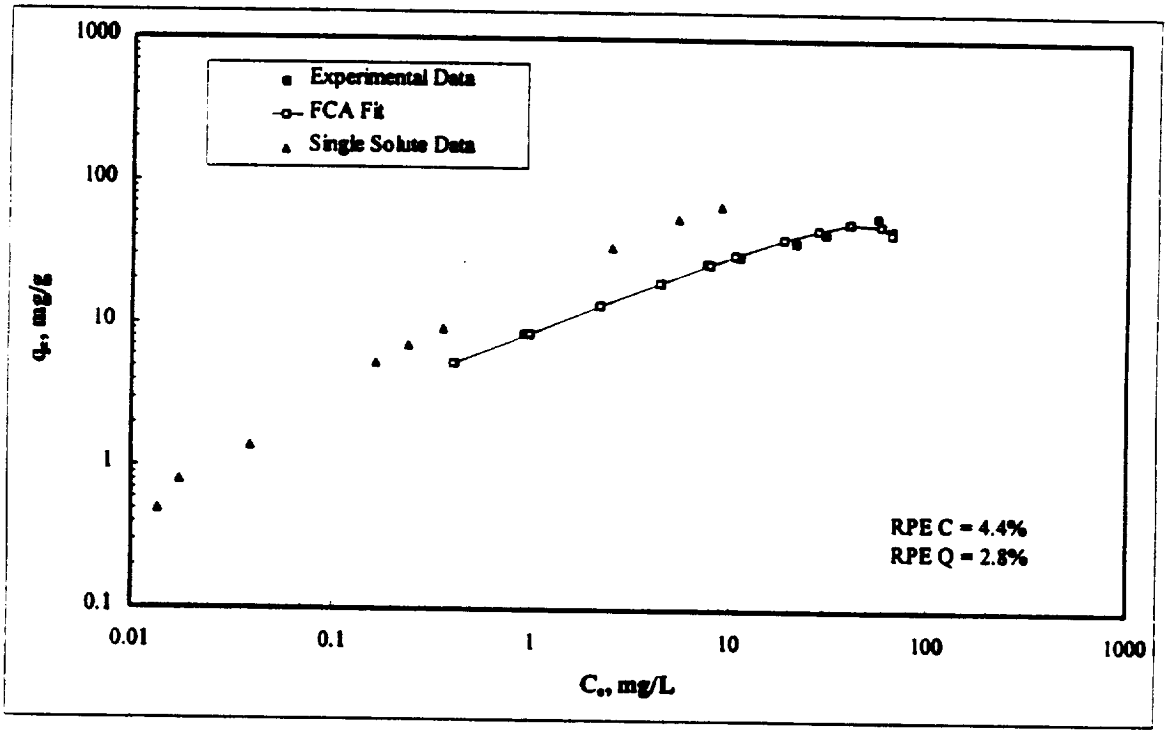

Figure 3-35. FCA fit of dilute ersatz water tracer (TCE) isotherm on XAD-4. Fit simultaneously with nondilute tracer isotherm.

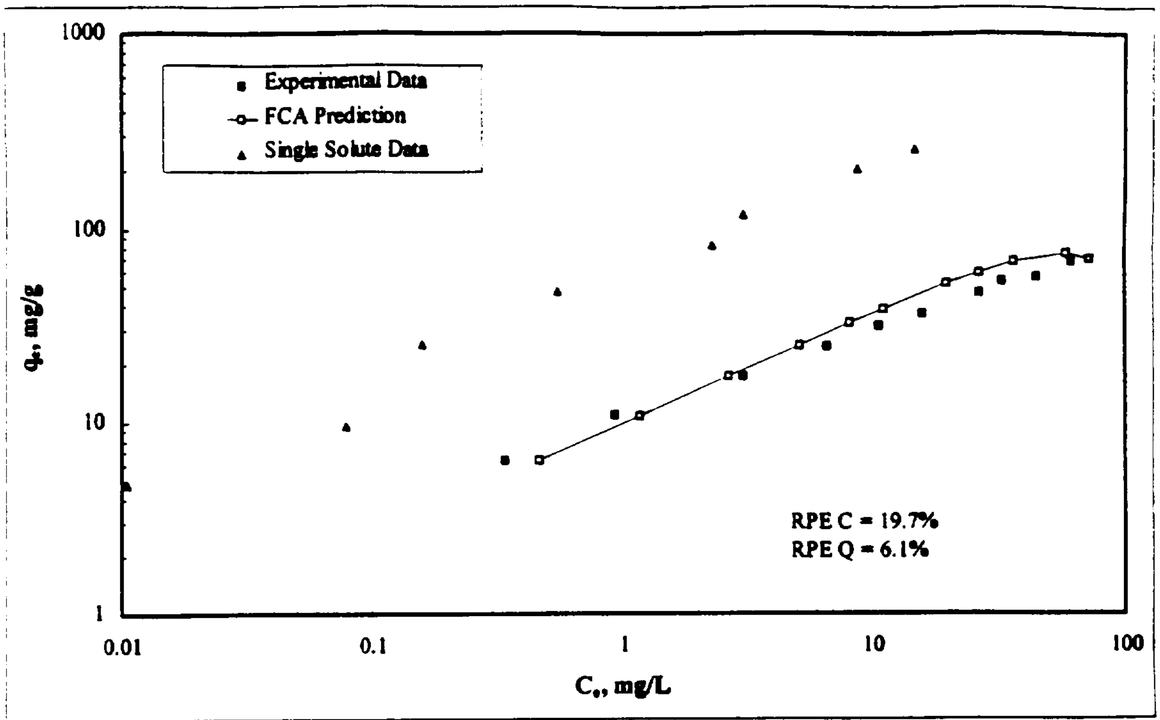

Figure 3-36. FCA prediction of toluene isotherm in ersatz water on XAD-4.

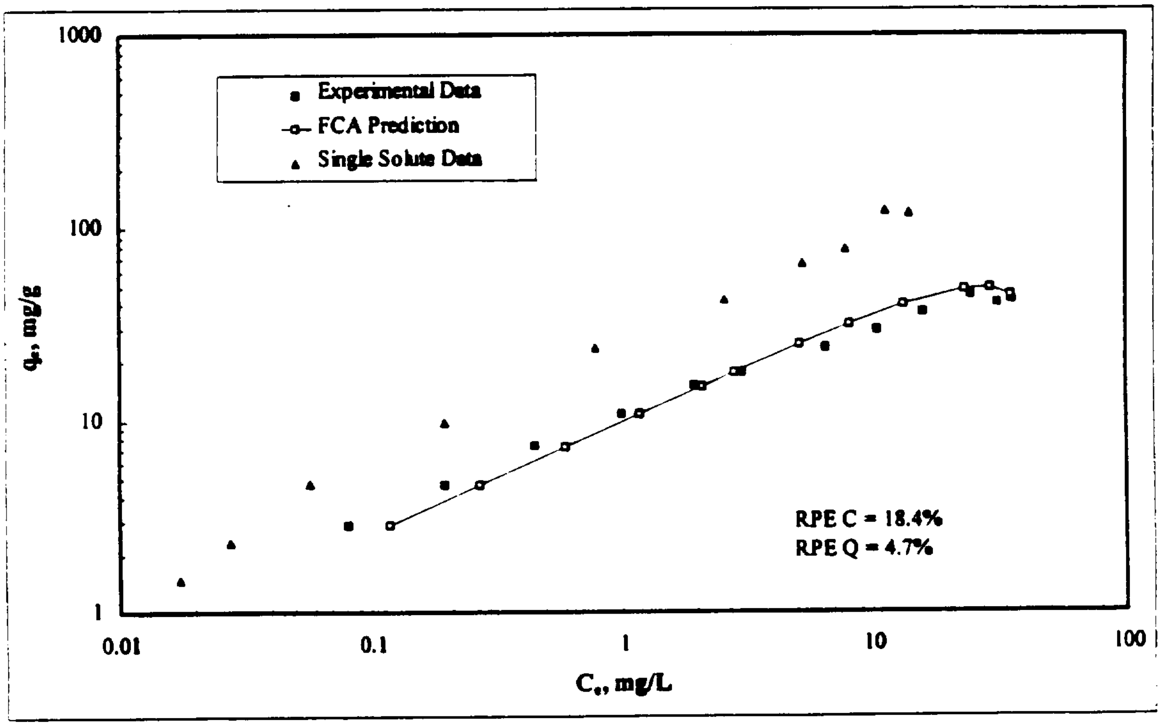

Figure 3-37. FCA prediction of toluene isotherm in dilute ersatz water on XAD-4.

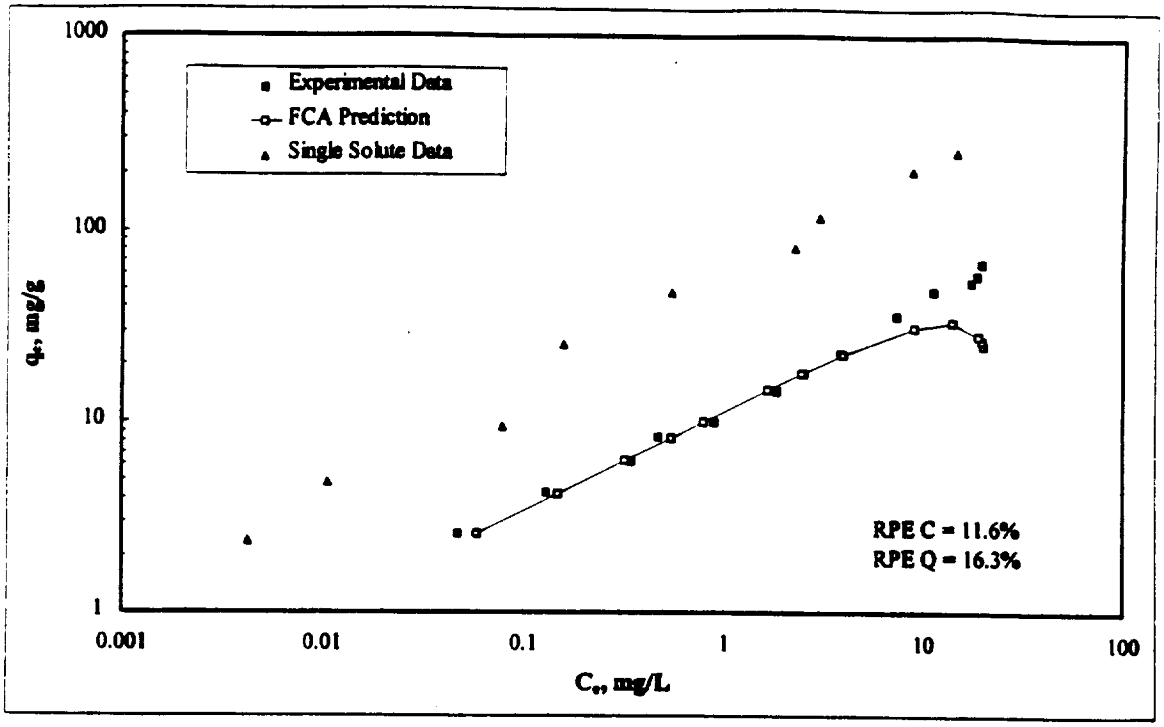

Figure 3-38. FCA prediction of m-xylene isotherm in ersatz water on XAD-4.

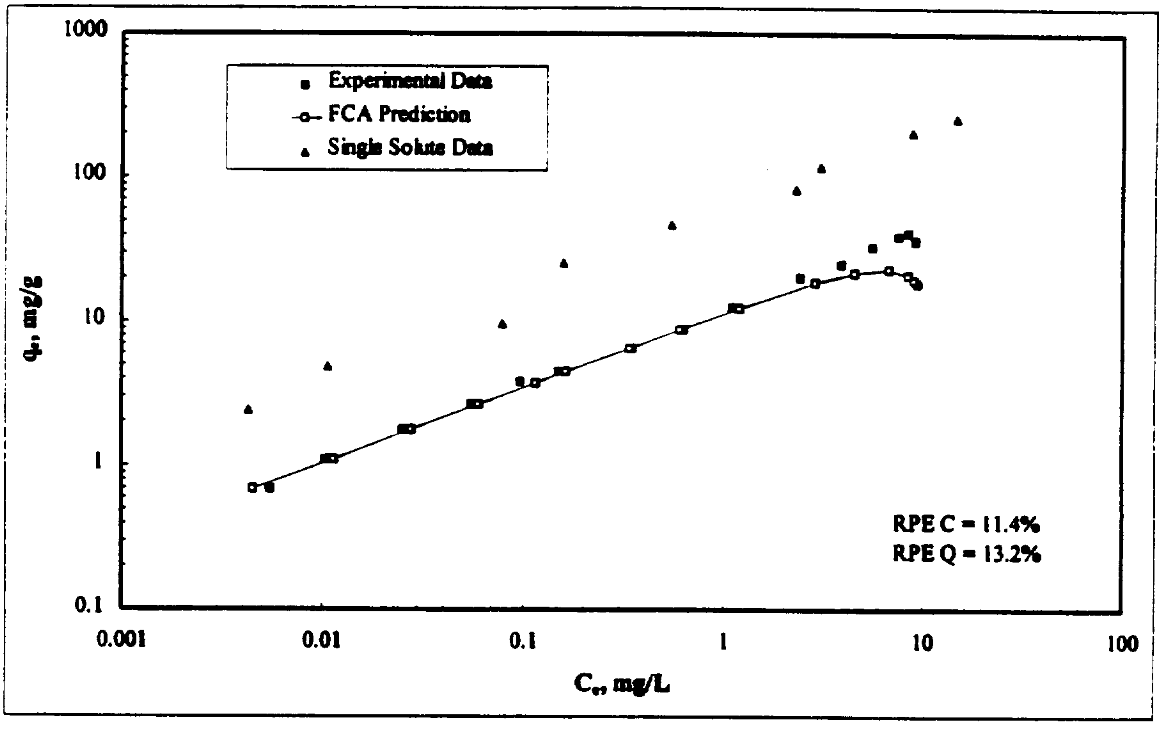

Figure 3-39. FCA prediction of m-xylene isotherm in dilute ersatz water on XAD-4.

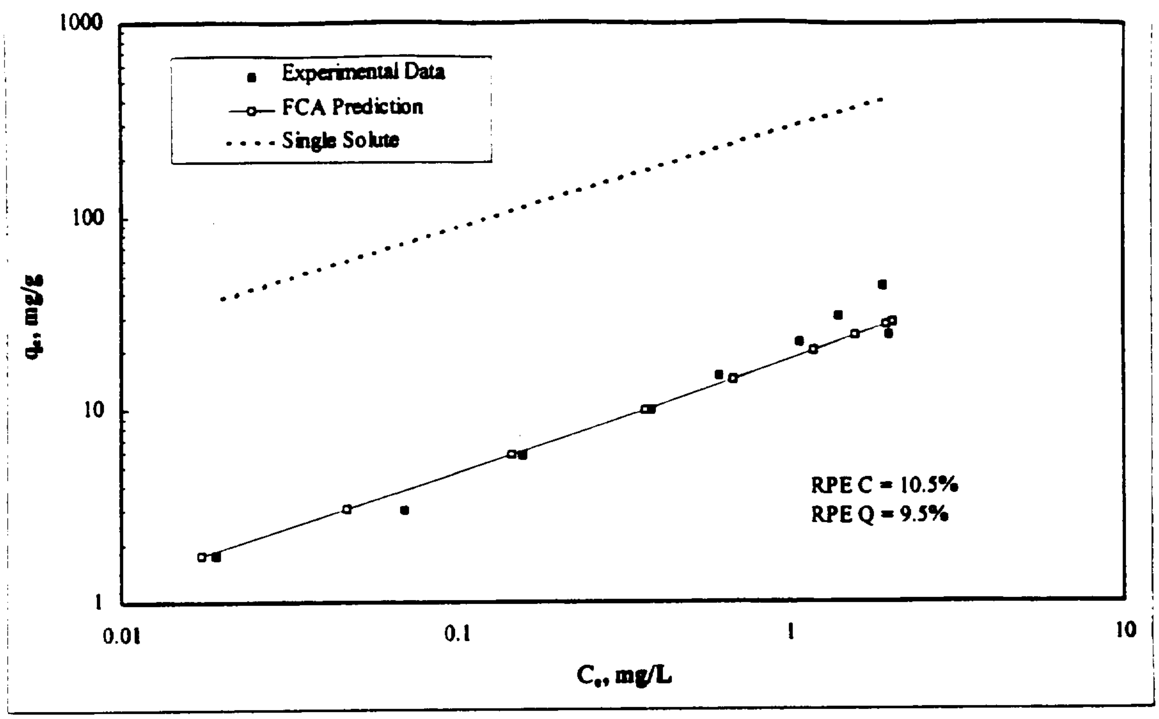

Figure 3-40. FCA prediction of 1,2,4-TCB isotherm in ersatz water on XAD-4.

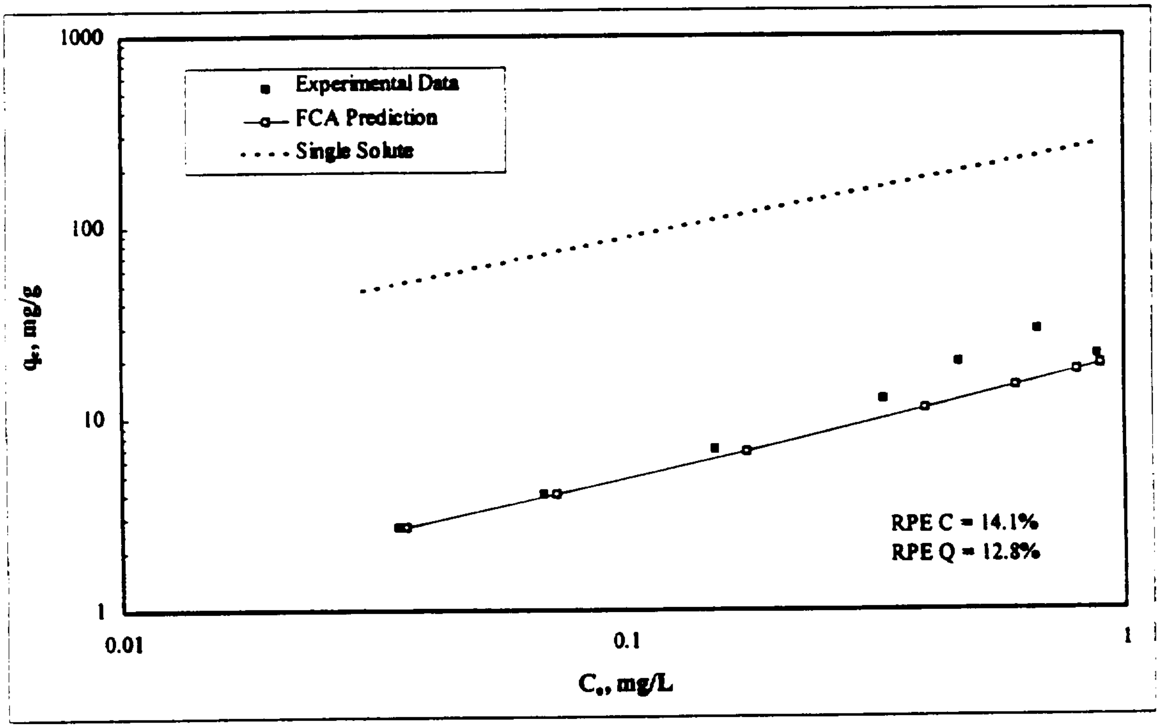

Figure 3-41. FCA prediction of 1,2,4-TCB isotherm in dilute ersatz water on XAD-4.

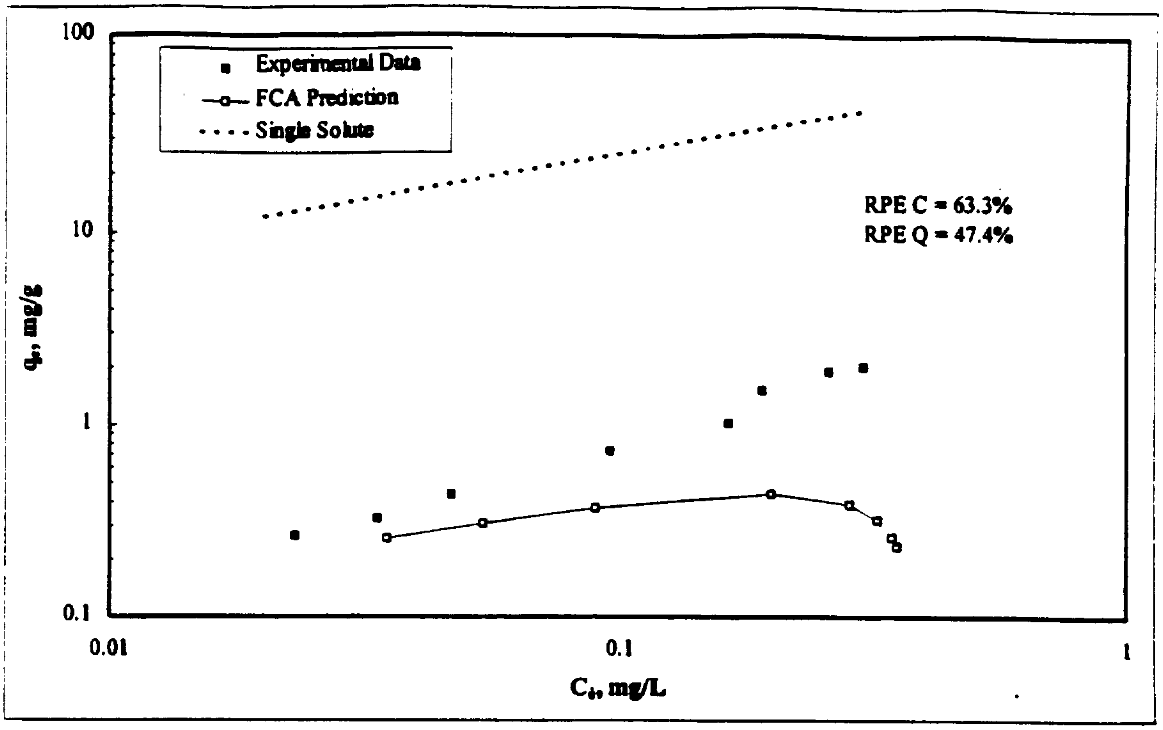

Figure 3-42. FCA prediction of naphthalene isotherm in ersatz water on XAD-4.

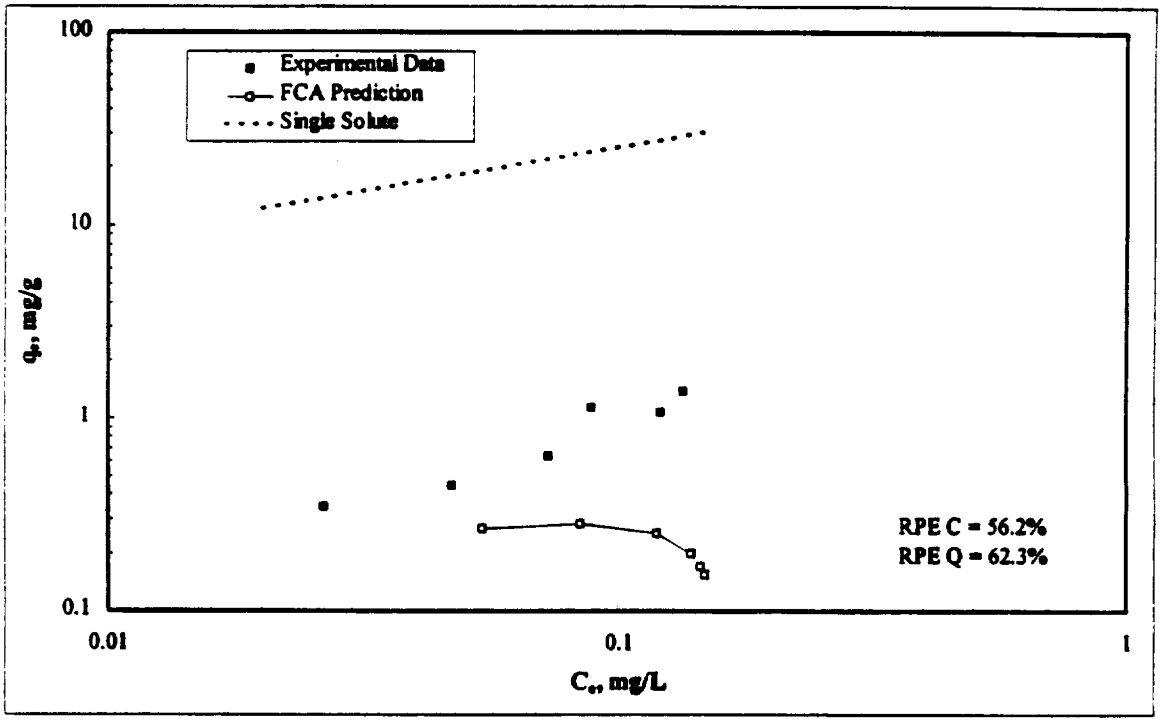

Figure 3-43. FCA prediction of naphthalene isotherm in dilute ersatz water on XAD-4.

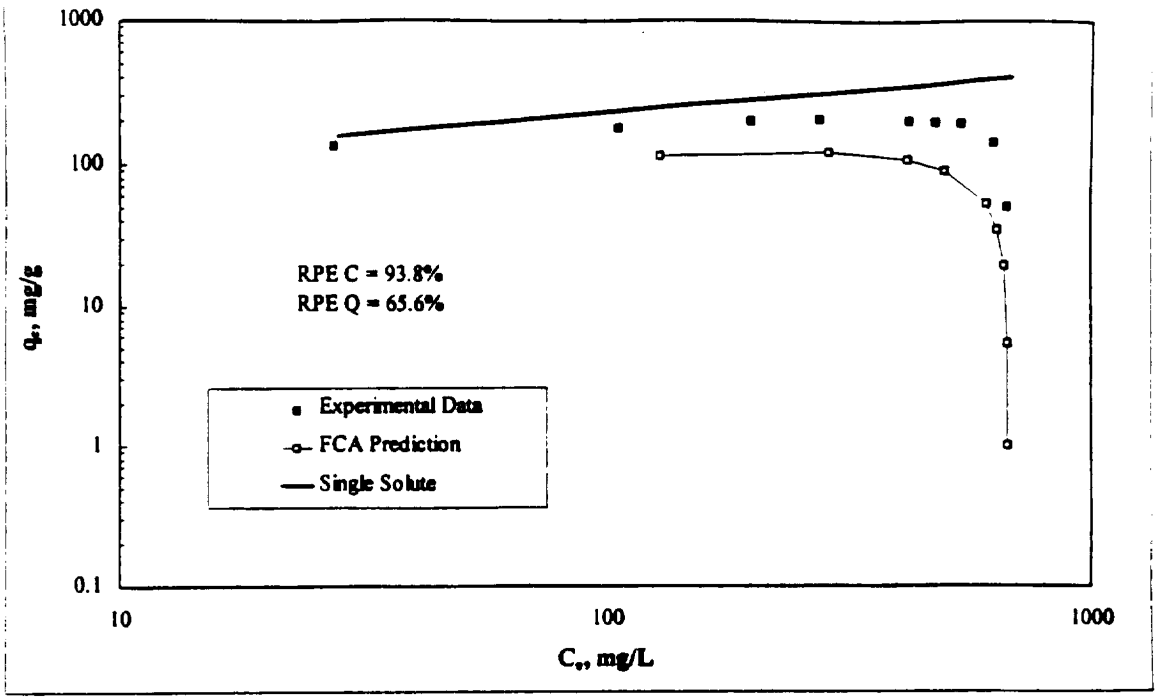

Figure 3-44. FCA prediction of SCMT isotherm in ersatz water on XAD-4.

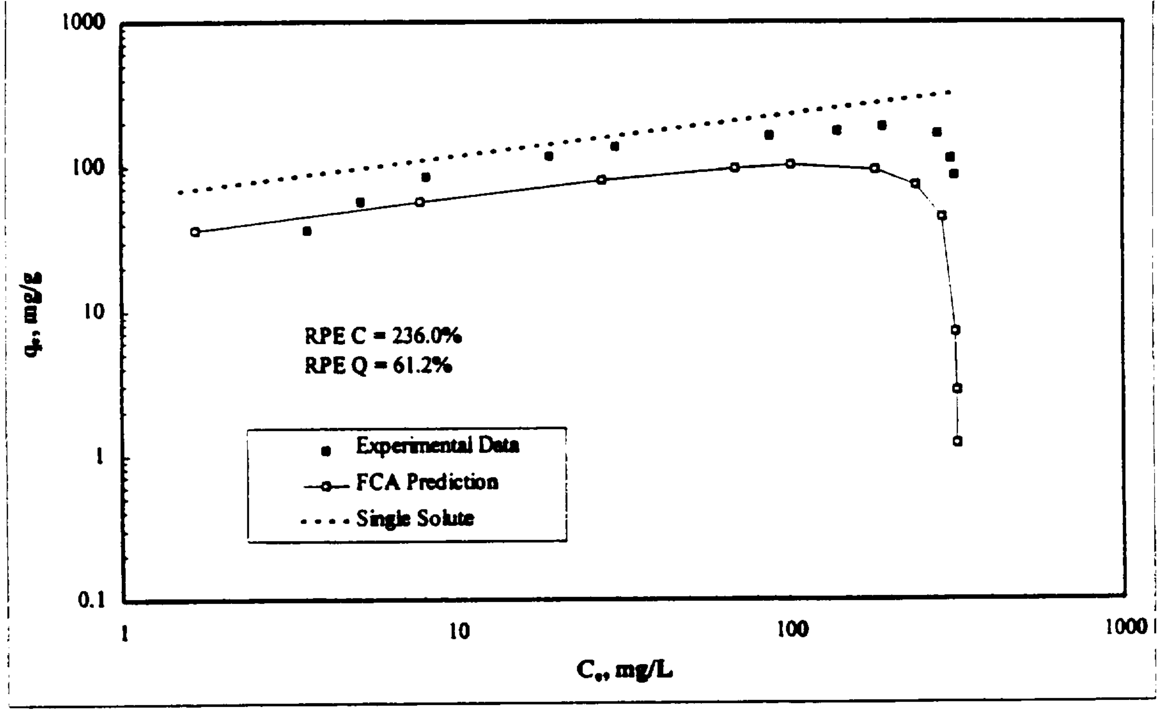

Figure 3-45. FCA prediction of SCMT isotherm in dilute ersatz water on XAD-4.

4.0 Fixed Bed Adsorption Model For The MFB

4.1 Pore and Surface Diffusion Model Equations

The transport of adsorbate molecules within adsorbent particles can occur by two mechanisms: surface diffusion and pore diffusion. Adsorbates may travel along the adsorbent surface by surface diffusion and through the fluid void space contained within the adsorbent pores by pore diffusion. The pore and surface diffusion model (PSDM) accounts for both of these intraparticle transport mechanisms. In the PSDM, Equations 4-1 through 4-9 describe the fate of an adsorbate, i, within a fixed bed adsorber (Friedman, 1984). The liquid-phase mass balance for each adsorbate in dimensionless form is:

$$-\frac{\partial \overline{C_i}(\bar{z},T)}{\partial \bar{z}} = \frac{1}{Dg_i+1}\frac{\partial \overline{C_i}(\bar{z},T)}{\partial T} + 3St_i\left[\overline{C_i}(\bar{z},T) - \overline{C_{p,i}}(\bar{r}=1,\bar{z},T)\right] \qquad (4\text{-}1)$$

The terms which appear in Equation 4-1 account for advective flow, accumulation of mass in the liquid phase, and transport from the liquid to solid phase by liquid phase mass transfer. The boundary condition for Equation 4-1 is:

$$\overline{C_i}(\bar{z}=0, T \geq 0) = 1 \qquad (4\text{-}2)$$

The initial condition for the liquid-phase mass balance (Equation 4-1) is:

$$\overline{C_i}\left[T(Dg_i+1) \leq \bar{z} \leq 1, T < \frac{1}{Dg_i+1}\right] = 0 \qquad (4\text{-}3)$$

The intraparticle mass balance is given as:

$$\frac{1}{\overline{r}^2}\frac{\partial}{\partial \overline{r}}\left[\overline{r}^2\left[\left(Ed_{p,i}-\frac{Dg_{p,i}}{Dg_{s,i}}Ed_{s,i}\right)\frac{\partial \overline{C_{p,i}}\left(\overline{r},\overline{z},T\right)}{\partial \overline{r}}+\left(Ed_{s,i}+\frac{Dg_{p,i}}{Dg_{s,i}}Ed_{s,i}\right)\frac{\partial \overline{X_i}\left(\overline{r},\overline{z},T\right)}{\partial \overline{r}}\right]\right]$$

$$=\frac{Dg_i}{Dg_i+1}\frac{\partial \overline{X_i}\left(\overline{r},\overline{z},T\right)}{\partial T} \tag{4-4}$$

The terms which appear in Equation 4-4 account for surface and pore diffusion, and accumulation in the intraparticle phase, respectively. The initial condition for Equation 4-4 is:

$$\overline{X_i}\left(0\le \overline{r}\le 1, 0\le \overline{z}\le 1, T=0\right)=0 \tag{4-5}$$

The boundary conditions for Equation 4-4 are:

$$\frac{\partial \overline{X_i}\left(\overline{r}=0, 0\le \overline{z}\le 1, T\ge 0\right)}{\partial \overline{r}}=0 \tag{4-6}$$

$$St_i\left[\overline{C_i}\left(\overline{z},T\right)-\overline{C_{p,i}}\left(\overline{r}=1,\overline{z},T\right)\right]=\frac{Dg_i}{Dg_i+1}\frac{\partial}{\partial T}\int_0^1 \overline{X_i}\left(\overline{r},\overline{z},T\right)\overline{r}^2 d\overline{r} \tag{4-7}$$

Equation 4-6 results from symmetry.

Equations 4-1 and 4-4 are coupled by assuming local equilibrium at the surface of the adsorbent. For single solute calculations, the Freundlich isotherm equation is used to relate the surface and pore concentrations within the adsorbent phase by:

$$\overline{X_i}\left(\overline{r},\overline{z},T\right)=\frac{Dg_{p,i}}{Dg_i}\overline{C_{p,i}}\left(\overline{r},\overline{z},T\right)+\frac{Dg_{s,i}}{Dg_i}\left[\overline{C_{p,i}}\left(\overline{r},\overline{z},T\right)\right]^{1/n_i} \tag{4-8}$$

For multicomponent calculations, the following non-linear equation which is derived from IAST is used to relate the surface and pore concentrations within the adsorbent phase by:

$$\overline{C_{p,j}}\left(\bar{r},\bar{z},T\right)=\left[\frac{\overline{X_i}\left(\bar{r},\bar{z},T\right)\overline{X_{e,j}}-\frac{\varepsilon_p}{\rho_a}\overline{C_{p,j}}\left(\bar{r},\bar{z},T\right)C_{o,j}}{C_{o,j}\sum_{j=1}^{m}\left[\overline{X_j}\left(\bar{r},\bar{z},T\right)\overline{X_{e,j}}-\frac{\varepsilon_p}{\rho_a}\overline{C_{p,j}}\left(\bar{r},\bar{z},T\right)C_{o,j}\right]}\right] \times\left[\frac{\sum_{k=1}^{m}\left[n_k\left[\overline{X_k}\left(\bar{r},\bar{z},T\right)\overline{X_{e,k}}-\frac{\varepsilon_p}{\rho_a}\overline{C_{p,j}}\left(\bar{r},\bar{z},T\right)C_{o,j}\right]\right]}{n_i K_i}\right] \tag{4-9}$$

Equations 4-1 through 4-9 represent a set of coupled nonlinear, partial differential equations that were solved numerically by orthogonal collocation (OC) (Finlayson, 1980). With the OC method, the dependence of concentration on position is described by a linear combination of orthogonal polynomials. These polynomials are used in integration and differentiation algorithms that only require values for the dependent variable, concentration, at specific collocation points. The collocation points are located at the roots of the polynomial approximations. Crittenden *et al.* (1986a) presented a detailed discussion of the model development and solution to model equations.

4.1.1 Dimensionless Groups Which Characterize The PSDM

Friedman (1984), Crittenden *et al.* (1986a), and Sontheimer *et al.* (1988) described the nature of the dimensionless groups appearing in the PSDM. These groups express the relative importance of competing kinetic mechanisms, or relative partitioning between the phases of thermodynamic states. Specifying values of these dimensionless coefficients determines a solution to the PSDM. The dimensionless groups characterizing the PSDM are given in Equations 4-10 through 4-17.

$$Dg_{s,i}=\frac{\rho_a q_{e,i}(1-\varepsilon)}{\varepsilon\, C_{o,i}} \tag{4-10}$$

$$Dg_{p,i} = \frac{\varepsilon_p(1-\varepsilon)}{\varepsilon} \qquad (4\text{-}11)$$

$$Dg_i = Dg_{s,i} + Dg_{p,i} \qquad (4\text{-}12)$$

$$Dg_t = \sum_{i=1}^{N}\left(Dg_{s,i} + Dg_{p,i}\right) \quad N = number\ of\ components \qquad (4\text{-}13)$$

$$St_i = \frac{k_{f,i}L(1-\varepsilon)}{vR\varepsilon} = \frac{k_{f,i}\tau(1-\varepsilon)}{R\varepsilon} \qquad (4\text{-}14)$$

$$Ed_{s,i} = \frac{LD_{s,i}Dg_{s,i}}{vR^2} = \frac{\tau D_{s,i}Dg_{s,i}}{R^2} \qquad (4\text{-}15)$$

$$Ed_{p,i} = \frac{LD_{p,i}Dg_{p,i}}{vR^2} = \frac{\tau D_{p,i}Dg_{p,i}}{R^2} \qquad (4\text{-}16)$$

$$D_i = \frac{D_{s,i}}{D_{p,i}} \qquad (4\text{-}17)$$

The surface solute distribution parameter, $Dg_{s,i}$, is a partitioning coefficient between the mass of adsorbate i on the adsorbent and the mass of adsorbate i in the liquid phase at equilibrium with $C_{0,i}$. It is based on the single solute capacity. As the adsorbate's affinity for the adsorbent phase increases, $Dg_{s,i}$ increases. $Dg_{s,i}$ is important in describing GAC adsorption as it is a measure of the relative adsorption strength of a compound.

The pore solute distribution parameter, $Dg_{p,i}$, is a partitioning coefficient between the mass of adsorbate i in the adsorbent pores and the mass of adsorbate i in the liquid phase. Since $Dg_{p,i}$ is a function of only the adsorbent properties, bed void fraction and the adsorbent void fraction, it is equal for all solutes in a given system.

Dg_i is the sum of $Dg_{s,i}$ and $Dg_{p,i}$, making Dg_i the total mass partitioning coefficient of adsorbate i in the adsorbent phase and the mass of adsorbate i in the liquid phase at equilibrium with $C_{0,i}$. Since $Dg_{s,i}$ is based on single solute capacities, $Dg_{p,i}$ will also be a single solute group. Dg_t is the total equilibrium mass partitioning for all solutes present.

Mass throughput, T, is the dimensionless time scale used in the fixed bed model. It may be expressed as the ratio of the mass of adsorbate i fed to the mass of adsorbate i adsorbed as a single component in equilibrium with $C_{o,i}$. T is defined as:

$$T = \frac{t}{\tau\left(Dg_t + 1\right)} \tag{4-18}$$

in which τ is the packed bed residence time.

The Stanton number, St, is a ratio of the rate of solute transport by external mass transfer to the rate by advection. As St_i increases, the spread in the mass transfer zone due to the external mass transfer becomes smaller. (The role of the Stanton number in single solute fixed bed adsorption may be estimated by ignoring other mass transfer mechanisms in the liquid phase mass balance and solving for the concentration profile assuming steady-state operation [Hand, 1984].)

The surface diffusion modulus, $Ed_{s,i}$, is the ratio of the rate of solute transport by intraparticle surface diffusion to that by advection. As $Ed_{s,i}$ increases, the spread in the mass transfer zone due to surface diffusion becomes smaller. As $Ed_{s,i}$ becomes much greater than 1/5 St_i, film transfer controls and as $Ed_{s,i}$ decreases well below 1/5 St_i, surface diffusion controls. In most fixed bed adsorption processes, the rate of film transfer is rarely the limiting mass transfer mechanisms and the Stanton number is usually large enough to be considered unimportant.

The pore diffusion modulus, $Ed_{p,i}$, compares the mass transport rate by pore diffusion to the advective rate. Like $Ed_{s,i}$, as $Ed_{p,i}$ increases, the spread in the mass transfer zone due to pore diffusion becomes smaller. Pore diffusion is generally an important mechanism for moderate to strongly adsorbed compounds in a multicomponent system. When there are weakly adsorbed organics present in the water that can preadsorb onto the surface of an adsorbent, surface diffusion may become negligible, and pore diffusion may become important for the compounds passing through the column after the weakly adsorbing compounds. This is especially true for strongly adsorbing compounds, because they migrate slowly through the bed which allows more time for the weakly and moderately adsorbed organics to preadsorb onto the adsorbent surface.

Another important dimensionless group is the Biot number. The Biot numbers for surface and pore diffusion controlled intraparticle diffusion describe the ratio of the external mass transfer rate to the intraparticle diffusion rates as follows:

$$Bi_{s,i} = \frac{St_i}{Ed_{s,i}} \tag{4-19}$$

$$Bi_{p,i} = \frac{St_i}{Ed_{p,i}} \tag{4-20}$$

When both Biot numbers are high (>20), then intraparticle diffusion resistance will control the mass transfer into the adsorbent. If either Biot number is low (<1), then film transfer resistance controls the rate of adsorption because intraparticle mass transport takes place by either surface or pore diffusion which act in parallel. Therefore, the faster of the two mechanisms will control the transport rate. For example, when $Ed_{s,i}$ or $Bi_{p,i}$ is much larger than $Ed_{p,i}$ or $Bi_{s,i}$, respectively, then surface diffusion will control the intraparticle mass transport rate, and the converse is also true.

4.2 Estimation Of Mass Transfer Parameters

The external or liquid phase mass transfer coefficient, $k_{f,i}$, was calculated using the Gnielinski correlation (Gnielinski, 1978):

$$k_{f,i} = \frac{\left(1 + 1.5 \times (1 - \varepsilon)\right) D_{L,i}}{d_p} \left[2 + 0.644 \, \mathrm{Re}^{1/2} \, Sc^{1/3} \right] \tag{4-21}$$

in which d_p is the diameter of the adsorbent particle, D_L is the liquid diffusivity of the adsorbate, and ε is the bed porosity. The liquid diffusivity was determined from a correlation given by Hayduk and Laudie (1974):

$$D_{L,i} = \frac{13.26\times10^{-5}}{\mu_L^{1.14}\, V_{m,i}^{0.589}} \tag{4-22}$$

in which $V_{m,i}$ is the molar volume of the adsorbate at the normal boiling point estimated from atomic volumes of Le Bas (Treybal, 1980) and μ_L is the viscosity of water. Sontheimer *et al.* (1988) discusses the application of these correlations to fixed bed adsorption processes.

The Reynolds (Re) and Schmidt (Sc) numbers are calculated by:

$$\mathrm{Re} = \frac{d_p v \rho_L}{\mu_L} \tag{4-23}$$

$$Sc = \frac{\mu_L}{\rho_L D_L} \tag{4-24}$$

in which d_p is the particle diameter, ρ_L is the density of water, and v is the interstitial fluid velocity.

The pore diffusivity for adsorbate i, $D_{p,i}$, was calculated from the adsorbate's liquid diffusivity using the following equation:

$$D_{p,i} = \frac{D_{L,i}\varepsilon_p}{\mu_i} \tag{4-25}$$

in which ε_p is the porosity of the adsorbent particle, and μ_i is the observed labyrinth factor or tortuosity for compound i. The particle porosity can be determined by experimental methods which are described by Sontheimer *et al.* (1988). The observed tortuosity is a parameter which depends on the adsorbent and adsorbates and can only be determined from kinetic experiments.

The surface diffusivity of adsorbate i, $D_{s,i}$, can be determined from batch rate tests as discussed by Hand *et al.* (1983) or estimated from various empirical correlations presented by Crittenden *et al.* (1987a). Based on kinetic data for a number of chlorinated alkanes, alkenes, and aromatic compounds, Crittenden *et al.* (1987a) developed a correlation for calculation of the surface diffusion coefficient. The surface diffusion coefficient was calculated by multiplying the pore diffusion flux by a correlating factor for each compound, the surface to pore diffusion flux ratio ($SPDFR_i$).

$$D_{s,i} = \frac{D_{L,i}\varepsilon_p C_{o,i}}{\mu_i \rho_a q_{o,i}} \times SPDFR_i \tag{4-26}$$

The SPDFR is the correlating parameter for determining $D_{s,i}$. The SPDFR is a useful correlating parameter, because it can be used to calculate $D_{s,i}$ values of similar compounds for a given adsorbent. The development and application of Equations 4-10 through 4-26 have been thoroughly discussed by Crittenden *et al.* (1987a) and Sontheimer *et al.* (1988).

4.2.1 Mass Transfer Parameter Correlations

Column experiments were performed on each of the adsorbents in the MFB design. The total empty bed contact time (EBCT) used in the experiments for each adsorbent was equal to that currently reported in the MFB design. The total EBCT for each adsorbent was divided up into four columns in series to investigate the effect of EBCT on the mass transfer parameters. The breakthrough curves from the column experiments were fit using the PSDM to determine the observed tortuosity and SPDFR for each adsorbate. To fit the column data with the PSDM, the breakthrough curves for each compound were integrated to determine the actual capacity observed in the column experiment. This capacity was then used in single solute PSDM calculations when fitting for the mass transfer parameters of each compound. This assured that the mass transfer parameter fitting was only being affected by the mass transfer parameters and not errors in capacity due to the multicomponent equilibrium description. The breakthrough data from each EBCT column was fit to determine if the mass transfer parameters were a function of EBCT. Correlations were developed based on the results from the fitting procedure to predict the SPDFR and tortuosity for FCs and compounds with no column breakthrough data available. The correlations were developed based on the Freundlich K value of the adsorbate since this is the most descriptive parameter for the FCs whose mass transfer parameters must be predicted.

4.3 Fixed Bed Model For TOC Removal In Unknown Mixtures

The kinetic model for TOC removal in unknown mixtures is based on the results of the TOC FCA analysis performed on the TOC isotherms. The TOC FCs determined from fitting the isotherms are simply input as the compounds present in the influent to the columns. IAST is used to predict the multicomponent equilibrium in the system between the TOC FCs. The mass transfer parameters for the TOC FCs are calculated using the correlations developed from the column breakthrough curves. The PSDM is run as a six component mixture (six TOC FCs) with a nonadsorbing fraction. The TOC contribution of each component is summed with the nonadsorbing fraction to get the overall TOC breakthrough profile from the column at any point during the run.

4.4 Fixed Bed Model For Target Compound Removal In Unknown Mixtures

The kinetic model for target compound removal in unknown mixtures is based on the results of the FCA applied to the tracer isotherms. The tracer FCs determined from fitting the isotherms are the compounds present in the influent to the columns along with the target compound of interest. IAST is used to predict the competitive adsorption interactions between the target compound and the tracer FCs. The mass transfer parameters are calculated using the correlations developed from the column breakthrough curves. The PSDM is run as a six component mixture (five FCs and the target compound). The PSDM output is the breakthrough of the target compound over time.

4.5 Fixed Bed Model For Adsorption Beds In Series Operation

The fixed bed model needed to include different adsorbent beds in series for modeling of the MFB. The FCA equilibrium description was developed in a manner to easily account for different adsorbent beds in series operation. The FCs were determined in a manner such that the effluent concentration of a FC from one bed was identical to the influent FC concentration to the next bed. The FC Freundlich K and 1/n values are simply changed as it moves into a different bed according to the isotherm fitting results (Tables 3-7 and 3-11). The mass transfer parameters for the FCs are calculated from the correlation based on Freundlich K values as the FCs pass between adsorbents.

4.6 Scope Of Adsorption Kinetics Experiments

All column experiments were performed using the procedure included as Appendix IV. Solutions were prepared and analyses were performed as outlined in Chapter 2. Samples from the column experiments were analyzed for TOC, TCE, toluene, m-xylene, 1,2,4-TCB, naphthalene, and pH. The physical properties of each adsorbent used in the column studies are included in Table 2-3.

One column study was performed with the purpose of verifying the ion exchange and adsorption models with both ion exchange and adsorption columns connected in series. The experimental apparatus included all of the ion exchange resins and adsorbents in the present MFB design at their currently reported EBCTs. The verification study was performed using the shower and handwash ersatz water. The column experiment data is included in Appendix VI.

4.7 Fixed Bed Adsorption Modeling Results

4.7.1 Mass Transfer Parameter Correlations

The breakthrough profiles from the adsorption column studies were fit using the PSDM to determine the optimum mass transfer parameters, μ_i and $SPDFR_i$, for each adsorbate in the ersatz water. The breakthrough profiles from all four EBCTs were fit to determine if the mass transfer parameters were a function of contact time for the adsorbents. The breakthrough curves were fit on a single solute basis using the integrated column capacity. The lower limit used for the SPDFR in the fitting procedure was 0.01 since a SPDFR of 0.01 means pore diffusion accounts for nearly 100 percent of the intraparticle mass transfer. The tortuosity was then altered to determine the best fit of the

Table 4-1. Ersatz water used in column experiments

Compound	Time average concentration, mg/L 580-26	APA	XAD-4
TCE	148.02	174.24	169.57
toluene	80.37	92.41	84.10
m-xylene	21.74	26.29	21.05
1,2,4-TCB	1.61	2.14	2.18
naphthalene	0.319	0.290	0.319
TOC	596.7	643.7	612.2
pH	9.3	9.0	9.0

breakthrough curves. The average influent concentrations to the adsorption columns are included in Table 4-1.

The results of fitting the 580-26 GAC column breakthrough curves are included in Table 4-2. The results indicate that pore diffusion controls the intraparticle mass transfer rate for all compounds except SCMT based on the SPDFR values obtained from fitting. There was no breakthrough observed for either the 1,2,4-TCB or naphthalene during the run time of the columns. SCMT broke through the columns first and had the highest concentration in the ersatz water. The other compounds passed through the column after SCMT had preadsorbed onto the adsorbent. The SCMT may have covered the surface of the adsorbent causing the surface diffusion mechanism to be virtually eliminated for the compounds passing through the column after SCMT. The correlation developed from the data predicts a SPDFR value of 0.01 for all compounds except SCMT which has a SPDFR of 1.0. The tortuosity predicted from the correlation is 5.0 for all compounds except SCMT which had an observed tortuosity of 1.0. The mass transfer parameters

Table 4-2. Mass transfer parameter fitting results for 580-26 ersatz columns.

	EBCT = 15.2 min.		EBCT = 30.7 min.		EBCT = 46.0 min.		EBCT = 60.8 min.	
Compound	SPDFR	Tortuosity	SPDFR	Tortuosity	SPDFR	Tortuosity	SPDFR	Tortuosity
TCE	0.01	5.0	0.01	5.0	0.01	5.0	0.01	5.0
Toluene	0.01	5.0	0.01	5.0	0.01	5.0	0.01	5.0
m-Xylene	0.01	5.0	0.01	5.0	0.01	5.0	0.01	5.0
1,2,4-TCB	NA	NA	NA	NA	NA	NA	NA	NA
Naphthalene	NA	NA	NA	NA	NA	NA	NA	NA
SCMT	1.00	1.0	1.00	1.0	1.00	1.0	1.00	1.0
NA means no column breakthrough data to fit								

were found to be independent of EBCT.

The mass transfer parameter fitting results for the APA GAC columns are presented in Table 4-3. Breakthrough of 1,2,4-TCB and naphthalene was only observed in the first APA column. The SPDFR results indicate that pore diffusion controls the intraparticle mass transfer rate for all compounds except SCMT as it did for the 580-26. The tortuosity required to fit the data decreased as the strength of the adsorbing compound increased. The correlation for the mass transfer parameters for APA was developed based on the Freundlich K value of the compound and is independent of EBCT. The SPDFR correlation involves setting the SPDFR of any compound to 0.01 except SCMT which was assigned a SPDFR of 1.0. The correlation developed from fitting the column data for prediction of tortuosity for compounds on APA based on Freundlich K value was the following:

$$\mu_i = \left\{ \begin{array}{l} 5.0 \text{ for } K_i \le 38 \\ -5.9 \times \mathrm{Log}_{10} K_i + 14.3 \text{ for } 38 < K_i < 183 \\ 1.0 \text{ for } K_i \ge 183 \end{array} \right\} \quad K\ units: \left(\frac{mg}{g}\right)\left(\frac{L}{mg}\right)^{\frac{1}{n}} \qquad (4\text{-}27)$$

The mass transfer parameter fitting results for the XAD-4 resin columns are presented in Table 4-4. Breakthrough of 1,2,4-TCB was observed only in the first column. Breakthrough of naphthalene was observed through the two XAD-4 columns with the shortest contact times. The fitting results for the SPDFR and tortuosity indicate that surface diffusion is about five times faster than pore diffusion. This may be due to the fact that XAD-4 is a macroporous adsorbent with larger pores than the granular activated carbons. The SPDFR of each FC and target compound on XAD-4 resin is simply set to 5.0 and the tortuosity is set equal to 1.0 for PSDM calculations based on the results of fitting the XAD-4 breakthrough curves. The mass transfer parameters are also independent of the EBCT based on the breakthrough curve fits.

4.7.2 580-26 GAC TOC Breakthrough Modeling With The TOC FCs

TOC breakthrough from the four 580-26 GAC columns was predicted using the 6 TOC FCs determined from fitting the 580-26 ersatz TOC isotherms and a nonadsorbing

Table 4-3. Mass transfer parameter fitting results for APA ersatz columns.

	EBCT = 4.1 min.		EBCT = 7.9 min.		EBCT = 12.0 min.		EBCT = 15.9 min.	
Compound	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**
TCE	0.01	5.0	0.01	5.0	0.01	5.0	0.01	5.0
Toluene	0.01	5.0	0.01	5.0	0.01	5.0	0.01	5.0
m-Xylene	0.01	2.0	0.01	2.0	0.01	2.0	0.01	2.0
1,2,4-TCB	0.01	1.0	NA	NA	NA	NA	NA	NA
Naphthalene	0.01	1.0	NA	NA	NA	NA	NA	NA
SCMT	1.00	1.0	1.00	1.0	1.00	1.0	1.00	1.0
NA means no column breakthrough data to fit								

Table 4-4. Mass transfer parameter fitting results for XAD-4 ersatz columns.

	EBCT = 4.4 min.		EBCT = 8.8 min.		EBCT = 13.0 min.		EBCT = 17.2 min.	
Compound	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**	**SPDFR**	**Tortuosity**
TCE	5.00	1.0	5.00	1.0	5.00	1.0	5.00	1.0
Toluene	5.00	1.0	5.00	1.0	5.00	1.0	5.00	1.0
m-Xylene	5.00	1.0	5.00	1.0	5.00	1.0	5.00	1.0
1,2,4-TCB	5.00	1.0	NA	NA	NA	NA	NA	NA
Naphthalene	5.00	1.0	5.00	1.0	NA	NA	NA	NA
SCMT	5.00	1.0	5.00	1.0	5.00	1.0	5.00	1.0
NA means no column breakthrough data to fit								

fraction. The mass transfer parameters of the TOC FCs (SPDFR and tortuosity) were determined using the correlations developed for 580-26 GAC in Section 4.7.1. The molar volume of all the TOC FCs was assumed to be 150 cm^3/mol for liquid diffusivity calculations. The initial concentration of each TOC FC was scaled on a TOC concentration basis to account for differences in the initial TOC of the ersatz water used in the isotherm and column experiments. The makeup of the ersatz water used for the 580-26 ersatz water column experiments is included in Table 4-1. The TOC FC parameters used to predict the 580-26 TOC breakthrough are included in Table 4-5.

The experimental TOC breakthrough profiles and PSDM predictions are compared for the four empty bed contact times studied in Figures 4-1 through 4-4. The model prediction for the 15.2 minute EBCT column agrees well with the data and appears to accurately describe the capacity and kinetics observed in the column. The model prediction for the 30.7 minute EBCT column is slightly later than the data. The model

Table 4-5. TOC FCs input to PSDM for ersatz column TOC breakthrough prediction

	Molecular	Percent	Molar	580-26 GAC			APA GAC			XAD-4 Resin		
Component	Weight	Carbon	Volume*	SPDFR	Tortuosity	C_0 mg/L	SPDFR	Tortuosity	C_0 mg/L	SPDFR	Tortuosity	C_0 mg/L
TOC FC1	357	60	150	1.00	1.0	681.33	1.00	1.0	747.75	5.00	1.0	711.11
TOC FC2	111	50	150	0.01	5.0	59.48	0.01	1.2	65.28	5.00	1.0	62.08
TOC FC3	111	50	150	0.01	5.0	62.06	0.01	1.0	68.12	5.00	1.0	64.78
TOC FC4	111	50	150	0.01	5.0	67.63	0.01	1.0	74.23	5.00	1.0	70.59
TOC FC5	111	50	150	0.01	5.0	85.71	0.01	1.0	94.07	5.00	1.0	89.46
TOC FC6	111	50	150	0.01	5.0	0.92	0.01	1.0	1.01	5.00	1.0	0.96

*Units are cm^3/mol

predictions for the 46.0 and 60.8 minute EBCT columns are also later than the experimental breakthrough. This indicates that the TOC capacity of the 580-26 GAC columns is slightly overpredicted with the 580-26 TOC FCs. The steepness of the breakthrough curve for both the model prediction and experimental data are similar implying that the mass transfer parameters used for the TOC FCs are adequate.

4.7.3 APA TOC Breakthrough Modeling With The TOC FCs

TOC breakthrough from the four APA columns was predicted using the six TOC FCs determined from fitting the APA ersatz TOC isotherms and a nonadsorbing fraction. The mass transfer parameters used for the TOC FCs were determined using the correlations developed in Section 4.7.1 for APA GAC. The molar volume of all the TOC FCs was assumed to be 150 cm^3/mol. The TOC FC initial concentrations from the isotherm fits were scaled so the overall TOC was equal to that of the ersatz water used in the APA column studies. The experimental TOC breakthrough profiles and the PSDM predictions are compared for the EBCTs studied for APA GAC in Figures 4-5 through 4-8. The mass transfer parameters used for the FCs describe the steepness of the breakthrough curves quite well. The model breakthrough prediction agrees well with the data for the 4.1 minute EBCT column. The predicted breakthrough is after the data for the 7.9, 12.0, and 15.9 minute EBCT columns. This indicates that the TOC FCs determined from fitting the APA TOC isotherms overpredict the APA GAC column capacity.

4.7.4 XAD-4 TOC Breakthrough Modeling With The TOC FCs

TOC breakthrough from the four XAD-4 columns was predicted using the six TOC FCs determined from fitting the XAD-4 ersatz TOC isotherms and a nonadsorbing fraction. The mass transfer parameters used for the XAD-4 TOC FCs were determined using the correlations developed from fitting the XAD-4 ersatz column breakthrough curves. The molar volume of the TOC FCs was assumed to be 150 cm^3/mol. The initial concentrations of the TOC FCs were again scaled to account for differences in overall TOC concentration from the XAD-4 ersatz isotherms and the column influent. The experimental TOC breakthrough profiles and the PSDM predictions are compared for the four EBCTs studied for XAD-4 in Figures 4-9 through 4-12. The model prediction agrees well with the data for the 4.4 minute EBCT column. The results for the 8.8, 13.0, and 17.2 minute EBCT columns indicate that the mass transfer parameters may be slightly off for the FCs on this adsorbent. The model predicted breakthrough begins slightly later than the experimental breakthrough but crosses the experimental breakthrough curve and then rises above the experimental breakthrough. The model predicted mass transfer is slightly too fast in these cases causing the predicted breakthrough curves to be steeper than the data. The capacity observed in the experimental columns is close to that of the model prediction.

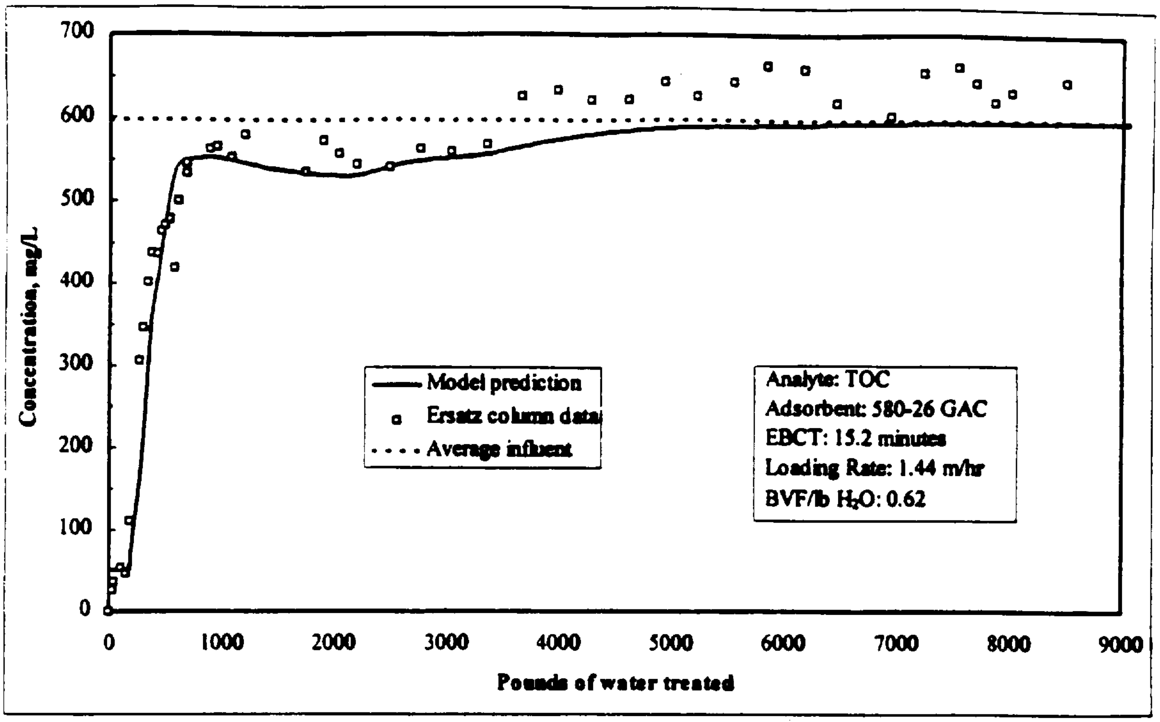

Figure 4-1. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on 580-26.

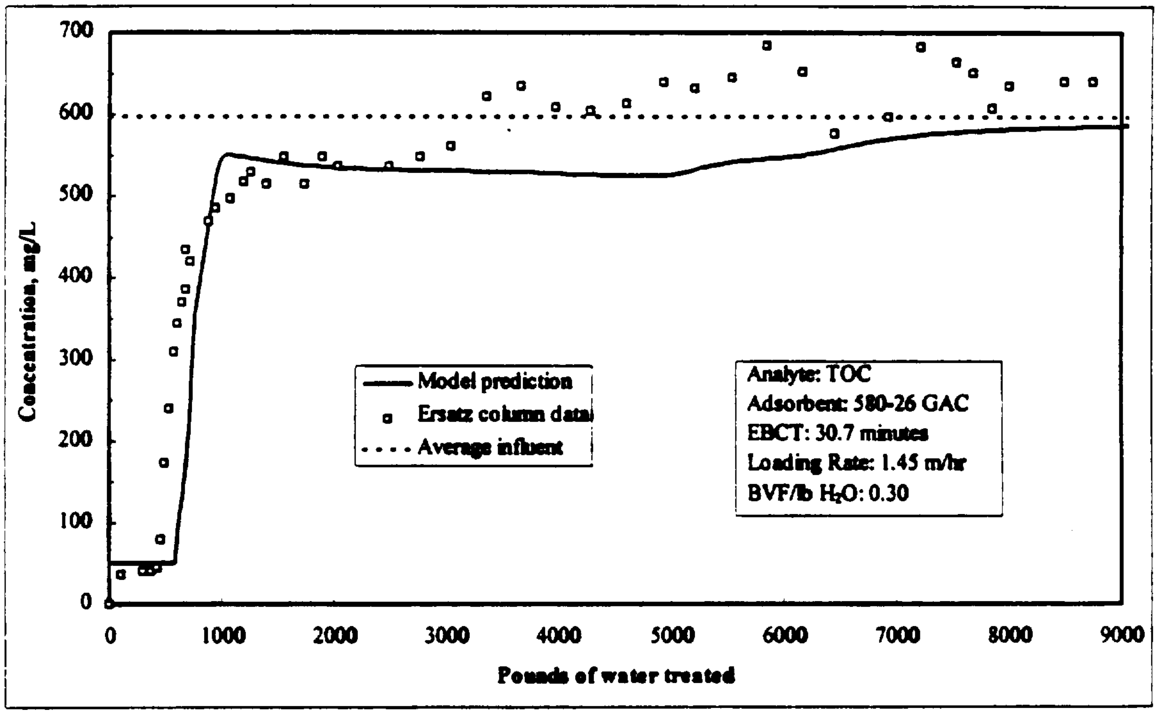

Figure 4-2. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on 580-26.

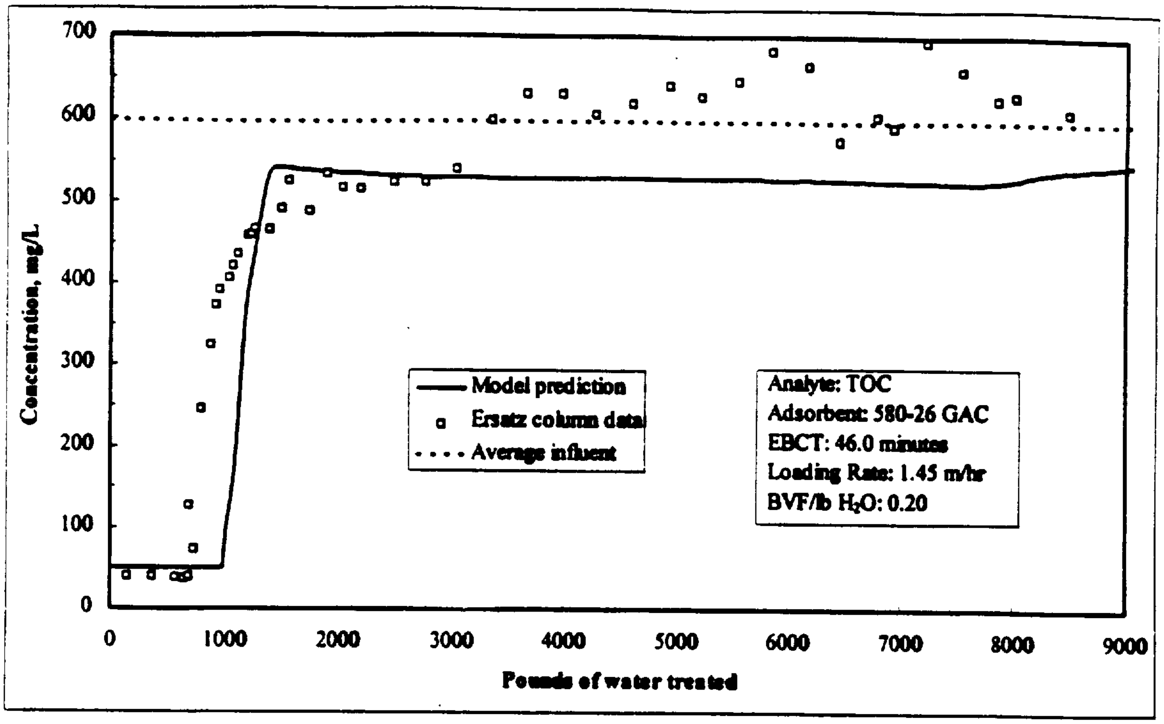

Figure 4-3. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on 580-26.

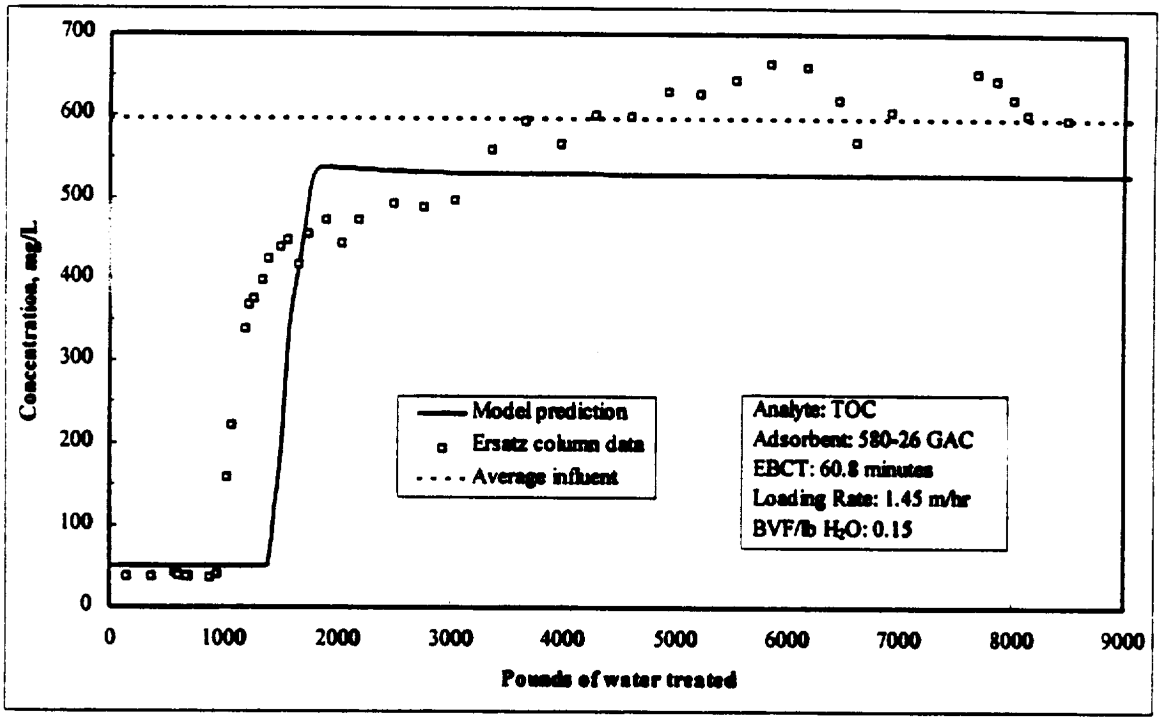

Figure 4-4. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on 580-26.

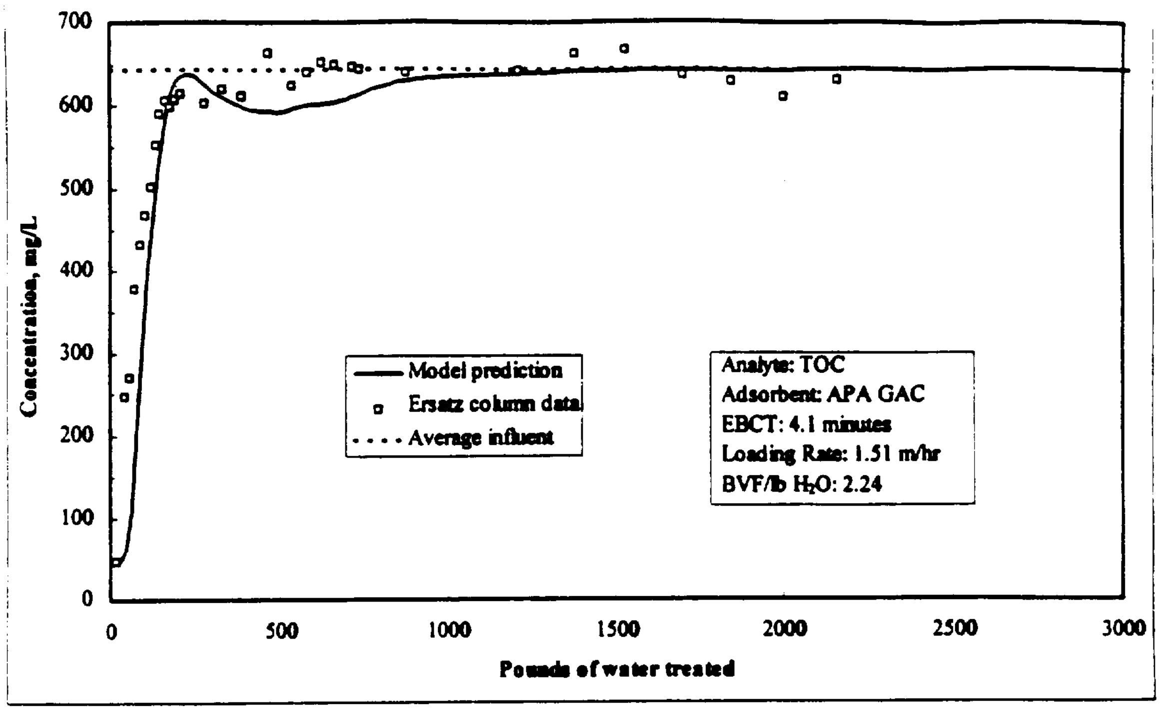

Figure 4-5. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on APA.

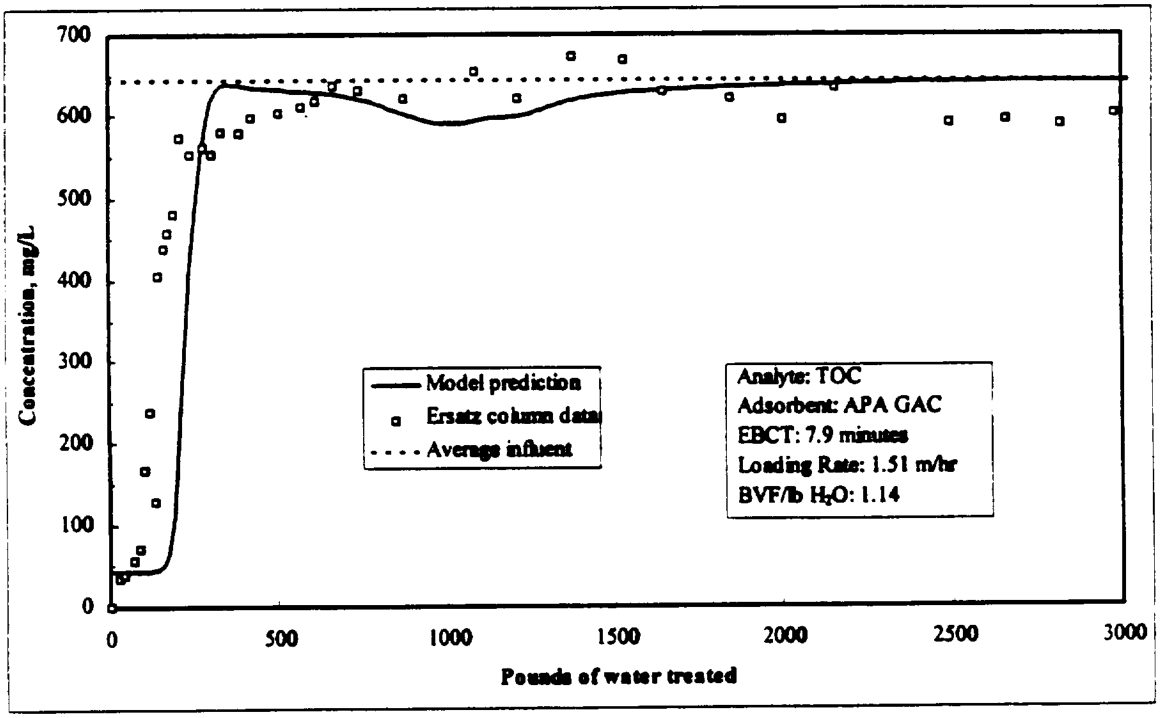

Figure 4-6. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on APA.

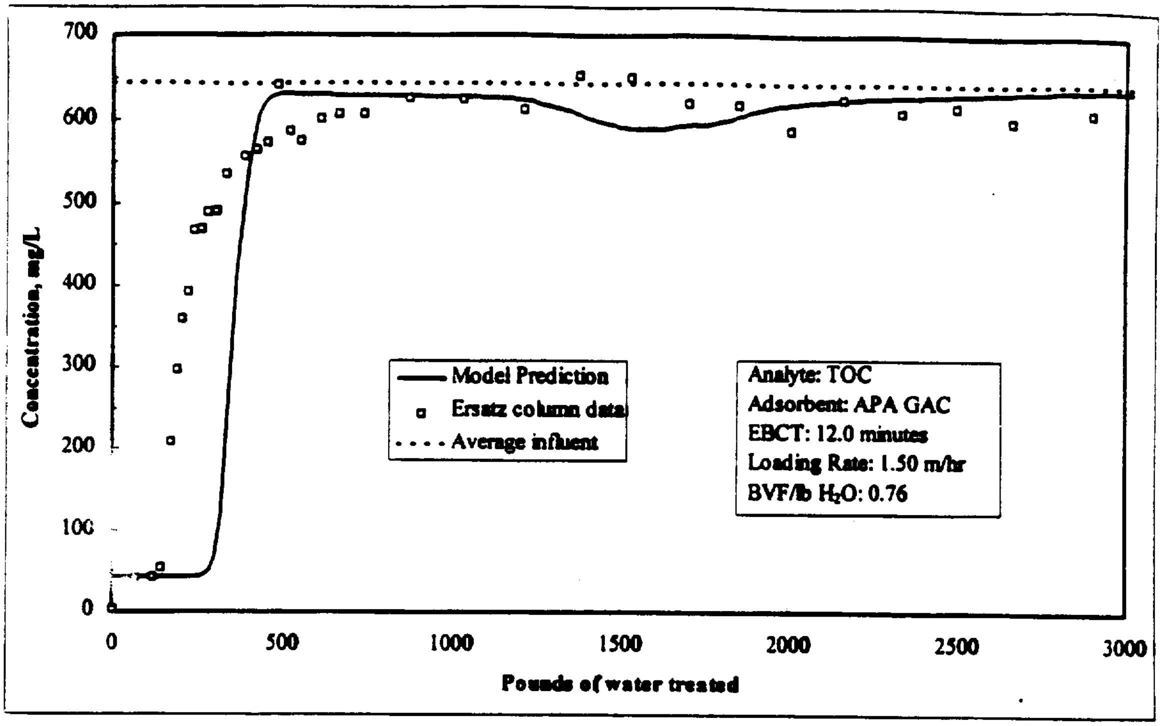

Figure 4-7. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on APA.

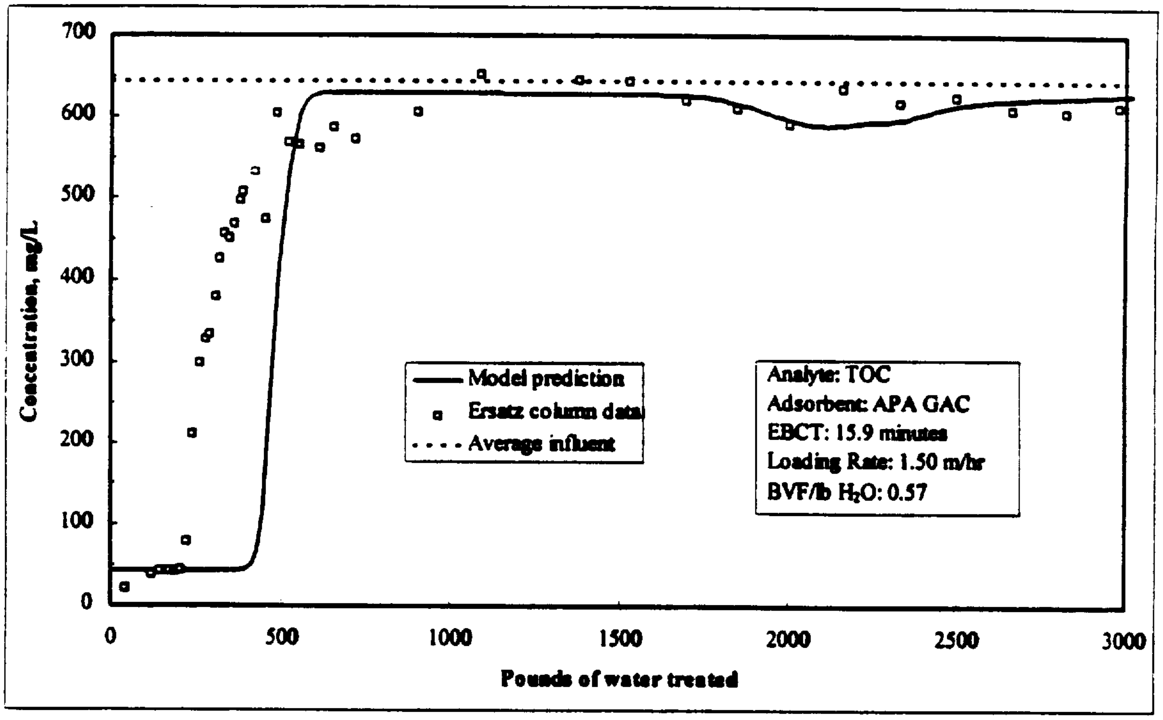

Figure 4-8. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on APA.

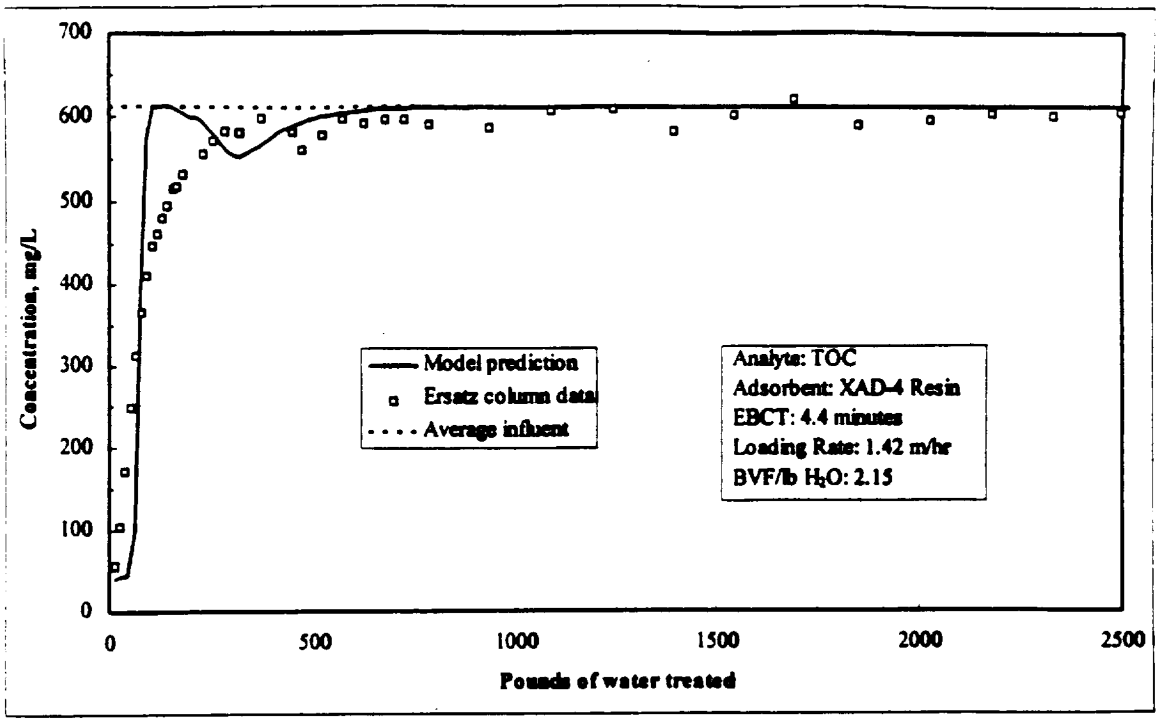

Figure 4-9. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on XAD-4.

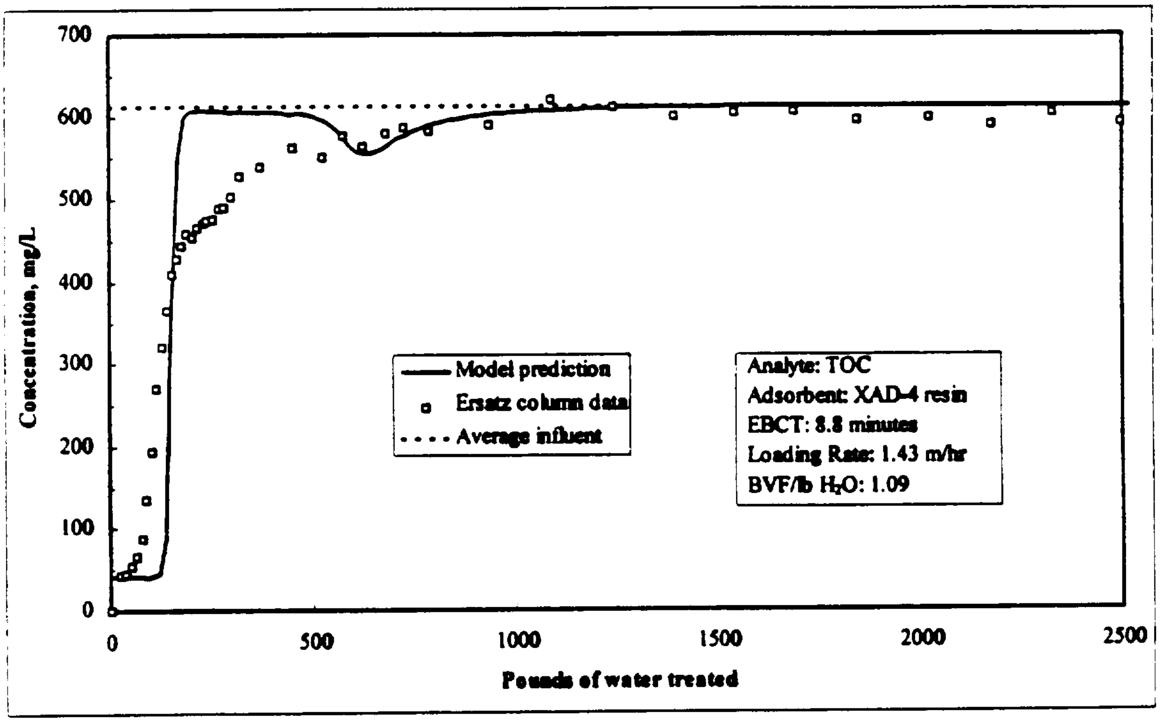

Figure 4-10. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on XAD-4.

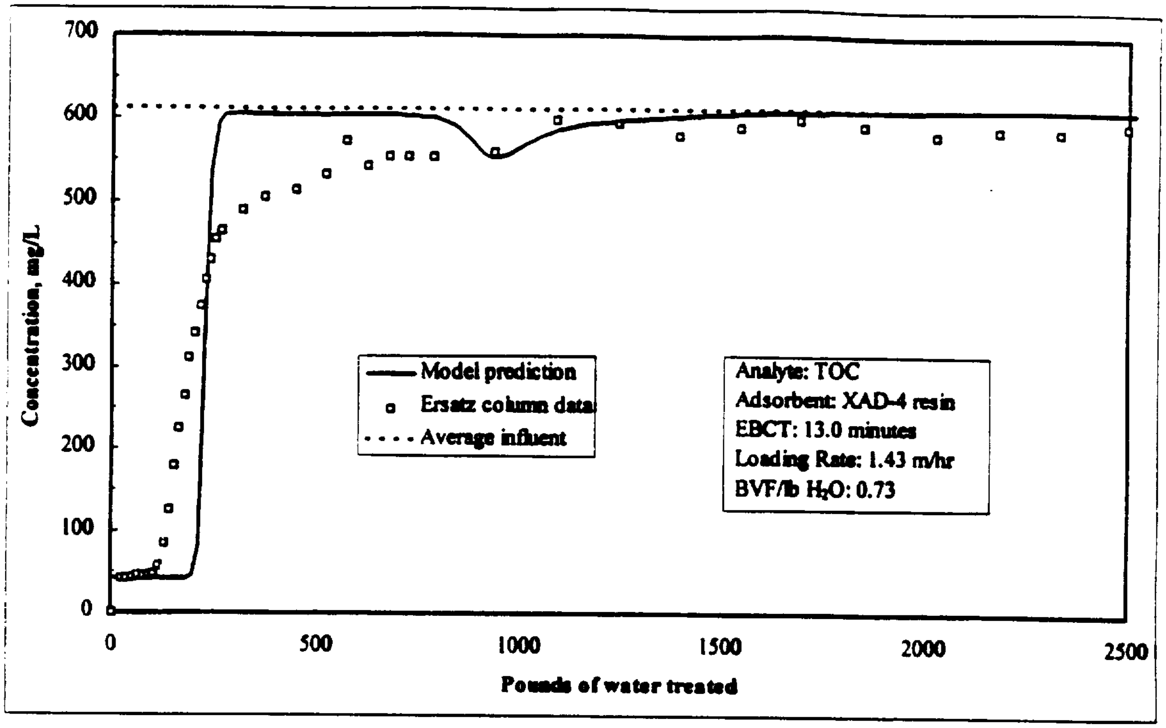

Figure 4-11. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on XAD-4.

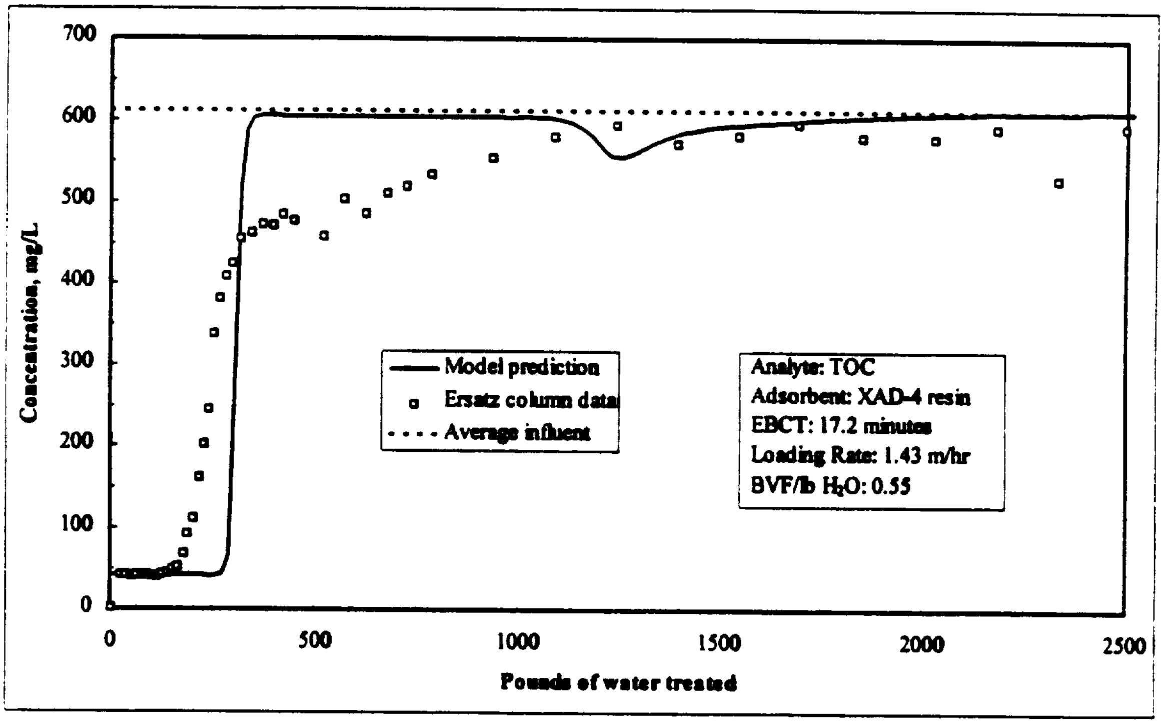

Figure 4-12. PSDM TOC breakthrough prediction using TOC FCs determined from simultaneous fitting of dilute and nondilute ersatz water TOC isotherms on XAD-4.

4.7.5 Target Compound Breakthrough From 580-26 GAC Fixed Beds

Target compound breakthrough from the four 580-26 GAC columns was predicted using the five tracer FCs (determined from fitting the 580-26 ersatz tracer isotherms) and the target compound in PSDM calculations. The mass transfer parameters of the tracer FCs (SPDFR and tortuosity) were determined using the correlations developed for 580-26 in Section 4.7.1. The molar volume of each FC was assumed to be 150 cm^3/mol for liquid diffusivity calculations. The initial concentration of each tracer FC was scaled to account for differences in the initial TOC of the ersatz water used in the isotherm and column experiments. The makeup of the ersatz water used for the 580-26 ersatz water column experiments was included in Table 4-1. The tracer FC parameters used for prediction of the target compound breakthrough profiles are included in Table 4-6. The FC Freundlich K and 1/n values were those determined from fitting the tracer isotherms included in Table 3-7. The target compounds in this case are the known constituents of the ersatz water.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 15.2 minute EBCT column in Figures 4-13 through 4-16. The prediction of SCMT breakthrough, Figure 4-13, agrees well with the data. The predicted breakthrough time corresponds well to the time of experimental breakthrough. The kinetic parameters describe the mass transfer well in the system as the shape of the prediction matches that of the data. However, the breakthrough at concentrations greater than the influent (overshoot) predicted by the model was not observed in the data. This may be due to diffusion interactions between the adsorbates not incorporated into the model. The prediction of TCE breakthrough, Figure 4-14, also compares very well with the data. The model effectively predicted both the capacity and kinetics of the

Table 4-6. Tracer FCs input to PSDM for ersatz column target compound breakthrough predictions.

Component	Molecular Weight	Percent Carbon	Molar Volume*	580-26 GAC			APA GAC			XAD-4 Resin		
				SPDFR	Tortuosity	C_o mg/L	SPDFR	Tortuosity	C_o mg/L	SPDFR	Tortuosity	C_o mg/L
Tracer FC 1	111	50	150	0.01	5.0	274.37	0.01	5.0	299.98	5.00	1.0	284.93
Tracer FC 2	111	50	150	0.01	5.0	19.75	0.01	3.75	21.59	5.00	1.0	20.51
Tracer FC 3	111	50	150	0.01	5.0	15.59	0.01	1.75	17.04	5.00	1.0	16.19
Tracer FC 4	111	50	150	0.01	5.0	41.57	0.01	1.0	45.45	5.00	1.0	43.17
Tracer FC 5	111	50	150	0.01	5.0	688.01	0.01	1.0	752.23	5.00	1.0	714.49

*Units are cm^3/mol

breakthrough. The prediction of toluene breakthrough, Figure 4-15, is not as close to the experimental data as the SCMT and TCE. The model prediction comes later than the experimental data. This may be due to a phenomenon known as counter diffusion. The PSDM assumes that there are no diffusion interactions between the solutes in the system. However, as the more strongly adsorbed compounds travel through the column, the column has been presaturated with the weaker adsorbing compounds and the weak compounds must diffuse out of the adsorbent pores to allow the stronger adsorbates to reach the surface. Toluene is a relatively strong adsorbing compound and counter diffusion may be an issue as the SCMT and TCE have migrated through the column ahead of it. This may cause the experimental data to breakthrough the column sooner than the model predicts for strongly adsorbing compounds. The predicted breakthrough for m-xylene, Figure 4-16, is also later than the experimental data. This may also be due to the issue of counter diffusion as m-xylene is even more strongly adsorbed than toluene so the column would also be preloaded with toluene before m-xylene was adsorbed. 1,2,4-TCB and naphthalene were never observed to break through any of the 580-26 GAC columns during the experiments. The target compound experimental breakthrough profiles and PSDM predictions are compared for the 30.7 minute EBCT column in Figures 4-17 through 4-20. The prediction for SCMT breakthrough, Figure 4-17, occurs slightly before the experimental data. This may be due to the mass transfer parameters as the prediction is steeper than the experimental data. The prediction for TCE shown in Figure 4-18 occurs just after the experimental breakthrough. The difference may be due to error in mass transfer parameters as the predicted capacity appears to be correct. The predictions for toluene and m-xylene shown in Figures 4-19 and 4-20 are both later than the experimental breakthrough. The capacity of toluene appears to be predicted correctly so the error in the prediction may be due to counter diffusion as explained earlier. The PSDM appears to overpredict the capacity for m-xylene in this case.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 46.0 minute EBCT column in Figures 4-21 through 4-24. The prediction of SCMT breakthrough, Figure 4-21, is very close to the experimental data. The model predictions for breakthrough of TCE, toluene, and m-xylene in Figures 4-22, 4-23, and 4-24 respectively, all occur at times later than the experimental breakthrough. The reason for the error in TCE and toluene predictions may again be counter diffusion with preadsorbed compounds. This did not occur for the TCE in the shorter contact time beds. However, as the EBCT increases and the waves get farther apart, the SCMT has more time to preadsorb onto the adsorbent before TCE is adsorbed. The PSDM again appears to overpredict the capacity for m-xylene in the column.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 60.8 minute EBCT column in Figures 4-25 through 4-28. The model accurately predicts the time of breakthrough for SCMT in Figure 4-25. The model prediction appears to have slightly faster kinetics than the experimental data as it has a steeper breakthrough profile. The results for the TCE, toluene, and m-xylene are similar to their results in the 46.0 minute EBCT column as the predictions are all after the data as shown in Figures 4-26, 4-27, and 4-28. However, the spreads between the predictions and the data are somewhat larger at this EBCT. This may be explained due to the longer time for preadsorption of the weaker compounds in the longer EBCT column.

The results of 580-26 ersatz column target compound breakthrough predictions indicate that the model works well for the weakly adsorbing compounds. Counter diffusion may explain the inaccuracy of the breakthrough predictions of the stronger adsorbing compounds. The effects of counter diffusion appear to increase with increases in EBCT. These effects could be fixed through further tuning of the mass transfer parameters. The PSDM may also overpredict the capacity for the most strongly adsorbed compounds in the system.

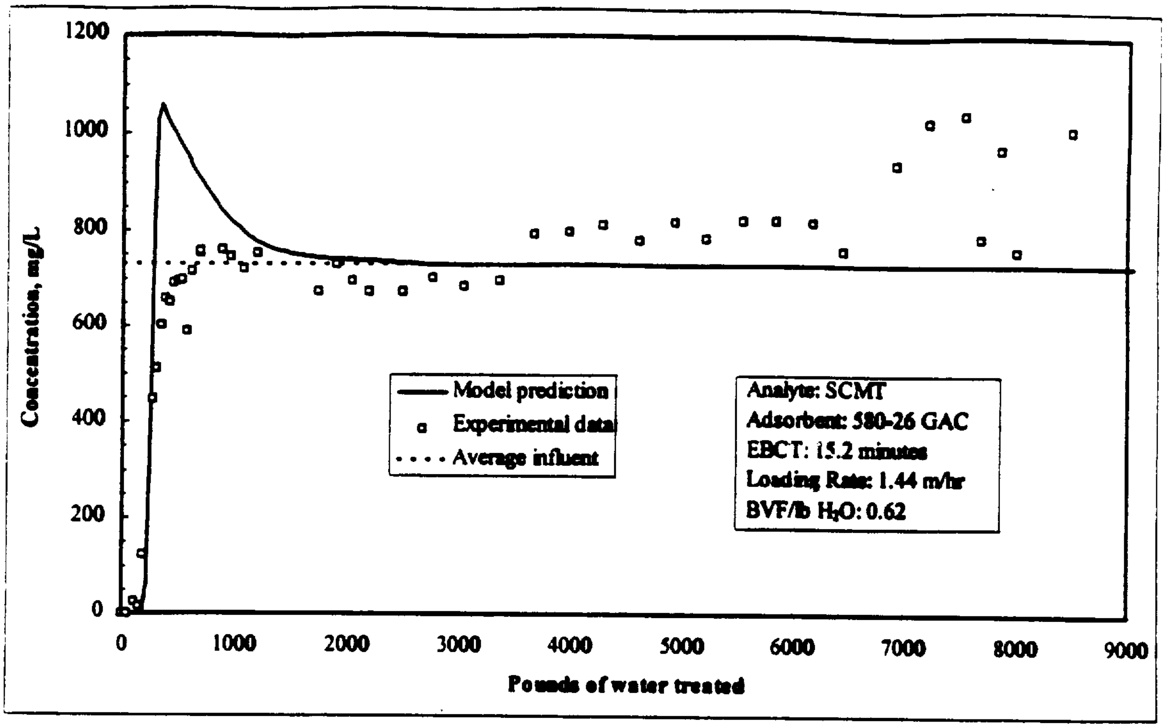

Figure 4-13. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

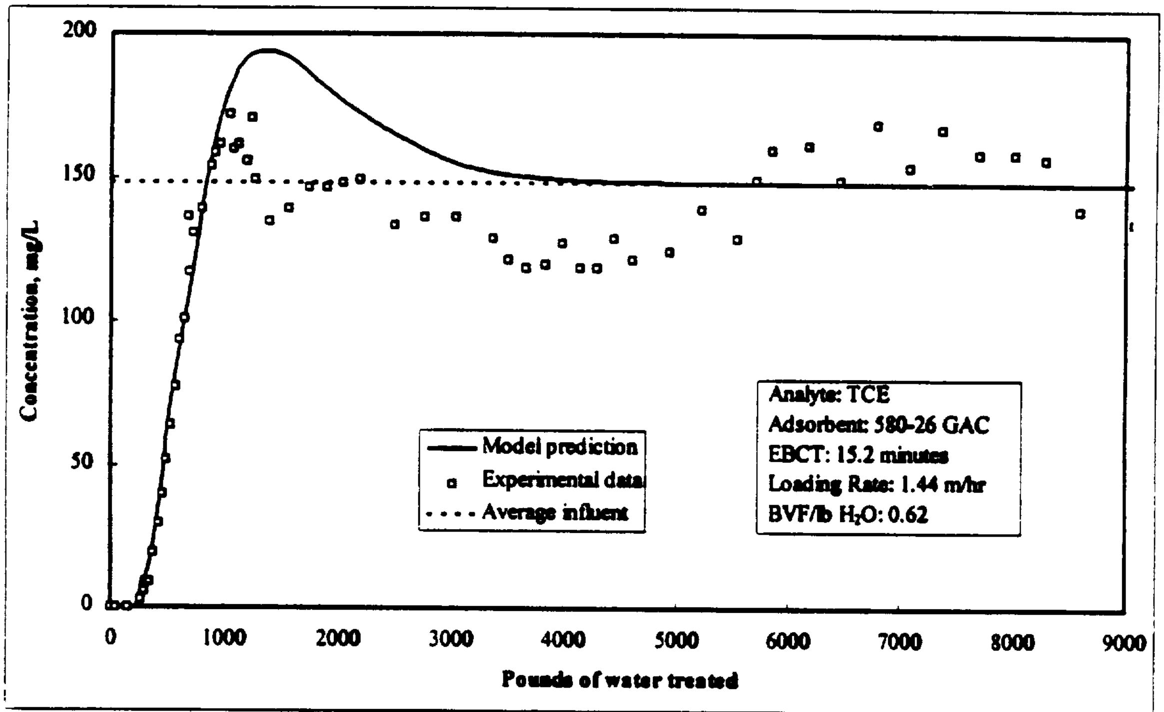

Figure 4-14. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

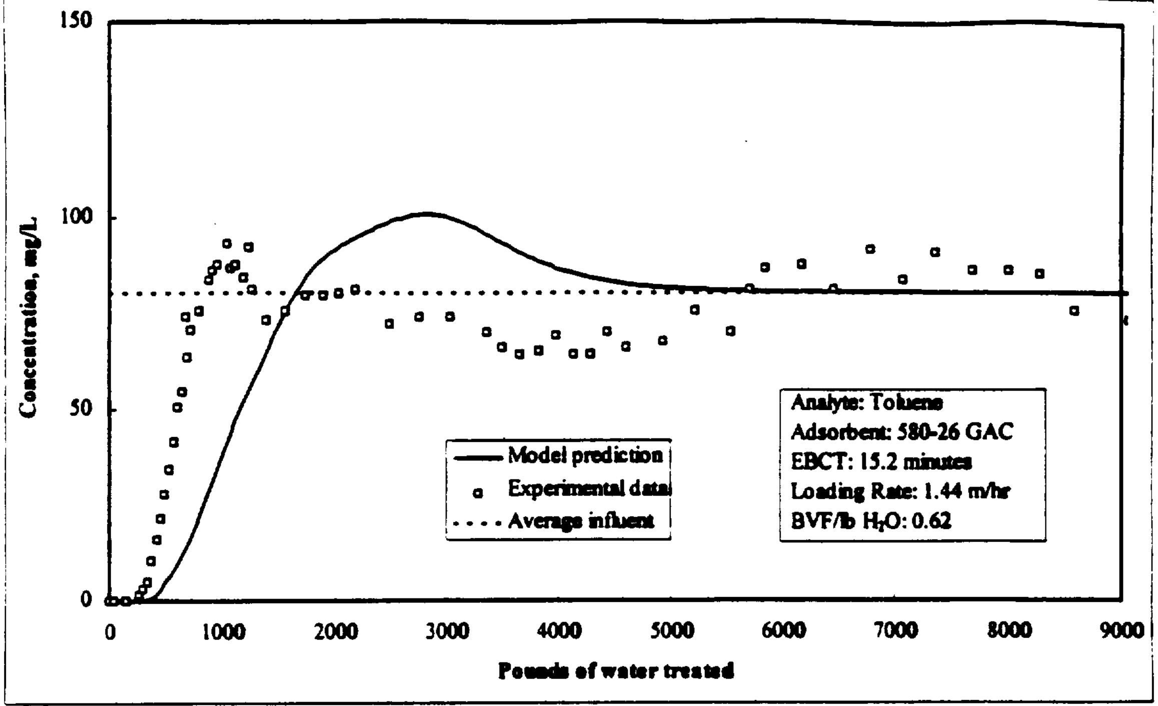

Figure 4-15. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

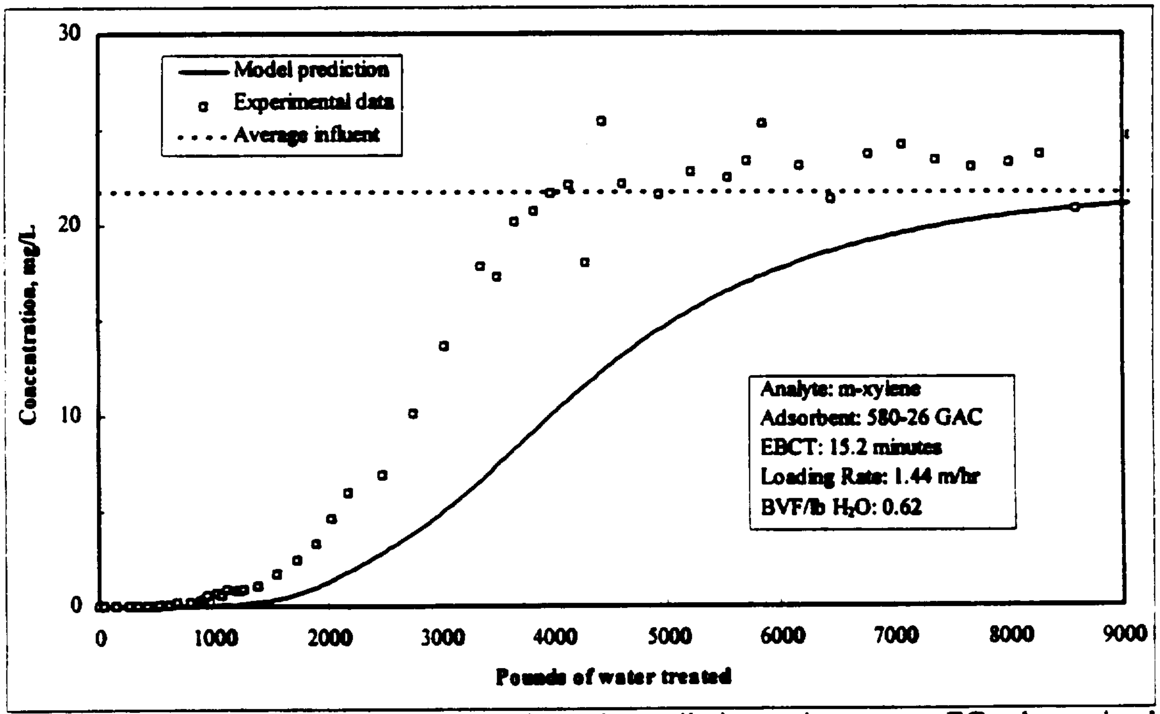

Figure 4-16. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

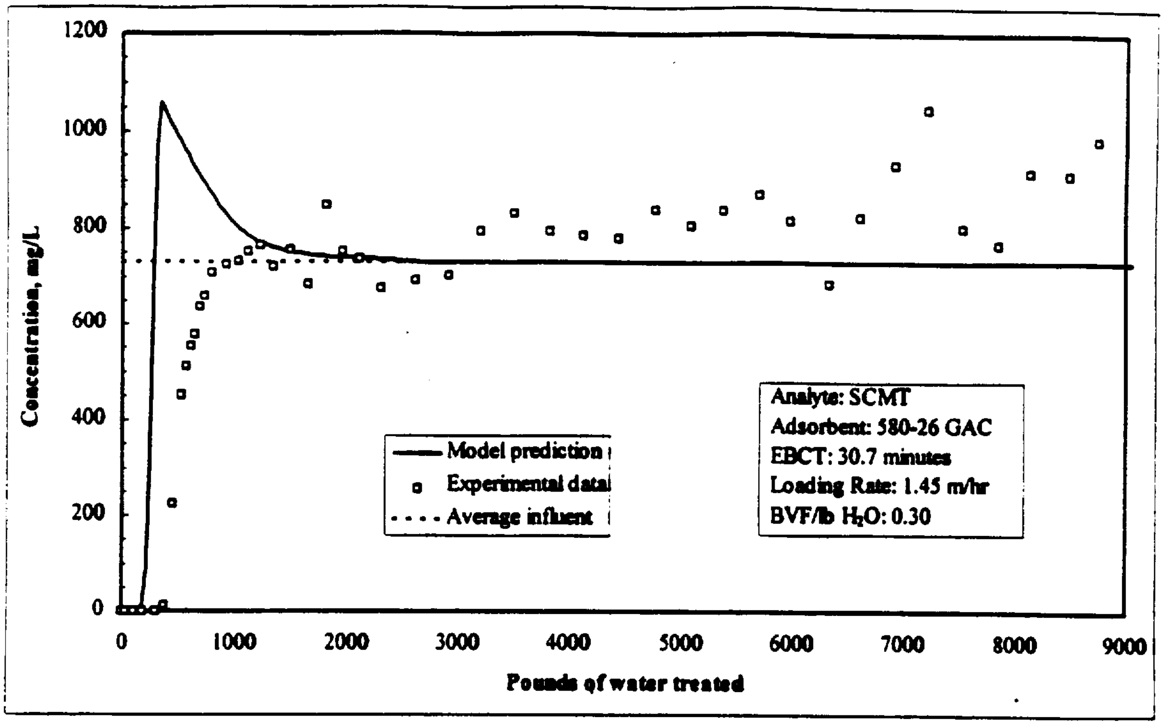

Figure 4-17. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

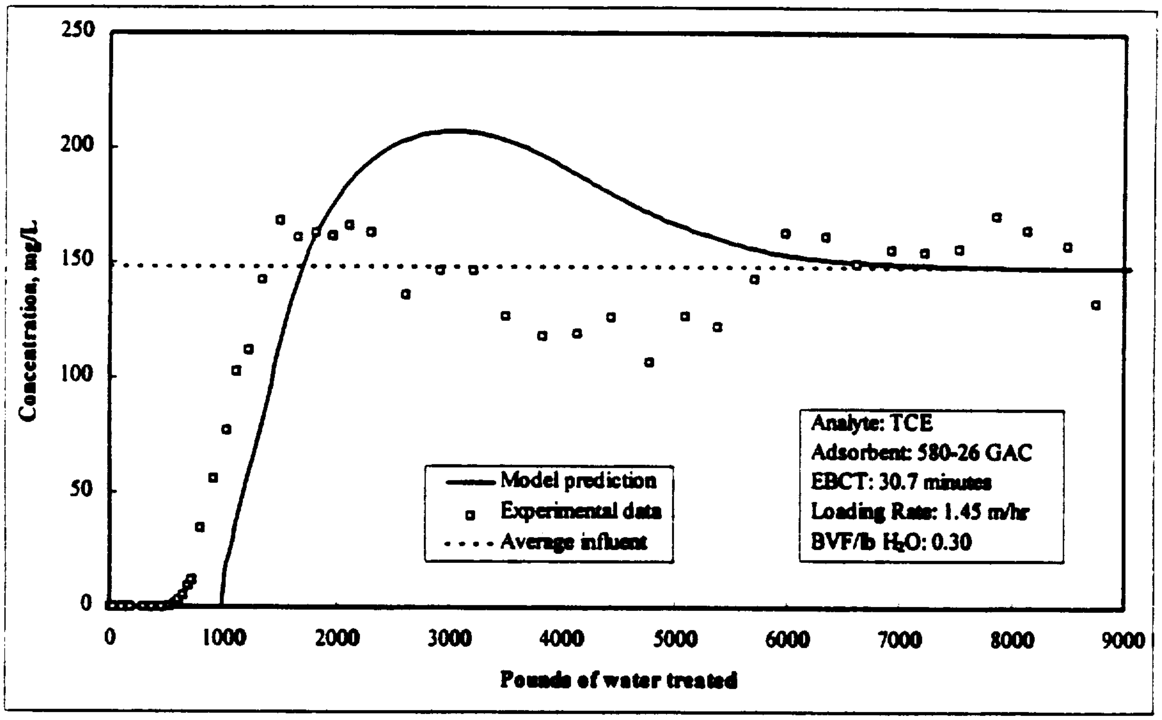

Figure 4-18. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

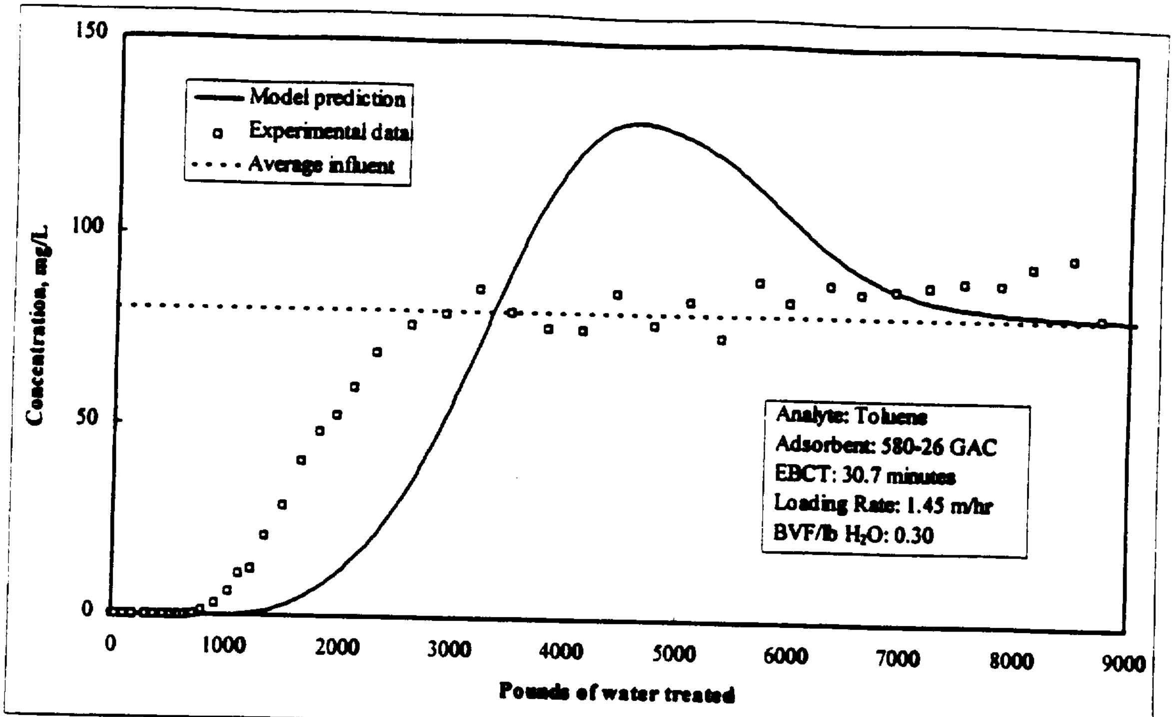

Figure 4-19. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

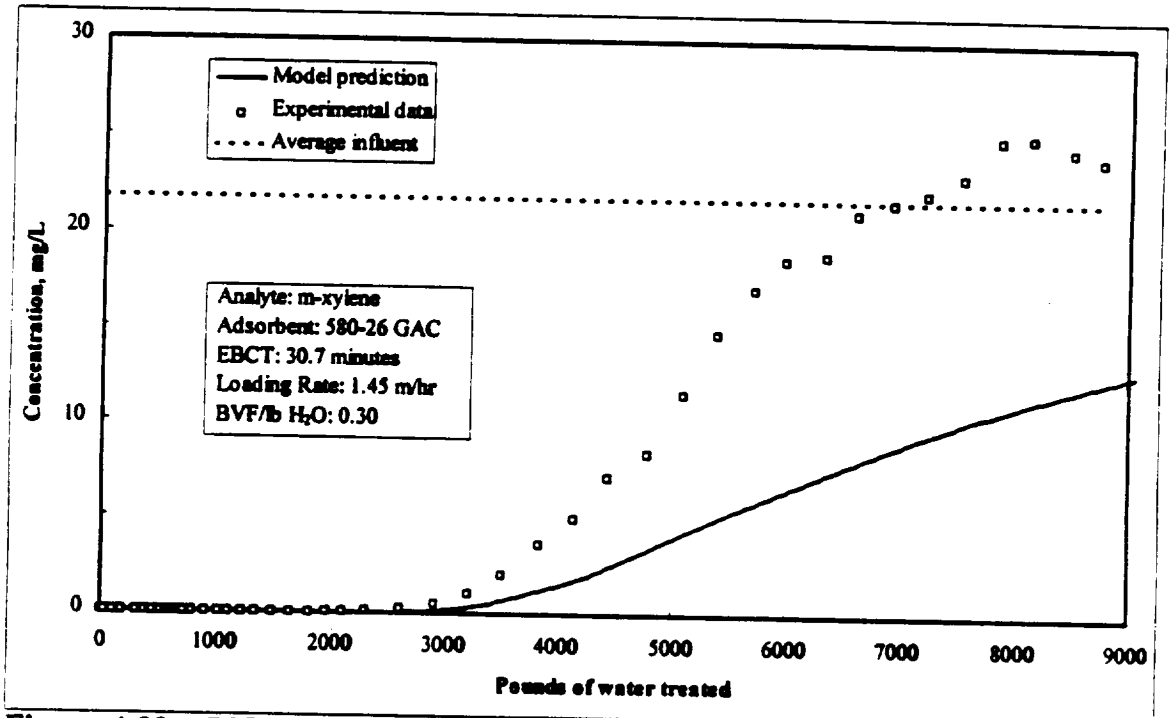

Figure 4-20. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

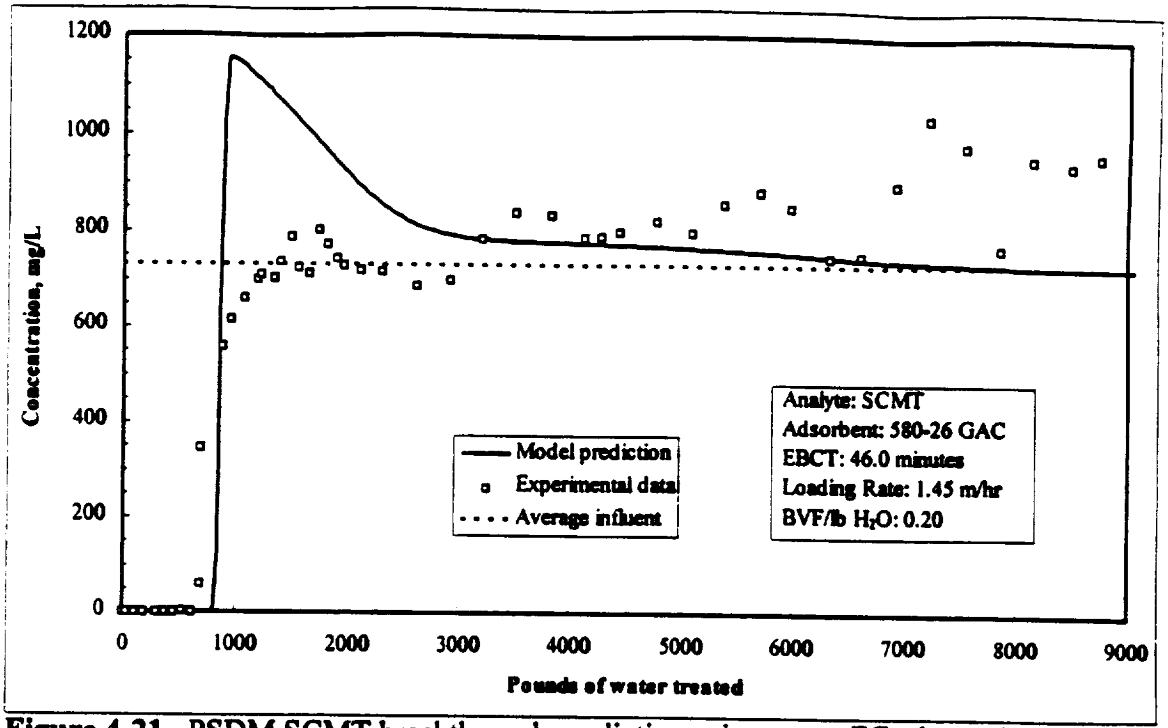

Figure 4-21. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

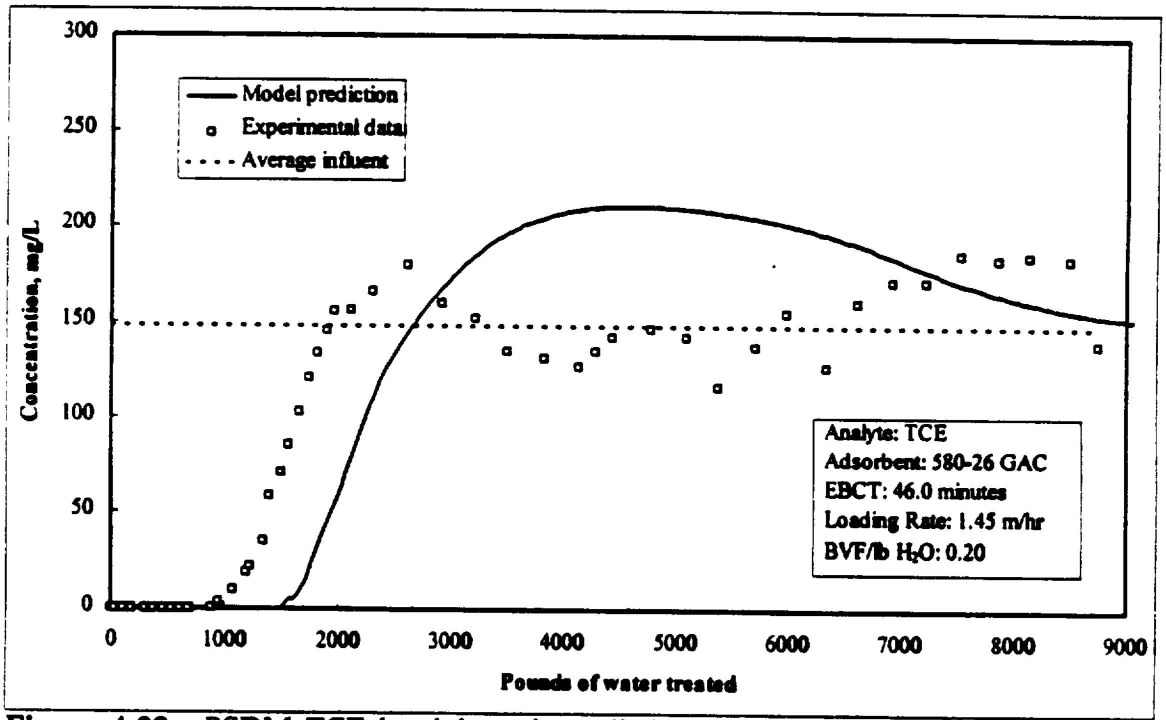

Figure 4-22. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

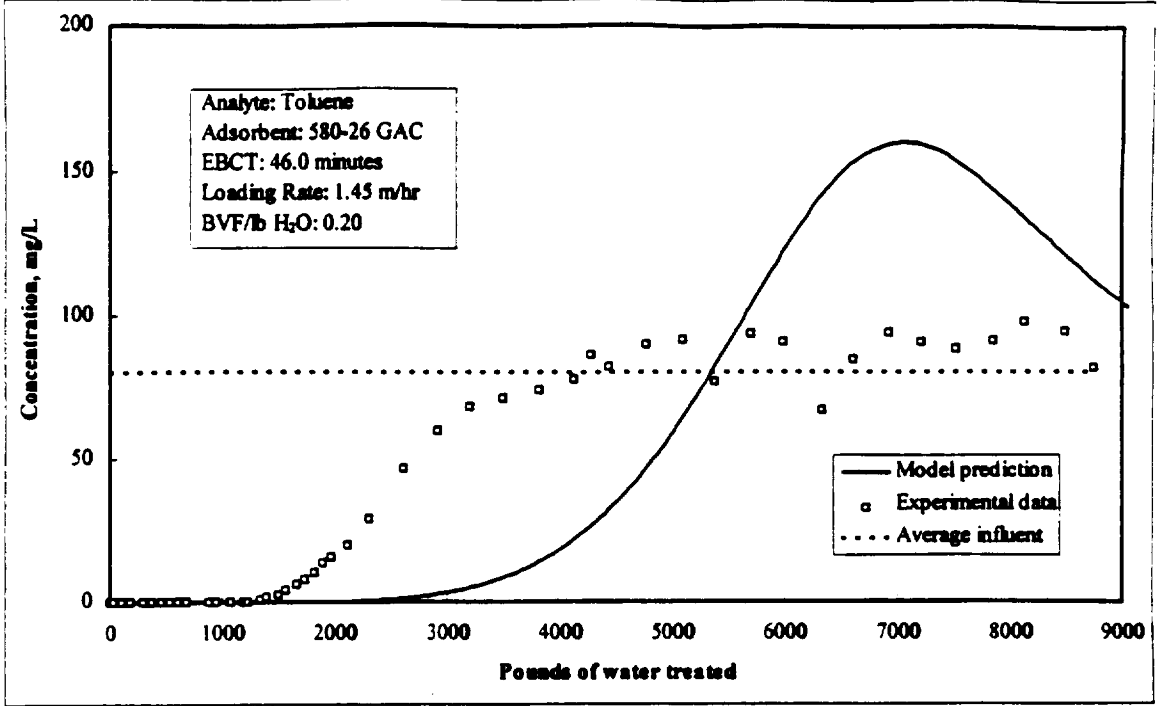

Figure 4-23. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

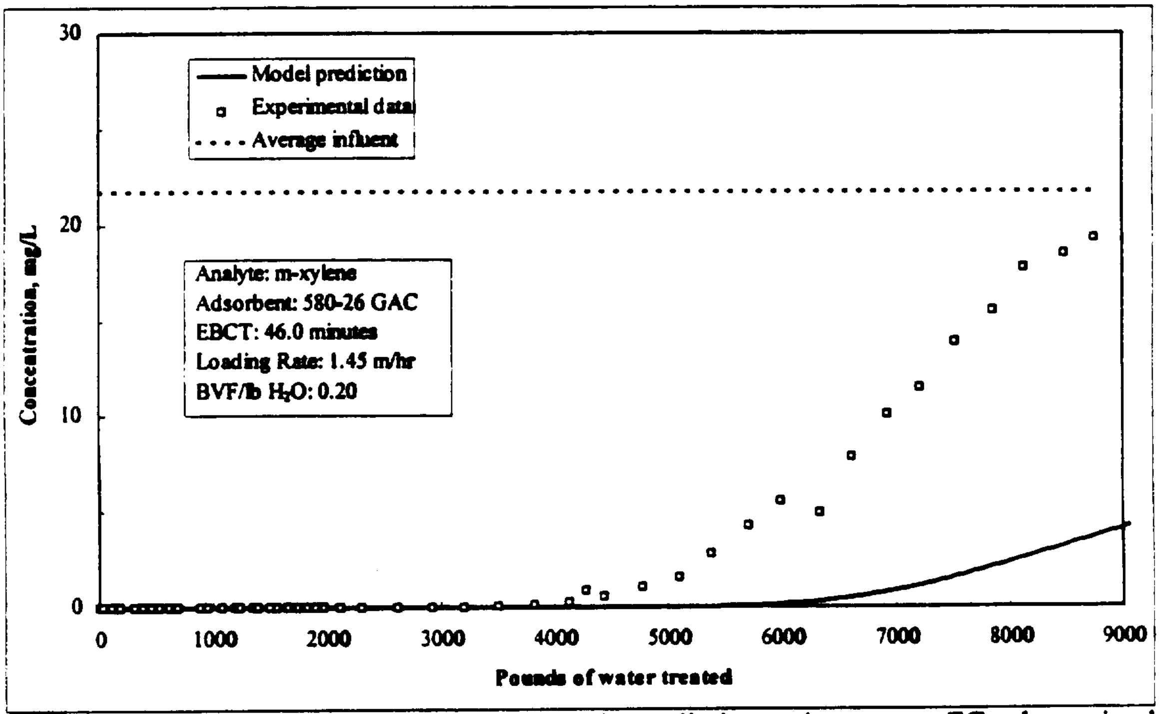

Figure 4-24. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

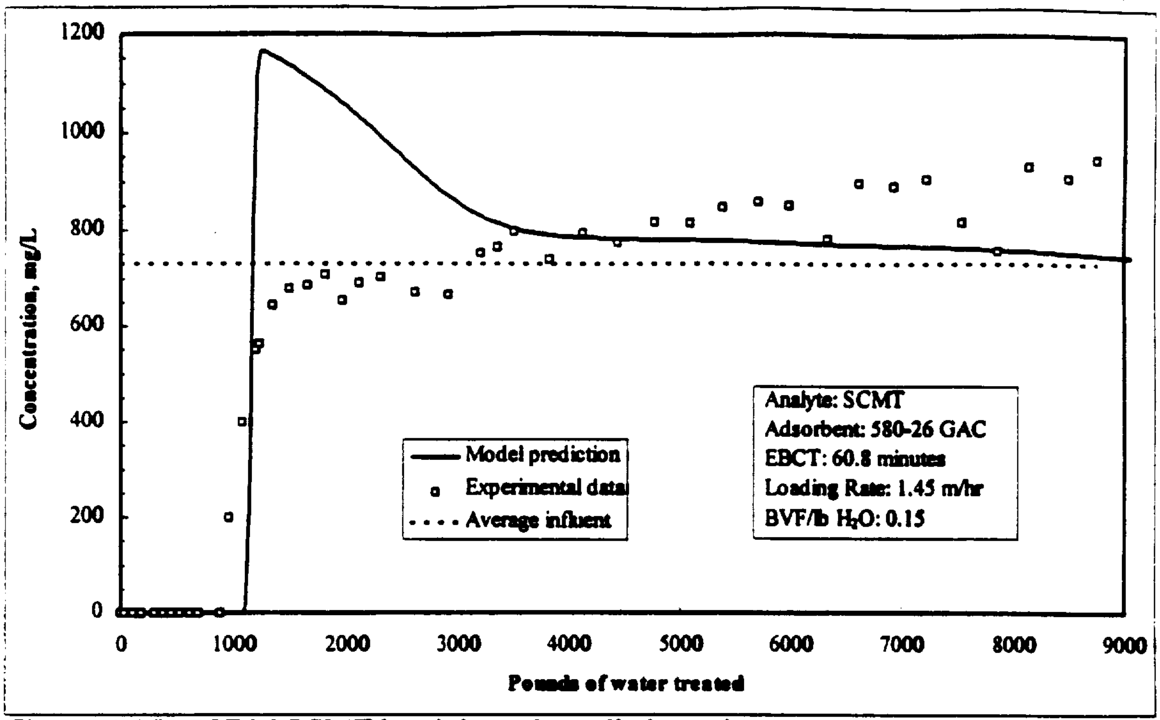

Figure 4-25. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

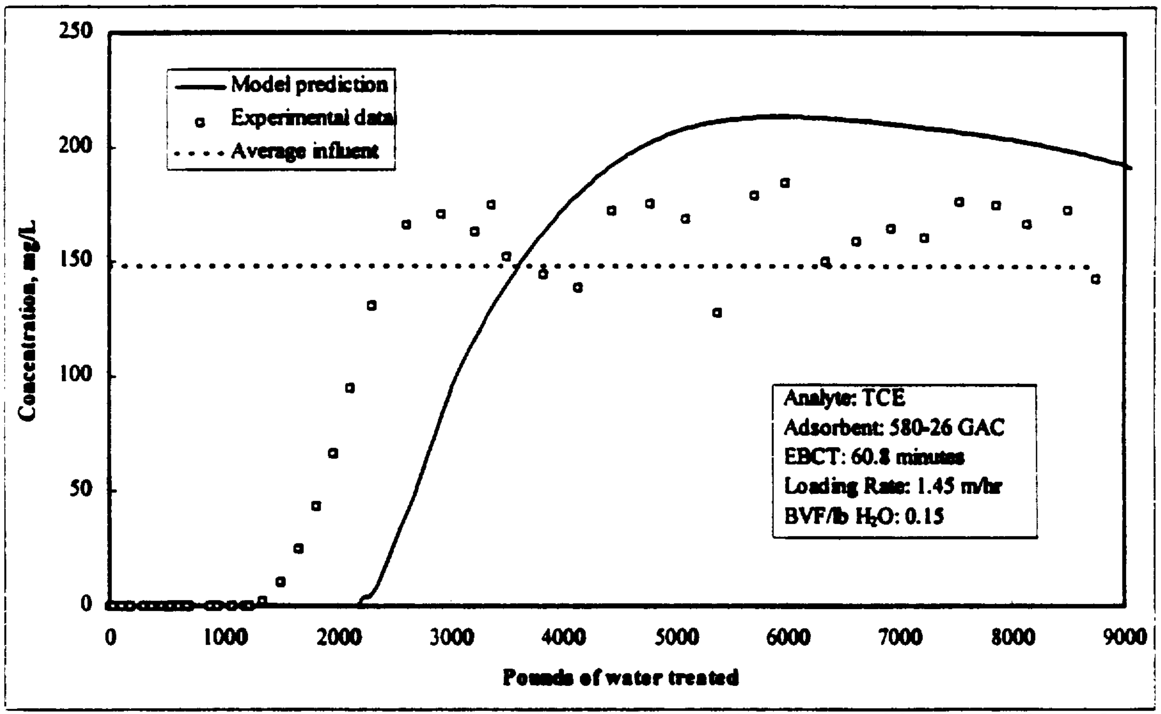

Figure 4-26. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

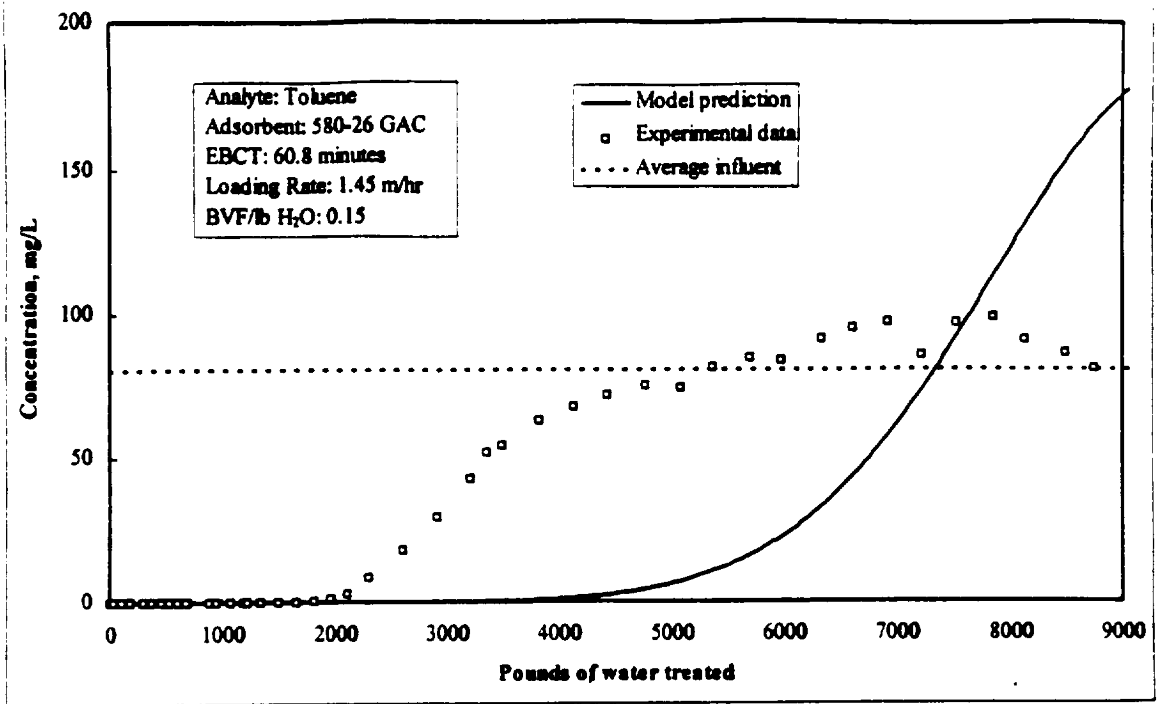

Figure 4-27. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

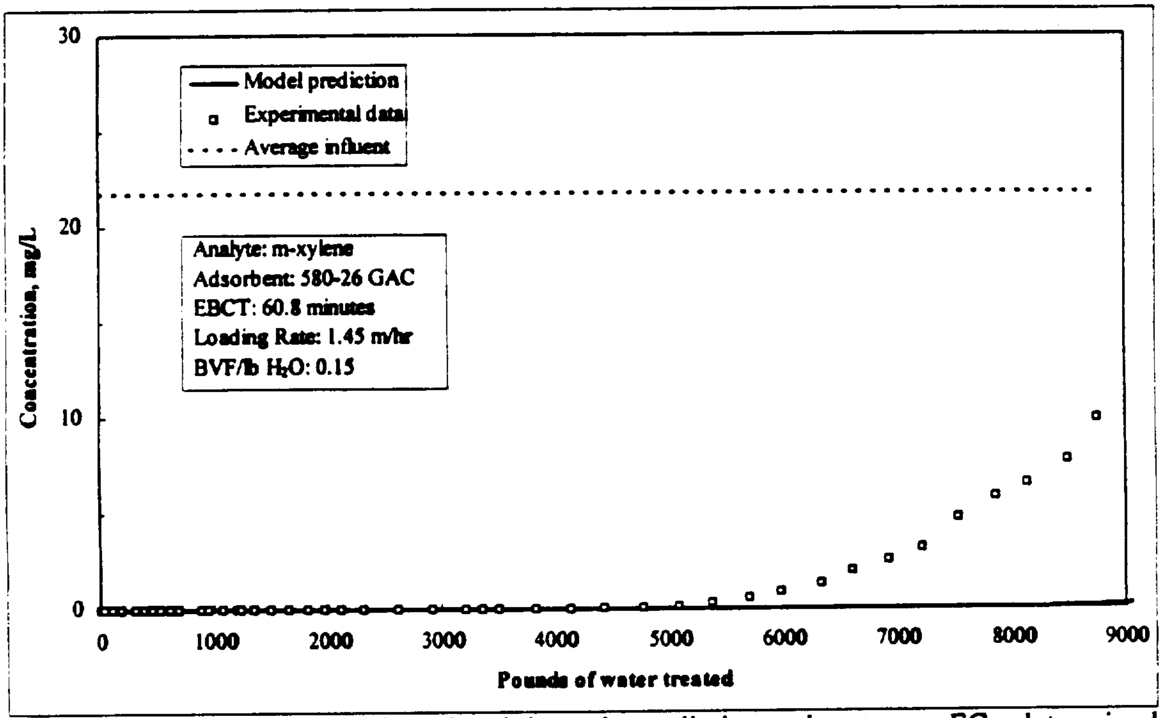

Figure 4-28. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on 580-26.

4.7.6 Target Compound Breakthrough From APA GAC Fixed Beds

Target compound breakthrough from the four APA GAC columns was predicted using the 5 tracer FCs (determined from fitting the APA ersatz tracer isotherms) and the target compound in PSDM calculations. The mass transfer parameters of the tracer FCs (SPDFR and tortuosity) were determined using the correlations developed for APA GAC in Section 4.7.1. The molar volume of each FC was assumed to be 150 cm^3/mol for liquid diffusivity calculations. The initial concentration of each tracer FC was scaled to account for differences in the initial TOC of the ersatz water used in the isotherm and column experiments. The makeup of the ersatz water used for the APA ersatz water column experiments is included in Table 4-1. The tracer FC parameters used for prediction of the target compound breakthrough profiles are included in Table 4-6.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 4.1 minute EBCT column in Figures 4-29 through 4-34. The prediction of SCMT breakthrough, Figure 4-29, coincides with the data. The predicted breakthrough time corresponds well to the time of experimental breakthrough. The kinetic parameters describe the mass transfer well in the system as the shape of the prediction matches that of the data. However, the breakthrough at concentrations greater than the influent (overshoot) predicted in the model was not observed in the data. The prediction of TCE breakthrough shown in Figure 4-30 also compares very well with the data. The model accurately predicted the breakthrough of toluene as shown in Figure 4-31. The model accurately predicted both the capacity and kinetics of the TCE and toluene breakthrough. The model prediction for m-xylene is compared to the experimental data in Figure 4-32. The capacity for m-xylene appears to be slightly underpredicted by the model. The capacity for naphthalene is greatly underpredicted by the model as shown in Figure 4-33. This indicates that the tracer FCs in IAST calculations predict a higher reduction in capacity for naphthalene than that observed in the column. This was also the case when the naphthalene isotherm was predicted in the ersatz water using the FCs in IAST calculations. The model predicts the breakthrough of 1,2,4-TCB to occur faster than the experimental data as shown in Figure 4-34. It is difficult to determine if the difference lies in the kinetics or the capacity since data is only available for a small part of breakthrough.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 7.9 minute EBCT column in Figures 4-35 through 4-38. Figure 4-35 shows that the model accurately predicts the breakthrough of SCMT. The breakthrough predictions for TCE and toluene shown in Figures 4-36 and 4-37 are close to the experimental breakthrough. The slight differences may be due to the mass transfer parameters. The predicted breakthrough for m-xylene, Figures 4-38, corresponds very well to the experimental breakthrough data except for the predicted overshoot which was not observed in the experimental data.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 12.0 minute EBCT column in Figures 4-39 through 4-42. The prediction of SCMT breakthrough, Figure 4-39, is very close to the experimental data. The model prediction for TCE shown in Figure 4-40 is also close to the experimental data. The model predictions for breakthrough of toluene and m-xylene in Figures 4-41 and 4-42 are both later than the experimental breakthrough data. The reason for this may again be counter diffusion with preadsorbed compounds. It may be seen as the EBCT in this case is larger than the first two APA columns evaluated.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 15.9 minute EBCT column in Figures 4-43 through 4-46. The model accurately predicts the time of breakthrough for SCMT in Figure 4-43. The model prediction appears to have slightly faster kinetics than the experimental data as it has a steeper breakthrough profile. The model accurately predicts the breakthrough of TCE as shown in Figure 4-44. The results for the toluene and m-xylene model predictions are shown in Figures 4-45 and 4-46 respectively. The model predictions occur after the experimental breakthrough in both cases. The separations are slightly larger than those observed in the 12.0 minute EBCT. This may be due to the longer time the adsorbent is exposed to the weakly adsorbing compounds before the strongly adsorbed compounds are present.

The results of the APA ersatz column target compound breakthrough predictions indicate that the model works well for all but the very strongly adsorbing compounds such as naphthalene and 1,2,4-TCB. Counter diffusion may be an issue at the longer contact times studied. The effects of counter diffusion appear to increase with increases in EBCT as well as the strength of the adsorbing compound.

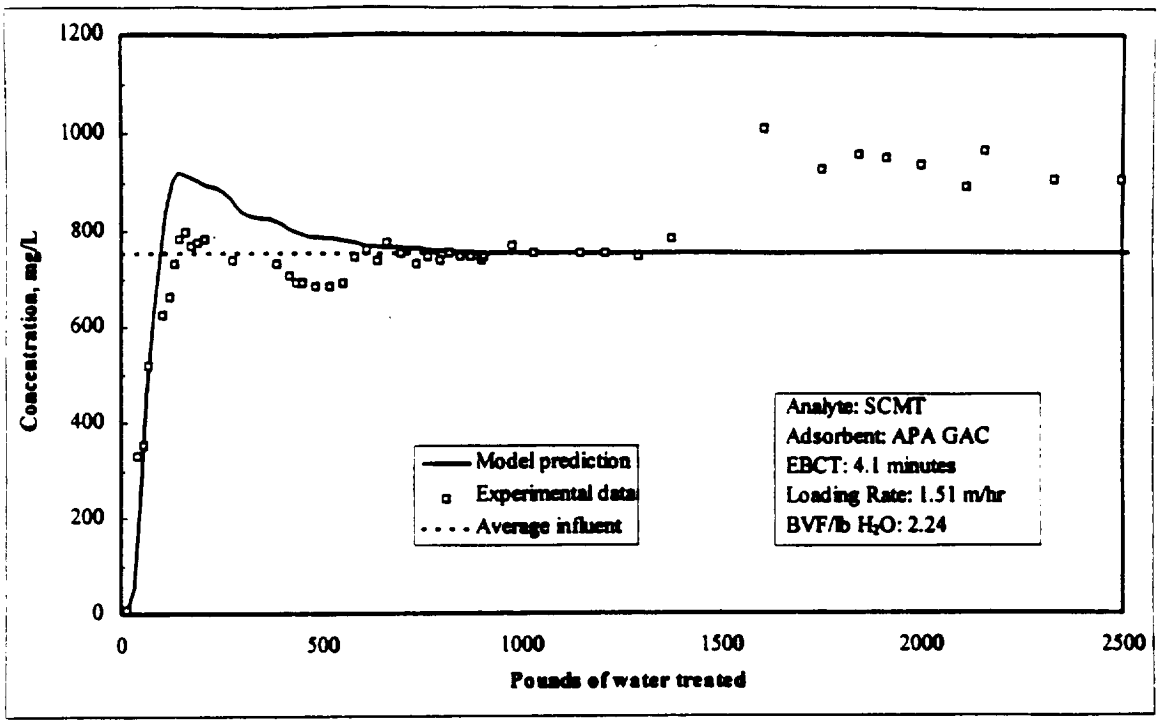

Figure 4-29. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

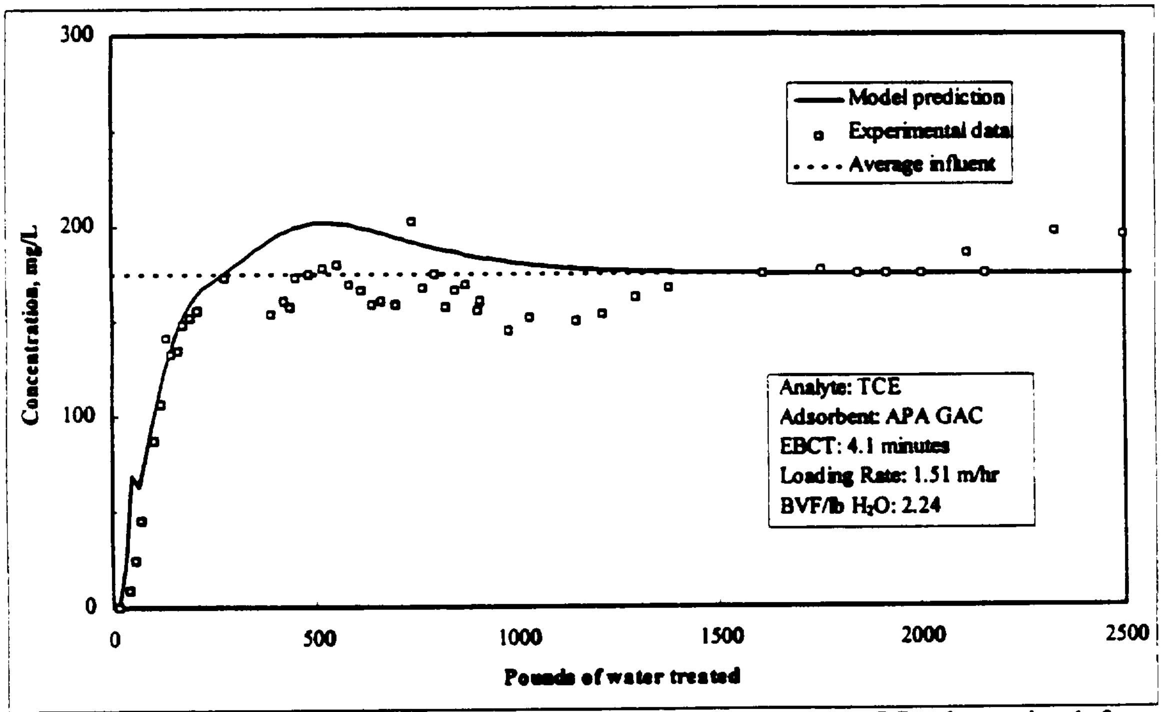

Figure 4-30. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

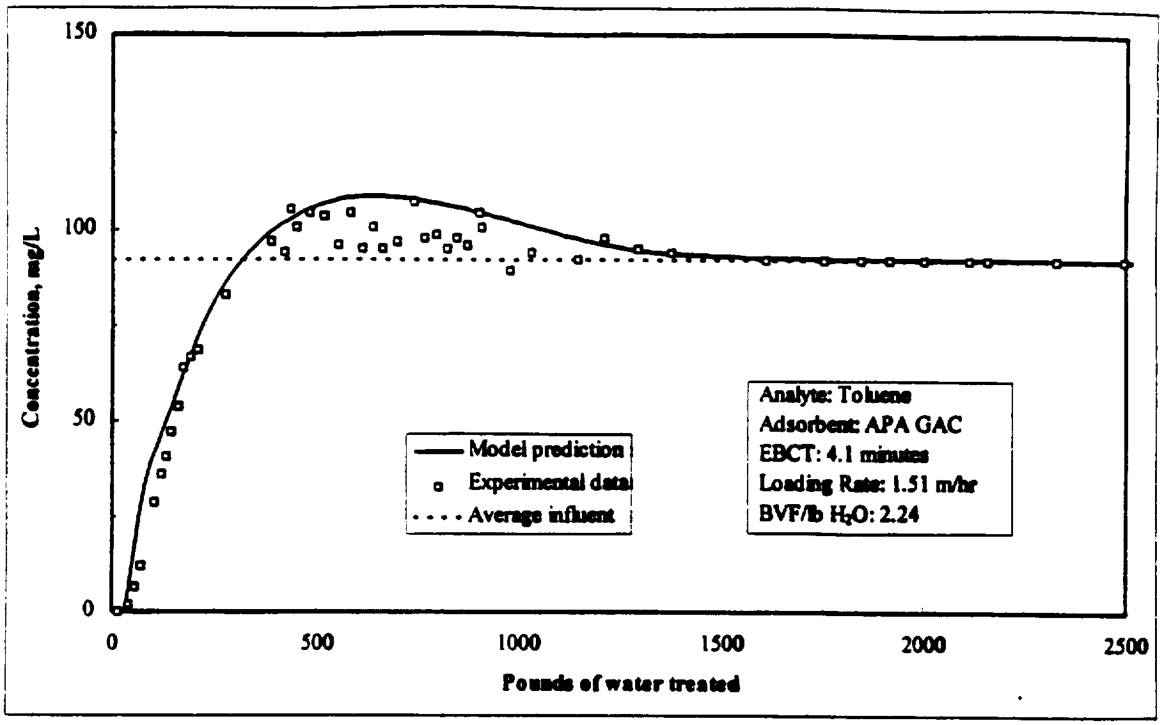

Figure 4-31. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

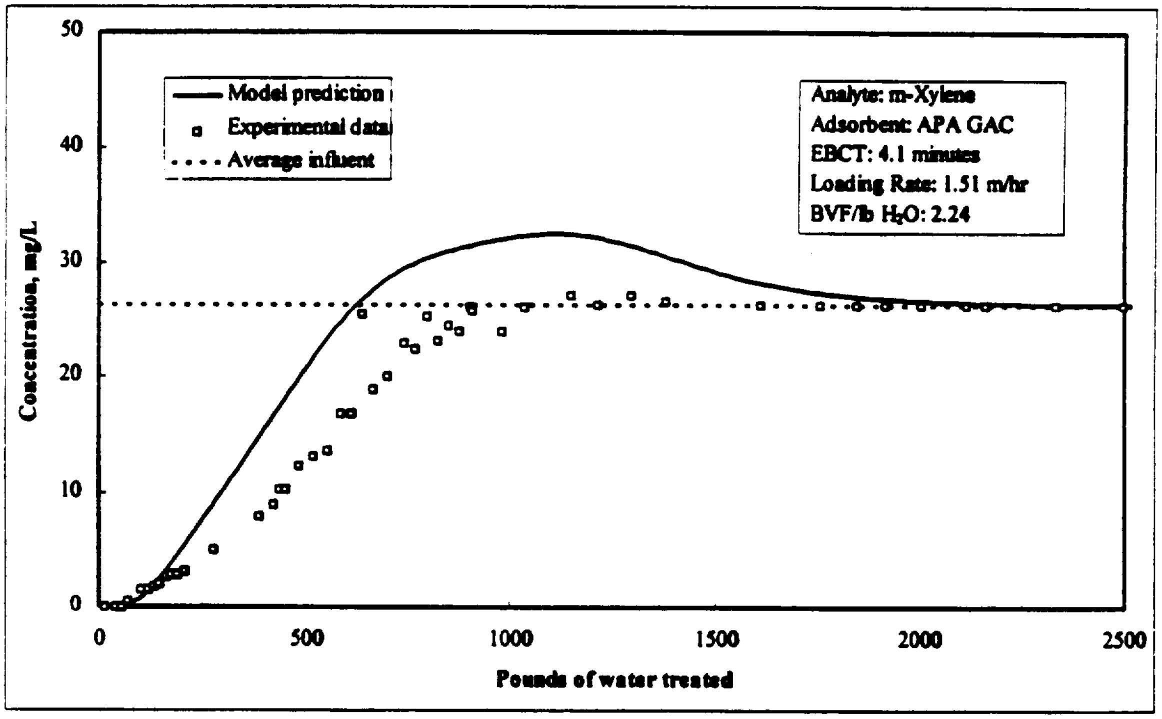

Figure 4-32. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

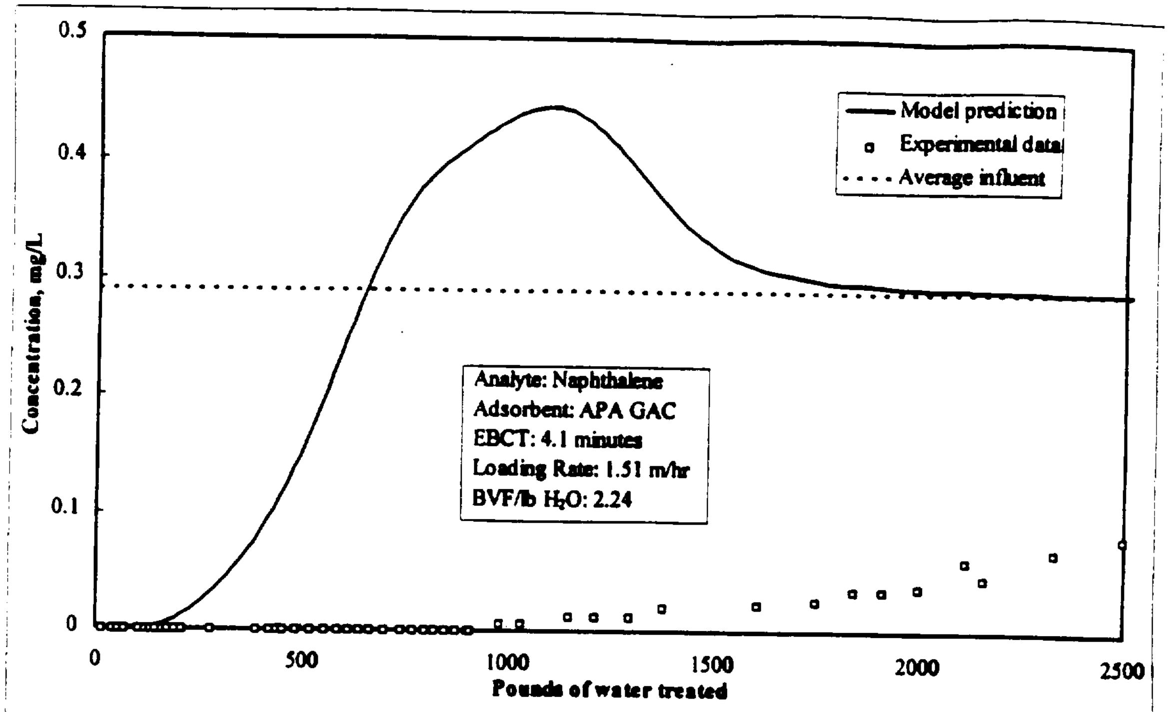

Figure 4-33. PSDM naphthalene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

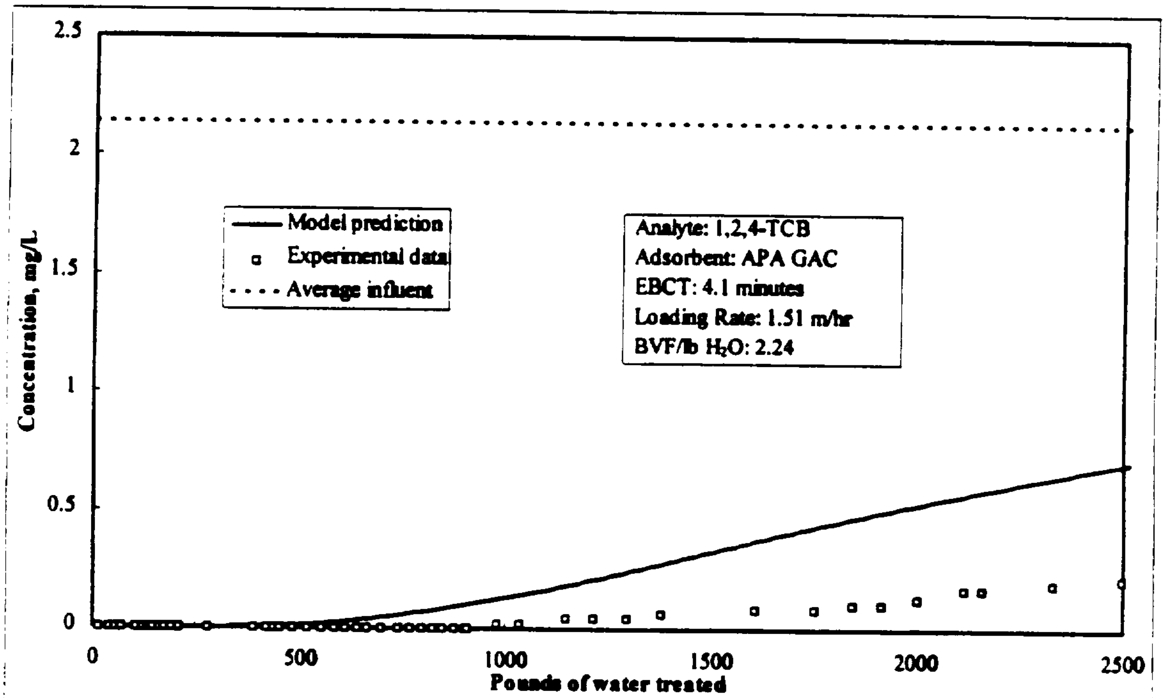

Figure 4-34. PSDM 1,2,4-TCB breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

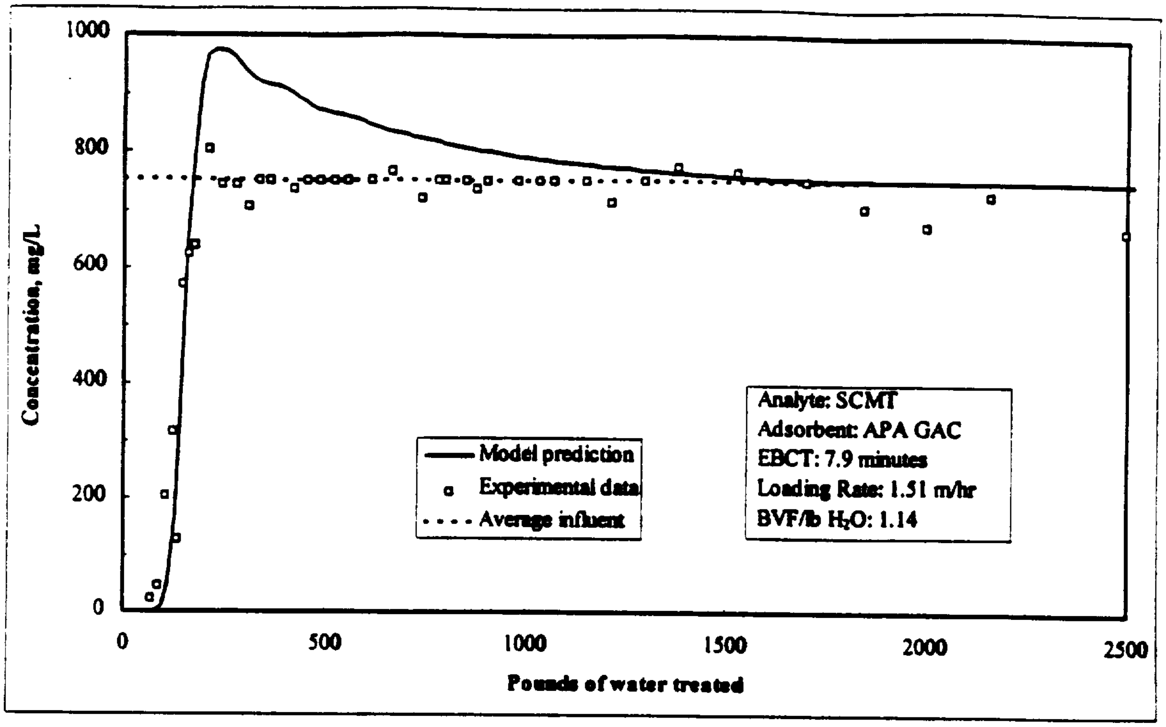

Figure 4-35. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

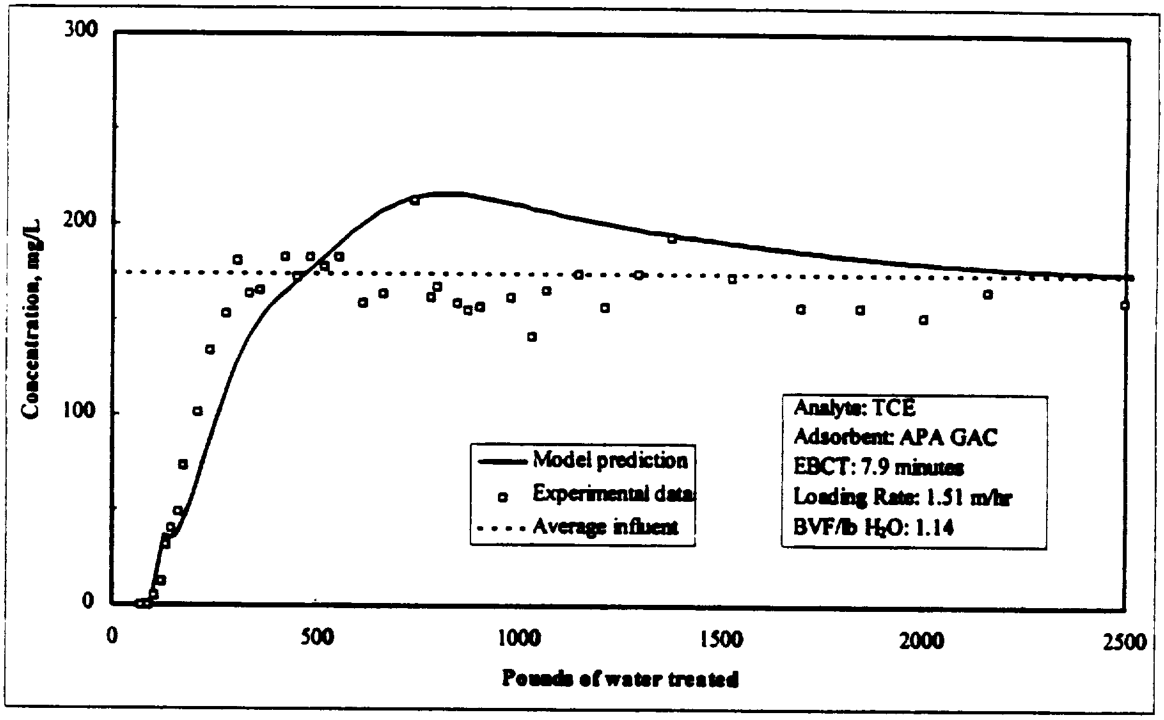

Figure 4-36. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

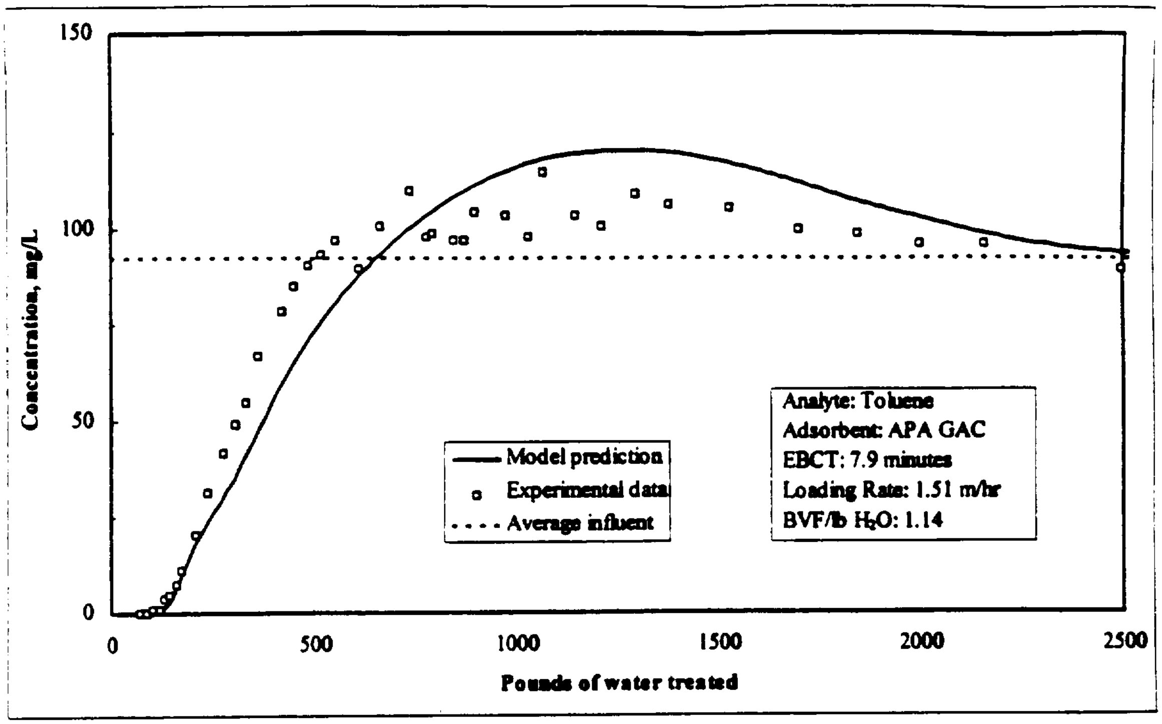

Figure 4-37. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

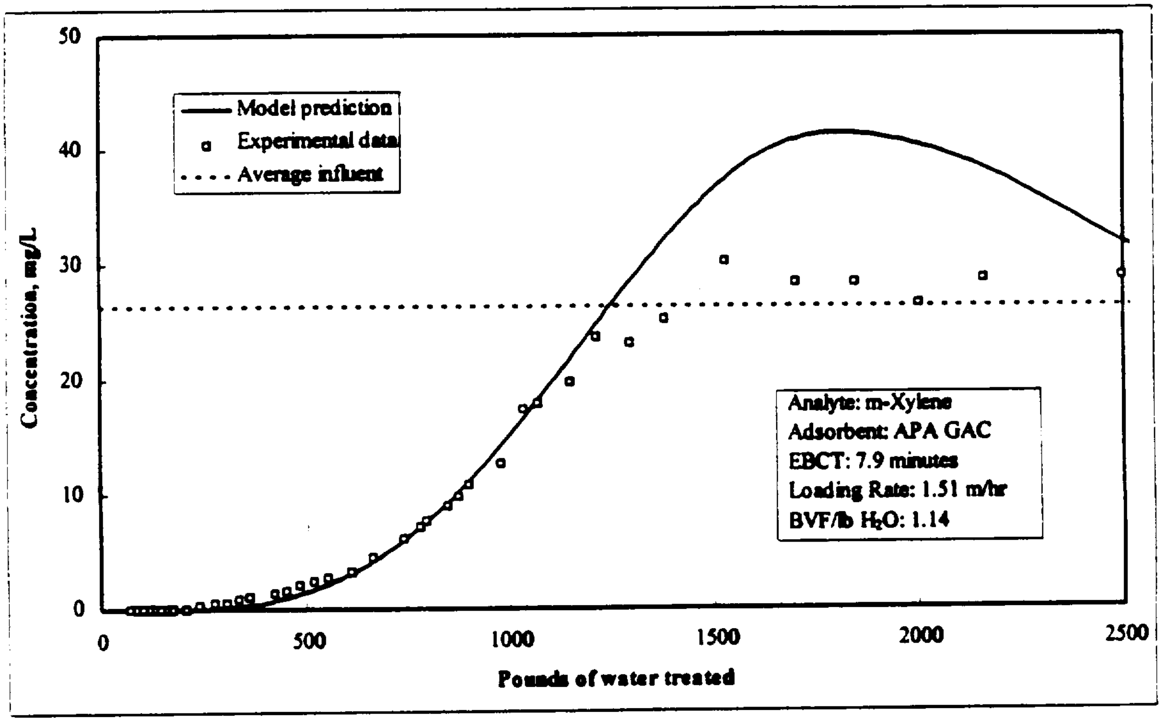

Figure 4-38. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

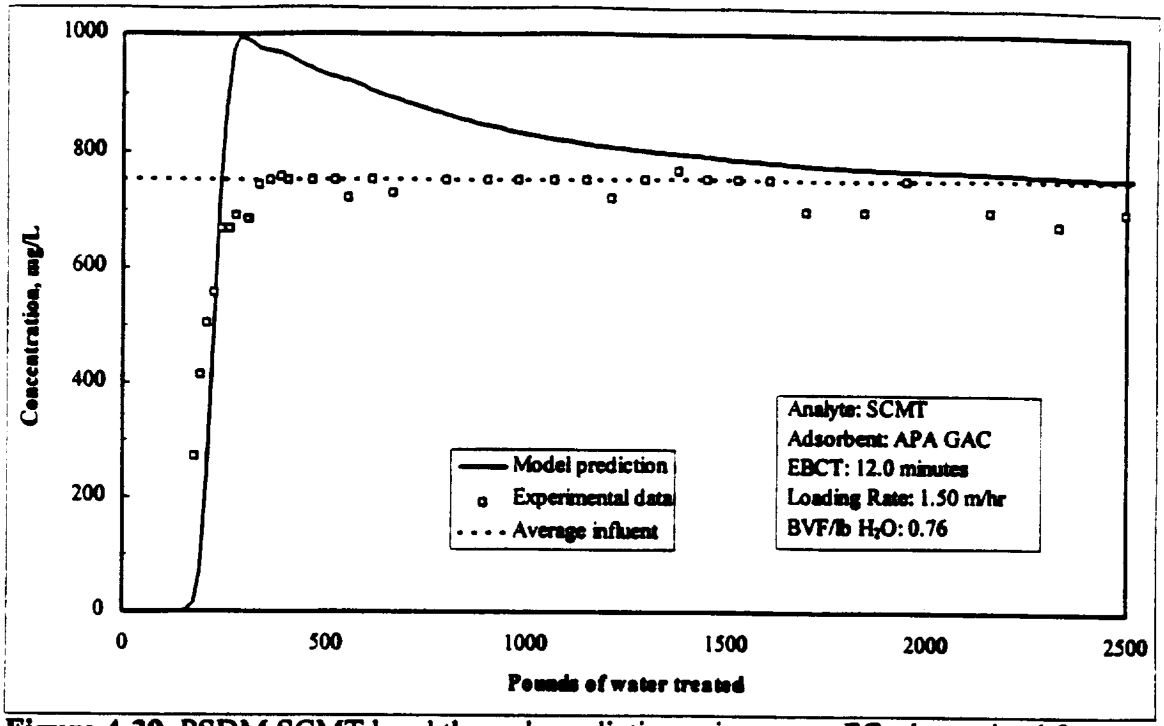

Figure 4-39. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

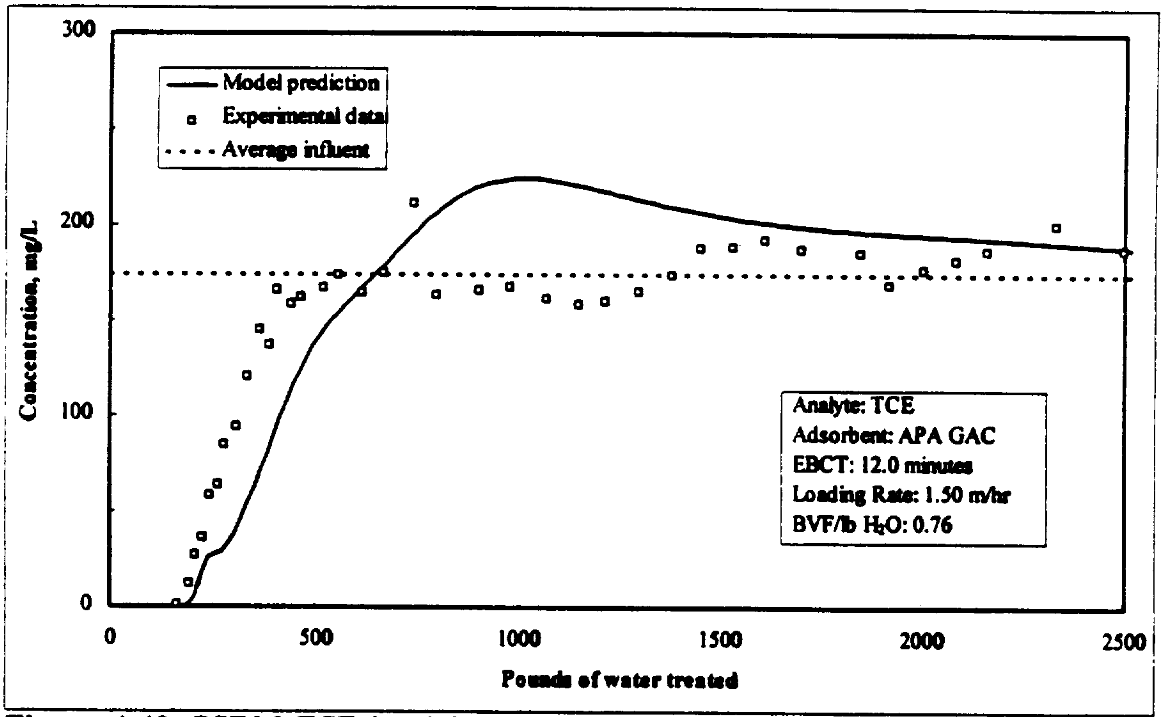

Figure 4-40. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

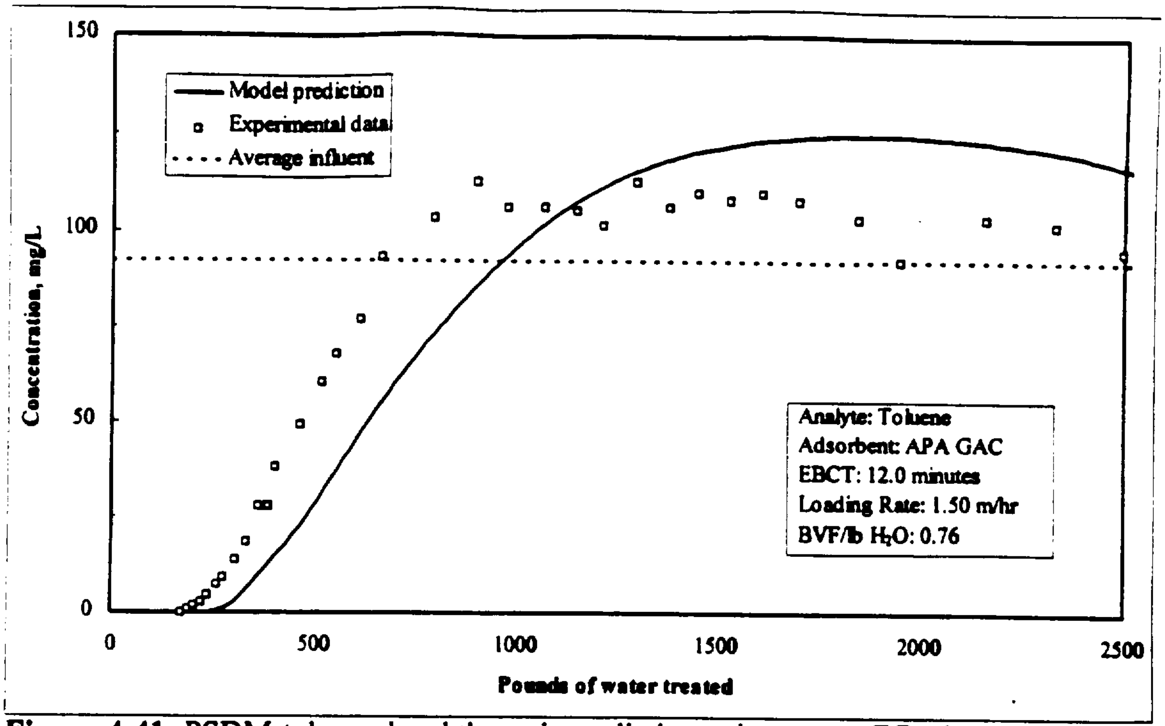

Figure 4-41. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

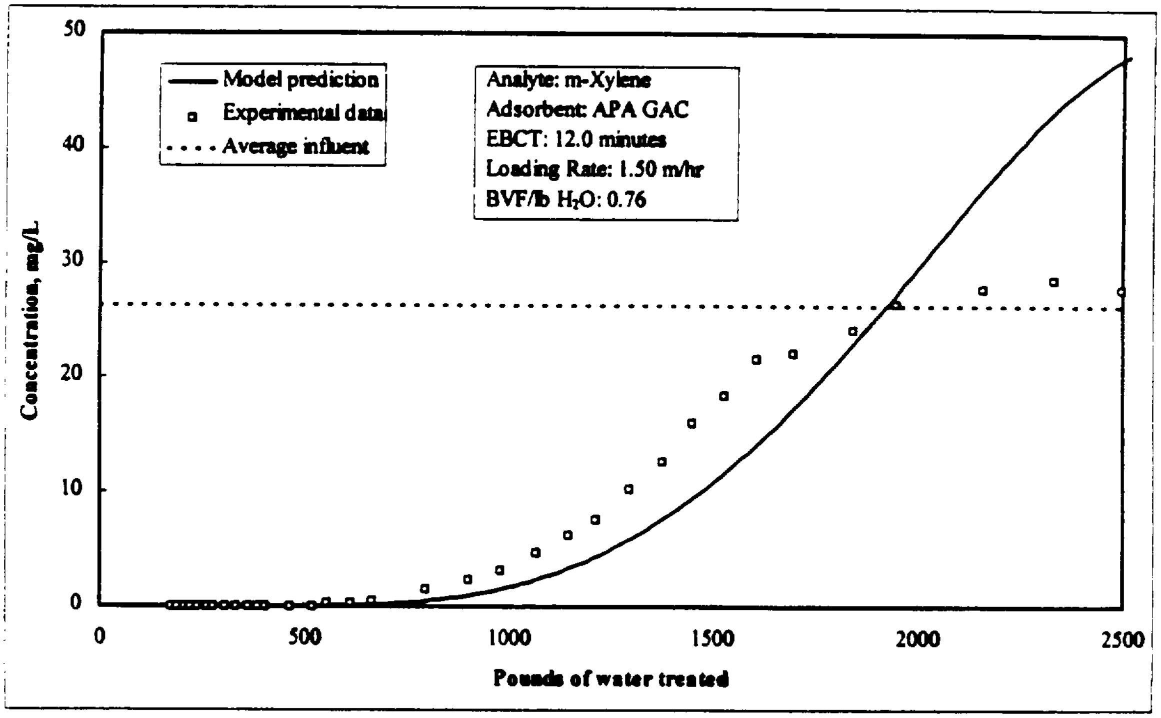

Figure 4-42. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

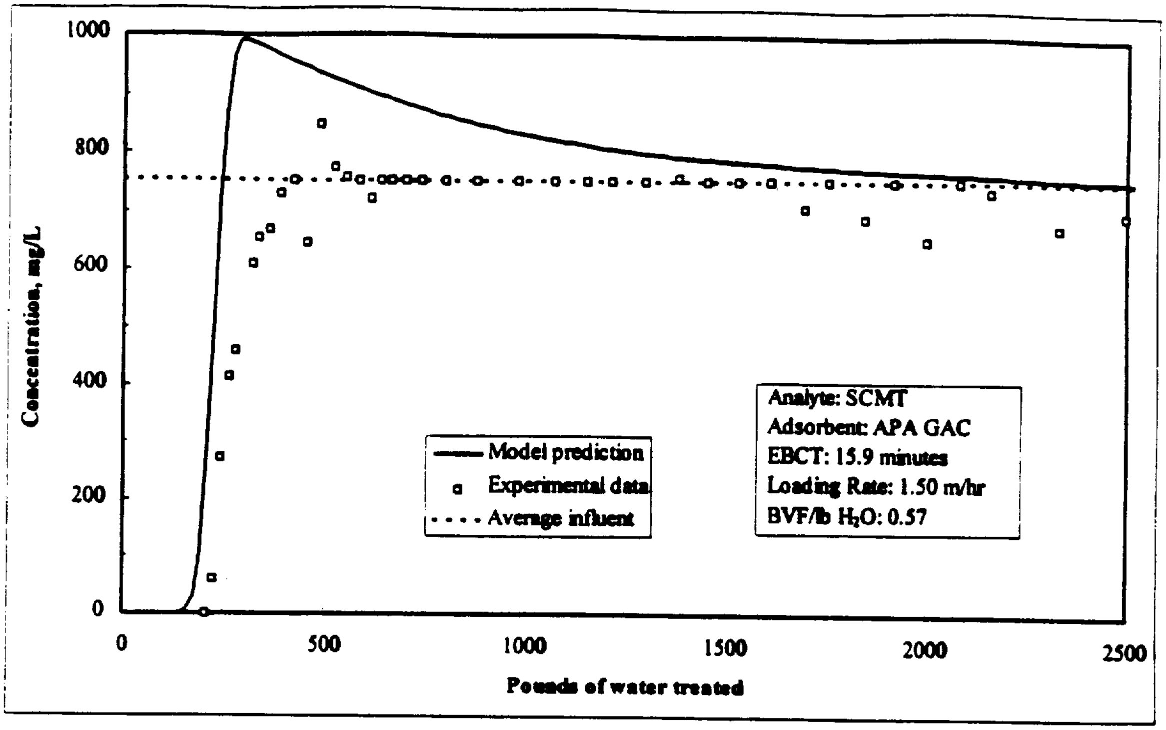

Figure 4-43. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

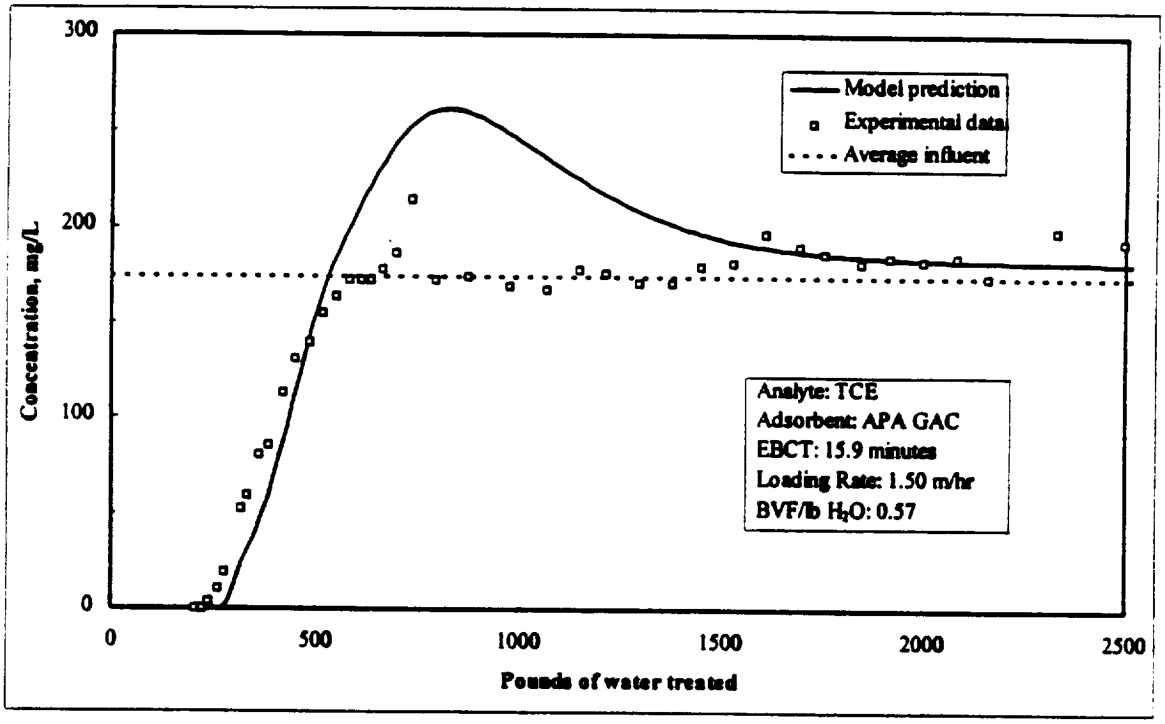

Figure 4-44. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

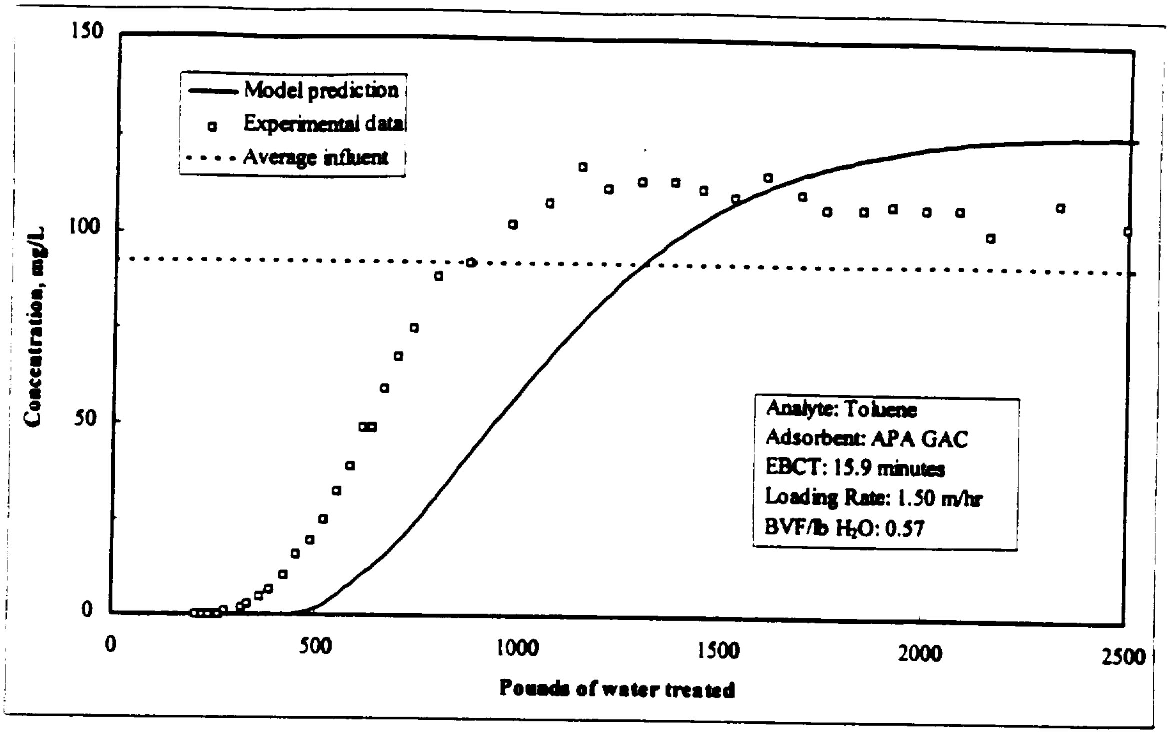

Figure 4-45. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

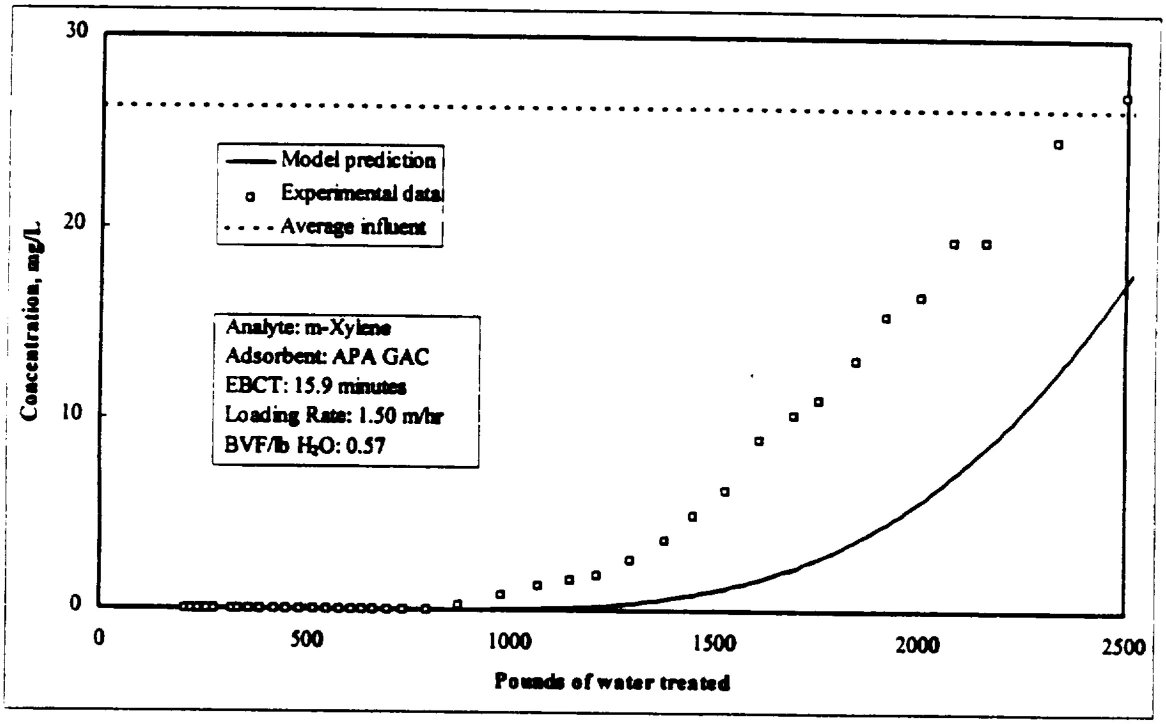

Figure 4-46. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on APA.

4.7.7 Target Compound Breakthrough From XAD-4 Resin Fixed Beds

Target compound breakthrough from the four XAD-4 resin columns was predicted using the 5 tracer FCs (determined from fitting the XAD-4 ersatz tracer isotherms) and the target compound in model calculations. The mass transfer parameters of the tracer FCs (SPDFR and tortuosity) were determined using the correlations developed for XAD-4 in Section 4.7.1. The molar volume of each FC was assumed to be 150 cm^3/mol for liquid diffusivity calculations. The initial concentration of each tracer FC was scaled to account for differences in the initial TOC of the ersatz water used in the isotherm and column experiments. The makeup of the ersatz water used for the XAD-4 ersatz water column experiments is included in Table 4-1. The tracer FC parameters used for prediction of the target compound breakthrough profiles are included in Table 4-6.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 4.4 minute EBCT column in Figures 4-47 through 4-52. The prediction of SCMT breakthrough, Figure 4-47, corresponds well with the data. The predicted breakthrough time corresponds well to the time of experimental breakthrough. The kinetic parameters describe the mass transfer well in the system as the shape of the prediction matches that of the data. However, the breakthrough at concentrations greater than the influent (overshoot) predicted in the model was not totally observed in the data. The prediction of TCE breakthrough shown in Figure 4-48 also compares very well with the data. The TCE model prediction again overpredicts the overshoot observed in the laboratory. The model predicted breakthrough of toluene slightly later than the data as shown in Figure 4-49. The error in the toluene prediction may be due to kinetics as the capacity observed appears to be correct. The model prediction for m-xylene is compared to the experimental data in Figure 4-50. The observed capacity for m-xylene is underpredicted by the model. The capacity for naphthalene is greatly underpredicted by the model as shown in Figure 4-51. This indicates that the tracer FCs predict a higher reduction in capacity for naphthalene than that observed in the column as they did for APA GAC as well. The breakthrough data for naphthalene also shows an abnormality as the effluent steps up to 20% of the influent suddenly and then levels off. This phenomenon corresponded to a time when o-xylene was released by the XAD-4 resin.

The model predicts the breakthrough of 1,2,4-TCB to occur faster than the experimental data as shown in Figure 4-52. It is difficult to determine if the difference lies in the kinetics or the capacity since data is only available for part of the breakthrough profile.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 8.8 minute EBCT column in Figures 4-53 through 4-57. Figure 4-53 shows that the model accurately predicts the breakthrough of SCMT. The breakthrough predictions for TCE and toluene shown in Figures 4-54 and 4-55 are both after the experimental breakthrough. The differences may be due to the mass transfer parameters. The predicted breakthrough for m-xylene, Figure 4-56, corresponds very well to the experimental breakthrough data except for the predicted overshoot which was not observed in the experiment. The model prediction for naphthalene shown in Figure 4-57 illustrates again that the model greatly underpredicts the capacity for naphthalene.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 13.0 minute EBCT column in Figures 4-58 through 4-62. The prediction of SCMT breakthrough, Figure 4-58, is very close to the experimental data. The model predictions for TCE, toluene, and m-xylene shown in Figures 4-59, 4-60, and 4-61 all occur after the experimental breakthrough. The model prediction did not predict the breakthrough of naphthalene well as shown in Figure 4-62.

The target compound experimental breakthrough profiles and PSDM predictions are compared for the 17.2 minute EBCT column in Figures 4-63 through 4-66. The model accurately predicts the time of breakthrough for SCMT in Figure 4-63. The model prediction appears to have slightly faster kinetics than the experimental data as it is steeper on breakthrough. The results for the TCE and toluene predictions are shown in Figures 4-64 and 4-65 respectively. The model predictions occur after the experimental breakthrough in both cases. The separations are slightly larger than those observed in the 13.0 minute EBCT column.

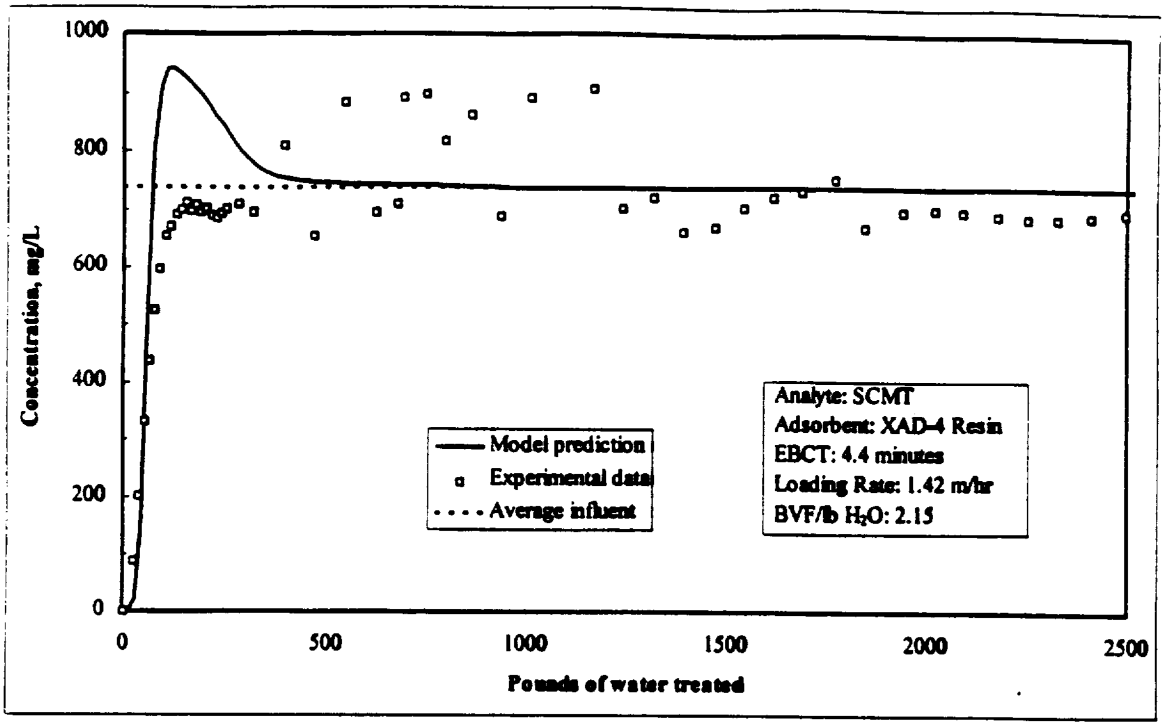

Figure 4-47. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

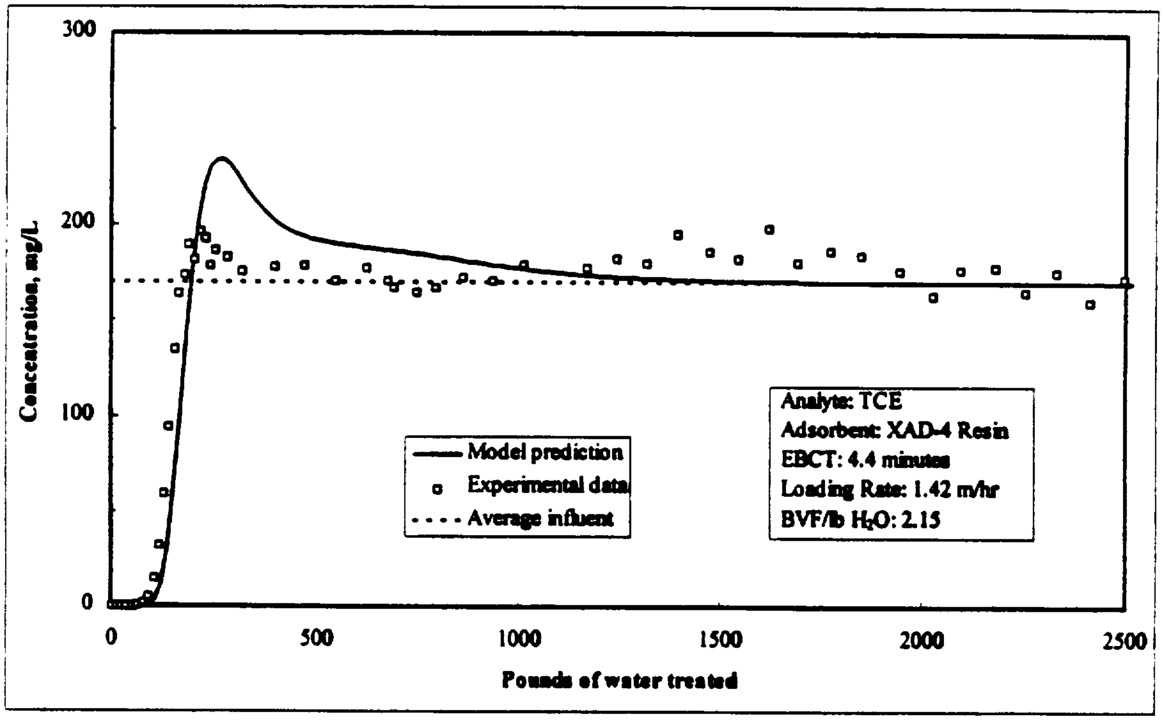

Figure 4-48. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

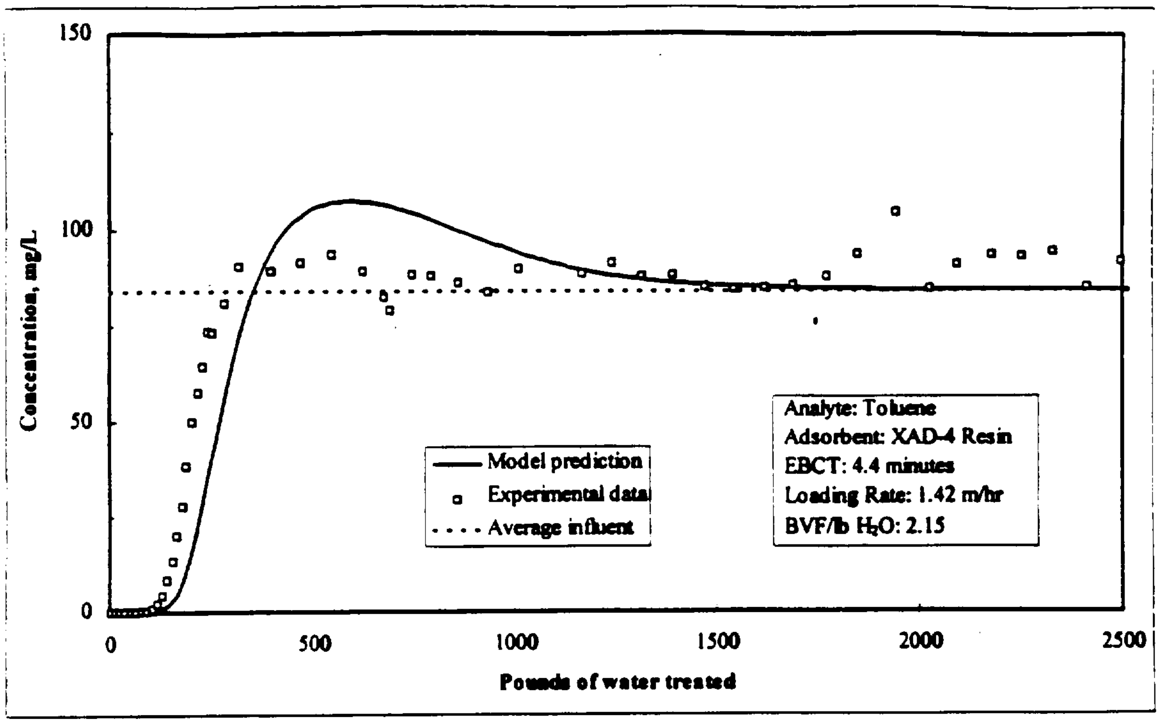

Figure 4-49. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

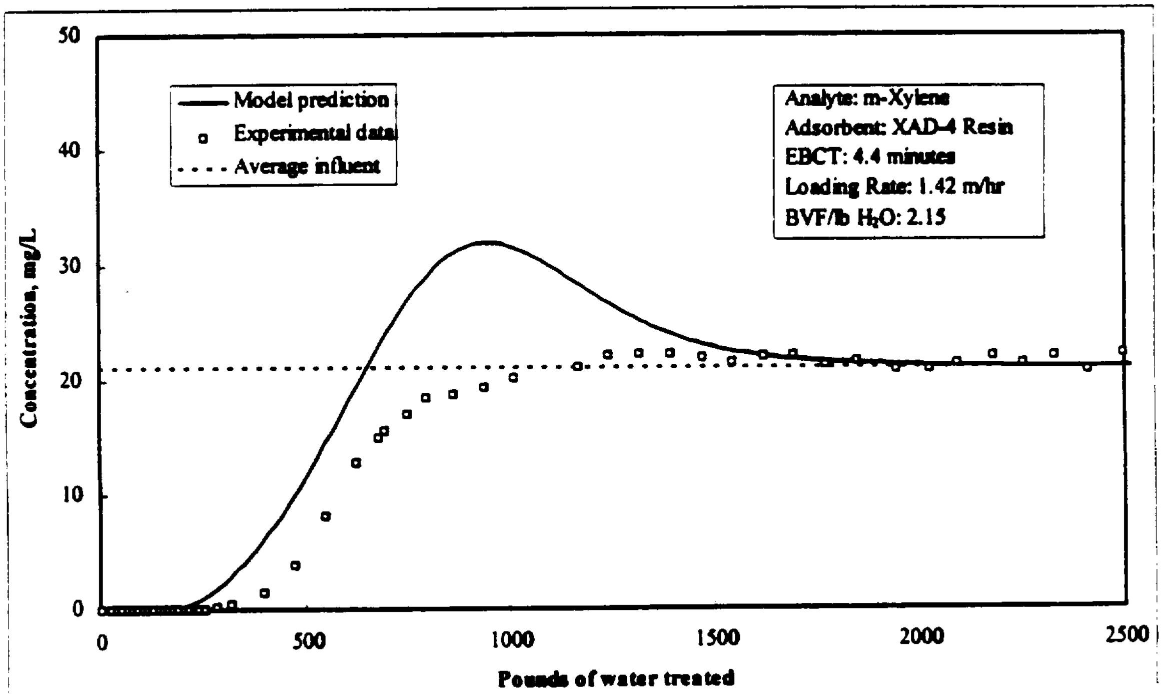

Figure 4-50. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

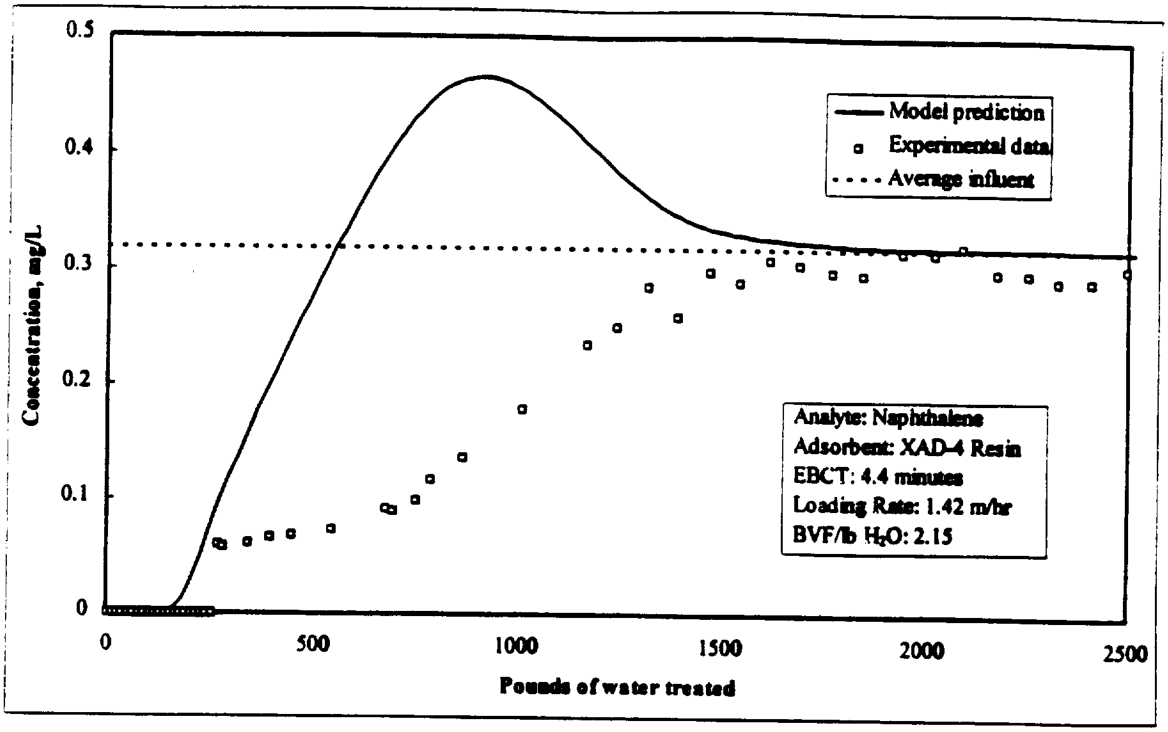

Figure 4-51. PSDM naphthalene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

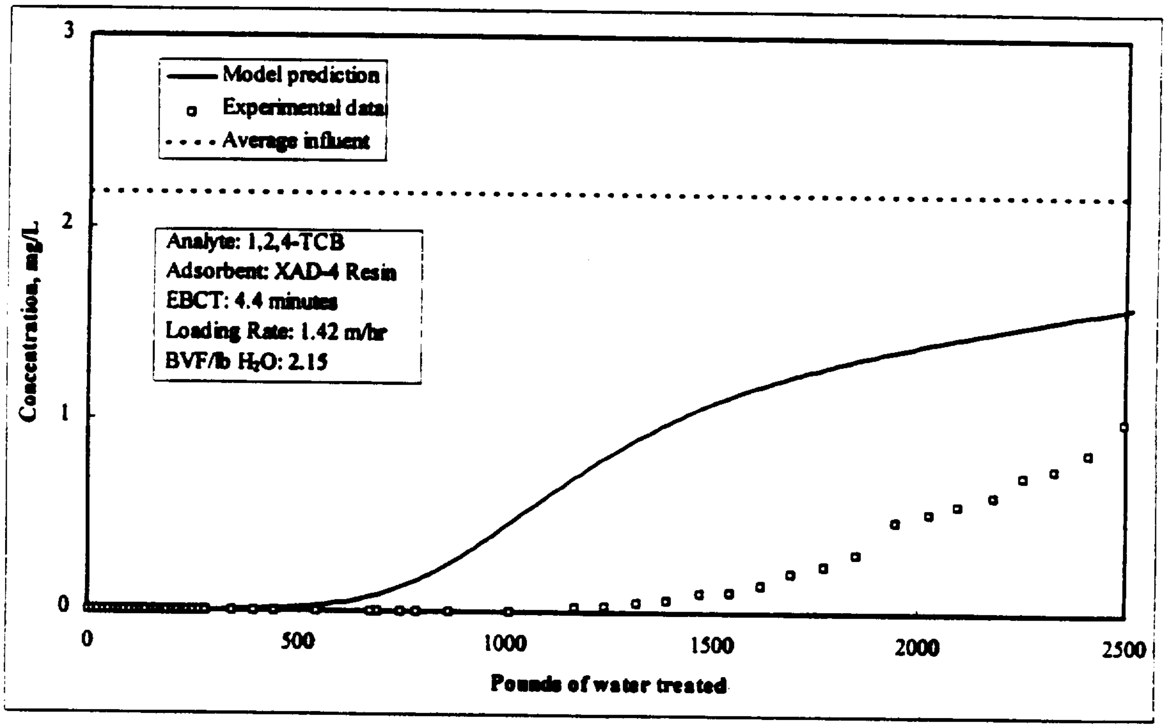

Figure 4-52. PSDM 1,2,4-TCB breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

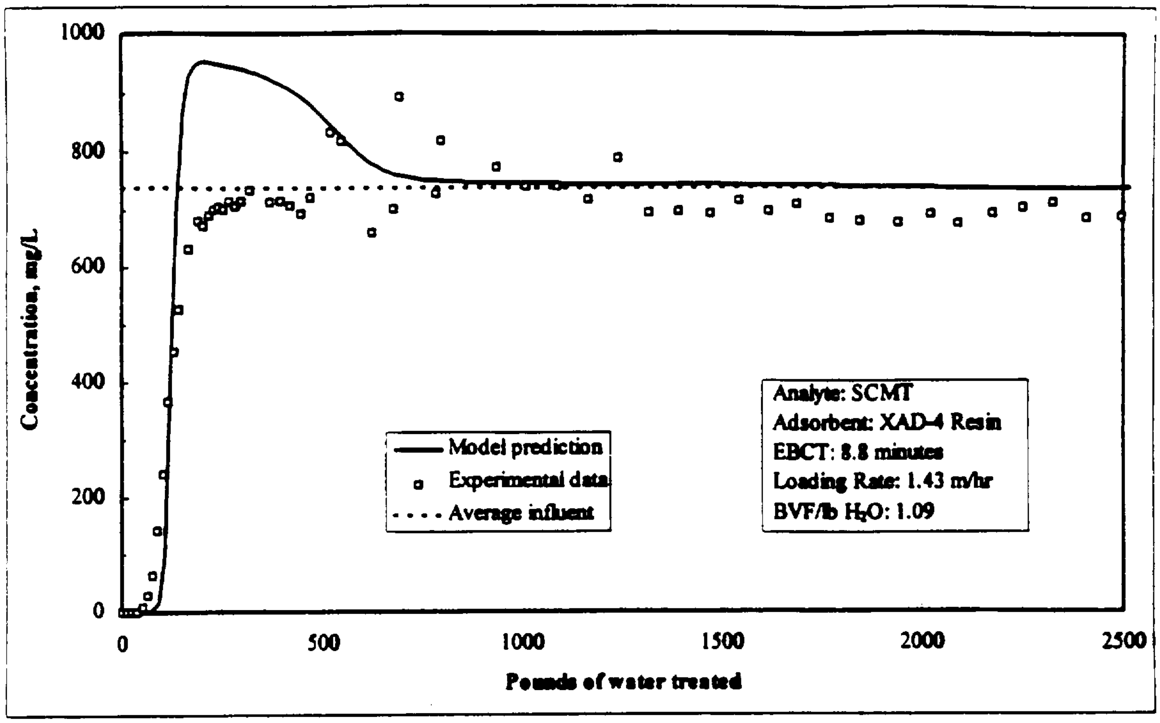

Figure 4-53. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

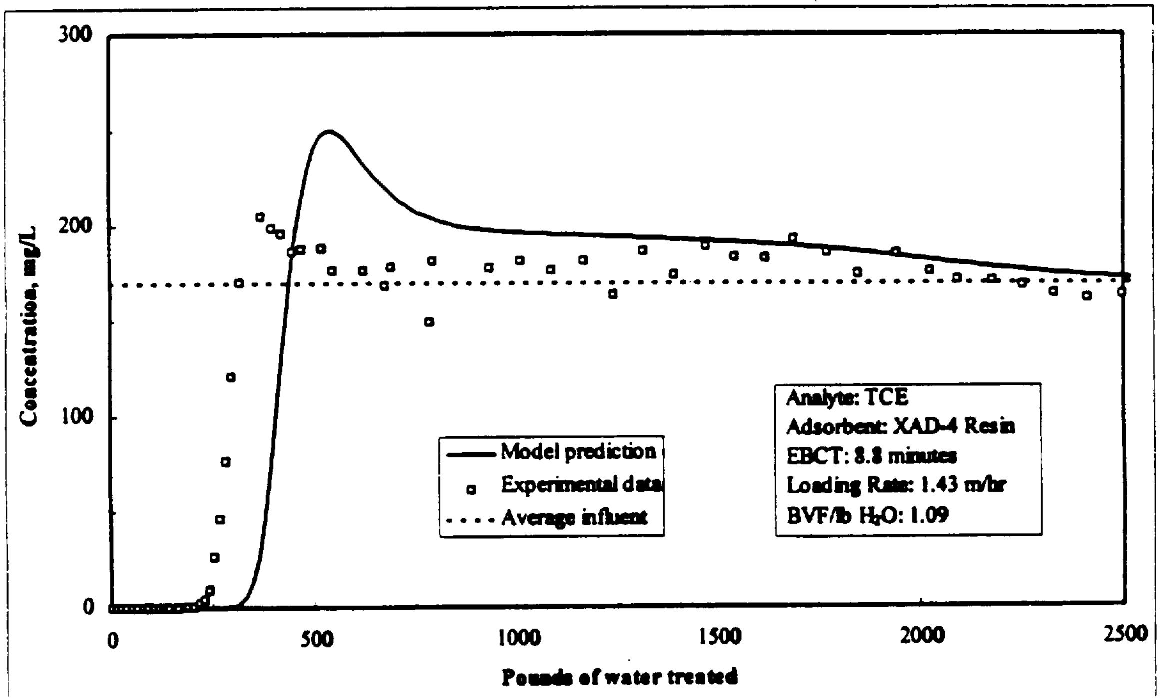

Figure 4-54. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

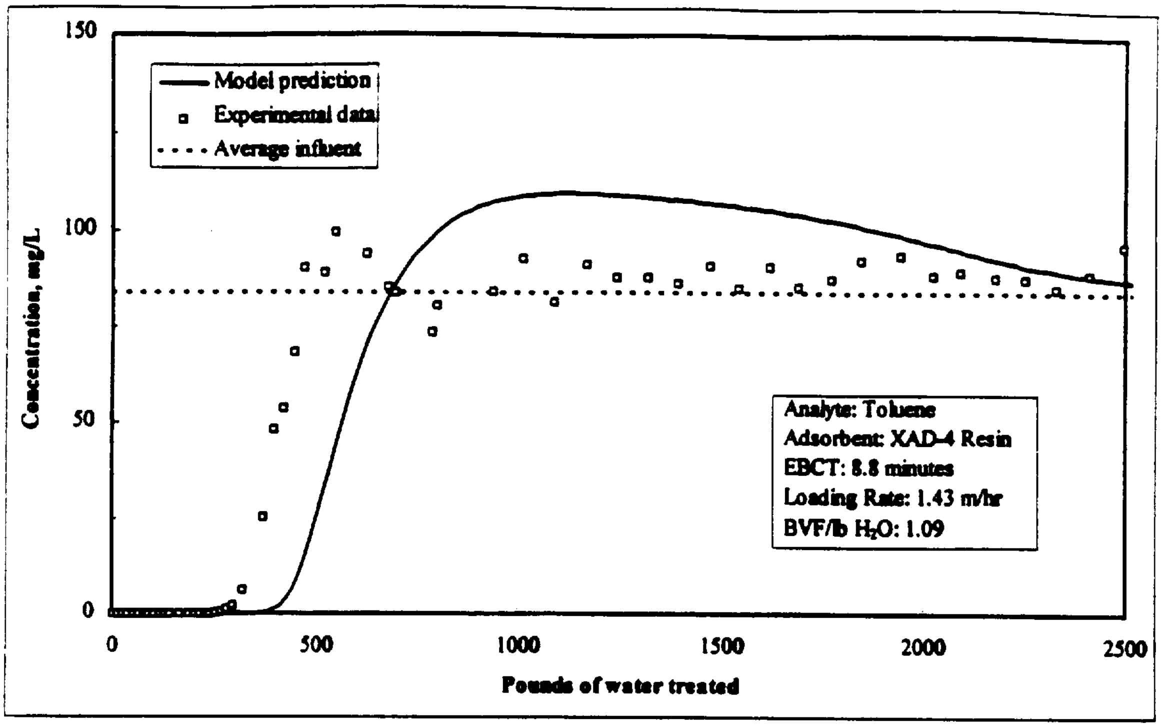

Figure 4-55. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

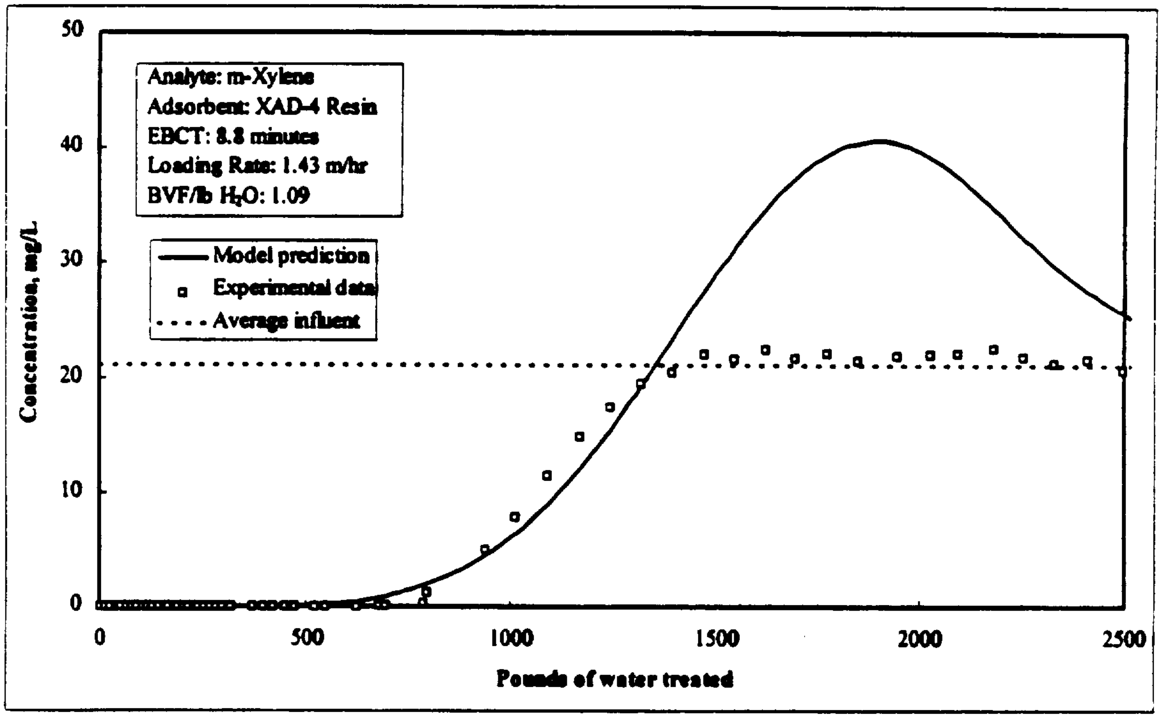

Figure 4-56. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

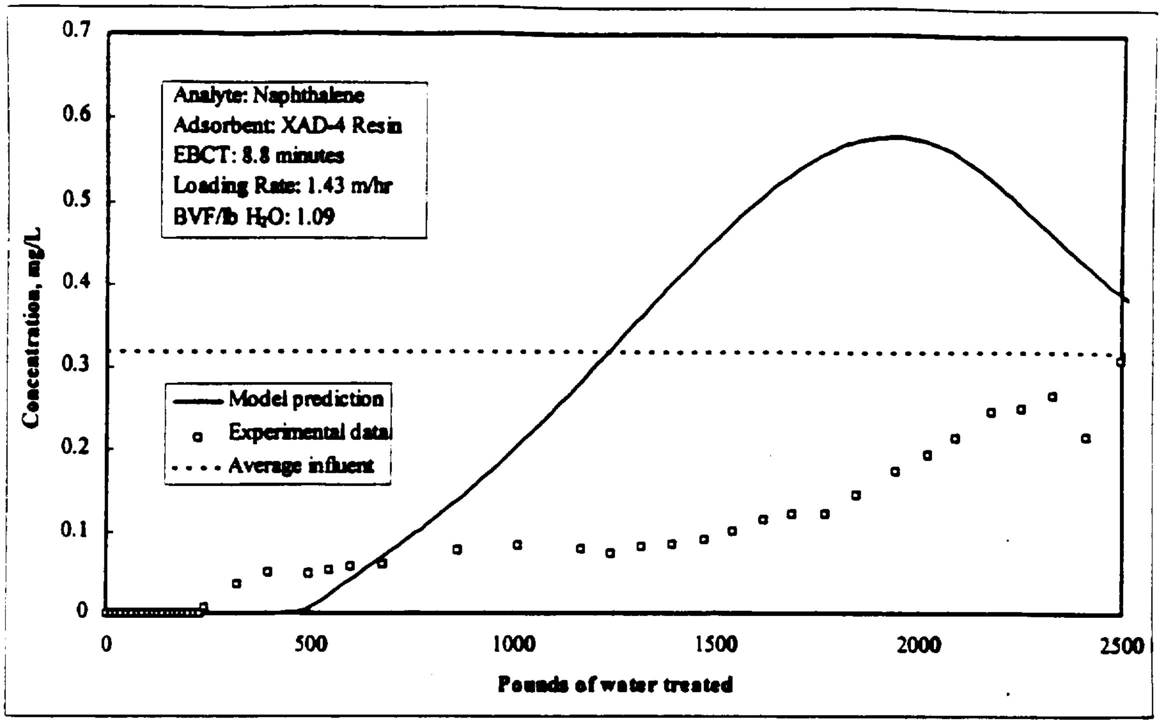

Figure 4-57. PSDM naphthalene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

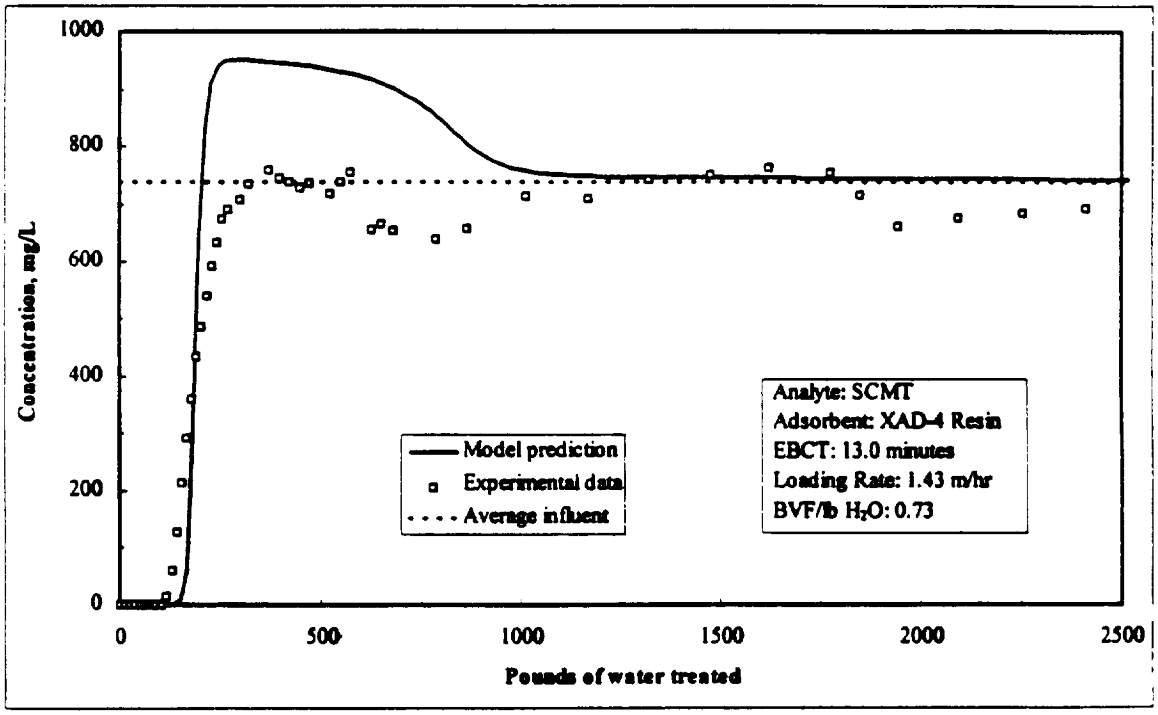

Figure 4-58. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

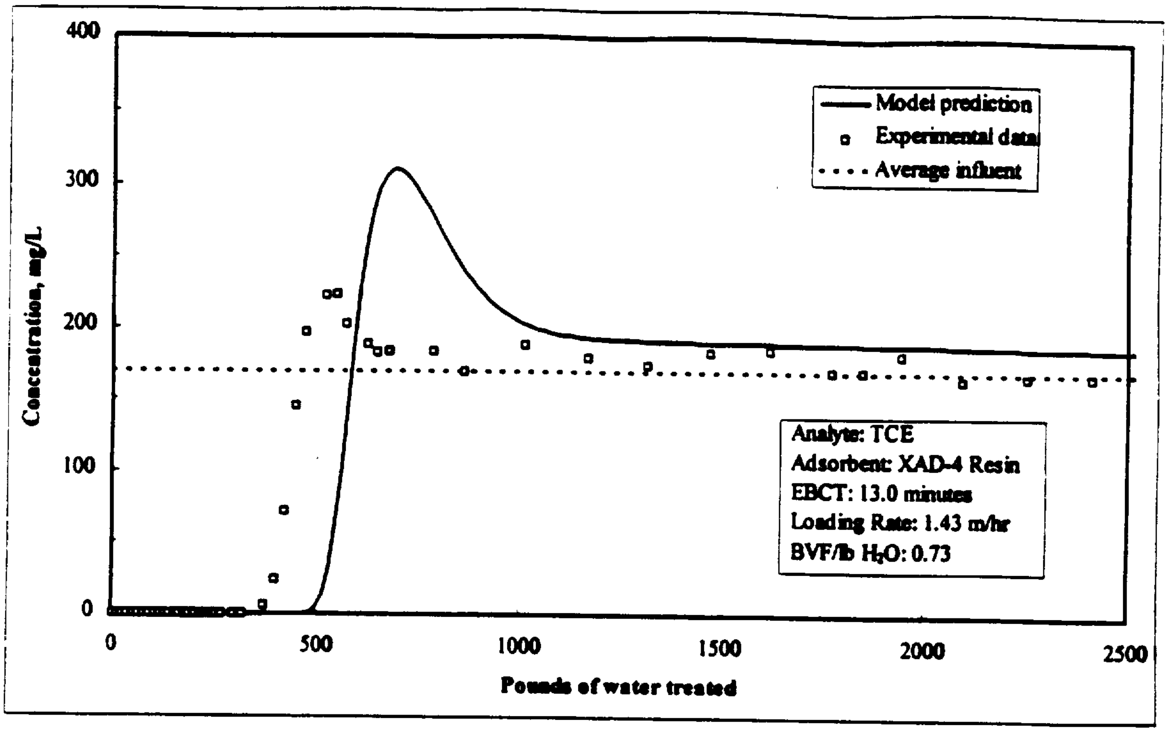

Figure 4-59. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

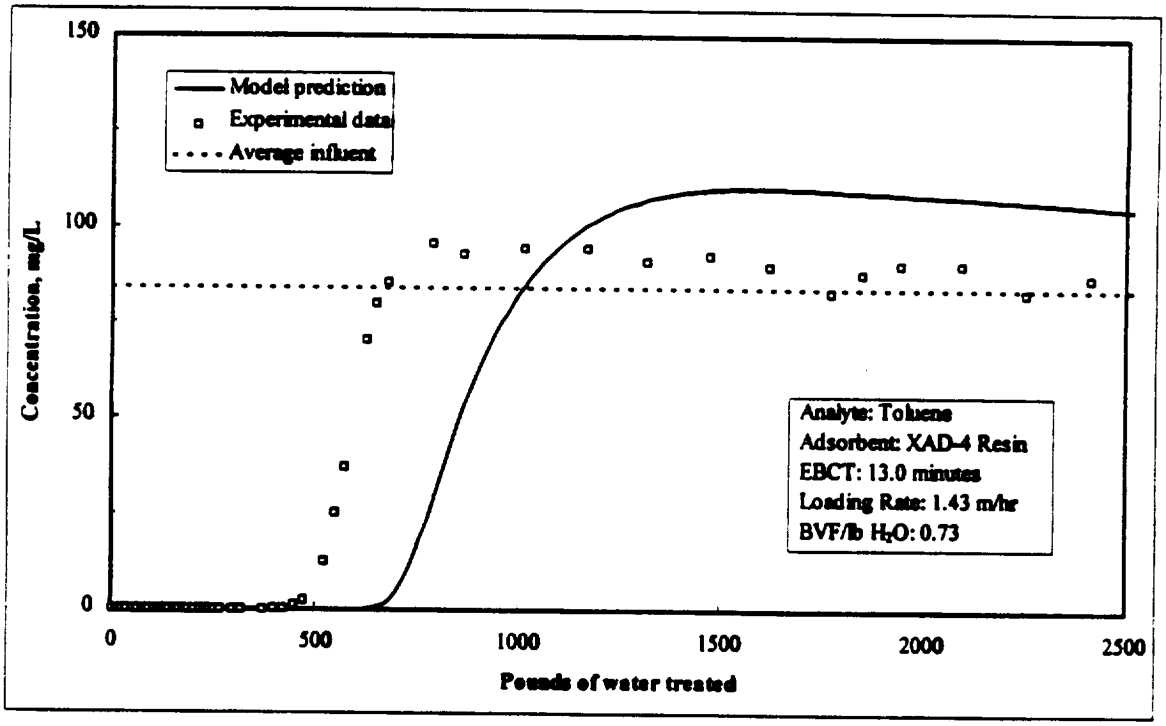

Figure 4-60. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

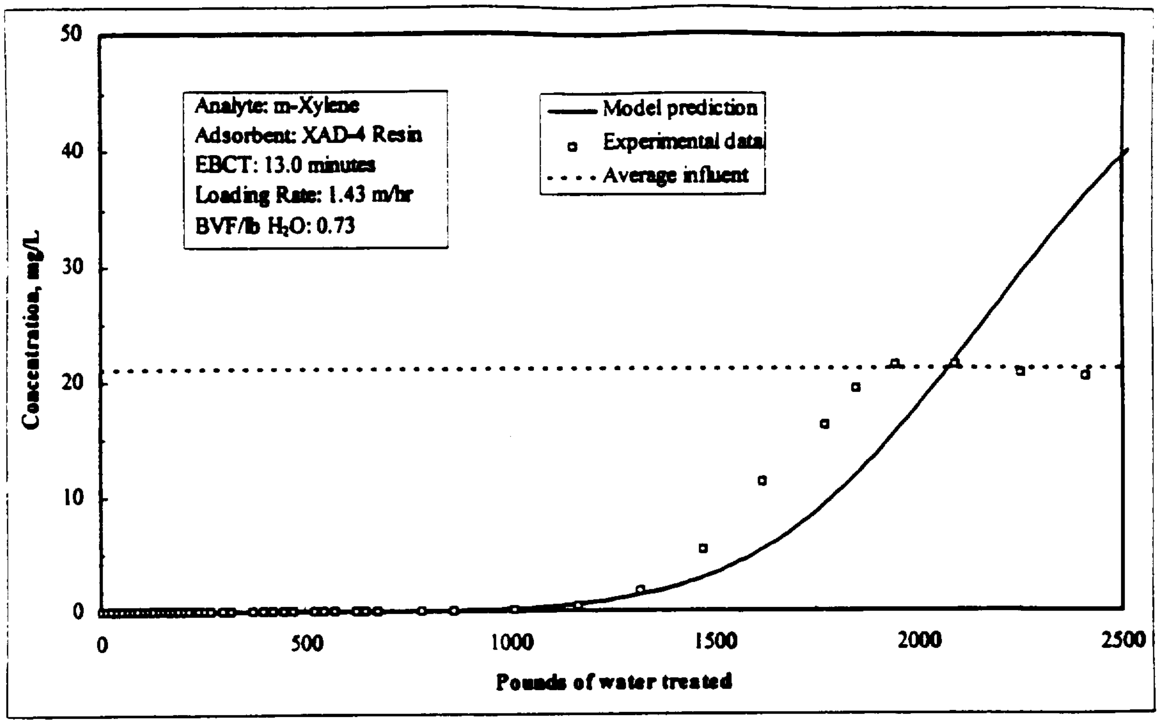

Figure 4-61. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

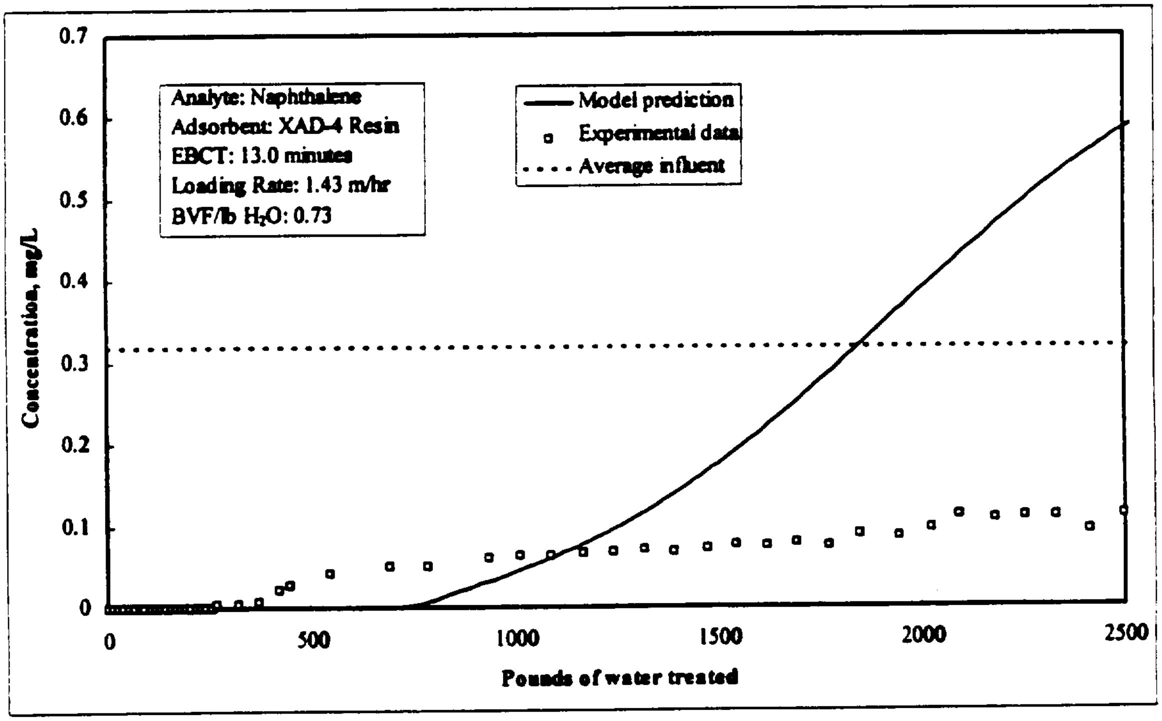

Figure 4-62. PSDM naphthalene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

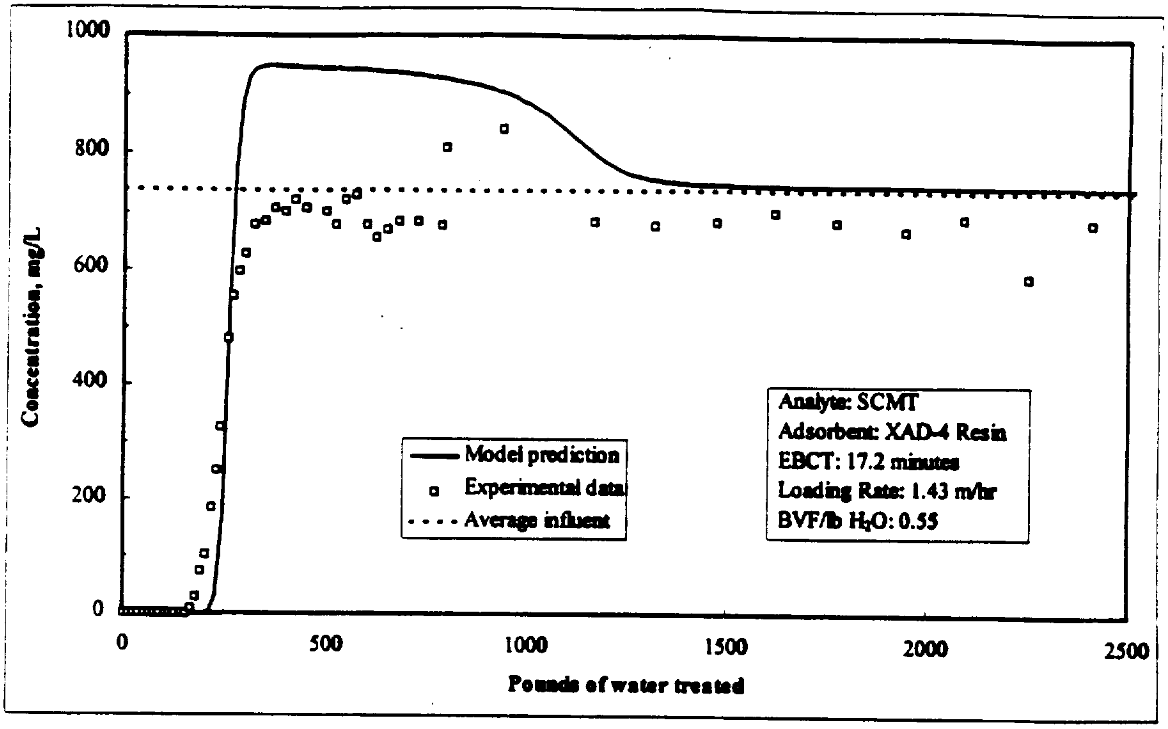

Figure 4-63. PSDM SCMT breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

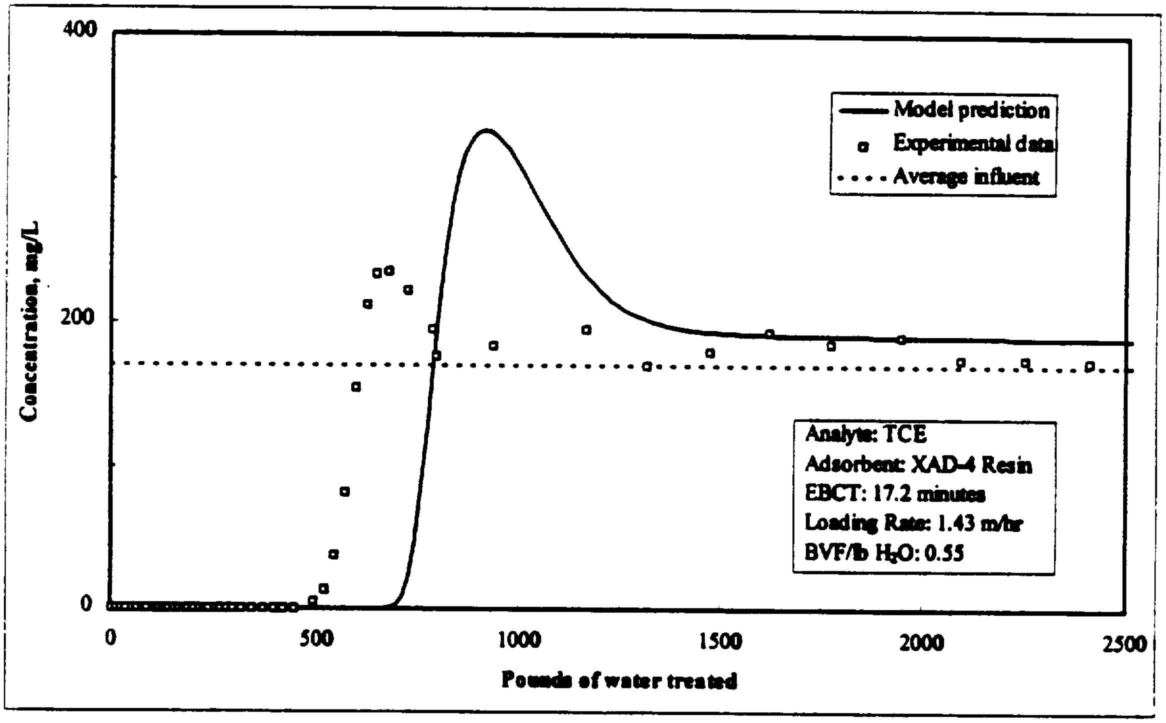

Figure 4-64. PSDM TCE breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

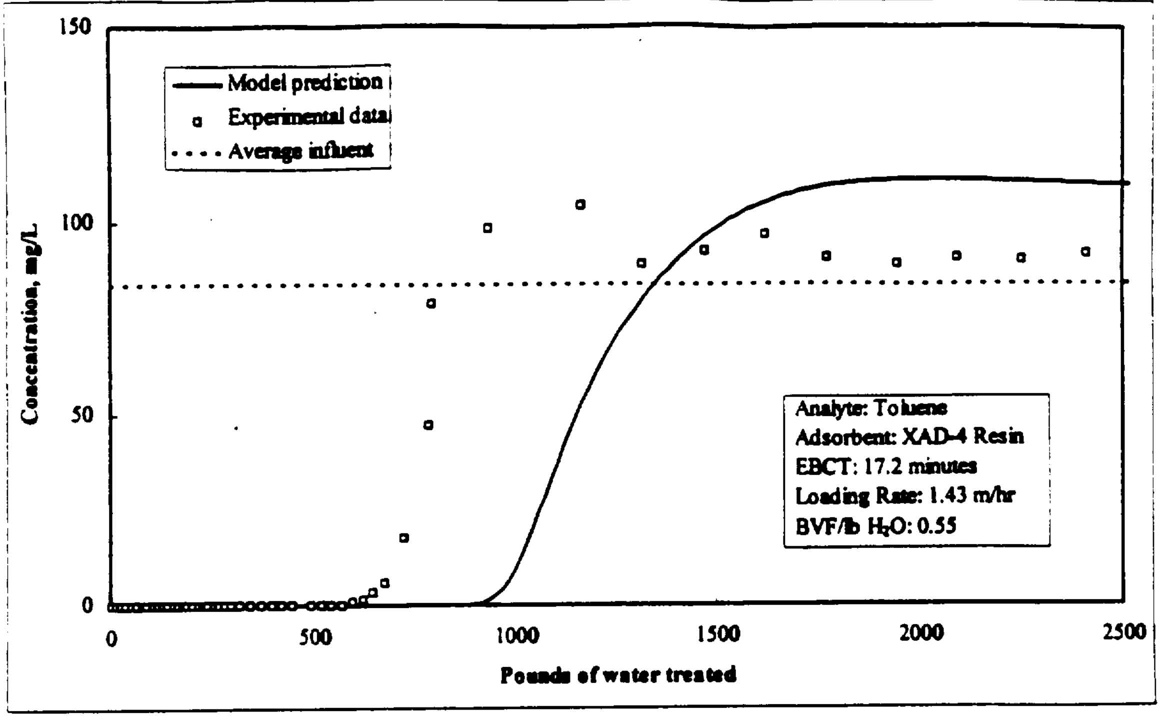

Figure 4-65. PSDM toluene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

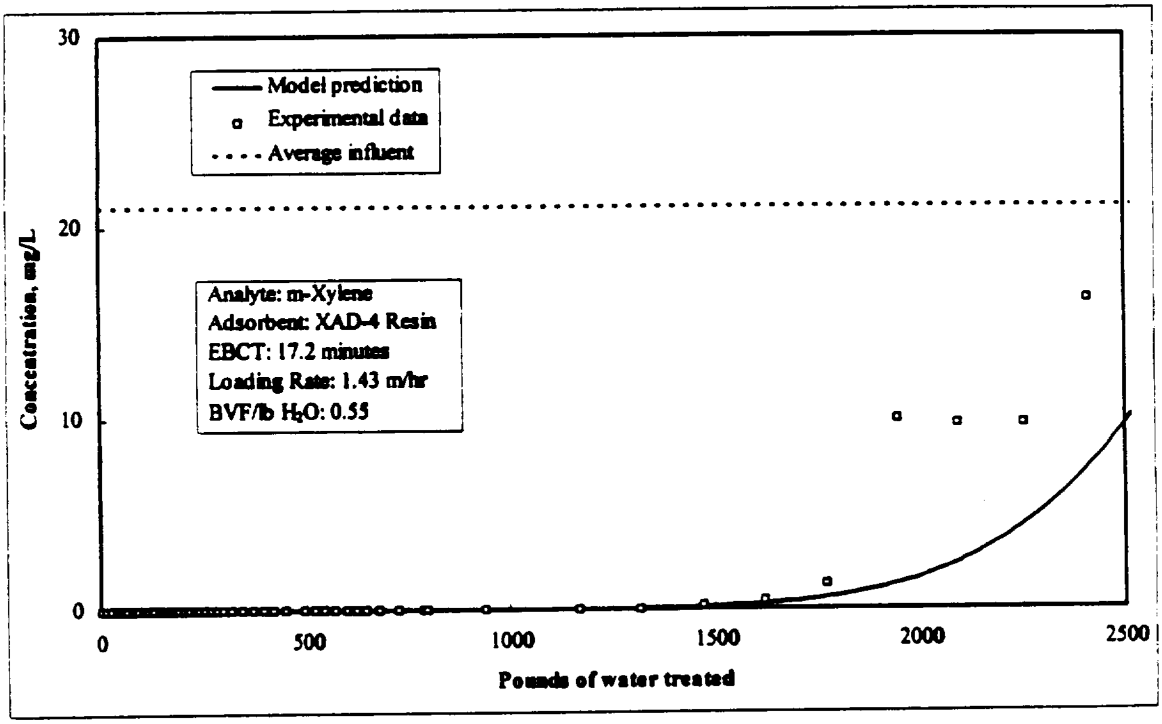

Figure 4-66. PSDM m-xylene breakthrough prediction using tracer FCs determined from simultaneous fitting of dilute and nondilute ersatz water TCE isotherms on XAD-4.

4.8 MFB Model Verification With Ersatz Water

One ersatz water experiment was performed using the entire MFB setup including ion exchange resins and adsorbents in their reported configuration (Figure 1-1). The purpose of the experiment was to verify the overall modeling approach for the MFB model. This experiment was also used to test and verify the approach used to model the different adsorption beds in series contained within the MFBs. The FCs used in the adsorption model were those determined from the ersatz TOC and tracer isotherms discussed previously. The FC initial concentrations were adjusted based on the differences in overall TOC between the ersatz water used for the verification column and that used for the isotherms. The nonadsorbing TOC concentration was determined from the known organic ion concentrations and a fraction of the TOC due to SCMT. The mass transfer parameters of the FCs were determined using the correlations developed in section 4.7.1. The FC liquid diffusivities were determined by assumming each FC had a molar volume of 150 cm^3/mol.

An additional step was added to the model for prediction of breakthrough from the verification column. The FCs were determined from isotherms on the ersatz water where SCMT and all other compounds were present. However, SCMT is removed in the MFB by the ion exchange resins for some time period ahead of the adsorption beds. The other nonpolar organics pass directly through the ion exchange resins to the adsorption beds. To solve this problem, the influent concentrations of the FCs to the adsorption beds were scaled depending on the concentration of SCMT in the ion exchange effluent. The FC initial concentrations were scaled down on a TOC concentration basis from their original values. When there was no SCMT breaking through the ion exchange beds, the total TOC of the FCs was equal to the nonadsorbing TOC concentration and the TOC due to the nonpolar organics. When SCMT broke through the ion exchange beds, the FC initial concentrations were increased to their original values determined from the TOC and tracer isotherm fitting.

4.8.1 MFB Model Verification Column TOC Breakthrough

The TOC FCs were used in the PSDM to predict the TOC breakthrough from the MFB verification column. The PSDM was run for the 580-26 GAC bed and the effluent concentrations were input to the PSDM as variable influent to the APA GAC bed and the APA effluent concentrations were input to the PSDM as variable influent to the XAD-4 resin bed. The TOC FCs Freundlich K and 1/n values were changed for each adsorbent between beds and their initial concentrations to the 580-26 GAC bed were adjusted as explained above to account for the SCMT being removed in the ion exchange resins.

The comparison of the TOC breakthrough data to the model prediction for the 580-26, APA, and XAD-4 beds in the MFB verification column are included in Figures 4-67, 4-68, and 4-69 respectively. The MFB model predicted partial TOC breakthrough through the 580-26 column at approximately 4000 pounds of water treated. The experimental TOC breakthrough did not occur until after 6000 pounds of water were treated. This occurred because the TOC FCs being input to the model during partial TOC breakthrough from the ion exchange resins were weaker adsorbing than the actual compounds entering the adsorbents at that time. This was a result of fitting the isotherms where SCMT was present and using those TOC FCs to predict this TOC breakthrough where SCMT was not present in the adsorbent bed influent for some time. The model accurately predicted the breakthrough of TOC after the SCMT broke through the ion exchange columns at approximately 6000 pounds of water treated. The results of the TOC breakthrough prediction through the APA bed included in Figure 4-68 are similar to those observed for 580-26. However, the two steps to breakthrough for APA are closer together than they were for the 580-26. The model predicts TOC breakthrough slightly sooner than the data for the XAD-4 bed plotted in Figure 4-69. The two step breakthrough was almost eliminated in this model prediction.

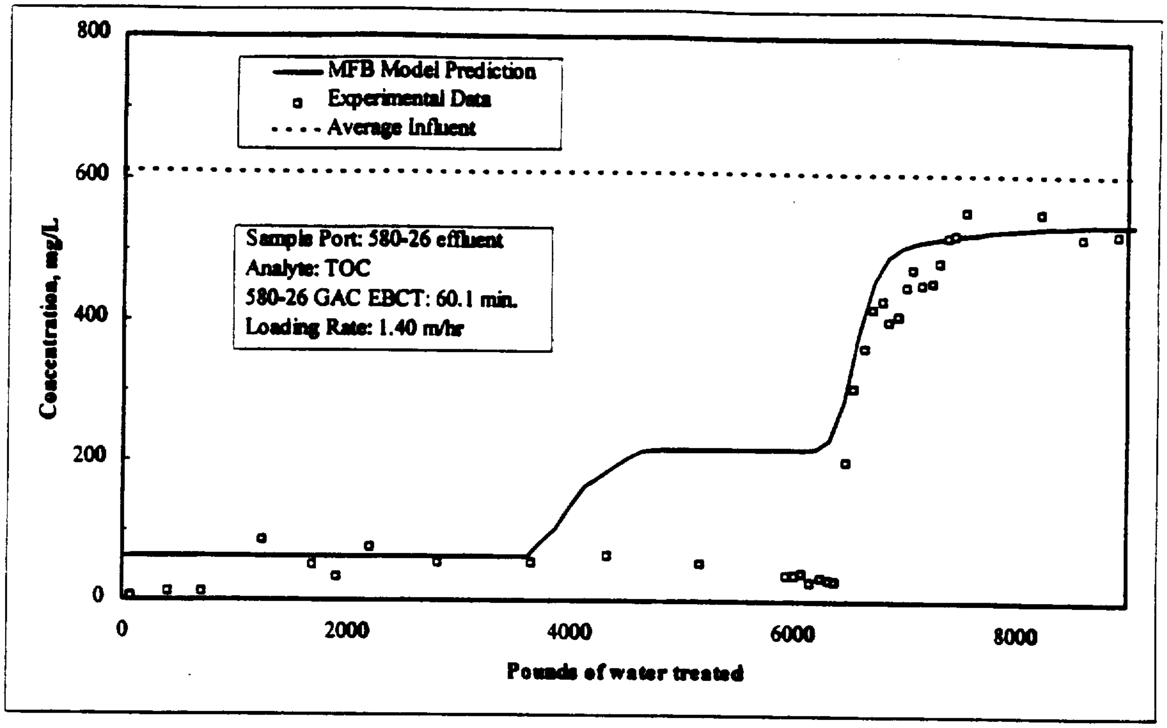

Figure 4-67. MFB model prediction of TOC breakthrough from 580-26 in the MFB model verification experiment.

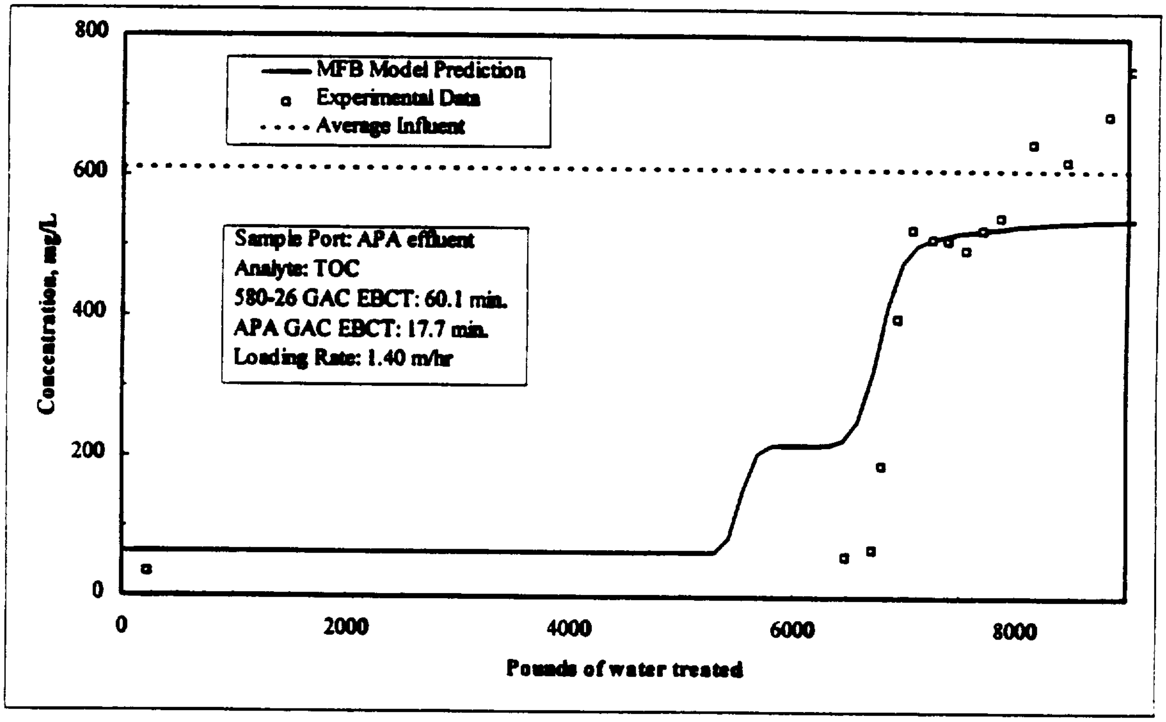

Figure 4-68. MFB model prediction of TOC breakthrough from APA in the MFB model verification experiment.

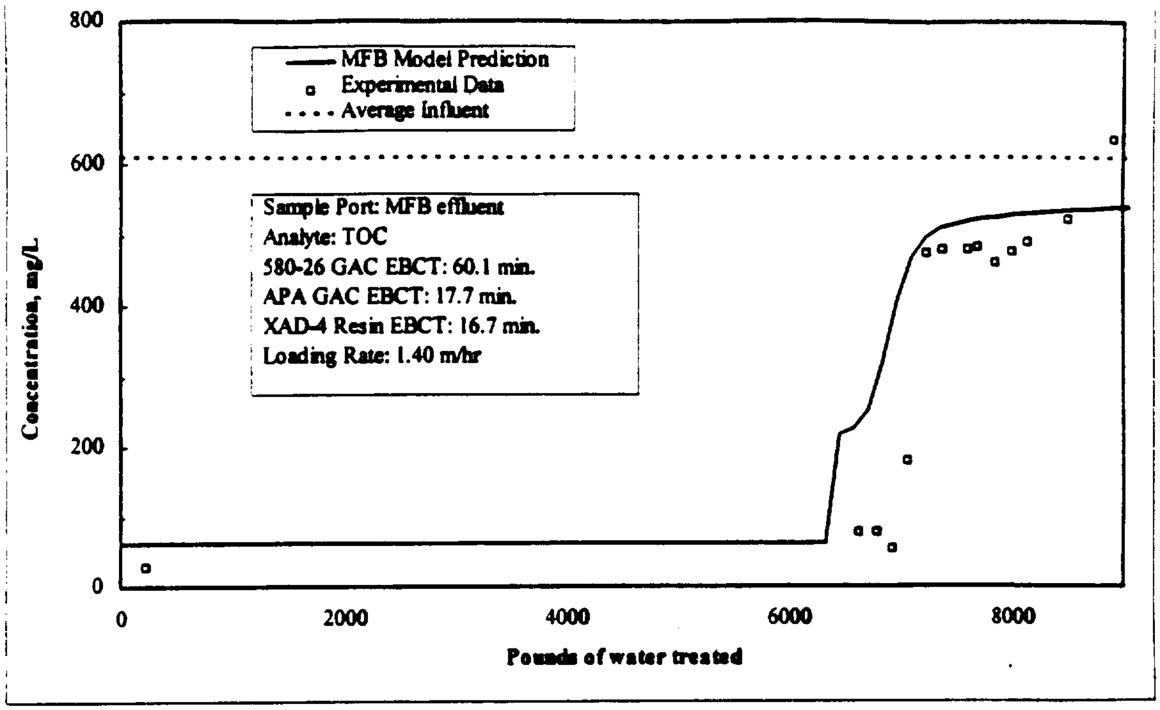

Figure 4-69. MFB model prediction of TOC breakthrough from XAD-4 in the MFB model verification experiment.

4.8.2 MFB Model Verification Column Target Compound Breakthrough

The tracer FCs were used to predict the breakthrough of target compounds from the MFB verification column. The PSDM was run for the 580-26 GAC bed and the effluent concentrations were input to the PSDM as variable influent to the APA GAC bed and the APA effluent concentrations were input to the PSDM as variable influent to the XAD-4 resin bed. The tracer FCs Freundlich K and 1/n values were changed for each adsorbent between beds and their initial concentrations to the 580-26 GAC bed were adjusted as explained above to account for the SCMT being held up in the ion exchange resins.

The results for the SCMT breakthrough prediction from the 580-26 bed in the MFB verification column are included in Figure 4-70. The model predicts the time of breakthrough for SCMT quite closely. The PSDM prediction appears to be slightly steeper than the data indicating that the kinetic parameters used for SCMT in the model may be slightly over estimated. This may be due to the initial holdup of SCMT in the ion exchange resin allowing the other organic compounds (TCE, toluene, m-xylene, 1,2,4-TCB, naphthalene) to have an opportunity to preadsorb onto the 580-26. The overshoot predicted by the model was not observed in the data. The model prediction for SCMT breakthrough from the APA bed is compared to the experimental data in Figure 4-71. The results are very similar to those explained for the 580-26 bed. The SCMT breakthrough prediction from XAD-4 is included in Figure 4-72. The results are again similar to those explained for the 580-26 bed.

The TCE breakthrough prediction from the 580-26 bed is compared to the experimental data in Figure 4-73. The model predicts TCE breakthrough sooner than was observed in the experimental data and with slower kinetics. The model prediction did not show the extremely large overshoot observed in the data. The TCE capacity achieved in the experimental column is very close to that achieved in the experiment. The error is most likely due to error in estimating the mass transfer parameters where SCMT was not present in the adsorbent for most of the run time. Figure 4-74 compares the model prediction for TCE breakthrough from the APA column to the experimental data. The results are nearly the same as those observed for the 580-26. The TCE model prediction is compared to the data for XAD-4 in Figure 4-75. The breakthrough through XAD-4 represents the effluent from the end of the MFB. The model prediction is close to the data but the kinetics again appear to need some adjustment. The time of breakthrough was predicted approximately 15% earlier than the data.

Figure 4-76 shows that the model predicts the breakthrough of toluene later than the experimental data for the 580-26 bed. The x-axis was extended past the experimental breakthrough to show the model prediction. It is difficult to determine whether the error is due to the kinetic parameters or the equilibrium description used in the model. The error is again partially due to the removal of SCMT in the ion exchange resins prior to its appearance in the adsorbent beds. Figures 4-77 and 4-78 compare the toluene model predictions to the data for the APA and XAD-4 beds. The results are very similar to those observed for the 580-26.

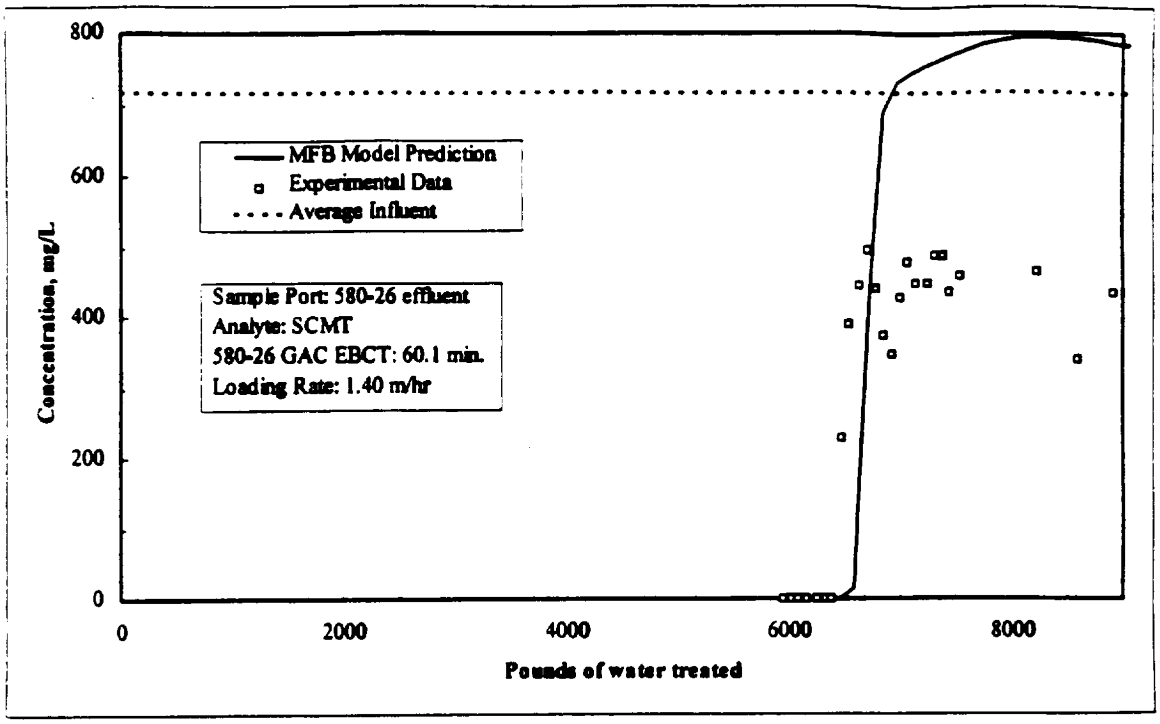

Figure 4-70. MFB model prediction of SCMT breakthrough from 580-26 in the MFB model verification experiment.

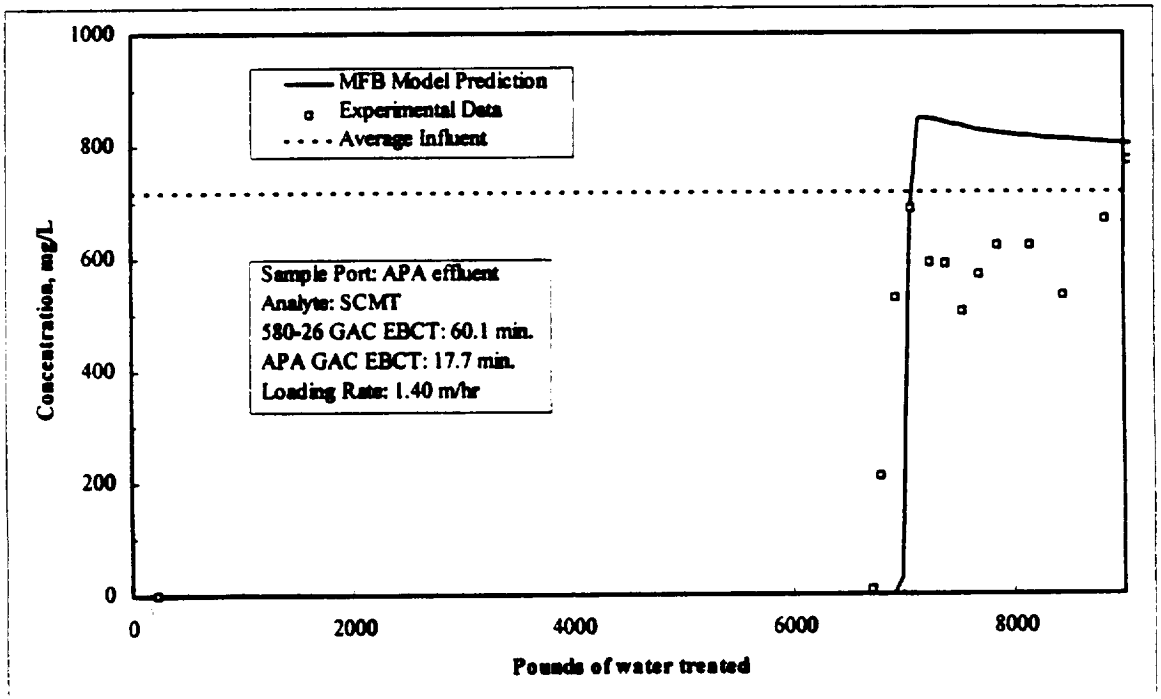

Figure 4-71. MFB model prediction of SCMT breakthrough from APA in the MFB model verification experiment.

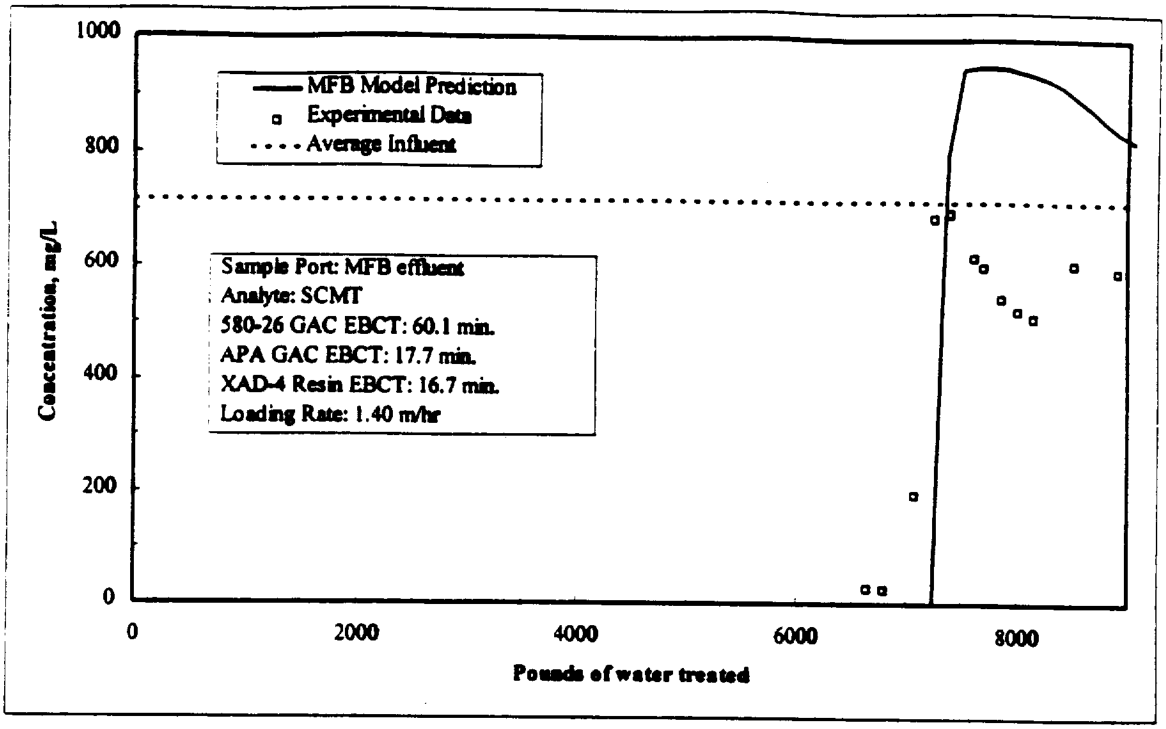

Figure 4-72. MFB model prediction of SCMT breakthrough from XAD-4 in the MFB model verification experiment.

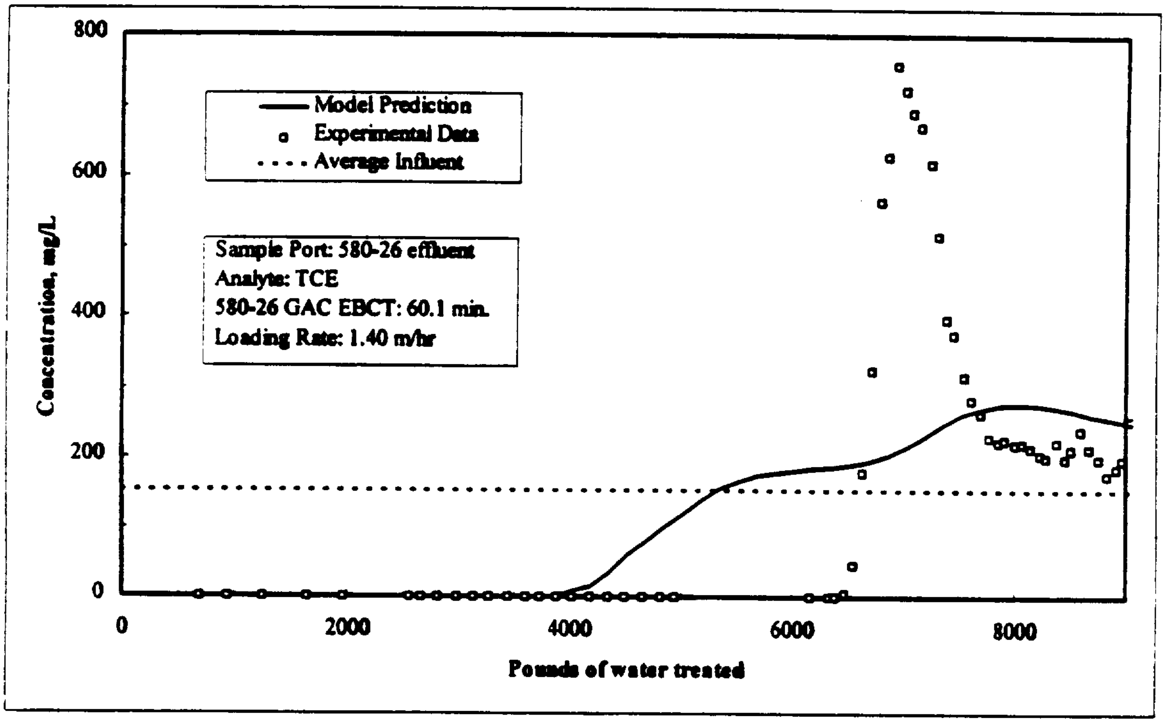

Figure 4-73. MFB model prediction of TCE breakthrough from 580-26 in the MFB model verification experiment.

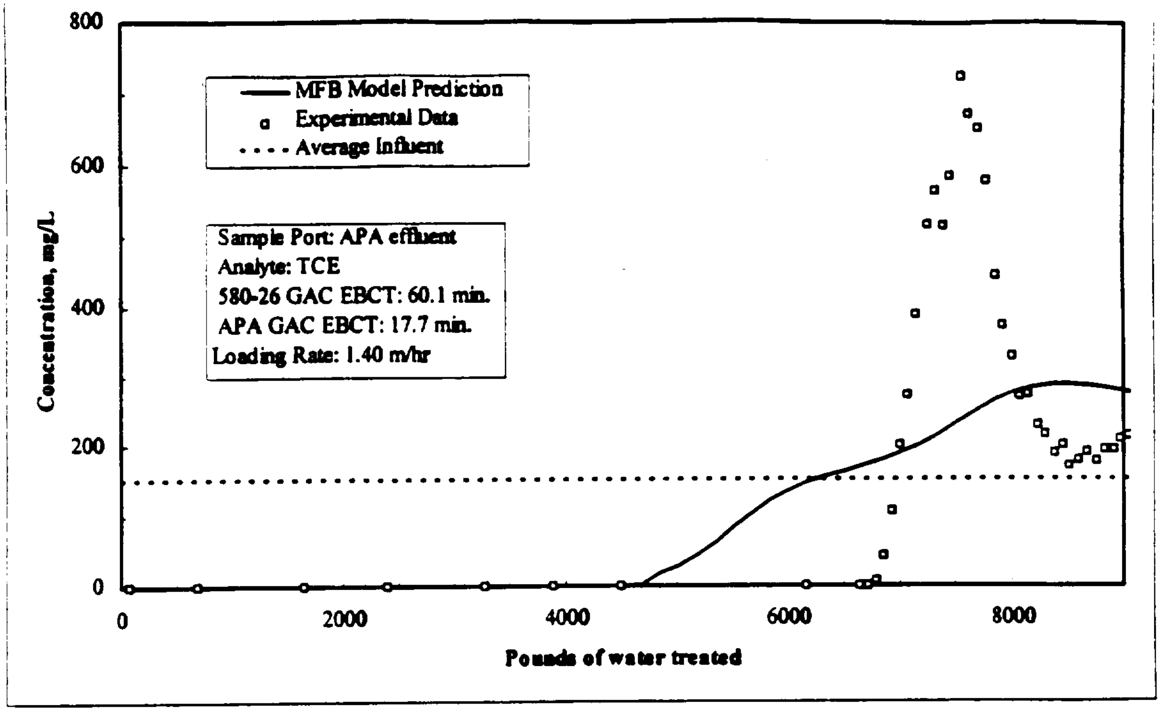

Figure 4-74. MFB model prediction of TCE breakthrough from APA in the MFB model verification experiment.

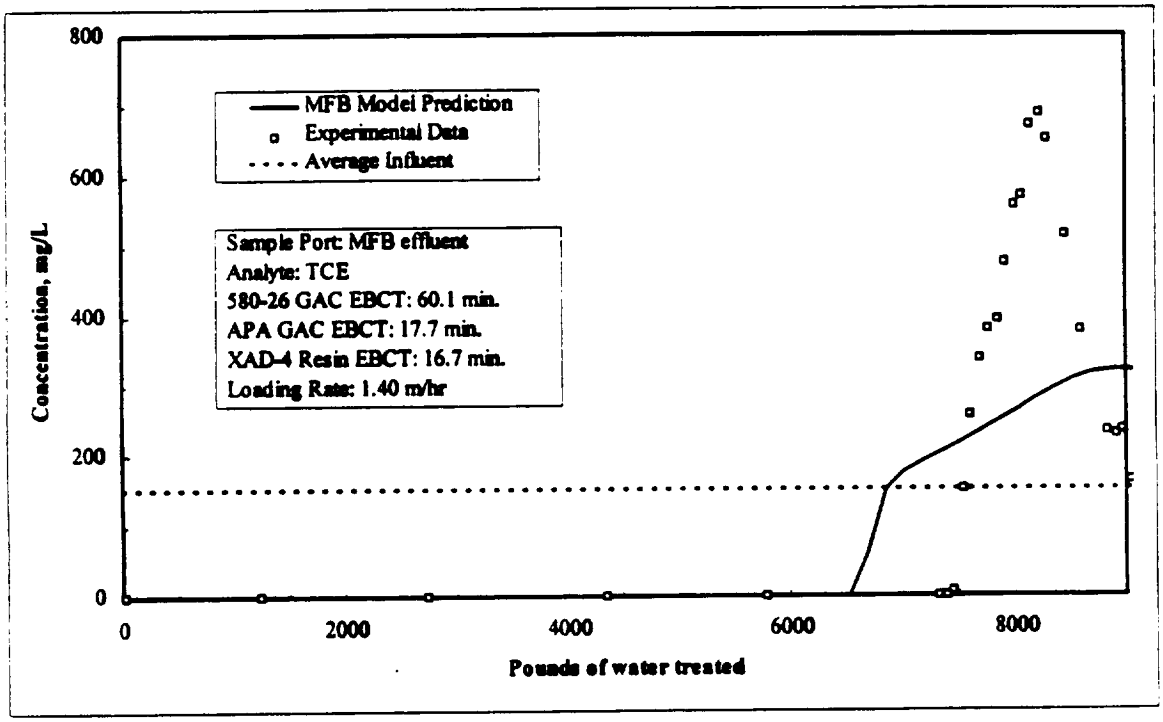

Figure 4-75. MFB model prediction of TCE breakthrough from XAD-4 in the MFB model verification experiment.

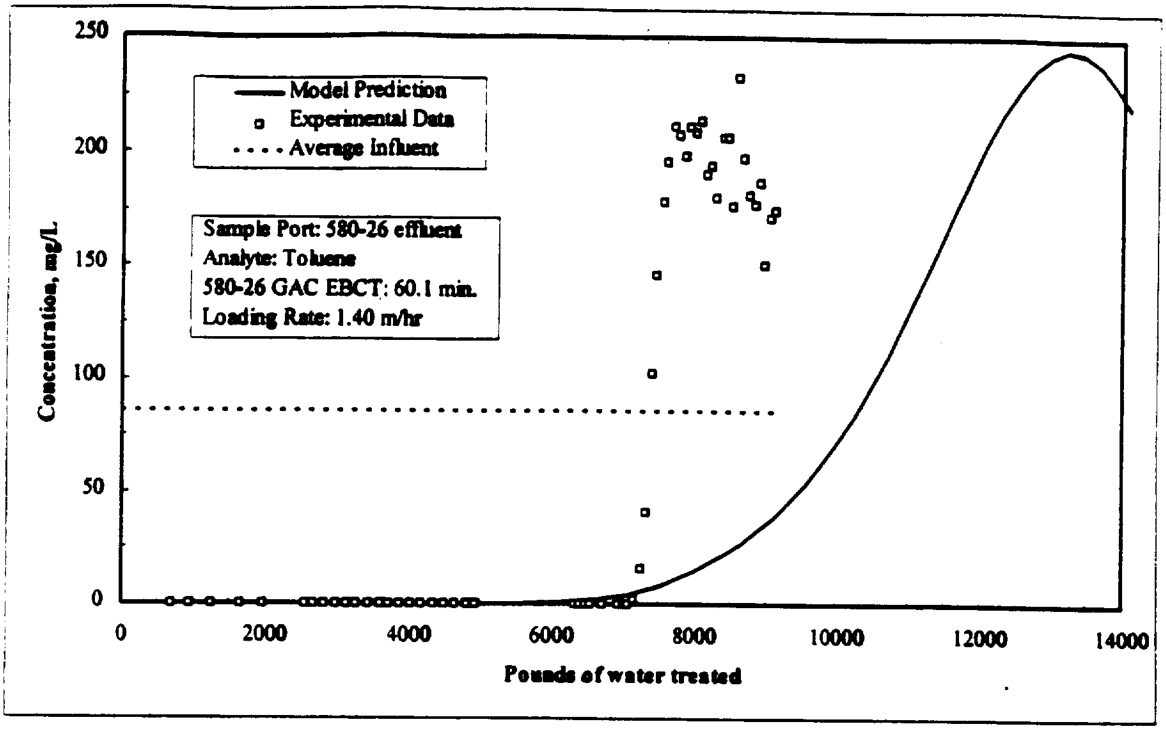

Figure 4-76. MFB model prediction of Toluene breakthrough from 580-26 in the MFB model verification experiment.

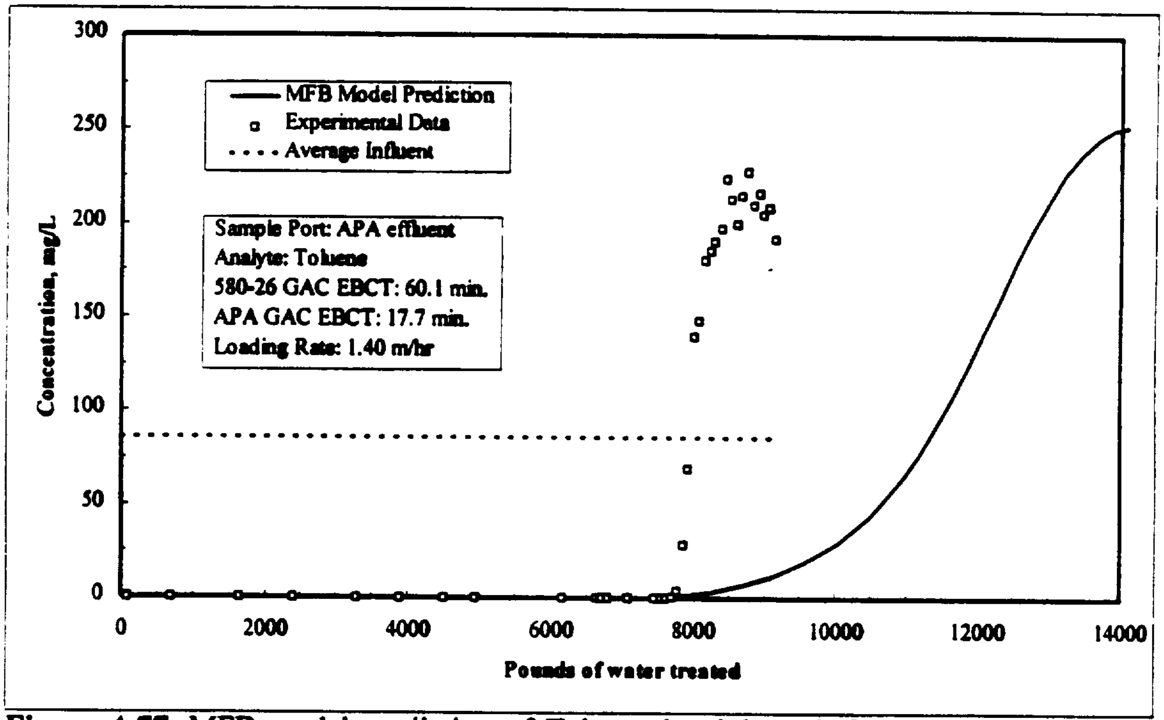

Figure 4-77. MFB model prediction of Toluene breakthrough from APA in the MFB model verification experiment.

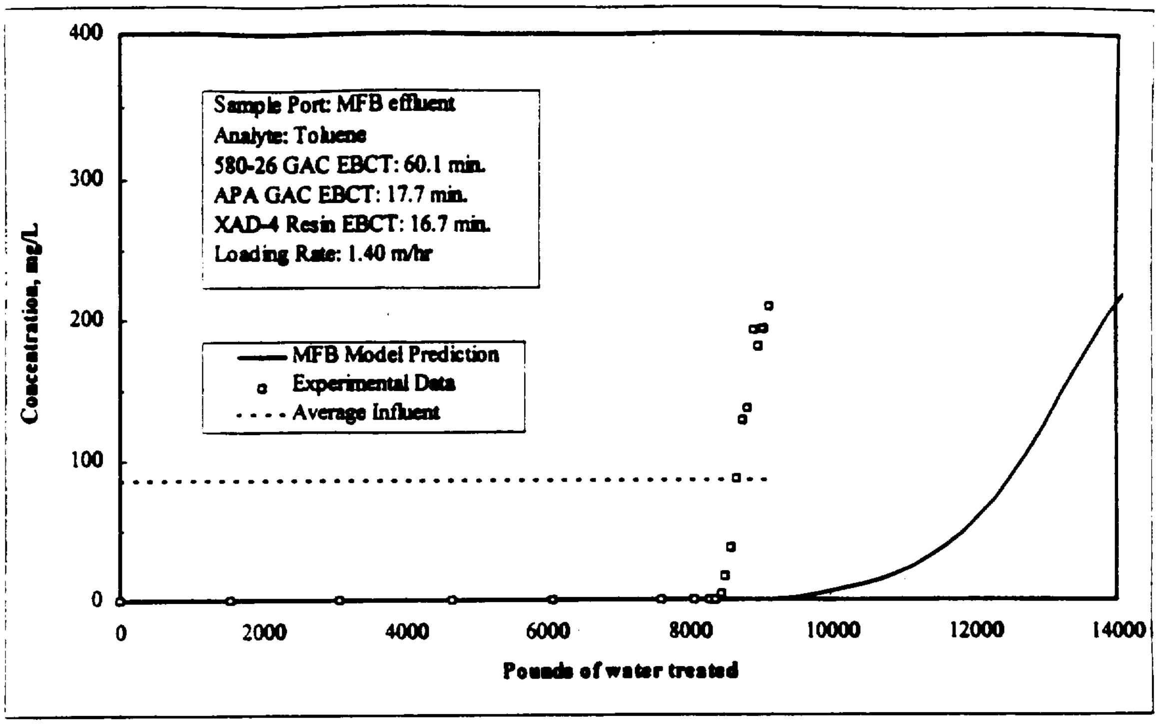

Figure 4-78. MFB model prediction of Toluene breakthrough from XAD-4 in the MFB model verification experiment.

5.0 Conclusions and Future Research Recommendations

A fixed bed adsorption model employing the FCA was developed for use in modeling the adsorption processes within the International Space Station multifiltration beds. This modeling approach was chosen because it can predict the TOC breakthrough as well as target compound breakthrough from the MFBs in an unknown mixture. The modeling approach was verified using an ersatz water made up to serve as a surrogate to the actual shower and handwash wastewater for experiments.

The three adsorbents currently included in the MFB design were evaluated in this study. Those adsorbents were 580-26 GAC, APA GAC, and XAD-4 resin. The shower and handwash ersatz water included SCMT, TCE, toluene, m-xylene, 1,2,4-TCB, and naphthalene as its adsorbable components. These compounds represent a distribution of relatively weakly to strongly adsorbing compounds. SCMT was included since it is reported to account for over 60% of the TOC in the actual shower and handwash wastewater. The ersatz water also contained ions representative of the actual shower and handwash wastewater.

Single solute isotherm data was available for each of the adsorbates in the ersatz water on each of the MFB adsorbents (Hand *et al.*, In Press). The isotherm data was obtained over a concentration range of approximately 10 µg/L to 10 mg/L and described using the Freundlich isotherm equation. The isotherms on the 580-26 and APA activated carbons were all linear on a log-log plot and the Freundlich equation fit the data well. The single solute isotherms on the XAD-4 resin exhibited some curvature on a log-log plot. For this reason, the XAD-4 resin Freundlich parameters were dependent on the concentration range fit.

A TOC isotherm was performed on the actual waste shower and handwash water to determine its TOC adsorption capacity. The isotherm revealed as expected that the shower and handwash wastewater was a multicomponent mixture with a nonadsorbing TOC fraction. Unfortunately, this was the only isotherm data obtained for the actual shower and handwash wastewater. More isotherms (dilute and nondilute TOC and tracer isotherms) should be performed to more accurately determine the competitive adsorption equilibrium characteristics of the actual shower and handwash wastewater.

An ersatz water was made up to mimic the TOC adsorption capacity of the actual waste shower and handwash water. A TOC isotherm was performed to verify that the TOC adsorption capacity of the ersatz water was similar to that of the actual waste shower and handwash water. Once verified as a suitable surrogate in this manner, the ersatz was treated as an unknown mixture for modeling efforts.

Isotherms were performed on each of the adsorbents using the ersatz water. The isotherms were analyzed for TOC and the individual constituents of the ersatz water. The FCA was applied to this isotherm data to determine the TOC and tracer FCs for each adsorbent. The FCs were determined from fitting the isotherm data in a manner which would facilitate beds in series modeling of the different adsorbents. The FCA was able to accurately fit the TOC isotherms for each of the adsorbents. This indicated that the TOC FCs used in IAST calculations accurately simulated the TOC adsorption capacity of the ersatz water.

The FCA was also able fit the tracer isotherms well for each of the adsorbents. The tracer FCs were tested in IAST calculations to see if the equilibrium of the other ersatz water constituents could be predicted based on the tracer fit. The results indicated that as the adsorbability of the compound increased, the accuracy of the model prediction to the data decreased. The model generally did a good job of predicting the equilibrium for TCE, toluene, and m-xylene. The equilibrium description consistently overpredicted the reduction in capacity for 1,2,4-TCB, naphthalene, and SCMT in the system. It was likely that the reduction in capacity was observed for naphthalene and 1,2,4-TCB since the strongly adsorbing compounds were already accounted for in the mixture by the FCs because a weakly adsorbing compound was fit. The reduction in capacity for SCMT was overpredicted because SCMT made up such a large percentage of the overall TOC of the mixture. A compound must make up a small amount of the TOC in the mixture because its adsorption potential is already accounted for by the FCs. The fits and predictions were more accurate for the XAD-4 resin than for either of the activated carbons. This may be due to the more uniform pore structure and macroporous matrix reported by the manufacturer for XAD-4 resin.

Column experiments were performed on each of the adsorbents using the ersatz water. The breakthrough curves for each of the known ersatz water constituents were fit on a single solute basis using the PSDM to determine the observed tortuosity and SPDFR for each compound. The fitting results were used to develop correlations for prediction of tortuosity and SPDFR for other target compounds on each adsorbent. The results indicated that pore diffusion was the controlling mass transfer mechanisms for both 580-26 and APA GACs for all compounds except SCMT. Surface diffusion was approximately five times more important than pore diffusion in describing the mass transfer for all compounds on the XAD-4 resin. The mass transfer parameter correlations were used to predict the mass transfer parameters for the FCs.

The TOC FCs were used in the PSDM to predict the TOC breakthrough from each of the adsorption columns. The results indicated that the model slightly overpredicted the capacity of the columns for TOC adsorption. These model calculations involve using the six TOC FCs determined from fitting the TOC isotherms in fixed bed calculations.

The tracer FCs were used in the PSDM with the known constituents of the ersatz water to predict breakthrough of those compounds. The model calculations involved using the target compound and the five tracer FCs determined from fitting the tracer isotherms in fixed bed calculations. The results were then compared to the experimental data to test the model. The model predictions were best for the weakly to moderately adsorbing compounds. As the strength of the adsorbing compound increased, the accuracy of the PSDM prediction consistently decreased. This is due to [illegible] mass transfer parameters and tracer FCs used in the system. The mass transfer parameters and tracer FCs could be tuned to better predict the breakthrough of the stronger compounds by fitting the breakthrough curves using a multicomponent PSDM simulation.

One experiment was performed using a series of adsorbents and ion exchange resins set up in the same configuration as the actual MFB design. This experiment was also performed with the ersatz water. The breakthrough of TOC and target compounds from the verification MFB was predicted with the fixed bed model and compared to the breakthrough data. The model predicted the TOC breakthrough slightly before the experimental data. The model did a good job of predicting the SCMT breakthrough. The breakthrough prediction began slightly after the data but was steeper than the data indicating that the mass transfer parameters used for the SCMT could use some fine tuning to get a better prediction. The model predicted TCE breakthrough occurred about 15% earlier than the data. The error here again appears to be due to the mass transfer parameters. The predicted breakthrough of toluene is significantly later than the experimental data. However, it is difficult to determine if the error is due to mass transfer parameters or capacity since only part of the breakthrough curve was observed during the experiment. The error in the MFB verification column predictions may have occurred since the SCMT was held up for some time period in the ion exchange resins but it was not held up in the experiments where the mass transfer parameter correlations were determined. This error could be corrected by adjusting the mass transfer parameters for this situation.

These results have shown that the FCA used in conjunction with the PSDM can predict breakthrough of both TOC and target compounds from the MFB. However, this verification was only on an ersatz water. The FCA should also be applied to urine distillate and humidity condensate water TOC and tracer isotherms. Further work should be done using the actual shower and handwash wastewater as well as mixtures of all the expected space station waste streams. The most important work would be done using a mixture of all of the potential waste streams aboard the ISS since the waste streams will be combined before treatment. Therefore, the main focus of future work should be on model verification using the combined mixture of all the space station waste streams. The final tuning of the mass transfer parameters used in the system could be performed in the actual water tests.

6.0 Nomenclature

$Bi_{p,i}$ = Biot number based on pore diffusivity (dimensionless)

$Bi_{s,i}$ = Biot number based on surface diffusivity (dimensionless)

BVF = bed volumes fed (dimensionless)

$C_{e,i}$ = equilibrium liquid phase concentration of component i (M/L^3)

$\overline{C_i}\left(\bar{z},T\right)$ = reduced adsorbate concentration in the bulk phase as a function of dimensionless axial position and dimensionless time (dimensionless); $C_i(z,t)/C_{o,i}$

$C_{o,i}$ = initial influent bulk phase concentration for component i (M/L^3)

$\overline{C_{p,i}}\left(\bar{r},\bar{z},T\right)$ = reduced adsorbate concentration in adsorbent pores as a function of dimensionless radial and axial position and dimensionless time (dimensionless); $C_{p,i}(r,z,t)/C_{o,i}$

$C_{s,i}$ = aqueous solubility of component i (M/L^3)

Dg_i = combined solute distribution parameter (dimensionless)

$Dg_{p,i}$ = pore solute distribution parameter (dimensionless)

$Dg_{s,i}$ = surface solute distribution parameter (dimensionless)

Dg_t = total solute distribution parameter (dimensionless)

D_i = ration of surface to pore diffusion transport (dimensionless)

D_L = free liquid diffusivity (L^2/t)

$D_{p,i}$ = pore diffusivity based on pre void fraction (L^2/t)

$D_{s,i}$ = surface diffusivity (L^2/t)

d = column diameter (L)

$EBCT$ = empty bed contact time; fluid residence time in the bed which is devoid of the adsorbent; V_B/Q, or L/V_s (t)

$Ed_{p,i}$ = pore diffusion modulus (dimensionless)
$Ed_{s,i}$ = surface diffusion modulus (dimensionless)
K_i = Freundlich isotherm capacity constant $[(M/L^3)(L^3/M)^{1/n}]$
$k_{f,i}$ = film transfer coefficiet (L/t)
$1/n_i$ = Freundlich isotherm intensity constant (dimensionless)
L = length of fixed bed (L)
m = number of components in PSDM simulation
M = mass of adsorbent added to isotherm (M)
$q_{e,i}$ = adsorbent phase concentration in equilibrium with the bulk liquid phase concentration (M/M)
$q_{o,i}$ = adsorbent phase concentration in equilibrium with the initial bulk liquid phase concentration (M/M); $K_iC_{o,i}^{1/ni}$
$\overline{q}_i(\overline{r},\overline{z},T)$ = reduced adsorbent phase concentration as a function of dimensionless radial and axial position and dimensionless time (dimensionless); $q_i(r,z,t)/q_{e,i}$
Q = fluid flowrate (L^3/t)
r = radial coordinate (L)
$\overline{r}$ = reduced radial coordinate (dimensionless); r/R
R = adsorbent radius (L)
Re = Reynolds number (dimensionless)
Sc = Schmidt number (dimensionless)
$SPDFR$ = Surface to Pore Diffusion Flux Ratio (dimensionless)
St_i = Stanton number (dimensionless)
t = elapsed time (t)
T = Reduced time, mass throughput (dimensionless)
v = interstitial velocity (L/t); V_s/ε
V = volume of isotherm bottle (L^3)
V_s = superficial velocity (L/t)

V_m = molar volume at normal boiling point (L^3/mol)

$X_{e,i}$ = total adsorbent phase concentration in equilibrium with initial bulk phase concentration (M/M); $q_{ei}(r,z,t)+[\varepsilon_p C_{o,i}(r,z,t)/\rho_a]$

$X_i(r,z,t)$ = total adsorbent phase concentration as a function of radial and axial position and time (M/M); $q_i(r,z,t)+[\varepsilon_p C_{p,i}(r,z,t)/\rho_a]$

$\overline{X_i}(\bar{r},\bar{z},t)$ = reduced total adsorbent phase concentration as a function of dimensionless radial and axial position and dimensionless time (dimensionless); $X_i(r,z,t)/X_{e,i}$

z = axial coordinate (m)

$\bar{z}$ = reduced axial coordinate (dimensionless); z/L

ε = bed porosity; fraction of volumetric space in reactor unoccupied by adsorbent, or void fraction (dimensionless)

ε_p = particle porosity, fraction of volumetric space in adsorbent phase unoccupied by adsorbent on the pore volume fraction (dimensionless)

ρ_a = apparent adsorbent density (includes intraparticle pore volume) (M/L^3)

ρ_b = adsorbent bulk density (includes all interparticle and intraparticle volume) (M/L^3)

ρ_L = density of water (M/L^3)

τ = fluid residence time in packed bed (t)

μ_l = observed tortuosity or labyrinth factor (dimensionless)

μ_L = viscosity of water (M/LxT)

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Appendix I. Multifiltration Bed Influent Wastewaters

Compound	Carbon	Humidity	Shower	Clothes	Urine
	Fraction	Condensate	Handwash	Wash	Distillate
		ug/L	ug/L	ug/L	ug/L
Total Organic Carbon (TOC)		50000	704000	101600	11100
Acenapthylene	0.947		10	8	
Acetaldehyde	0.545	170		26	330
Acetic Acid	0.4	8000	10800	11000	990
Acetone	0.621	500	60	98	353
Acetophenone	0.8				2.2
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	0.837			47	
4-Acetyl morpholine	0.558	2100			
Acetyloxyoctadecenoic acid, Methyl ester	0.704			5	
Adipate	0.493				22
Alphahydroxybenzeneneacetic acid ester	0.651				33
Amine(unknown)	0.6	170			
2-Amino benzoic acid methyl ester	0.636				1
Benzaldehyde	0.792	10			9
Benzene	0.923	1		1	
Benzeneacetic acid	0.706	4	64		24
Benzene ethanol	0.787	50		8	
Benzene methanol	0.778	380			
Benzoic Acid	0.689	150	50	60	660
Benzophenone	0.857	5			
2H-1-Benzopyran-2-one	0.74	4			
Benzothiazole	0.622	40		8	
Benzyl alcohol	0.778	200		5	33
1,1-Biphenyl-2-ol	0.847	10			
Bis(2-ethylhexyl)phthalate	0.738	10	150	15	33
Bis(1-methylethyl)ester hexadecanoic acid	0.626	30			
Bis(2-methypropyl)phthalate	0.691	6			
1,3-Butanedoid	0.533	14			6
Butanoic acid	0.545	70	44800	3040	1320
2-Butanol	0.649	1000	1600		
2-Butanone	0.667	50			34
2-Butoxyethanol	0.61	900	8	23	9
2-Butoxyethoxyethanol	0.593	500		18	
Butylated hydroxy anisole	0.733	60		14	
Butylbenzylphthalate	0.731	4			9
(1-Butylheptl) benzene	0.879			23	
(1-Butyloctyl) benzene	0.878			40	
Butyraldehyde	0.666	25			
Butyrolactone	0.558				22
C12 Alcohol	0.774			20	
C12+Aldehyde-methyloxime	0.723		20		
C11+ Alkylsubstituted benzene	0.878			75	
C4-Substituted cyclohexanol	0.784	20			
C5-7 Ketone	0.697				11
Caffeine	0.495		50	25	
Caprolactam	0.637	12000	1700	17	110
Carbon Disulfide	0.273	500			
4-Chloro aniline	0.565		10		
Chlorobenzene	0.352			14	
2-Chloroethanol phosphate	0.135	160			
Chloroform	0.101				18
1-Chloro-4-isocyanato benzene	0.549		9		

Chloromethylphenol	0.59				21
Chlorophenol	0.561	7			30
Cholesterol	0.839		1400	310	
Cis-p-menth-2-ene-1.8-diol	0.706				5
Cotinine	0.682		10		
Crotonaldehyde	0.685	10			
Cyclohexanone	0.734	100			
2-Cyclohexen-1-ol	0.72	1			
2-Cyclohexen-1-one	0.734	5			
1-(1-Cyclohexen-1-yl)ethanone	0.774				25
Cyclopentanone	0.714				5
Decanoic acid	0.69	100	40	23	12
Decanoic acid, Methyl ester	0.71		10		
1-Decanol	0.759		100		
1,4-diacetylbenzene	0.741	12			
Butyl amine	0.744	1000			51
di-n-Butylphthalate	0.593	100	5	7	
2,4-Dichloroaniline	0.645		5		
Dichlorobenzoic acid	0.44	20			
2,4-Dichlorophenol	0.442				15
Diethylene glycol	0.453	3			
Diethylene glycol diecetate	0.505	400			
Diethylphthalate	0.649	320	12	10	22
Dihydroacetic acid	0.387	4			
2,3-Dihydrobenzofuran	0.8				34
Dihydro-5,5-dimethyl-2(3H)-furanone	0.632				97
Dihydro-5-ethenyl-5-methyl-2H-furanone	0.667				72
Dihydro-5-ethyl-2H-furanone	0.632	28			121
1,3-Dihydro-2H-indol-2-one	0.722				9
Dihydro-5-methyl-2(3H)-furanone	0.612	33	30		212
2,3-Dihydro-4-methyl-1H-indole	0.812				10
1-(Dimethylamino)-2-propanol	0.588	85			
a,a-Dimethyl benzenemethanol	0.787	150			
Dimethylbenzyl alcohol	0.794	100			7
(3,3-Dimethyldecyl) benzene	0.873			28	
Dimethyl disulfate	0.25[illegible]				14
4-(1,1-Dimethylethyl)-benzoic acid	0.741	16			
3-(1,1-Dimethylethyl)-phenol	0.8	50			
2,2-Dimethyl-1-(2-hydroxy-1-methylethyl)					
-propyl ester propanoic acid	0.667	73			
3,7-Dimethyl-1,5-octadien-3-ol	0.779	10			11
Dimethylphthalate	0.619	40			39
2,2-dimethyl propanoic acid	0.448	50			
2,3-Dimethylpyrazine	0.667				11
Dimethyl sulfide	0.387		25		
Dimethyl sulfone	0.255	140	76	75	75
Dimethylsulfoxide	0.307		10	9	
Dimethyltetrahydropyranone	0.656				8
2,6-Dinitrotoluene	0.454	80			
1,6-Dioxacyclododecane-7,12-dione	0.631	450			
Dipropyleneglycol methyl ether	0.568	50		12	
Docosane	0.852	10			
Docosanoic acid	0.776		80		
Docosanoic acid, methyl ester	0.78		190		
Dodecanal, o-methyloxime	0.732		440		
Dodecanoic acid	0.72	50	2250	160	78
Dodecanoic acid, methyl ester	0.729		900		
Dodecanol	0.774	6	160	43	

Eicosane	0.851	21			
Eicosanoic acid	0.769		180	41	
Eicosanoic acid, methyl ester	0.773		250		
2,2-[1,2-Ethaneoxybis(oxy)] bis-ethanoldiacetate	0.513	200			
Ethanol	0.522	7000	2400	500	3850
Substituted ethanone	0.65	40			
2-Ethoxyethanol	0.533	200			
Ethoxyethanol acetate	0.545	100			
Ethoxyethoxy ethanol	0.537	500		15	
Ethoxyethoxy ethanol acetate	0.539	25			
1-(2-Ethoxypropoxy)-2-propanol	0.592	130			
Ethylacetate	0.545				3
Ethyl benzene	0.905			8	
2-Ethyl-1-butanol	0.706				110
(1-Ethyldecyl) benzene	0.878			28	
Ethelene glycol	0.386	3000	790	310	
2-Ethyl hexanoic acid	0.667	500	4	21	5
2-Ethylhexanol	0.738	40	10	6	11
2-Ethylhexylphthalate	0.738			63	
4-Ethyl-2-methoxyphenol	0.71				5
4-ethyl morpholine	0.73	6600	910		187
1-Ethylnonyl) benzene	0.879			25	
1-Ethylpiperidine	0.743	26			
Formaldehyde	0.4	6000	120	120	127
Formic Acid	0.261	3000	3500		4400
Freon 113	0.141				
2-Furan methanol	0.612				65
2-(3H)-furanone	0.571	7		7	
Furanone, alkyl substituted	0.714				17
Glycerol	0.391	1400	110		
Glycol ether	0.3	420			
Glycolic acid	0.316	4000	3000		220
Hendecanoic acid	0.702		90		22
Heneicosanoic acid, methyl ester	0.776		40		
Heptacosane	0.853			46	
Heptadecane	0.85		5		
Heptadecanoic acid	0.755		130	48	
Heptadecanoic acid, methyl ester	0.761		50		
Heptanoic acid	0.646	200	3	6	11
4-Heptanol	0.724				6
4-Heptanone	0.737				41
Hexacosane	0.852	3		23	
Hexadecanoic acid	0.75	5	2450	340	3
9-Hexadecanoic acid, eicosyl ester	0.809		75	53	
Hexadecanoic acid, hexadectyl ester	0.799		90		
Hexadecanoic acid, methyl ethyl ester	0.626	26	600	9	
Hexadecanoic acid, octadectyl ester	0.803		50		
Hexadecanol	0.793		46	53	24
Hexadecenoic acid	0.756		230	190	11
Hexadecenoic acid, methyl ester	0.761	11	200		
2,4-Hexadienedioic acid	0.507	9			
Hexanal, o-methoxime	0.651		1360		
Hexanedioic acid, bis(1-metyhylethyl) ester	0.939	20			
2,5-Hexanedione	0.632				5
Hexanoic acid	0.621	200	13	10	18
Hexanoic acid, methyl ester	0.646		5		0
2-Hexanol	0.706		95	110	114
3-Hexanone	0.72				5

Hexenal	0.61	13			
1-Hexen-3-ol	0.7195	3			
4-Hydroxybenzoic acid	0.609	2			
Hydroxybenzoic acid, methyl ester	0.568	13	305	10	
3-Hydroxy-2-butanone	0.545	20			
Hydroxybutyric acid	0.462			180	488
Hydroxymethoxybenzaldehyde	0.632	9			21
1-(4-Hydroxy-3-methoxyphenol) ethanone	0.651				13
4-Hydroxy-4-methyl-2-pentanone	0.621	200	130	36	5
1-(2-Hydroxy-5-methylphenyl) ethanone	0.8	14			100
Hydroxyphenylacetic acid, choroethyl ester	0.56				30
Hydroxyphenylethanone	0.706				8
3-(2-Hydroxyphenyl)-2-propenoic acid	0.663				10
1-Hydroxy-2-propanone	0.486	30			46
Hydroxypropoxy propanol	0.537	400			0
Substituted hydroxyquinoline	0.755	40			0
Indole	0.821		210		11
Iodoacetic acid	0.129			21	14
1-(3H)Isobenzofuranone	0.716	20			5
Isobutyric acid	0.545	640			
Isocitric acid	0.375	575			
Isophorone	0.783	18			
Isoketoglutaric acid	0.411		80		
Lactic acid	0.4	3250	30000	15000	154
Methacrylic acid	0.558	5			
Methanol	0.375	1000	1400	434	1900
2-Methoxyethanol	0.474	100			
2-(2-Methoxyethoxy) ethanol	0.5	50			
1-(2-Methoxy-1-methylethoxy)-2-propanol	0.564	100			
Methoxymethylpropanol	0.582	100			
Methoxy phenol	0.677	150			32
1-(4-Methoxyphenol)-ethanone	0.72				58
3-Methoxy-1,2-propanediol	0.453	70			
2-Methoxy-4-(1-propenyl)-phenol	0.732				13
1-(2-Methoxypropoxy)-2-propanol	0.568	100		11	
2-Methylbenzaldehyde	0.8				7
Methylbenzoic acid	0.706	22			
3-Methyl butanoic acid	0.588	25			190
3-Methyl-2-butanone	0.697				3
3-Methylcyclopentanone	0.735				8
(1-Methyldecyl) benzene	0.879			40	7
2-Methyl-2,2-dimethyl-1-(2-hydroxy propyl)					
- propionic acid	0.667	25			
2-Methyl-2,2-dimethyl-1-(2-hydroxy,1methylethyl)					
-propyl esterpropionic aci	0.667	24		12	
2-Methyl-2,2-dimethyl-1-(2-hydroxy,1-methyl)					
-propionic acid	0.667	50			
2-Methyl, 1-(1,1,-dimethyl)-2-methyl					
-1,3-propanediyl ester propionic acid	0.667	25			
Methylene chloride	0.141	5			17
Methyl-2-heptanol	0.76		20		
2-Methyl-3-hydroxy-2,2,4-trimethylpentyl					
-ester propionic acid	0.556	50		13	
Methylisopropylcyclohexanol	0.769	37			
Methyl methacrylate	0.6				11
Methyl-(methylethenyl)-2-cyclohexen-1-one	0.81	10			12
5-methyl-2-(1-methylethyl)-phenol	0.8	200			110
Methyloxime	0.261		42		

14-Methyl-pentadecanoic acid.methyl ester	0.756		8		
2-Methyl-2,4-pentanediol	0.61	425			
4-Methyl pentanoic acid	0.62	6			
2-Methyl-3-pentanone	0.719				18
4-Methyl-3-penten-2-one	0.735			8	
Methyl phenol	0.778	300			268
2-Methyl propanoic acid	0.545	25	7	6	105
2-Methyl-2-propenoic acid	0.558	50			
Methyl pyrazine	0.638				12
1-Methyl-2-pyrrolidinone	0.606	100	550		
12-Methyl-tetradecanoic acid	0.744		30		
(1-Methylundecyl) benzene	0.877			3	
Morpholine	0.551	500			
Substituted Morpholine	0.6	220			
Morpholine ethanamine	0.549	130			
N,N-di-n-butylformamide	0.688	250		10	
N,N-diethyl-3-methylbenzamide	0.754	20			
N,N-diethyl-m-toluamide	0.754	23			
N,N-dimethylacetamide	0.552	40		4	
N,N-dimethylbenzylamine	0.8	40			3
N,N-dimethylthioformamide	0.493	400	4	13	
N,N-dimethylthioformamide	0.404	40			
n-Butyl ether	0.738	5			
N-Butylbenzenesulfonamide	0.563	20			
N-Methyl-2-pyrrolidinone	0.605	1200	4	18	
N-Nitrosodimethyl amine	0.324	30			
N-Nitrosomorpholine	0.414	6			
Nicotine	0.74		17		
Nitrophenol (ortho)	0.518	6			57
Nonacosane	0.853			25	
Nonadecanoic acid, methyl ester	0.769		47		
Nonanoic acid	0.683	30	16	21	
Octacosane	0.853	20		35	
9,12-Octadecadienoic acid, methyl ester	0.775		47		
Octadecanoic acid	0.76		410	330	
Octadecanoic acid, methyl ester	0.765		2450	153	
Octadecanol	0.799		100	116	
Octadecenoic acid	0.765		2800	1100	
Octadecenoic acid, methyl ester	0.77		360	12	
9-Octadecen-1-ol	0.857		39		
Octanoic acid	0.667	300	35	14	7
1-octanol	0.738			41	
Octenoic acid	0.676				142
Oxalic acid	0.267	200	80	310	880
4-Oxo-pentanoic acid	0.517	20			
1,1-Oxybis (2-ethoxy) ethane	0.592	100		8	
1,1-Oxybis-2-propanol	0.537	50			
Pantolactone	0.554				36
Pentachlorophenol	0.271	4			
Pentacosane	0.852	20		14	
Pentadecanoic acid	0.744		230	75	
Pentadecanoic acid, methyl ester	0.75		185		
Pentadecanol	0.714		53	306	
Pentadecenoic acid	0.75		30	58	
2,4-Pentanedione	0.6				11
Pentanoic acid	0.588	100	2	2	13
2-Pentanone	0.698				5
2,5,8,11,14-Pentaoxapentadecane	0.541	50	12		

Phenol	0.766	300	410	7	103
2-Phenoxyethanol	0.696	50		4	
2-Phenoxy-1-propanol	0.711	22			
Phenyl acetic acid, alpha methyl-4-isobutyl	0.757				40
Phenylacetonitrile	0.82		140		171
1,1-(phenylene)bis ethanone	0.714	27			
2-phenylethanol	0.787	100			13
1-Phenylethanone	0.806	120			7
Phenyl propanoic acid	0.72				7
Phosphoric acid triethyl ester	0.396	35			
Phthalate ester	0.65	120	240		
1,2-Propanediol	0.473	5000	440	3400	396
1-Propanol	0.6		260	200	
2-Propanol	0.6	300		200	275
Propionic acid	0.486	12000	17800	13000	2530
2-Propoxyethanol	0.577	300			
Pyrene	0.95				2
2-Pyridinamine	0.638				15
1H-pyrrole	0.896				7
Pyruvic acid	0.409		180		220
Sodium coconut acid-n-methyl taurate (SCMT)	0.525		425200		
Sodium dodectyl benzene sulfonate	0.621			98000	
Squalene	0.877		7700	2040	3
4-(tert-butyl) benzoic acid	0.741	6			
3-tertbutyl phenol	0.8	60			5
Tetrachloroethene	0.145		4	11	
Tetracosane	0.852	20		18	
Tetracosanoic acid, methyl ester	0.785		140		
Tetradecanal, o-methyloxime	0.747		100		
Tetradecanoic acid	0.736	7	1570	120	1
Tetradecanoic acid, 3 hydroxy-methyl ester	0.698		4		
Tetradecanoic acid, methyl ester	0.744		750	10	
Tetradecanol	0.784		85	206	5
Tetradecene	0.857			5	
Tetradecenoic acid	0.743			90	
Tetraethylene glycol diacetate	0.518	2			
Tetraethylene glycol monoacetate	0.508		4		
Tetrahydro-5,6-dimethyl-2H-pyran-2-one	0.656				106
Tetrahydro-6-methyl-2H-pyran-2-one	0.632	45			75
Tetrahydrothiophene-1,1-dioxide (sulfolane)	0.4	28			
4-(2,2,3,3) Tetramethylbutyl phenol	0.816				7
Tetramethylurea	0.517	31			
Tetraoxadodecane	0.539				
Toluene	0.913	1	1000	5	
Total Amino Acids	0.442		275	320	374
Total Protein	0.5	1300	23000	19700	1100
Tri(2-chlorethoxy)phosphate	0.254	120			
Triacontane	0.853			96	
Triacotanoic acid	0.773		95		
Triacosane	0.852	16		5	
Tri(2-chloroethoxy)phosphate	0.254	150			
Trichloropropene	0.25		3	21	
Tricosanoic acid, methyl ester	0.783		37		
Tridecanoic acid	0.729		12	16	
Tridecanoic acid, methyl ester	0.737		42		
Triethoxyphosphate	0.396	26			
Triethylene glycol	0.5	5			
Triethylene glycol diacetate	0.513	46	3		

Trimethylbenzylalcohol	0.8				9
Triumethylcyclohexenemethanol	0.779	41			14
Trimethyl-2-cyclopenten-1-one	0.787				8
2,2,4-Trimethyl-1,3-pentanediol	0.738	60			
1-(2,4,6-trimethylphenyl)ethanone	0.761	8			
Trimethylpyrazine	0.688				8
1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6-trione	0.578	12			
Undecanoic acid	0.709	10			
1-Undecene	0.851		9		
Urea	0.2	1000	15000	19600	3300
Vanillin	0.632	7			13
Vinyl benzylalcohol	0.806			16	
Aluminum	NA	25			25
Ammonium	NA	14000	6723	2630	1400
Arsenic	NA		10.8	20	3
Barium	NA		10.8	10	12
Bicarbonate	NA	30000	17604	22760	1700
Bromide	NA	50	54	100	
calcium	NA	55	3574.8		100
Carbon dioxide	NA				
Chloride	NA	200	125280	91880	1100
Chromium	NA				8
Copper	NA		75.6		10
Cyanide	NA				280
Fluoride	NA	220	2376	75	160
Iodide	NA				110
Iodine	NA				
Iron	NA		129.6	110	45
Lead	NA	10			3
Magnesium	NA		421.2	430	28
Manganese	NA		10.8		3
Mercury	NA	3			
Nickel	NA		21.6		16
Nitrate	NA	150	270	140	110
Nitrite	NA	190		100	120
Phosphate	NA		3375	660	480
Potassium	NA	95	18122.4	9450	450
Selenium	NA				3
Sodium	NA	665	135000	78720	1070
Sulfate	NA	240	17820	6810	1240
Zinc	NA	3		30	8
Volume (l/day)		9.25	27.22	49.9	8.13
note: all values are in ppb unless noted					

Appendix II. Determination of Adsorbent Physical Properties

The following procedures were used to determine the densities and porosities of the various adsorbents used in experiments.

1.0) Physical properties determination for 580-26 and APA GAC

1.1) Experimental procedure

(A.) Weigh sample of dry adsorbent

(B.) Weigh empty 50 ml volumetric flask

(C.) Completely wet adsorbent by placing it in methanol overnight.

(D.) Remove adsorbent from methanol and remove excess methanol from adsorbent surface with adsorbent pad.

(F.) Transfer wetted adsorbent into previously weighed 50 ml volumetric and weigh.

(G.) Fill volumetric with adsorbent inside to 50 ml mark with methanol and weigh.

(H.) Place filled volumetric flask in an oven and dry for 24 hours at 110°C or until constant weight is achieved. Place the volumetric flask with adsorbent in a decicator to cool. Weigh flask and dried adsorbent. Check to see that dried adsorbent weight equals A to assure no adsorbent lost through procedure.

1.2) Adsorbent physical properties calculations

(a.) Weight of wet adsorbent g) = F - B

(b.) Volume of wet adsorbent (mL) = $50ml - \left(\frac{G-F}{\rho_{methanol}}\right)$

(c.) Weight of dry adsorbent (g) = A

(d.) Apparent density, ρ_{ap} (g/ml) = $\frac{c}{b}$

(e.) Material density, ρ_m (g/ml) = $\frac{c}{\left(b - \frac{(a-c)}{\rho_{methanol}}\right)}$

(f.) Particle porosity, $\varepsilon_p = 1 - \frac{\rho_{ap}}{\rho_m}$

2.0) Physical properties determination for XAD-4 resin

2.1 Experimental Procedure

A similar procedure to 1.0 is followed for XAD-4 resin. XAD-4 resin, however, was stored in a wetted form so wetting the adsorbent with methanol was not required. Therefore, steps A, C, and D were omitted for determination of the physical properties for XAD-4. The dry weight was obtained from step H above for XAD-4..

2.2 Physical properties calculations

The same calculations as those in section 1.2 for adsorbents were used except the density of water was used in place of the density of methanol since the XAD-4 was water wetted.

Appendix III. Equilibrium Isotherm Procedure

Equilibrium isotherms are used to determine the liquid phase and solid phase concentrations of adsorbates at equilibrium with an adsorbent. The liquid phase concentration (C_e) is measured directly. The solid phase concentration (q_e) is determined by a mass balance on the isotherm bottle:

$$q_e = \frac{V}{M}(C_0 - C_e)$$

where V is the isotherm bottle volume and M is the adsorbent mass.

1.0) Cleaning procedure for isotherm equipment

All equipment used in experiments was cleaned with the following procedure or that set forth by Sievers Co. (Boulder, CO) for ultra low level TOC analysis.

A.) All equipment is washed with Micro, a phosphate free laboratory cleaner.

B.) The equipment is rinsed with Milli-Q water several times and then air dried. The Milli-Q UV system consists of:

1.) Activated carbon cartridges to remove dissolved organics.

2.) Ion exchange cartridges to remove ionic species.

3.) 185 nm and 254 nm UV lamp for disinfection and organic oxidation.

4.) A membrane filter to remove particulates greater than 0.22 μm.

C.) The equipment is rinsed with ethanol and air dried.

D.) All glassware is baked in a 250° C forced air oven for one hour. All teflon and stainless steel apparatus was dried at 105° C in a forced air oven for one hour.

2.0) Preparation of adsorbents for isotherms

2.1) Powdered adsorbent preparation (580-26 and APA)

A.) Separate an adequate amount of adsorbent from the cleaned adsorbent to perform all the necessary isotherms.

B.) Completely crush all the adsorbent to be used for the isotherm experiments to a 200 by 400 (USTM) sieve size using a mortar and pestle for crushing.

C.) Place the powdered adsorbent in isotherm bottles so that they are approximately 1/3 full. Fill the remaining volume with Milli-Q water and shake for a few minutes, then centrifuge each bottle for at least 1/2 hour at 2300 rpm.

D.) Pour off supernatant. This will remove the fine suspended particles that may interfere with the final isotherm analysis.

E.) Place the isotherm bottles containing the adsorbent in the oven at 105° C overnight (16-20 hours). Cool in a desiccator.

F.) Store adsorbent in airtight, borosilicate, dark glass bottles in the dark until ready to use.

2.2) XAD-4 resin preparation

A.) XAD-4 resin was used in its uncrushed form for isotherm experiments. XAD-4 resin was rinsed with Milli-Q water until the effluent rinse water exhibited nondetectable carbonate concentrations to remove sodium carbonate added to the adsorbent to inhibit biological growth in shipping and storage.

3.0) Weighing procedure

3.1) XAD-4 adsorbent resin weighing procedure

A.) Prior to weighing, the resin was transferred to an absorbent pad to remove excess water.

B.) The weight of the resin was found by first weighing a piece of weighing paper, adding the approximate resin dosage, and re-weighing the weighing paper subsequent to resin placement in the bottle.

C.) To determine the percent solids of the resin, three solids samples were taken during the weighing procedure (beginning, middle, and end). The solids determination consisted of:

1.) Solids samples were weighed directly from the absorbent pad (as were the isotherm samples).

2.) Samples were dried at 110°C for 8 hours and cooled in a desiccator.

3. Dry samples were weighed to determine the difference in weight due to water.

3.2) Powdered adsorbent weighing procedure

A.)The powdered adsorbents were weighed out using procedure 3.1 except step 3.1 A was omitted.

4.0) Ersatz Solution Preparation and Handling

A.)Saturated solutions of the organic constituents are pumped into 100 L Tedlar bags.

B.)Ionic components were injected into the Tedlar bags.

C.)Stainless steel hose valve and a septum unit sealed the solution and were used for pumping purposes. Teflon tubing was used to directly pump the solution into isotherm bottles and columns.

5.0) Isotherm bottle filling

A.)The resin or powdered adsorbent dosages were added to the isotherm bottles.

B.)The bottles plus resin or adsorbent were weighed then filled with solution and capped with teflon septa. A procedure is used to fill the bottles that causes the least amount of solution agitation. The teflon tube from the tedlar gas bag is not allowed to come into contact with the solution in the isotherm bottle since adsorbent or ion exchange resin can cling to the teflon tube and change the dosage. To prevent loss of adsorbent resin from the isotherm bottle when they are capped, approximately 1 ml of headspace is left in the bottle. Two isotherm bottles containing only the filling solution were taken at the start and end of all isotherms as blanks to determine initial concentration. Two additional bottles containing only the filling solution were taken in the middle of the isotherms to determine if volatilization of adsorbate was occurring during the filling process. The blanks were all taken in duplicate and one was analyzed at the beginning of the equilibration period and one was analyzed at the end as controls to monitor volatilization or microbial degradation of the solutes during equilibration.

D.)The filled bottles were re-weighed to determine the exact volume of solution added.

6.0) Equilibration and Sampling

A.) The isotherm bottles were tumbled at 18 rpm at room temperature for a minimum time period of 7 to 10 days.

B.) The isotherm bottles were then removed from the tumbler and centrifuged to settle all adsorbent to the bottom of the isotherm bottle. The supernatant was then sampled and analyzed for pH and the adsorbates of interest.

Appendix IV. Column Procedure For Kinetic Studies

1.0) Cleaning procedure for isotherm equipment

All equipment used in experiments was cleaned with the following procedure or that set forth by Sievers Co. (Boulder, CO) for ultra low level TOC analysis.

A.) All equipment is washed with Micro, a phosphate free laboratory cleaner.

B.) The equipment is rinsed with Milli-Q water several times and then air dried. The Milli-Q UV system consists of:

1.) Activated carbon cartridges to remove dissolved organics.

2.) Ion exchange cartridges to remove ionic species.

3.) 185 nm and 254 nm UV lamp for disinfection and organic oxidation.

4.) A membrane filter to remove particulates greater than 0.22 mm.

C.) The equipment is rinsed with ethanol and air dried.

D.) All glassware is baked in a 250° C forced air oven for one hour. All teflon and stainless steel apparatus was dried at 105° C in a forced air oven for one hour.

2.0) Column set-up

A.) Columns with an inner diameter of 5.0 cm were capped with a Teflon end cap. The adsorbent was retained with 150 mesh stainless steel screen at one end, and attached to a pump with Teflon tubing for solution introduction on the other end.

B.) The desired amount of adsorbent was slurried into the column with Milli-Q water.

C.) The adsorbents were degassed by applying a vacuum to the top of the column and agitating the adsorbent until no air bubbles were observed to be coming out of the adsorbent particles.

D.) The solutions were pumped downflow through the columns. The exact flow rate was determined gravimetrically.

E.) The height of the adsorbent bed was measured regularly to determine any change in bed size and for calculation of EBCT.

3.0) Sampling

A.) The column influent and effluent was collected at the desired intervals, 50 mL per sample. The exact time of sampling was recorded.

B.) The compounds of interest were monitored with the methods included in Chapter 2.

Appendix V. Ersatz Isotherm Data

Table AV-1. 580-26 Shower and Handwash Ersatz Verification Data for Figure 3-1.

CHEMICAL COMPOUND. . . . . TOC
ADSORBENT TYPE. 580-26
ISOTHERM TYPE. . . . . Virgin
PARTICLE SIZE. . . . . 200 x 400 mesh

Actual Shower and Handwash Water

EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
32.6	21.5
33.4	25.6
33.4	36.7
35.7	60.0
36.5	78.2
40.7	117.7
49.4	162.5
77.1	211.3
116.0	298.2
162.0	334.3
224.0	281.2
267.0	240.2

Shower and Handwash Ersatz Water

EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
37.6	50.5
38.6	78.9
38.7	143.5
50.5	213.2
74.9	268.0
317.8	688.3

Table AV-2. 580-26 Ersatz TOC Isotherm Data for Figure 3-2.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	6.7-9.8
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2507	0.0161	574.3	560.98	207.4
0.2498	0.0285	574.3	524.43	437.1
0.2499	0.0496	574.3	489.83	425.6
0.2515	0.0896	574.3	517.1	160.7
0.2504	0.1231	574.3	485.5	180.7
0.2499	0.1712	574.3	446.6	186.3
0.2479	0.2321	574.3	381.1	206.4
0.2493	0.3239	574.3	284.6	223.0
0.2501	0.4421	574.3	168.3	229.7
0.2507	0.6125	574.3	64.6	208.6
0.2492	0.8428	574.3	44.0	156.8
0.2483	1.1540	574.3	41.9	114.5
0.2486	1.5022	574.3	44.1	87.7
BLANK 1		569.2		
BLANK 2		551.1		
BLANK 4		561.6		
BLANK 5		610.1		
BLANK 6		579.7		

Table AV-3. 580-26 Dilute Ersatz TOC Isotherm Data for Figure 3-3.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2448	0.0888	276.4	210.8	180.7
0.2470	0.1171	276.4	194.1	173.6
0.2422	0.1530	276.4	129.0	233.4
0.2438	0.1993	276.4	79.3	241.2
0.2474	0.2615	276.4	45.2	218.7
0.2441	0.3399	276.4	21.1	183.4
0.2430	0.5808	276.4	18.9	107.8
0.2456	0.9928	276.4	22.0	62.9
BLANK 1		280.6		
BLANK 3		262.6		
BLANK 6		286.0		

Table AV-4. APA Ersatz TOC Isotherm Data for Figure 3-5.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.4-9.6
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2510	0.0895	573.4	479.4	263.8
0.2505	0.1258	573.4	456.6	232.6
0.2501	0.1702	573.4	413.9	234.4
0.2481	0.2357	573.4	338.2	247.6
0.2494	0.3259	573.4	242.7	253.1
0.2475	0.4439	573.4	145.8	238.4
0.2494	0.6132	573.4	61.3	208.3
0.2500	0.8119	573.4	42.0	163.6
0.2485	1.1582	573.4	36.2	115.3
0.2477	1.5878	573.4	30.9	84.6
BLANK 1		578.6		
BLANK 2		568.9		
BLANK 3		571.8		
BLANK 4		563.2		
BLANK 5		569.9		
BLANK 6		588.2		

Table AV-5. APA Dilute Ersatz TOC Isotherm Data for Figure 3-6.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND.. TOC
ADSORBENT TYPE.. APA
ISOTHERM TYPE.. Virgin
PARTICLE SIZE.. 200x400 Mesh
TEMPERATURE, Deg C.. 23
pH.. 7.3-9.3
EQUILIBRATION TIME, Days.. 10
BACKGROUND WATER MATRIX.. Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2490	0.0060	263.9	258.8	212.2
0.2521	0.0517	263.9	190.5	357.8
0.2528	0.0876	263.9	185.8	225.6
0.2500	0.1179	263.9	155.6	229.7
0.2485	0.1528	263.9	124.5	226.7
0.2502	0.2007	263.9	84.5	223.7
0.2498	0.2635	263.9	45.8	206.7
0.2495	0.3398	263.9	26.9	174.0
0.2506	0.4473	263.9	18.9	137.3
0.2499	0.5855	263.9	17.1	105.3
0.2498	0.7662	263.9	20.6	79.3
BLANK 1		262.4		
BLANK 2		254.0		
BLANK 3		265.3		
BLANK 4		269.8		
BLANK 5		267.8		

Table AV-6. XAD-4 Ersatz TOC Isotherm Data for Figure 3-8.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	7.8-10.1
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2526	0.0020	582.0	579.3	351.0
0.2512	0.0277	582.0	560.3	197.2
0.2500	0.0903	582.0	513.8	188.8
0.2500	0.1805	582.0	437.4	200.2
0.2514	0.2496	582.0	385.6	197.8
0.2512	0.3193	582.0	342.3	188.5
0.2503	0.4852	582.0	240.5	176.1
0.2499	0.5947	582.0	186.3	166.3
0.2500	0.7985	582.0	125.0	143.1
0.2491	1.1934	582.0	72.6	106.3
0.2450	1.9175	582.0	52.0	67.7
0.2427	3.2611	582.0	49.9	39.6
BLANK 1		588.3		
BLANK 2		579.3		
BLANK 3		579.5		
BLANK 4		559.3		
BLANK 5		578.2		
BLANK 6		607.4		

Table AV-7. XAD-4 Dilute Ersatz TOC Isotherm Data for Figure 3-9.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C.	21
pH	8.0-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2513	0.0016	271.4	266.7	744.5
0.2508	0.0137	271.4	264.7	122.7
0.2509	0.0310	271.4	252.9	149.6
0.2504	0.0583	271.4	230.8	174.3
0.2503	0.1699	271.4	156.9	168.8
0.2486	0.2553	271.4	118.4	149.0
0.2498	0.3568	271.4	81.8	132.7
0.2495	0.5303	271.4	42.3	107.8
0.2497	0.6388	271.4	34.0	92.8
0.2485	0.9057	271.4	26.0	67.3
0.2473	1.3458	271.4	23.2	45.6
0.2465	2.1333	271.4	21.8	28.8
0.2428	3.4194	271.4	20.1	17.8
BLANK 1		272.3		
BLANK 2		280.3		
BLANK 3		275.0		
BLANK 4		269.8		
BLANK 5		266.8		
BLANK 6		264.1		

Table AV-8. 580-26 Ersatz TCE Isotherm Data for Figure 3-10.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND. . . . . TCE
ADSORBENT TYPE. 580-26
ISOTHERM TYPE. . . . . Virgin
PARTICLE SIZE. . . . . 200x400 Mesh
TEMPERATURE, Deg C. 23
pH. 6.7-9.8
EQUILIBRATION TIME, Days. 10
BACKGROUND WATER MATRIX. . . . . Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2487	0.00469	145.702	144.726	51.770
0.2500	0.00928	145.702	144.581	30.191
0.2499	0.04958	145.702	145.009	3.494
0.2515	0.08959	145.702	136.738	25.165
0.2504	0.12311	145.702	124.657	42.804
0.2499	0.17120	145.702	105.541	58.622
0.2479	0.23206	145.702	91.028	58.406
0.2493	0.32394	145.702	65.704	61.565
0.2501	0.44207	145.702	47.896	55.334
0.2507	0.61247	145.702	25.174	49.335
0.2492	0.84283	145.702	9.941	40.141
0.2483	1.15400	145.702	4.749	30.328
0.2486	1.50219	145.702	2.268	23.737
BLANK 1		137.872		
BLANK 2		145.311		
BLANK 3		140.689		
BLANK 4		150.907		
BLANK 5		145.180		
BLANK 6		154.254		

Table AV-9. 580-26 Dilute Ersatz TCE Isotherm Data for Figure 3-11.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2471	0.0162	78.836	75.676	48.225
0.2455	0.0293	78.836	73.589	43.957
0.2466	0.0499	78.836	68.398	51.621
0.2448	0.0888	78.836	59.735	52.653
0.2470	0.1171	78.836	52.933	54.630
0.2422	0.1530	78.836	45.557	52.689
0.2438	0.1993	78.836	36.087	52.303
0.2474	0.2615	78.836	25.404	50.542
0.2441	0.3399	78.836	15.482	45.495
0.2472	0.4445	78.836	7.328	39.766
0.2430	0.5808	78.836	3.592	31.481
0.2474	0.7600	78.836	2.017	25.006
0.2456	0.9928	78.836	1.078	19.235
BLANK 1		78.366		
BLANK 2		75.092		
BLANK 3		80.747		
BLANK 4		81.707		
BLANK 6		78.268		

Table AV-10. 580-26 Ersatz Toluene Isotherm Data for Figure 3-12.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	6.7-9.8
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2487	0.0047	86.833	84.519	122.731
0.2507	0.0161	86.833	86.260	8.944
0.2498	0.0285	86.833	75.517	99.068
0.2499	0.0496	86.833	73.360	67.902
0.2515	0.0896	86.833	61.179	72.015
0.2504	0.1231	86.833	53.348	68.105
0.2499	0.1712	86.833	42.967	64.031
0.2479	0.2321	86.833	32.632	57.901
0.2493	0.3239	86.833	20.165	51.306
0.2501	0.4421	86.833	12.707	41.937
0.2507	0.6125	86.833	5.033	33.483
0.2492	0.8428	86.833	1.270	25.298
0.2483	1.1540	86.833	0.406	18.596
0.2486	1.5022	86.833	0.160	14.344
BLANK 1		86.384		
BLANK 3		83.305		
BLAN K4		91.324		
BLANK 5		83.563		
BLANK 6		89.589		

Table AV-11. 580-26 Dilute Ersatz Toluene Isotherm Data for Figure 3-13.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10 .
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2443	0.0053	39.670	38.406	58.664
0.2479	0.0093	39.670	37.375	60.935
0.2471	0.0162	39.670	38.249	21.687
0.2455	0.0293	39.670	35.761	32.748
0.2466	0.0499	39.670	32.499	35.460
0.2448	0.0888	39.670	21.884	49.028
0.2470	0.1171	39.670	18.161	45.362
0.2422	0.1530	39.670	13.814	40.936
0.2438	0.1993	39.670	8.511	38.122
0.2474	0.2615	39.670	5.439	32.379
0.2441	0.3399	39.670	2.516	26.680
0.2472	0.4445	39.670	0.675	21.685
0.2430	0.5808	39.670	0.233	16.500
0.2474	0.7600	39.670	0.135	12.869
0.2456	0.9928	39.670	0.055	9.800
BLANK 1		40.386		
BLANK 2		39.386		
BLANK 3		37.622		
BLANK 4		40.765		
BLANK 6		40.191		

Table AV-12. 580-26 Ersatz m-Xylene Isotherm Data for Figure 3-14.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	580-26.
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	6.7-9.8
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2500	0.0093	24.860	21.792	82.670
0.2507	0.0161	24.860	20.497	68.099
0.2498	0.0285	24.860	17.219	66.898
0.2499	0.0496	24.860	14.113	54.167
0.2515	0.0896	24.860	8.927	44.727
0.2504	0.1231	24.860	6.547	37.247
0.2499	0.1712	24.860	4.263	30.065
0.2479	0.2321	24.860	2.484	23.904
0.2493	0.3239	24.860	1.237	18.180
0.2501	0.4421	24.860	0.642	13.701
0.2507	0.6125	24.860	0.225	10.084
BLANK 1		24.747		
BLANK 2		25.510		
BLANK 3		24.466		
BLANK 4		24.841		
BLANK 5		25.075		
BLANK 6		24.522		

Table AV-13. 580-26 Dilute Ersatz m-Xylene Isotherm Data for Figure 3-15.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2443	0.0053	11.147	10.179	44.938
0.2479	0.0093	11.147	9.403	46.301
0.2471	0.0162	11.147	8.358	42.568
0.2455	0.0293	11.147	6.697	37.286
0.2466	0.0499	11.147	4.746	31.656
0.2448	0.0888	11.147	1.784	25.811
0.2470	0.1171	11.147	1.493	20.361
0.2422	0.1530	11.147	0.849	16.304
0.2438	0.1993	11.147	0.510	13.015
0.2474	0.2615	11.147	0.245	10.312
0.2441	0.3399	11.147	0.083	7.945
0.2472	0.4445	11.147	0.038	6.178
0.2430	0.5808	11.147	0.014	4.658
BLANK 1		10.537		
BLANK 2		11.593		
BLANK 3		11.225		
BLANK 4		11.324		
BLANK 6		11.058		

Table AV-14. 580-26 Ersatz 1,2,4-TCB Isotherm Data for Figure 3-16.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	1,2,4-TCB
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	6.7-9.8
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2477	0.00279	1.629	1.072	49.455
0.2487	0.00469	1.629	0.921	37.558
0.2500	0.00928	1.629	0.538	29.400
0.2507	0.01606	1.629	0.331	20.258
0.2498	0.02853	1.629	0.211	12.420
0.2499	0.04958	1.629	0.088	7.767
0.2515	0.08959	1.629	0.029	4.492
0.2504	0.12311	1.629	0.010	3.294
0.2499	0.17120	1.629	0.010	2.364
BLANK 1		1.630		
BLANK 2		1.598		
BLANK 3		1.622		
BLANK 4		1.694		
BLANK 5		1.536		
BLANK 6		1.696		

Table AV-15. 580-26 Dilute Ersatz 1,2,4-TCB Isotherm Data for Figure 3-17.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	1,2,4-TCB
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2392	0.0027	0.608	0.278	29.437
0.2443	0.0053	0.608	0.186	19.607
0.2479	0.0093	0.608	0.104	13.396
0.2471	0.0162	0.608	0.052	8.480
0.2455	0.0293	0.608	0.021	4.919
BLANK 1		0.673		
BLANK 2		0.602		
BLANK 3		0.613		
BLANK 6		0.544		

Table AV-16. 580-26 Ersatz Naphthalene Isotherm Data for Figure 3-18.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	6.7-9.8
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2477	0.00279	0.333	0.230	9.184
0.2487	0.00469	0.333	0.195	7.317
0.2500	0.00928	0.333	0.121	5.724
0.2507	0.01606	0.333	0.072	4.085
0.2498	0.02853	0.333	0.043	2.546
0.2499	0.04958	0.333	0.022	1.571
0.2515	0.08959	0.333	0.005	0.922
0.2504	0.12311	0.333	0.004	0.670
BLANK 1		0.336		
BLANK 2		0.315		
BLANK 3		0.350		
BLANK 4		0.328		
BLANK 5		0.343		
BLANK 6		0.328		

Table AV-17. 580-26 Dilute Ersatz Naphthalene Isotherm Data for Figure 3-19.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	7.2-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2392	0.0027	0.101	0.054	4.188
0.2443	0.0053	0.101	0.034	3.081
0.2479	0.0093	0.101	0.021	2.110
0.2471	0.0162	0.101	0.012	1.349
0.2455	0.0293	0.101	0.004	0.806
BLANK 1		0.103		
BLANK 2		0.101		
BLANK 3		0.098		
BLANK 6		0.102		

Table AV-18. APA Ersatz TCE Isotherm Data for Figure 3-22.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND... TCE
ADSORBENT TYPE.. APA
ISOTHERM TYPE... Virgin
PARTICLE SIZE... 200x400 Mesh
TEMPERATURE, Deg C.. 23
pH.. 7.4-9.6
EQUILIBRATION TIME, Days.. 10
BACKGROUND WATER MATRIX... Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2505	0.1258	153.066	151.547	3.027
0.2501	0.1702	153.066	128.354	36.322
0.2481	0.2357	153.066	111.788	43.452
0.2494	0.3259	153.066	85.901	51.406
0.2475	0.4439	153.066	64.046	49.639
0.2494	0.6132	153.066	42.154	45.109
0.2500	0.8119	153.066	19.377	41.166
0.2485	1.1582	153.066	9.200	30.868
0.2477	1.5878	153.066	4.616	23.159
BLANK 1		154.521		
BLANK 2		152.210		
BLANK 3		152.191		
BLANK 4		155.130		
BLANK 5		151.324		
BLANK 6		153.020		

Table AV-19. APA Dilute Ersatz TCE Isotherm Data for Figure 3-23.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	7.3-9.3
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2490	0.0060	72.543	71.676	36.089
0.2507	0.0284	72.543	64.696	69.208
0.2521	0.0517	72.543	60.925	56.691
0.2528	0.0876	72.543	56.389	46.634
0.2500	0.1179	72.543	49.870	48.079
0.2485	0.1528	72.543	46.031	43.117
0.2502	0.2007	72.543	38.162	42.865
0.2498	0.2635	72.543	29.204	41.084
0.2495	0.3398	72.543	19.663	38.825
0.2506	0.4473	72.543	11.274	34.323
0.2499	0.5855	72.543	6.775	28.072
0.2498	0.7662	72.543	3.889	22.382
0.2499	1.0084	72.543	1.730	17.549
BLANK 1		71.507		
BLANK 2		71.050		
BLANK 3		74.855		
BLANK 4		71.522		
BLANK 5		72.229		
BLANK 6		74.098		

Table AV-20. APA Ersatz Toluene Isotherm Data for Figure 3-24.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	7.4-9.6
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME Liters	DRY WEIGHT Grams	INITIAL CONC. mg/L	EQ. LIQ-PHASE CONC. mg/L	EQ. SOL-PHASE CONC. mg/g
0.2510	0.0502	85.520	76.885	43.199
0.2510	0.0895	85.520	66.797	52.528
0.2505	0.1258	85.520	63.400	44.055
0.2501	0.1702	85.520	53.083	47.675
0.2481	0.2357	85.520	38.633	49.355
0.2494	0.3259	85.520	28.960	43.289
0.2475	0.4439	85.520	16.856	38.288
0.2494	0.6132	85.520	7.321	31.804
0.2500	0.8119	85.520	2.710	25.499
0.2485	1.1582	85.520	0.871	18.162
0.2477	1.5878	85.520	0.330	13.290

BLANK 1	84.269
BLANK 2	87.056
BLANK 3	85.916
BLANK 4	82.072
BLANK 5	82.808
BLANK 6	90.998

Table AV-21. APA Dilute Ersatz Toluene Isotherm Data for Figure 3-25.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C.	23
pH	7.3-9.3
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2490	0.0060	41.254	40.734	21.635
0.2496	0.0161	41.254	36.558	72.989
0.2507	0.0284	41.254	36.493	41.987
0.2521	0.0517	41.254	33.434	38.158
0.2528	0.0876	41.254	26.092	43.770
0.2500	0.1179	41.254	19.734	45.634
0.2485	0.1528	41.254	16.740	39.867
0.2502	0.2007	41.254	12.052	36.409
0.2498	0.2635	41.254	7.121	32.356
0.2495	0.3398	41.254	3.762	27.527
0.2506	0.4473	41.254	1.554	22.240
0.2499	0.5855	41.254	0.631	17.339
0.2498	0.7662	41.254	0.330	13.342
0.2499	1.0084	41.254	0.142	10.188
BLANK 1		41.678		
BLANK 2		42.394		
BLANK 3		42.259		
BLANK 4		39.164		
BLANK 5		40.397		
BLANK 6		41.632		

Table AV-22. APA Ersatz m-Xylene Isotherm Data for Figure 3-26.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.4-9.6
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2494	0.0027	21.631	20.765	80.227
0.2508	0.0053	21.631	20.481	54.587
0.2505	0.0090	21.631	19.283	65.533
0.2520	0.0161	21.631	17.767	60.637
0.2521	0.0281	21.631	16.807	43.240
0.2510	0.0502	21.631	13.341	41.478
0.2510	0.0895	21.631	9.940	32.800
0.2505	0.1258	21.631	6.969	29.203
0.2501	0.1702	21.631	4.898	24.595
0.2481	0.2357	21.631	3.060	19.549
0.2494	0.3259	21.631	1.697	15.257
0.2475	0.4439	21.631	0.868	11.578
0.2494	0.6132	21.631	0.357	8.652
0.2500	0.8119	21.631	0.093	6.632
0.2485	1.1582	21.631	0.025	4.636
0.2477	1.5878	21.631	0.010	3.373
BLANK 1		23.040		
BLANK 2		19.882		
BLANK 3		22.771		
BLANK 4		20.687		
BLANK 5		21.970		
BLANK 6		21.438		

Table AV-23. APA Dilute Ersatz m-Xylene Isotherm Data for Figure 3-27.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.3-9.3
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2501	0.0029	9.870	9.584	24.757
0.2490	0.0060	9.870	9.020	35.382
0.2501	0.0100	9.870	9.431	11.027
0.2496	0.0161	9.870	7.305	39.872
0.2507	0.0284	9.870	6.596	28.879
0.2521	0.0517	9.870	4.467	26.366
0.2528	0.0876	9.870	2.558	21.109
0.2500	0.1179	9.870	1.617	17.501
0.2485	0.1528	9.870	1.130	14.214
0.2502	0.2007	9.870	0.681	11.456
0.2498	0.2635	9.870	0.350	9.025
0.2495	0.3398	9.870	0.145	7.140
0.2506	0.4473	9.870	0.056	5.498
0.2499	0.5855	9.870	0.018	4.205
0.2498	0.7662	9.870	0.009	3.215
BLANK1		10.152		
BLANK2		9.668		
BLANK3		10.550		
BLANK4		9.246		
BLANK5		9.863		
BLANK6		9.743		

Table AV-24. APA Ersatz 1,2,4-TCB Isotherm Data for Figure 3-28.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	1,2,4-TCB
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.4-9.6
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2494	0.0027	1.472	1.065	37.667
0.2508	0.0053	1.472	0.827	30.571
0.2505	0.0090	1.472	0.559	25.470
0.2520	0.0161	1.472	0.374	17.218
0.2521	0.0281	1.472	0.211	11.293
0.2510	0.0502	1.472	0.117	6.774
0.2510	0.0895	1.472	0.041	4.014
0.2505	0.1258	1.472	0.023	2.884
0.2501	0.1702	1.472	0.010	2.148
BLANK 1		1.521		
BLANK 2		1.508		
BLANK 3		1.414		
BLANK 4		1.464		
BLANK 5		1.390		
BLANK 6		1.531		

Table AV-25. APA Dilute Ersatz 1,2,4-TCB Isotherm Data for Figure 3-29.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	1,2,4-TCB
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.3-9.3
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2501	0.0029	0.652	0.358	25.349
0.2490	0.0060	0.652	0.252	16.623
0.2501	0.0100	0.652	0.135	12.947
0.2496	0.0161	0.652	0.085	8.798
0.2507	0.0284	0.652	0.042	5.377
BLANK 1		0.615		
BLANK 2		0.729		
BLANK 3		0.666		
BLANK 6		0.596		

Table AV-26. APA Ersatz Naphthalene Isotherm Data for Figure 3-30.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.4-9.6
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME Liters	DRY WEIGHT Grams	INITIAL CONC. mg/L	EQ. LIQ-PHASE CONC. mg/L	EQ. SOL-PHASE CONC. mg/g
0.2494	0.0027	0.279	0.207	6.664
0.2508	0.0053	0.279	0.173	5.032
0.2505	0.0090	0.279	0.120	4.446
0.2520	0.0161	0.279	0.084	3.069
0.2521	0.0281	0.279	0.050	2.053
0.2510	0.0502	0.279	0.024	1.274
0.2510	0.0895	0.279	0.009	0.757
0.2505	0.1258	0.279	0.005	0.547
BLANK 1		0.294		
BLANK 2		0.277		
BLANK 3		0.272		
BLANK 4		0.269		
BLANK 5		0.281		
BLANK 6		0.281		

Table AV-27. APA Dilute Ersatz Naphthalene Isotherm Data for Figure 3-31.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	23
pH	7.3-9.3
EQUILIBRATION TIME, Days	1.0
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2501	0.0029	0.157	0.088	5.892
0.2490	0.0060	0.157	0.059	4.066
0.2501	0.0100	0.157	0.036	3.032
0.2496	0.0161	0.157	0.022	2.098
BLANK 1		0.147		
BLANK 2		0.154		
BLANK 3		0.161		
BLANK 5		0.164		
BLANK 6		0.182		

Table AV-28. XAD-4 Ersatz TCE Isotherm Data for Figure 3-34.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND. . . . . TCE
ADSORBENT TYPE. XAD4
ISOTHERM TYPE. . . . . Virgin
PARTICLE SIZE. . . . . 0.3-1.2 mm
TEMPERATURE, Deg C. 23
pH. 7.8-10.1
EQUILIBRATION TIME, Days. 1.0
BACKGROUND WATER MATRIX. . . . . Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2526	0.0019	154.185	154.152	4.282
0.2525	0.0478	154.185	144.782	49.686
0.2500	0.0903	154.185	121.311	91.001
0.2500	0.1805	154.185	94.490	82.658
0.2514	0.2496	154.185	79.756	74.973
0.2512	0.3193	154.185	67.088	68.512
0.2503	0.4852	154.185	41.923	57.910
0.2499	0.5947	154.185	32.250	51.237
0.2500	0.7985	154.185	22.073	41.363
0.2491	1.1934	154.185	11.003	29.886
0.2450	1.9175	154.185	4.077	19.179
0.2427	3.2611	154.185	1.665	11.351
BLANK 1		153.589		
BLANK 2		158.429		
BLANK 3		150.496		
BLANK 4		153.468		
BLANK 5		146.487		
BLANK 6		162.640		

Table AV-29. XAD-4 Dilute Ersatz TCE Isotherm Data for Figure 3-35.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	8.0-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2508	0.0137	75.169	74.425	13.630
0.2509	0.0310	75.169	73.500	13.499
0.2504	0.0583	75.169	64.454	46.003
0.2518	0.0907	75.169	54.696	56.829
0.2503	0.1699	75.169	39.618	52.390
0.2486	0.2553	75.169	30.064	43.920
0.2498	0.3568	75.169	21.096	37.854
0.2495	0.5303	75.169	11.079	30.154
0.2497	0.6388	75.169	7.491	26.456
0.2485	0.9057	75.169	4.408	19.416
0.2473	1.3458	75.169	2.168	13.415
0.2465	2.1333	75.169	0.908	8.581
0.2428	3.4194	75.169	0.408	5.308
BLANK 1		75.150		
BLANK 2		79.558		
BLANK 4		73.866		
BLANK 5		72.524		
BLANK 6		74.750		

Table AV-30. XAD-4 Ersatz Toluene Isotherm Data for Figure 3-36.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND. . . . . Toluene
ADSORBENT TYPE. XAD4
ISOTHERM TYPE. . . . . Virgin
PARTICLE SIZE. . . . . 0.3-1.2 mm
TEMPERATURE, Deg C. 23
pH. 7.8-10.1
EQUILIBRATION TIME, Days. 10
BACKGROUND WATER MATRIX. . . . . Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2526	0.0019	85.581	85.555	3.374
0.2514	0.0070	85.581	84.803	27.940
0.2525	0.0478	85.581	72.337	69.988
0.2500	0.0903	85.581	61.015	68.003
0.2500	0.1805	85.581	44.648	56.680
0.2514	0.2496	85.581	32.408	53.562
0.2512	0.3193	85.581	26.431	46.529
0.2503	0.4852	85.581	15.708	36.044
0.2499	0.5947	85.581	10.612	31.502
0.2500	0.7985	85.581	6.602	24.728
0.2491	1.1934	85.581	3.024	17.232
0.2450	1.9175	85.581	0.931	10.816
0.2427	3.2611	85.581	0.340	6.344
BLANK 1		80.495		
BLANK 2		85.978		
BLANK 3		83.736		
BLANK 4		89.021		
BLANK 5		85.371		
BLANK 6		88.885		

Table AV-31. XAD-4 Dilute Ersatz Toluene Isotherm Data for Figure 3-37.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	8.0-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2506	0.0070	40.537	40.336	7.229
0.2508	0.0137	40.537	39.989	10.036
0.2509	0.0310	40.537	35.251	42.745
0.2504	0.0583	40.537	30.989	40.989
0.2518	0.0907	40.537	24.335	44.974
0.2503	0.1699	40.537	15.739	36.544
0.2486	0.2553	40.537	10.391	29.354
0.2498	0.3568	40.537	6.492	23.833
0.2495	0.5303	40.537	2.997	17.663
0.2497	0.6388	40.537	1.942	15.087
0.2485	0.9057	40.537	0.991	10.851
0.2473	1.3458	40.537	0.449	7.367
0.2465	2.1333	40.537	0.196	4.661
0.2428	3.4194	40.537	0.080	2.873
BLANK 1		41.581		
BLANK 2		42.053		
BLANK 3		38.313		
BLANK 4		40.470		
BLANK 5		40.333		
BLANK 6		40.475		

Table AV-32. XAD-4 Ersatz m-Xylene Isotherm Data for Figure 3-38.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	XAD4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	7.8-10.1
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2507	0.0027	20.298	19.570	67.995
0.2514	0.0070	20.298	18.665	58.617
0.2517	0.0133	20.298	17.438	53.927
0.2525	0.0478	20.298	11.145	48.365
0.2500	0.0903	20.298	7.317	35.932
0.2500	0.1805	20.298	3.880	22.733
0.2514	0.2496	20.298	2.512	17.916
0.2512	0.3193	20.298	1.848	14.513
0.2503	0.4852	20.298	0.891	10.011
0.2499	0.5947	20.298	0.472	8.331
0.2500	0.7985	20.298	0.342	6.248
0.2491	1.1934	20.298	0.129	4.210
0.2450	1.9175	20.298	0.047	2.587

BLANK 1	20.3395
BLANK 2	20.3246
BLANK 3	20.8641
BLANK 4	19.4180
BLANK 5	20.7021
BLANK 6	20.1380

Table AV-33. XAD-4 Dilute Ersatz m-Xylene Isotherm Data for Figure 3-39.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	m-Xylene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23.
pH	8.0-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2508	0.0030	9.608	9.180	36.115
0.2506	0.0070	9.608	8.465	40.942
0.2508	0.0137	9.608	7.482	38.930
0.2509	0.0310	9.608	5.563	32.706
0.2504	0.0583	9.608	3.873	24.618
0.2518	0.0907	9.608	2.397	20.014
0.2503	0.1699	9.608	1.100	12.537
0.2486	0.2553	9.608	0.623	8.749
0.2498	0.3568	9.608	0.347	6.483
0.2495	0.5303	9.608	0.150	4.450
0.2497	0.6388	9.608	0.096	3.718
0.2485	0.9057	9.608	0.055	2.621
0.2473	1.3458	9.608	0.025	1.761
0.2465	2.1333	9.608	0.010	1.109
0.2428	3.4194	9.608	0.005	0.682
BLANK 1		10.338		
BLANK 2		9.633		
BLANK 3		9.084		
BLANK 4		9.167		
BLANK 5		10.004		
BLANK 6		9.421		

Table AV-34. XAD-4 Ersatz 1,2,4-TCB Isotherm Data for Figure 3-40.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	1,2,4-TCB
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	7.8-10.1
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2526	0.0019	2.255	1.915	44.069
0.2507	0.0027	2.255	1.996	24.127
0.2514	0.0070	2.255	1.412	30.255
0.2517	0.0133	2.255	1.081	22.132
0.2512	0.0277	2.255	0.614	14.898
0.2525	0.0478	2.255	0.385	9.882
0.2500	0.0903	2.255	0.158	5.803
0.2500	0.1805	2.255	0.070	3.025
0.2512	0.3193	2.255	0.019	1.758
BLANK 1		2.270		
BLANK 2		2.143		
BLANK 3		2.301		
BLANK 4		2.325		
BLANK 5		2.302		
BLANK 6		2.186		

Table AV-35. XAD-4 Dilute Ersatz 1,2,4-TCB Isotherm Data for Figure 3-41.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND.. 1,2,4-TCB
ADSORBENT TYPE.. XAD-4 Resin
ISOTHERM TYPE.. Virgin
PARTICLE SIZE.. 0.3-1.2 mm
TEMPERATURE, Deg C.. 23.
pH.. 8.0-9.9
EQUILIBRATION TIME, Days.. 10
BACKGROUND WATER MATRIX.. Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2513	0.0016	1.015	0.882	21.306
0.2508	0.0030	1.015	0.669	29.218
0.2506	0.0070	1.015	0.468	19.603
0.2508	0.0137	1.015	0.332	12.513
0.2509	0.0310	1.015	0.152	6.980
0.2504	0.0583	1.015	0.069	4.060
0.2518	0.0907	1.015	0.035	2.719
BLANK 1		0.992		
BLANK 2		0.926		
BLANK 3		1.045		
BLANK 4		1.050		
BLANK 6		1.061		

Table AV-36. XAD-4 Ersatz Naphthalene Isotherm Data for Figure 3-42.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	23
pH	7.8-10.1
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2514	0.0070	0.360	0.304	2.015
0.2517	0.0133	0.360	0.259	1.903
0.2512	0.0277	0.360	0.192	1.528
0.2525	0.0478	0.360	0.165	1.032
0.2500	0.0903	0.360	0.096	0.731
0.2500	0.1805	0.360	0.047	0.434
0.2514	0.2496	0.360	0.033	0.329
0.2512	0.3193	0.360	0.023	0.265
BLANK 1		0.349		
BLANK 2		0.351		
BLANK 3		0.366		
BLANK 4		0.365		
BLANK 5		0.367		
BLANK 6		0.362		

Table AV-37. XAD-4 Dilute Ersatz Naphthalene Isotherm Data for Figure 3-43.

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C.	23 .
pH	8.0-9.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Dilute Shower/Handwash Ersatz

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2508	0.0030	0.150	0.134	1.380
0.2506	0.0070	0.150	0.121	1.071
0.2508	0.0137	0.150	0.088	1.139
0.2509	0.0310	0.150	0.073	0.630
0.2504	0.0583	0.150	0.047	0.444
0.2518	0.0907	0.150	0.026	0.344
BLANK 1		0.144		
BLANK 2		0.144		
BLANK 3		0.152		
BLANK 4		0.153		
BLANK 6		0.159		

Appendix VI. Ersatz Column Experiment Data

Table AVI-1. 580-26 Column Influent Data For Figures 4-1 to 4-4 and 4-13 to 4-28.

Time Averaged Influent Concentrations	
Trichloroethylene (TCE)	148.02 mg/L
Toluene	80.37 mg/L
m-Xylene	21.74 mg/L
1,2,4-Trichlorobenzene (TCB)	1.610 mg/L
Naphthalene	0.319 mg/L
Total Organic Carbon (TOC)	596.7 mg/L
Time Averaged Flowrate	48.5 ml/min
Operating Temperature	23 +/- 2 C

Run Time (days)	Flowrate (ml/min)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.00	48.5	145.70	69.07	21.74	1.224	0.279	575.3	9.21
0.72	48.4						577.8	9.33
1.16	48.4	143.90	74.41	21.42	1.309	0.302	591.7	9.23
1.74	48.5						561.0	
2.20	48.5	152.50	76.42	21.79	1.349	0.335	619.9	9.42
2.73	48.4						587.6	
3.18	48.4	137.80	71.02	20.37	1.417	0.302	579.6	9.53
3.72	48.5						587.4	
4.21	48.5	149.20	70.97	21.37	1.337	0.278	581.8	9.38
4.72	48.4						594.1	9.44
5.19	48.4	138.50	72.02	20.73	1.494	0.270	565.9	
5.96	48.3						591.1	
6.72	48.0	133.70	73.23	21.09	1.210	0.275	577.6	9.11
7.25	48.0						592.0	7.80
7.74	48.4	151.70	73.99	21.81	1.308	0.279	585.3	
8.17	48.4						584.9	
8.71	48.8	139.10	67.12	20.65	1.411	0.278	587.5	9.39
9.71	48.2	152.80	61.51	19.44	1.379	0.246	525.7	9.32
10.11	48.2	175.60	64.88	20.50	1.352	0.268	538.2	
10.73	48.5						528.7	
11.28	48.5	135.26	72.66	22.30	1.334	0.286	543.2	9.41
11.78	48.0	125.10	66.69	22.22	1.455	0.276	552.1	8.78
12.75	48.0	128.40	71.64	21.59	1.333	0.283	551.5	
13.71	48.0		69.24				551.7	
14.20	48.3	132.30	70.51	21.95	1.279	0.276	541.2	
14.98	48.3	123.10		22.22	1.567	0.266	568.0	9.46
16.16	50.0						540.1	
16.97	47.2	133.57	74.20	22.92	1.249	0.284	537.2	
17.93	48.6						546.9	
18.97	47.6	130.29	74.13	21.75	1.417	0.299	592.5	
19.73	48.9						555.9	9.56
20.85	48.9	126.20	75.03	22.10	1.231	0.299	551.7	
21.82	46.9						597.9	
22.77	48.5	120.30	78.40	18.74	1.803	0.357	601.6	
23.80	47.9	108.30	70.94	17.46	1.822	0.299	592.0	9.51
24.85	47.8						605.9	9.68
25.85	48.2	109.80	70.14	18.58	1.911	0.314	610.3	
26.84	47.9						610.3	
27.80	47.7						599.5	
28.80	47.9	110.99	73.94	19.40	1.672	0.292	578.4	
29.94	47.9						586.5	9.32
31.01	47.9	109.00	70.19	20.30	1.723	0.348	608.5	
32.02	50.3						619.9	
33.08	49.7	115.07	74.05	19.04	1.694	0.303	586.9	
33.88	47.8						590.5	
34.96	49.6	153.42	89.87	24.66	1.669	0.222	619.5	9.60

Table AVI-1 Continued

Run Time (days)	Flowrate (ml/min)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
35.99	50.4	148.50	80.76	25.28	1.830	0.232	612.7	
37.06	48.6	178.60	87.51	26.20	1.689	0.242	619.2	
37.96	50.8						663.8	
38.90	49.9	173.80	87.70	27.79	1.875	0.289	720.6	
40.08	50.0						623.7	9.61
41.19	49.5	180.30	84.84	19.68	1.804	0.464	580.2	
41.94	48.0						497.0	
42.98	48.5	180.10	86.99	19.66	1.604	0.429	538.3	
44.07	49.0						582.9	9.53
45.02	49.0	172.90	91.77	18.48	1.504	0.435	582.1	
45.98	47.9						581.6	
46.91	48.0	182.90	88.31	18.50	1.517	0.429	597.4	
47.83	49.3						583.5	
48.94	49.2	185.70	96.39	24.35	1.860	0.363	616.8	
49.93	49.9						601.2	9.45
51.04	49.0	182.20	93.17	24.80	1.777	0.312	607.9	
52.03	47.8						641.9	9.23
52.83	47.3	187.50	98.44	25.73	1.741	0.326	645.3	
53.79	48.0						701.1	
55.17	48.0	180.35	104.10	24.16	1.878	0.381	639.0	
55.81	48.0						640.1	9.51
56.83	47.7	178.40	100.89	23.66	2.020	0.341	745.5	
57.99	48.4	130.04	80.83	23.89	1.942	0.303	668.8	
59.02	49.5	159.70	96.90	23.91	2.008	0.279	632.6	9.35

Table AVI-2. 580-26 Column Effluent Data For Figures 4-1 and 4-13 to 4-16.

Bed Parameters	
Adsorbent	580-26 GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.651 g/ml
Bed Length	0.364 m
Bed Diameter	5.08 cm
Weight of GAC	0.2592 kg
EBCT	15.2 minutes

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.00	0.00					0.0	6.22
0.19	0.00	0.00	0.00			25.4	6.21
0.31	0.00	0.00	0.00			36.1	6.20
0.71	0.01	0.00	0.00			52.8	6.74
0.96	0.01	0.00	0.00			47.0	7.90
1.16	0.01	0.01				111.3	6.48
1.74	2.33	0.14	0.01			306.6	6.35
1.96	5.22	0.38				346.5	6.19
2.19	9.55	0.91				401.9	
2.44	19.38	1.97	0.01			438.8	
2.73	29.94	3.82	0.00			437.3	7.02
2.95	39.67	5.33	0.02			464.9	
3.18	52.35	7.69				471.9	
3.44	63.37	10.23	0.04			478.6	6.74
3.72	77.44	13.85				418.8	6.79
3.96	93.49	16.69	0.08			500.1	8.25
4.21	101.01	20.31					8.67
4.45	116.90	24.67	0.12			534.2	8.52
4.72	130.67	28.06					9.23
4.44	135.50	30.54	0.20			545.3	9.29
5.19	139.00	36.13	0.21				9.24
5.73	154.30	44.32	0.29			563.0	9.20
5.96	158.50	46.78	0.36				9.42
6.17	161.20	54.55	0.56			565.6	9.17
6.72	171.30	69.15	0.69				9.43
6.97	160.10	56.56	0.54			552.0	9.35
7.25	161.70	66.40	0.86				9.36
7.74	154.80	66.90	0.79			579.4	9.35
7.96	169.60	66.94	0.81				
8.17	148.80	61.81	0.86				
8.71							
9.02	134.64	63.21	1.05				
9.71							
10.11	138.50	70.72	1.68				9.43
10.73							
11.28	146.60	71.01	2.43			535.5	
11.78							
12.31	147.10	73.02	3.29			572.1	
12.75							
13.21	147.40	75.92	4.62			556.3	9.39
13.71							
14.20	149.20	76.92	5.97			544.4	
14.98							
16.16	133.80	73.91	6.92			540.2	
16.97							
17.93	136.00	76.06	10.14			562.8	

Table AVI-2 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
19.73	135.60	79.07	13.64			559.7	
20.85							
21.82	128.60	77.92	17.83			567.9	9.45
22.77	121.40	74.75	17.29				
23.80	118.35	79.21	20.21			626.7	
24.85	119.46	79.62	20.77				
25.85	126.80	79.91	21.67			633.9	
26.84	118.30	81.56	22.08				
27.81	117.90	61.33	18.02			621.2	
28.81	128.37	78.40	25.46				
29.94	120.90	80.32	22.18			622.5	
32.02	123.70	78.20	21.60			644.1	9.43
33.88	139.10	77.26	22.76			626.3	
35.99	128.30	73.04	22.46			643.4	
37.06	148.90	88.31	23.31				
37.96	160.40	87.27	25.33			664.3	
40.08	161.00	87.53	23.09			659.3	
41.94	150.00	85.44	21.37			619.3	9.67
44.07	168.10	85.55	23.68				
45.02						602.5	
45.98	153.50	90.11	24.21				
46.91						654.5	
47.83	166.90	83.45	23.40				
48.94						662.3	
49.93	158.70	90.39	23.02			643.3	
51.04						620.5	
52.03	158.30	96.29	23.29			631.8	9.59
53.79	156.40	96.85	23.70				
55.17						644.4	
55.81	138.40	91.05	20.88				
56.83						784.5	
58.99	134.15	85.66	24.68	0.003	0.003		
60.02						639.9	

Table AVI-3. 580-26 Column Effluent Data For Figures 4-2 and 4-17 to 4-20.

Bed Parameters	
Adsorbent	580-26 GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.651 g/ml
Bed Length	0.741 m
Bed Diameter	5.06 cm
Weight of GAC	0.5336 kg
EBCT	30.7 minutes

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.00						0.7	6.06
0.71						36.4	
0.96							6.90
1.16							6.09
1.96						40.2	
2.19							7.60
2.44						40.1	7.07
2.73						45.5	8.65
2.95						79.3	8.37
3.18	0.01					173.3	
3.44	0.09					240.1	6.24
3.72	0.51					308.9	
3.96	1.30	0.00				344.5	
4.21	2.86					370.3	
4.45	4.98	0.03				385.6	6.44
4.72	9.46	0.16				421.4	6.42
4.44	11.93	0.19				435.8	
5.19	18.40	0.43					
5.73	34.68	1.34				470.4	
5.96	43.66	2.12					
6.17	55.97	3.15				486.2	6.32
6.72	66.73	5.06					
6.97	77.25	6.15				497.0	
7.25	72.35	8.01					
7.74	102.30	10.68				518.4	
7.96	102.90	12.18					6.51
8.17	111.70	12.08				529.1	7.86
8.71	121.10	17.09					8.66
9.02	142.70	20.59				514.6	9.00
9.71							9.22
10.11	168.40	28.70				548.7	
10.73							9.44
11.28	161.20	40.32				515.1	
12.31						547.6	
13.21		52.44	0.04			537.1	
14.20	166.30	60.02	0.06				
16.16	163.20	69.12	0.13			536.9	9.63
17.93	135.58	76.62	0.25			548.4	
19.73	146.50	79.73	0.49			560.7	
21.82	146.60	86.24	1.04			621.9	9.50
22.77	136.30	82.61	1.24				
23.80	126.70	80.22	2.02			635.5	
24.85	135.10	88.85	2.54				
25.85	118.00	76.29	3.63			609.4	
26.84	0.00	85.10	4.26				
27.81	118.60	76.00	4.98			604.6	
28.81	128.14	84.75	6.23				

Table AVI-3 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
29.94	126.00	85.34	7.18			613.6	
31.01	131.60	85.76	8.25				
32.02	106.70	77.32	8.37			638.8	8.09
33.08	125.50	78.69	10.62				
33.88	126.40	83.69	11.55			631.7	
34.96	123.20	82.27	12.79				
35.99	122.10	74.24	14.74			644.7	
37.06	142.70	77.82	15.45				
37.96	142.75	89.18	17.07			683.8	
40.08	163.30	83.92	18.63			651.9	
41.94	161.30	88.61	18.89			577.1	9.46
44.07	149.63	86.56	21.11				
45.02						597.5	
45.98	156.00	87.26	21.67				
46.91						683.4	
47.83	154.95	88.73	22.14				
48.94						664.3	
49.93	156.60	89.73	23.02			650.5	
51.04						606.8	
52.03	170.66	89.56	24.99			634.5	9.51
53.79	164.42	94.26	25.12				
55.17						640.1	
55.81	157.70	96.69	24.46				
56.83						641.2	
58.99	132.84	81.10	23.98				
60.02						642.0	

Table AVI-4. 580-26 Column Effluent Data For Figures 4-3 and 4-21 to 4-24.

Bed Parameters	
Adsorbent	580-26 GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.651 g/ml
Bed Length	1.114 m
Bed Diameter	5.05 cm
Weight of GAC	0.8143 kg
EBCT	46.0 minutes

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.00							9.02
0.19							6.49
0.96						40.5	6.67
1.16							6.96
1.74							9.34
1.96							9.56
2.19							9.27
2.44						39.9	9.23
2.73							9.12
2.95							9.09
3.18							8.96
3.44							8.92
3.72						38.6	
4.21						37.9	
4.45						40.6	9.10
4.72						73.5	
4.44						127.8	9.43
5.19						245.5	
5.73	0.43					324.5	
5.96	0.43					372.5	
6.17	1.09					392.5	
6.72	3.87					406.8	
6.97	5.96	0.01				421.3	
7.25	9.86					434.9	
7.74	17.00	0.09				458.2	
7.96	19.44					460.4	
8.17	22.17	0.19				466.8	6.36
8.71	28.75	0.54					
9.02	35.22	0.80				465.9	
9.71	58.64	1.74				492.0	
10.11	70.72	2.63				526.2	
10.73	86.01	4.21					
11.28	102.84	6.09				488.2	
11.78	120.92	7.74				0.0	
12.31	134.12	10.34				535.3	
12.75	145.61	13.54					
13.21	155.96	15.83				517.6	9.39
14.20	156.60	19.88				516.4	
16.16	166.90	28.93				525.0	
17.93	180.30	46.73	0.01			524.6	
19.73	160.30	60.09	0.01			541.6	
21.82	152.20	68.27	0.02			599.3	9.61
22.77	151.60	72.66					
23.80	135.30	71.14	0.07			631.0	
25.85	131.20	73.90	0.12			630.0	
27.81	127.20	77.87	0.25			605.6	
28.81	135.03	86.40	0.89				

Table AVI-4 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
29.94	142.42	82.12	0.53			618.5	
32.02	146.67	90.16	1.04			640.8	9.81
33.88	142.44	91.58	1.57			628.3	
35.99	116.90	76.98	2.80			646.8	
37.96	137.65	93.76	4.27			683.2	
40.08	155.85	91.04	5.55			664.8	
41.94	126.89	66.78	4.95			576.0	9.46
44.07	161.36	84.71	7.83			604.0	
45.02						592.1	
45.98	172.45	94.16	10.08				
46.91						694.8	
47.83	172.21	90.83	11.46				
48.94						659.3	
49.93	186.22	88.54	13.90				
51.04						624.6	
52.03	183.93	91.22	15.55			629.6	9.36
53.79	185.91	97.79	17.77				
55.17						609.9	
55.81	183.72	94.63	18.52				
56.83						833.5	
58.99	139.26	81.67	19.35				
60.02						613.5	

Table AVI-5. 580-26 Column Effluent Data For Figures 4-4 and 4-25 to 4-28.

Bed Parameters

Adsorbent	580-26 GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.651 g/ml
Bed Length	1.474 m
Bed Diameter	5.05 cm
Weight of GAC	1.085 kg
EBCT	60.8 minutes

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.000							9.24
0.188							6.50
0.958						36.9	
1.160							6.74
1.736							8.68
1.958							8.96
2.195							9.94
2.438						37.1	9.79
2.729							9.64
2.948							9.41
3.177							9.30
3.438							9.40
3.719						41.3	9.00
3.958						38.9	7.63
4.208							9.12
4.448						37.9	9.15
4.438						37.0	8.77
5.729						35.7	
6.167						40.1	
6.715						158.4	
6.965						221.5	
7.743	0.07					338.9	
7.958						368.7	
8.167	0.24	0.00				375.9	6.08
8.708						399.5	
9.021	2.31	0.01				425.6	
9.708						439.9	
10.115	10.19	0.01				447.4	
10.729						417.6	
11.278	24.83	0.13				454.6	
12.313	43.22	0.56				471.8	
13.208	66.45	1.13				443.1	6.16
13.708							6.15
14.201	94.62	2.75				472.1	6.25
14.979							6.34
16.160	130.89	8.56				492.2	6.87
16.965							9.46
17.930	166.13	17.98				487.9	9.37
18.972							9.38
19.729	170.78	29.40				496.4	9.41
21.823	163.06	42.77				558.9	9.65
22.771	174.60	51.84					
23.802	152.30	54.05	0.00			593.9	
25.854	144.50	63.02	0.01			565.8	
27.805	138.60	67.60	0.02			601.3	
28.805	140.60	76.45					
29.938	171.97	72.06	0.04			599.5	

Table AVI-5 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-Xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
32.021	175.03	75.15	0.08			628.8	9.56
33.875	168.30	74.49	0.14			626.3	
35.990	127.80	81.19	0.31			643.4	
37.958	178.80	84.53	0.54			664.3	
40.083	184.36	83.61	0.89			659.3	
41.938	150.20	91.33	1.32			619.3	9.71
42.979						568.4	
44.073	158.55	94.76	1.96				
45.021						605.6	
45.979	164.31	97.08	2.53				
47.833	160.20	85.35	3.15				
48.938						711.8	
49.927	176.35	96.70	4.71			652.8	
51.042						643.5	
52.031	174.91	98.44	5.81			620.3	9.45
52.833						601.9	
53.792	166.70	90.70	6.50				
55.067						596.8	
55.813	172.55	86.10	7.70				
56.833						822.3	
58.990	142.59	81.09	9.88				
60.021						609.2	

Table AVI-6. APA Column Influent Data For Figures 4-5 through 4-8 and 4-29 to 4-46.

Time Averaged Influent Concentrations	
Trichloroethylene (TCE)	174.24 mg/L
Toluene	92.41 mg/L
m-Xylene	26.29 mg/L
1,2,4-Trichlorobenzene (TCB)	2.138 mg/L
Naphthalene	0.29 mg/L
Total Organic Carbon (TOC)	643.7 mg/L
Time Averaged Flowrate	50.1 ml/min
Operating Temperature	23 +/- 2 C

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
0.00	144.13	87.18	24.66	2.54	0.28	606.3	9.12
0.76	141.00	97.03	27.48	2.10	0.31	688.1	
0.84	174.02	90.15	28.26			683.2	
1.40	162.38	96.04	24.05	2.09	0.31		
1.91	175.15	90.53	23.88	2.88	0.26	622.3	8.98
2.38	149.71	94.61	23.88	2.13	0.30		
2.75	149.15	97.86	24.74	2.17	0.29		
3.27	149.37	87.81	25.58	1.92	0.32	630.8	
3.77	159.09	97.10	26.23	1.73	0.28		9.06
4.28	190.33	103.65	25.36			644.7	
4.76	164.21	96.07	24.60	1.94	0.31		
5.18	163.18	101.87	21.99	2.06	0.33	650.8	
5.68	152.68	94.95	25.50	2.59	0.33		9.14
6.18	151.02	93.97	26.53	1.88	0.31		
6.73	151.04	98.06	23.64	2.09	0.33	664.0	
7.23	159.87	91.04	28.41	2.08	0.34		
7.64	163.41	93.50	25.88	1.91	0.33	648.0	8.85
8.16	164.51	95.66	27.40	1.96	0.32		
8.68	158.94	91.43	22.25	2.05	0.30	660.7	
9.14	171.84	83.61		2.47			
9.63	182.23	86.15	22.55	2.53		655.1	8.94
10.13	202.44	97.07	25.16	2.48			
10.71	199.50	87.69	27.53	2.31		633.2	
11.09	175.40	90.16	27.04	2.70			
11.66	190.54	91.31	28.37	2.67		623.5	9.10
12.11	191.47	90.33	27.81	2.16	0.25		
12.64	180.89	81.76	25.37	2.06	0.26	606.1	
13.15	205.38	86.97	28.04	2.13	0.26		
13.63	201.52	84.91	27.63	2.17	0.24	636.5	8.82
14.20	200.41	91.20	28.18	1.98	0.26		
14.71	189.88	86.90	28.36	1.90	0.30		
15.24	192.90	90.96	28.98	1.93	0.29		
15.75	190.14	89.48	28.73	1.86	0.27	664.5	9.13
16.28	192.72	96.80	34.25	2.02	0.29		
16.80	187.25	91.84	29.77	1.79	0.27		
17.29	182.64	92.71	30.04	2.05	0.28		
17.80	178.60	91.46	29.21	2.04	0.28	625.7	8.87
18.28	161.40	97.33	31.42	2.08	0.29		
18.80	163.30	100.25	32.59	2.14	0.29		

Table AVI-7. APA Column Effluent Data For Figures 4-5 and 4-29 to 4-34.

Bed Parameters

Adsorbent	APA GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.674 g/ml
Bed Length	0.1020 m
Bed Diameter	5.03 cm
Weight of GAC	0.0745 kg
EBCT	4.1 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
0.10	0.03					47.6	9.12
0.18	1.24	0.23					
0.26	9.14	2.22	0.05			247.2	
0.35	23.68	6.34				271.2	
0.44	44.87	11.60	0.64			379.0	
0.55	70.70	21.91				431.8	
0.65	87.49	29.05	1.52			468.2	9.44
0.76	105.71	36.17	1.70			502.2	
0.84	140.84	40.61	1.86			553.8	
0.91	131.70	46.72	2.15			590.8	
1.02	134.70	53.80	2.56			606.8	
1.10	148.30	63.42	2.97			599.9	
1.20	151.93	66.79	2.93			608.4	
1.31	155.15	68.55	3.20			615.6	
1.40	165.00	68.55	4.26				
1.52	161.00	79.48	4.74				
1.65	160.92	80.35	4.49				9.46
1.75	171.84	83.61	5.00			604.2	
1.92	195.01	87.91	5.59				
2.10	152.47	89.95				620.6	
2.19	156.60	95.08	7.85				
2.28	158.37	97.83	7.12				
2.44	152.67	97.03	7.82			611.9	
2.65	160.53	94.68	8.96				
2.75	157.40	105.75	10.24				9.63
2.84	172.35	100.93	10.30				
2.93						664.5	
3.05	174.70	104.49	12.36				
3.27	178.50	103.72	13.15				
3.38						625.7	
3.48	180.14	96.03	13.72				
3.68	169.23	104.30	16.70			640.4	9.55
3.85	165.66	95.52	16.80				
3.93						652.0	
4.02	159.37	101.15	25.60				
4.18	161.17	95.43	18.88			649.7	
4.40	158.81	96.93	19.90				
4.51						646.6	
4.65	201.80	107.20	22.89			643.9	
4.83	166.65	98.16	22.47				
5.01	174.14	98.89	25.13				
5.17	156.20	94.98	23.17				
5.33	165.54	97.60	24.55				
5.50	168.25	95.85	23.90			638.9	
5.67	155.76	104.13	26.03				
5.71	160.92	100.38	25.68				
6.16	144.31	89.91	23.80	0.019	0.006		

Table AVI-7 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
6.50	151.10	93.94	26.05	0.021	0.007		
6.72	164.12	103.47	27.87	0.033			
7.22	149.06	92.20	26.98	0.039	0.011		
7.63	154.14	97.91	26.39	0.038	0.011	642.6	9.56
8.15	161.31	95.37	27.20	0.047	0.012		
8.33							
8.67	168.06	94.03	26.43	0.054	0.019	662.0	9.58
9.12				0.055	0.014		
9.36		96.17	29.53				
9.61				0.087		666.8	9.63
9.89	173.98						
10.12				0.083	0.024		
10.36		101.17	28.78				
10.69						636.9	9.67
11.03	175.18			0.090	0.027		
11.61				0.101	0.034	628.9	9.10
11.82		94.63	27.46				
12.05				0.110	0.036		
12.26	171.73						
12.59				0.121	0.038	610.8	9.41
12.33		91.26	33.23				
13.30	184.73			0.174	0.060		
13.58				0.165	0.047	631.5	9.30
14.15		89.89	28.61				
14.66	196.56			0.200	0.070		
15.71	194.47			0.210	0.080		
16.23	182.70	92.97	28.26				
16.75				0.240	0.090		
17.24	207.75	105.11	33.23				
17.75	213.84	96.90	33.36	0.342	0.087		
18.75	191.08	110.37	34.93	0.386	0.115		
19.01	185.78	110.40	34.68	0.442	0.123		

Table AVI-8. APA Column Effluent Data For Figures 4-6 and 4-35 to 4-38.

Bed Parameters	
Adsorbent	APA GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.674 g/ml
Bed Length	0.199 m
Bed Diameter	5.04 cm
Weight of GAC	0.1496 kg
EBCT	7.9 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
0.01						0.7	7.43
0.18						35.2	
0.26						39.5	
0.44						56.6	
0.55						71.3	
0.65	4.99	1.00				167.7	9.73
0.76	12.96	1.25				238.4	
0.84	31.77	3.24				128.7	
0.91	39.47	4.66				405.6	6.63
1.02	48.51	7.21				438.4	
1.10	72.64	11.54	0.01			457.6	
1.21			0.09			480.1	
1.31	101.15	20.25				572.8	8.35
1.51	134.02	31.78	0.19			552.1	
1.75	153.55	41.87				562.1	9.42
1.92	180.51	48.91	0.44			552.7	
2.10	164.32	54.86				580.8	
2.27	164.68	66.99	1.09				
2.37	168.36	89.95					
2.43			1.20			578.5	
2.65	183.35	78.47	1.40			597.9	9.58
2.84	171.79	85.35	1.67				
3.05	183.30	90.91	2.08				
3.17						604.0	
3.27	177.90	93.12	2.32				
3.48	183.36	96.88	2.53				
3.58						610.2	9.45
3.85	158.72	89.87	3.23			618.1	
4.18	163.92	100.97	4.46			636.2	
4.65	212.17	109.79	6.13			630.8	9.52
4.91	162.03	97.68	7.14				
5.01	166.70	98.43	7.71				
5.17			8.99				
5.33	159.09	97.17	9.03				
5.50	154.32	96.76	9.68			620.7	
5.67	157.08	103.98	10.90				
6.16	161.68	103.56	12.75				
6.35	159.88	111.47					
6.50	140.41	97.79	17.32				
6.72	165.89	114.33	17.80				
6.84	172.92		17.67			653.6	
7.22	173.39	103.55	19.62				
7.63	155.97	100.88	23.68			620.3	9.67
8.15	174.32	109.36	23.26				
8.67	194.14	106.37	25.22			672.8	9.58
9.61	171.65	105.48	30.18			668.2	9.67
10.36						629.9	

Table AVI-8 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
10.69	157.21	99.64	28.43				9.71
11.61	157.30	98.85	28.44			620.6	9.62
12.59	151.20	95.81	26.67			594.3	9.60
13.58	165.10	95.93	28.62			634.0	9.50
14.15			28.67				
15.71	161.06	89.50	29.02			590.1	
16.75	166.30	82.52	26.08			595.0	
17.75	164.04	91.10	29.93			589.1	
18.75	149.29	93.12	30.98			601.3	

Table AVI-9. APA Column Effluent Data For Figures 4-7 and 4-39 to 4-42.

Bed Parameters	
Adsorbent	APA GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.674 g/ml
Bed Length	0.299 m
Bed Diameter	5.05 cm
Weight of GAC	0.2248 kg
EBCT	12.0 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
0.02						3.0	
0.44						41.5	
0.76						43.7	
0.91						54.8	
1.02	1.43	0.04					
1.10						209.2	
1.20	12.12	0.64				297.5	
1.30	27.20	1.82				359.0	
1.40	36.55	2.51				392.6	
1.51	58.90	4.67				467.3	
1.65	64.09	7.22				469.2	7.40
1.75	85.27	9.22				489.6	6.82
1.92	94.58	13.47				491.1	
2.10	120.67	18.09				534.8	8.60
2.27	144.82	27.80					
2.43	137.11	28.14				557.0	7.67
2.54	166.25	37.53					
2.65						566.4	9.51
2.75	158.52	43.15					
2.84						574.6	
2.92	162.32	48.80					
3.05						642.4	
3.27	167.31	60.12				588.1	
3.38			0.21				
3.48	173.82	67.91	0.21			575.9	
3.85	164.81	76.84	0.35			601.6	
4.18	175.61	93.14	0.55			607.0	
4.65	211.71	103.77				607.5	9.53
5.01	163.81	103.60	1.55				
5.50						626.0	
5.67	166.00	112.60	2.48				
6.16	168.08	106.38	3.22				
6.50						624.5	
6.72	161.46	106.19	4.70				9.54
7.22	158.73	105.67	6.33				
7.63	160.53	101.90	7.72			612.7	8.98
8.15	165.50	112.42	10.21				
8.67	174.26	106.53	12.54			654.1	9.65
9.12	188.04	109.65	16.10				
9.61	188.95	108.47	18.30			651.4	9.72
10.12	192.43	110.13	21.45				
10.69	187.87	107.95	22.21			621.3	9.65
11.61	185.50	103.44	24.16			619.7	9.67
12.06	168.84						
12.26			26.61				
12.59	177.25	102.07				588.6	9.64
12.83			26.79				
13.10	182.10						

Table AVI-9 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
13.58	187.32	103.61	27.89			625.8	9.60
14.66	200.61	101.87	28.68			610.2	
15.71	187.85	95.48	27.78			617.5	
16.75	189.77	100.00	28.58			599.9	
17.75	159.38						
18.23		86.66	29.05			611.0	
18.75	166.62	86.45	28.81				

Table AVI-10. APA Column Effluent Data For Figures 4-8 and 4-43 to 4-46.

Bed Parameters

Adsorbent	APA GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.674 g/ml
Bed Length	0.399 m
Bed Diameter	5.05 cm
Weight of GAC	0.300 kg
EBCT	15.9 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
0.27						21.7	7.21
0.76						39.6	
0.91						43.4	
1.09						43.7	
1.20						42.8	
1.30						44.4	
1.40	0.45					79.7	
1.51	3.28	0.02				211.5	
1.64	10.12	0.12				299.5	7.94
1.75	19.48	0.63				327.8	
1.83		0.72				334.2	
1.92		0.97				380.0	
2.01	52.06	1.72				427.0	
2.10	58.50	2.65				457.3	6.73
2.18		3.41				451.2	
2.27	79.38	4.34				469.2	
2.37						497.5	
2.43	85.47	6.12				508.1	6.60
2.54		8.27					
2.65	113.36	9.98				532.2	9.31
2.75		13.11					
2.84	129.84	15.60				474.0	
3.05	140.14	19.79				604.2	
3.27	154.26	25.32				569.0	
3.47	163.20	32.65				564.9	
3.67	171.83	38.96					9.57
3.85	173.14	49.12				561.2	
3.93			0.02				
4.01	173.14	49.12					
4.11			0.03			587.4	
4.18	176.95	59.26					
4.40	187.07	67.79					
4.51			0.07			572.7	9.53
4.64	215.00	74.78					
4.91			0.11				
5.01	172.78	88.56					
5.50			0.24				
5.66	163.82	100.24				606.0	
6.16	168.33	102.14	0.91				
6.72	166.48	107.67	1.20				9.55
6.84						651.8	
7.22	177.12	117.35	1.64				
7.63	175.60	112.10	1.77				9.74
8.15	169.92	113.51	2.63				
8.67	171.13	113.32	3.68			645.5	9.72
9.12	178.83	111.99	4.99				

Table AVI-10 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	pH
9.61	181.76	109.93	6.35			642.9	9.66
10.12	196.44	115.66	9.02				
10.66	189.46	111.03	10.18			620.8	9.70
11.04	185.59	107.07	10.97				
11.61	181.59	106.81	13.18			609.9	9.61
12.06	184.46	108.16	15.63				
12.59	182.29	107.19	16.58			590.8	9.64
13.10	183.91	107.25	19.42				
13.58	174.85	100.90	19.53			635.5	9.58
14.15		94.28	22.98				
14.66	198.69	109.44	24.69			617.4	9.64
15.71	193.29	103.79	27.06			624.6	9.67
16.75	187.84	99.64	26.88			609.4	9.62
17.75		87.17	27.87			606.5	
18.23	162.20						
18.75		89.10	28.82			613.4	

Table AVI-11. XAD-4 Column Influent Data For Figures 4-9 to 4-12 and 4-47 to 4-66.

Time Averaged Influent Concentrations	
Trichloroethylene (TCE)	169.57 mg/L
Toluene	84.10 mg/L
m-Xylene	21.05 mg/L
1,2,4-Trichlorobenzene (TCB)	2.177 mg/L
Naphthalene	0.319 mg/L
Total Organic Carbon (TOC)	612.2 mg/L
o-Xylene	0.03 mg/L
Time Averaged Flowrate	47.8 ml/min
Operating Temperature	23 +/- 2 C

Run Time days	Flowrate ml/min	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
0.01	48.2	159.50	77.17	19.66	2.197	0.323	584.8	0.03	8.98
0.93	48.1	179.50	83.72	21.60	2.084	0.310	607.8	0.03	
1.02	47.1	174.88	88.32	21.22	2.240	0.360	595.7	0.03	
1.51	47.1	174.53	81.56	21.19	2.110	0.340	612.7	0.03	9.10
2.10	46.9	170.07	81.89		2.046	0.344		0.03	
2.62	46.9	162.73	81.46	19.84	2.124	0.360	602.9	0.03	
3.10	46.8	167.82	87.82	20.73	2.052	0.325		0.03	
3.60	46.1	188.21	85.23	20.20	1.798	0.324	616.3	0.03	9.22
4.11	46.6	161.84	92.58	20.08	2.143	0.324		0.02	
4.57	46.8	166.08	86.95	19.97	2.036	0.338	602.6	0.03	
4.78	47.5	170.66	81.30	20.22	1.596	0.365		0.04	
5.18	46.1	184.57	82.31	21.85	1.764	0.366	604.2	0.03	8.90
5.70	47.4	176.30	82.13	21.64	1.467	0.372		0.03	
6.18	47.0	180.83	81.51	21.87	1.822	0.368	619.2	0.03	
6.67	47.1			22.65	1.945	0.286		0.03	
7.18	47.1	177.74	91.61	21.54	2.760	0.337	624.0	0.03	9.12
7.70	47.2	170.10	87.07	20.83	2.690	0.316		0.03	
8.19	46.6	184.47	94.74	22.74		0.311	619.2	0.03	
8.69	47.2	180.92	91.69	22.25	2.570	0.318		0.03	
9.18	48.2	192.29	86.40	24.29	1.945	0.286	607.2	0.03	9.04
9.71	46.2	186.00	82.59	23.45	2.149	0.297			
10.18	47.1	188.00	79.80	22.61	1.994	0.298	615.4	0.03	
10.81		180.73	86.12	20.43		0.280		0.03	
11.16		190.24	77.68	20.19	1.894	0.273	623.5	0.03	9.08
11.69		189.40	81.05	23.64	2.187	0.298		0.03	
12.19		181.96	86.75	22.49	2.680	0.328	583.1		
13.16		172.89	93.92	22.16	2.310	0.309		0.03	
13.69	48.4	175.28	90.82	21.32	2.320	0.308	621.5	0.03	8.96
14.14		167.12	93.50	21.94	2.320	0.314		0.03	
14.70	48.2	177.38	92.61	21.38	2.250	0.299	617.4		
15.19		160.97	89.63	21.50	2.440	0.334		0.03	
15.69	48.4	159.71	89.66	21.52	2.370	0.319	622.7	0.03	8.75
16.23		163.15	89.92	22.87	2.310	0.310		0.03	
16.80	48.6	146.87	91.13	22.77	2.340	0.312	625.2	0.03	
17.14		164.34	92.47	23.23	2.310	0.315		0.03	
17.74		172.26	81.11	21.89	2.090	0.289	625.2	0.03	9.16
18.19		170.95	84.81	22.02	2.010	0.271		0.03	9.03

Table AVI-12. XAD-4 Column Effluent Data For Figures 4-9 and 4-47 to 4-52.

Bed Parameters	
Adsorbent	XAD-4 Resin
Particle Radius	0.060 cm
Particle Porosity	0.572
Apparent Density	0.443 g/ml
Bed Length	0.1040 m
Bed Diameter	5.08 cm
Dry Weight of Adsorbent	0.0708 kg
EBCT	4.4 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
0.01							0.059	
0.10						56.3	0.090	
0.18						103.5		
0.26						171.6	0.180	9.21
0.35						248.7	0.287	
0.43	0.62					312.3	0.494	
0.52	1.63	0.20				365.6	0.523	
0.59	5.06	0.39				409.8	0.625	
0.69	14.70	1.00				446.8	0.947	
0.77	32.23	2.08				460.2	1.340	
0.85	59.53	4.46				479.2	1.670	
0.94	94.74	8.24				494.1	2.260	
1.02	134.48	13.22				513.7	2.960	
1.10	163.52	19.92				517.1	3.360	9.16
1.18	173.27	27.83				531.2	3.630	
1.25	189.26	38.40					4.100	
1.34	181.29	49.92					4.680	
1.43	196.44	57.65					4.780	
1.51	192.42	64.41				555.6	5.080	
1.58	178.18	73.40					5.320	
1.68	186.36	73.14				572.0	5.390	
1.77			0.11		0.060		6.140	
1.86	182.52	80.81	0.16		0.058	583.0	5.890	
1.96								9.02
2.10	175.39	90.52	0.37			582.6	5.490	
2.27			0.56		0.061		6.350	
2.44						598.9		
2.62	177.49	89.10	1.39		0.066		6.110	
2.95			3.05		0.068	583.7	5.700	
3.10	178.41	91.33	3.86			561.5	5.020	
3.44						579.6		
3.60	170.53	93.46	8.15		0.073		3.820	9.10
3.77						598.3		
4.11	176.90	89.12	12.76			592.0	2.220	
4.47	170.19	82.28	14.97		0.092	595.6	1.490	
4.57	166.94	79.08	15.52		0.090		1.270	
4.78						596.3		
4.94	164.39	88.40	17.00		0.099		0.856	
5.18					0.117	590.3	0.616	
5.25	166.63	87.92	18.43				0.502	
5.70	172.36	85.99	18.74		0.137		0.286	
6.18	170.41	83.72	19.37			588.1		9.18
6.67	178.91	89.87	20.18		0.179		0.101	
7.18						607.6		
7.70	176.86	88.70	21.10	0.023	0.235		0.063	
8.19	182.04	91.49	22.15	0.033	0.251	608.8	0.054	
8.69	179.85	87.93	22.19	0.050	0.286		0.049	
9.18	195.05	88.22	22.23	0.062	0.260	583.5	0.040	

Table AVI-12 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
9.71	185.97	85.22	21.96	0.097	0.299		0.041	
10.18	181.92	84.54	21.52	0.106	0.290	602.3	0.038	
10.68	198.13	85.03	21.98		0.310			
11.16	180.50	85.53	22.13	0.205	0.306	621.0	0.036	
11.69	186.35	87.69	21.27	0.244	0.299		0.036	
12.19	183.87	93.38	21.62	0.305	0.297	591.2		8.95
12.83	176.11	104.27	20.92	0.477	0.317		0.035	
13.36	162.85	84.42	20.86	0.521	0.316	597.0	0.034	
13.80	176.68	90.66	21.44	0.560	0.322		0.033	
14.37	177.69	93.21	21.97	0.615	0.299	603.0	0.034	
14.86	164.87	92.96	21.41	0.718	0.298		0.033	
15.36	175.26	94.27	22.06	0.750	0.292	600.8	0.031	
15.90	159.64	85.02	20.78	0.842	0.292		0.032	
16.47	171.93	91.73	22.18	1.000	0.303	605.0	0.031	9.02
16.81	162.69	86.32	21.33	1.090	0.294		0.030	
17.41	160.04	90.24	21.60	1.160	0.275	595.8	0.029	
17.85	181.10	89.89	21.92	1.340	0.304		0.031	

Table AVI-13. XAD-4 Column Effluent Data For Figures 4-10 and 4-53 to 4-57.

Bed Parameters	
Adsorbent	XAD-4 Resin
Particle Radius	0.060 cm
Particle Porosity	0.572
Apparent Density	0.443 g/ml
Bed Length	0.2080 m
Bed Diameter	5.06 cm
Dry Weight of Adsorbent	0.1359 kg
EBCT	8.8 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
0.01						0.5		
0.18						42.5		
0.26						44.3		
0.35						55.2		
0.43						66.7		
0.52						88.1		
0.59						135.7	0.220	9.00
0.69						194.1	0.245	
0.77						269.9	0.291	
0.85						321.0		
0.93		0.03				365.6	0.400	
1.02						409.0		
1.10	0.05	0.02				428.4	0.467	9.30
1.18						443.6		
1.25	0.43					459.1	0.606	
1.34	0.88	0.02				454.3	0.601	
1.43	2.31					465.7	0.860	
1.51	4.22	0.07				472.2		
1.58	9.44	0.14	0.01		0.007	474.9		
1.68	26.25	0.45				476.4	1.240	
1.77	46.50	0.73				488.9		
1.86	76.82	1.16				489.6		
1.96	120.98	2.25				503.6		8.90
2.10	170.30	6.27			0.037	527.7	3.350	
2.27	215.64	12.48						
2.44	205.07	25.44				539.4	3.330	
2.62	198.73	48.00			0.050		5.130	
2.77	195.45	53.79						
2.95	186.57	68.31				562.7		
3.10	187.55	90.56					5.190	
2.27			0.01		0.049		6.020	
3.44						550.1		
3.60	176.77	99.64	0.03		0.053		6.080	
3.77						576.8		
3.95			0.03		0.057		6.920	
4.11	176.69	94.01				564.0	5.760	9.14
4.47	168.23	85.51	0.08		0.061	579.4	6.770	
4.57	178.64	83.93					6.440	
4.77						586.5		
5.18	149.14	73.59	0.35			581.8	5.040	
5.70	181.27	80.49	1.28		0.078		6.400	
6.18						589.9	6.250	
6.67	177.83	84.19	5.07		0.083		4.870	
7.18	181.66	92.83	7.91			619.8	3.870	
7.70	176.70	81.53	11.50		0.079		2.630	
8.19	181.69	91.49	14.88		0.074	611.2	1.610	
8.69	163.82	87.93	17.53		0.082		0.973	9.23
9.18	186.35	88.06	19.56		0.085	599.3	0.522	
9.71	173.81	86.34	20.45		0.091		0.291	

Table AVI-13 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
10.18	188.61	91.15	22.02		0.101	603.9	0.183	
10.68	183.51	85.32	21.58		0.115		0.128	
11.16	182.73	90.78	22.39		0.122	605.4		
11.69	192.32	85.60	21.74		0.122		0.068	
12.19	185.93	87.76	22.17		0.146	595.1		
12.83	174.98	92.59	21.54		0.174		0.091	
13.36	185.08	93.97	21.96		0.195	597.5	0.050	9.16
13.80	175.78	88.67	21.97	0.012	0.214		0.045	
14.37	171.64	89.61	22.15	0.012	0.247	589.2	0.047	
14.86	171.25	87.98	22.58	0.015	0.251		0.045	
15.36	168.25	87.74	21.86	0.017	0.267	604.4	0.043	
15.90	164.21	85.24	21.25	0.022	0.216		0.039	
16.47	161.53	88.93	21.58	0.030	0.310	592.6	0.042	
16.81	163.87	96.21	20.68	0.029	0.274		0.038	
17.41	161.74	83.39	21.07	0.035	0.294	596.4	0.037	8.98
17.85	168.65	85.96	21.35	0.035	0.284		0.035	

Table AVI-14. XAD-4 Column Effluent Data For Figures 4-11 and 4-58 to 4-62.

Bed Parameters	
Adsorbent	XAD-4 Resin
Particle Radius	0.060 cm
Particle Porosity	0.572
Apparent Density	0.443 g/ml
Bed Length	0.309 m
Bed Diameter	5.05 cm
Dry Weight of Adsorbent	0.1994 kg
EBCT	13.0 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
0.01						0.6		
0.18						41.2		
0.26						41.7		
0.35						42.5		9.30
0.43						45.4		
0.52						44.0		
0.59						46.3		
0.68						47.0		
0.76						58.3	0.124	
0.85						85.2		
0.93						125.9		
1.01						178.7		
1.10						224.8		
1.18						265.5		
1.25						310.5		
1.34						341.5		
1.43						374.0		
1.51						405.9		
1.58						430.3		
1.68						455.3	0.585	9.15
1.77	0.03				0.005	465.0	0.570	
1.96	0.07	0.02	0.01				0.573	
2.10	0.12	0.02	0.01		0.005	490.3	0.570	
2.27	0.84						0.600	
2.44	5.79	0.03	0.01		0.007	506.1	0.830	
2.62	24.03	0.17					1.440	
2.77	71.41	0.28	0.01		0.021		1.890	
2.95	144.88	1.11	0.01		0.027	514.4	2.700	
3.10	197.10	2.56					2.960	
3.27	225.01	5.86					3.140	
3.44	222.45	12.66				533.1	3.430	
3.60	223.43	25.17	0.02		0.042		4.400	
3.77	202.43	37.34				573.9	3.920	8.87
3.95	191.53	53.76					4.180	
4.11	188.17	70.48				542.7	4.590	
4.27	182.59	80.04					4.560	
4.47	183.39	85.36				554.4	4.850	
4.57		82.13	0.02		0.051		5.760	
4.78						554.0		
5.18	183.39	95.60	0.02		0.050	555.2	6.170	
5.70	184.43						6.720	
6.18	169.25	92.82	0.04		0.061	560.7	7.200	
6.67	181.47	93.29	0.36		0.064		7.240	
7.18	188.26	94.55	0.07		0.063	599.1	7.380	
7.70	178.45	103.57	0.17		0.066		7.530	
8.19	179.27	94.41	0.40		0.067	594.9	7.040	
8.69	184.86	99.93	0.92		0.070		6.900	8.46
9.18		90.90	1.75		0.067	579.8	6.360	
9.71	183.09	90.49	3.39		0.072		5.820	

Table AVI-14 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
10.18		92.58	5.40		0.077	590.2	4.710	
10.68	187.48	89.88	8.16		0.075		3.780	
11.16		89.70	11.24		0.079	600.0	2.690	
11.69	185.29	88.82	13.78		0.075		1.700	
12.19		82.89	16.20		0.089	593.6		
12.83	170.76	87.97	19.38		0.086		0.443	
13.36	181.49	90.53	21.38		0.096	582.3	0.196	
13.80	179.11	91.65	21.30		0.112		0.185	
14.37	164.34	90.58	21.38		0.108	588.1	0.214	
14.86	170.80	89.97	19.38		0.111		0.221	
15.36	166.69	82.94	20.66		0.111	586.4	0.185	9.15
15.90	162.11	85.85	21.57		0.093		0.134	
16.47	166.68	86.94	20.37		0.113	594.8	0.092	
16.82	162.73	85.53	20.97		0.102		0.078	
17.41	159.63	90.59	21.80		0.110	588.1	0.055	9.10
17.85	173.31	93.23	22.48		0.118		0.049	

Table AVI-15. XAD-4 Column Effluent Data For Figures 4-12 and 4-63 to 4-66.

Bed Parameters	
Adsorbent	XAD-4 Resin
Particle Radius	0.060 cm
Particle Porosity	0.572
Apparent Density	0.443 g/ml
Bed Length	0.411 m
Bed Diameter	5.05 cm
Dry Weight of Adsorbent	0.2641 kg
EBCT	17.2 minutes

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
0.01						0.9		
0.18						41.4		9.12
0.26						42.0		
0.35						41.3		
0.43						42.0		
0.52						42.7		
0.59						41.3		
0.68						41.1		
0.76						40.7		
0.84						43.0		
0.93						44.3		
1.02						49.1		
1.10						52.9		
1.18						67.9		9.06
1.25						92.9		
1.34						112.2		
1.43						161.4		
1.51						201.2		
1.58						245.2		
1.68						338.1	0.329	
1.77						381.7		
1.86						408.9		
1.96						425.0	0.473	
2.10						454.9	0.574	
2.27						462.4		
2.44	0.08				0.005	472.7	0.563	
2.62						471.3	0.591	
2.77	0.08				0.006	484.1		9.23
2.95						476.5		
3.10	0.78						0.726	
3.27	4.20	0.03			0.006		0.807	
3.44	13.71	0.04			0.007	457.7	1.020	
3.60	36.95	0.14					1.290	
3.77	81.73	0.31				503.2	1.840	
3.95	154.62	0.82					2.440	
4.11	211.71	1.97				486.1	2.770	
4.27	233.38	2.98					3.090	
4.47	235.78	6.06				510.6	3.280	
4.57	230.70	9.73					3.560	
4.78	222.70	17.71				518.3	3.730	
4.94	204.39	16.98					3.870	
5.18	194.21	46.99				533.3	4.250	
5.70	175.78	78.81					4.580	8.98
6.18			0.01		0.047	553.0	6.010	
6.67	183.79	98.54						
7.18			0.02		0.067	580.1	6.810	
7.70	182.32	78.53					7.900	
8.19	194.88	103.97	0.04		0.061	593.6	7.280	
8.69	192.93	99.22	0.05		0.059		6.800	

Table AVI-15 Continued

Run Time days	TCE mg/L	Toluene mg/L	m-Xylene mg/L	1,2,4-TCB mg/L	Naphthalene mg/L	TOC mg/L	o-Xylene mg/L	pH
9.18	169.68	88.96			0.060	571.0	7.260	
9.71	192.97	95.66			0.071		7.690	
10.18	179.48	92.72	0.28		0.066	581.2	7.640	
10.68	174.58	91.94	0.36		0.069		7.660	
11.16	193.67	96.86	0.33		0.070	595.8	7.310	
11.69		90.20	0.63		0.073		6.970	
12.19	184.13	90.94	1.23		0.076	580.1		
12.83	178.07	91.57	4.60		0.074		4.630	9.10
13.36	189.51	89.48	9.82		0.075	578.4	2.970	
13.80	176.73	84.97	11.43		0.075		2.840	
14.37	174.31	90.59	9.72		0.077	591.0	3.030	
14.86	172.54	94.03	9.69		0.076		3.540	
15.36	174.18	90.33	9.66		0.076	529.0	3.250	
15.90	172.25	86.52	12.26		0.072		2.340	
16.47	173.07	91.51	16.30		0.090	593.0	1.510	
16.82	169.39	84.04	16.84		0.082		0.948	
17.41	158.44	85.08	18.95		0.090	582.0	0.523	8.10
17.85	165.34	86.33	19.94		0.090		0.322	

Table AVI-16. MFB Model Verification Experiment Influent Data for Figures 4-67 to 4-78.

Run Time (days)	Flow (ml/min)	TOC	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	pH
0.51	47.9		177.2	106.4	22.83	2.4	0.312	
1.51	48							
2.50	47.7	628.73						6.5
3.50	46.4	626.32						6.89
4.52	46.5	652.94	153.8	93.14	21.79	2.53	0.318	6.69
5.50	46	649.27						6.79
6.52	46.2	629.54						6.4
7.55	46	583.35						6.39
8.56	45.8	595.33	162	97.13	21.32	2.19	0.294	6.37
9.51	43.5	571.94						6.35
10.53	46.9	636.74						6.38
11.53	46.6	600.52						6.32
12.55	44.5					2.1	0.263	
14.50	47.6	509.2						6.44
15.73	47.9	648.9						6.43
16.76	47.4	577.13	157.3.	92.33	21.66	2.06	0.298	6.43
17.52	48.6	723.91						6.53
18.50	48.4	698.59						6.47
19.64	48.7	621.98	162.8	87.41	22.75	1.87	0.33	6.33
20.59	47.6	611.5						6.31
21.52	48.2	593.86						6.28
22.60	48.6	676.7						6.4
23.71	48.4	627.1						6.35
24.59	49.1	574.2	135.2	82.31	21.79	1.93	0.38	6.34
26.52	48.2	600.38						6.32
27.52	48.6	595.66						6.34
28.60	48.6	613.46	176.9	90.84	25.45	1.5	0.4	6.32
29.60	48.4	610.54						6.35
30.65	48.4	576.53						6.34
31.67	47.7	589.82						6.34
32.52	48	583.54	130.6	89.72	22.39			6.35
32.77	48.3	619.76						
33.66		610.99						6.33

Table AVI-16 Continued

Run Time (days)	Flow (ml/min)	TOC	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)
34.63		530.9					
35.73	48.8	702.9					
40.58	48		141.6	64.91	17.83	1.72	0.336
41.69			122	81.56	18.78	1.6	0.394
42.65	48.4		133.7	75.2	19.67	1.72	0.346
43.72	49.2		133.8	101	23.94	1.91	0.314
44.76	49.2						
45.66	48.3		133.9	71.11	20.53	1.77	0.348
46.56			143.6	85.79	21.84	2.04	0.411
47.75			133.2	70.82	28.35	2.03	0.355
48.66	48		153.7	70.33	31.25	1.93	0.375
49.68			148.6	79.81	24.25	1.77	0.343
50.67			146.2	88.53	22.4	2.09	0.523
51.71	49.4		146.1	79.14	25.28	2.32	0.537
52.70	48.4		148.7	78.47	22.8	2.38	0.601
53.66	48.7		154.3	76.5	22.96	2.15	0.537
54.58	48		153.5	60.28	20.47		
55.67	48.4		198.8	72.38	21.07	2.86	0.594
56.57	48.5		173.1	70.03	20.98	2.72	0.501
57.64	48.6		161.6	87.19	19.18	1.81	0.452
58.69	48.2		169.5	78.96	21.35	1.8	0.547
59.59	47.2		176.6	73.83	20.84	1.94	0.515

Table AVI-17. 580-26 Column Effluent Data from MFB Model Verification Experiment for Figures 4-67, 4-70, 4-73, and 4-76.

Bed Parameters	
Adsorbent	580-26 GAC
Particle Radius	0.042 cm
Particle Porosity	0.68
Apparent Density	0.651 g/ml
Bed Volume, ml	2890.2
Bulk Density, g/ml	0.370
Wet Weight of Adsorbent, g	1084.3
Dry Weight of Adsorbent, g	1069.3
Total EBCT, min	60.1

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.67							10.11
1.51							10.18
3.16							9.87
4.52	ND	ND	ND	ND	ND		
4.86							9.62
6.17	ND	ND	ND	ND	ND		
7.55							8.29
8.15	ND	ND	ND	ND	ND		
10.82	ND	ND	ND	ND	ND		7.13
12.90	ND	ND	ND	ND	ND		
13.82							8.75
16.76	ND	ND	ND	ND	ND		
17.52	ND	ND	ND	ND	ND		7.81
18.50	ND	ND	ND	ND	ND		
19.64	ND	ND	ND	ND	ND		
20.59	ND	ND	ND	ND	ND		
21.52	ND	ND	ND	ND	ND		
22.60	ND	ND	ND	ND	ND		
23.08							7.46
23.71	ND	ND	ND	ND	ND		
24.55	ND	ND	ND	ND	ND		
25.53	ND	ND	ND	ND	ND		
26.48	ND	ND	ND	ND	ND		
27.48	ND	ND	ND	ND	ND		
27.99							8.16
28.56	ND	ND	ND	ND	ND		
29.56	ND	ND	ND	ND	ND		
30.60	ND	ND	ND	ND	ND		
31.63	ND	ND	ND	ND	ND		
32.48	ND	ND	ND	ND	ND		
32.96							7.63
38.08							7.92
39.13						37.14	
39.59						36.9	
40.00						40.5	
40.53	ND	ND	ND	ND	ND	26.12	
41.16						33.38	
41.64	ND	ND	ND	ND	ND	29.6	
42.01	ND	ND	ND	ND	ND	29.24	
42.61	5.09	ND	ND	ND	ND	200.34	
43.06	45.64	ND	ND	ND	ND	304.21	
43.68	178.4					361.88	
44.18	324.8	ND	ND	ND	ND	418.23	
44.72	564.7					429.73	
45.10	629					400.52	

Table AVI-17 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
45.61	757.8	0.007				408.25	
46.13	723.4	0.0255				450.06	
46.51	691.4	0.172				475.19	
47.04	670.6	1.86				454.45	
47.71	618.1	15.983				457.73	
48.13	516.8	41.051				485.78	
48.61	397	102.65				520.57	
49.00	375.5	146.24				524.81	
49.64	316	178.62	ND	ND	ND	557.41	
50.04	281.9	195.86					
50.63	261.8	210.89					
51.09	228.5	207.44					
51.67	221.2	198.38					
52.08	225.7	210.94					
52.66	217.7	208.47					
53.08	219.7	213.73	ND	ND	ND		
53.61	214.1	190.76					
54.13	204.1	194.17				555.78	
54.54	199.8	180.9	ND	ND	ND		
55.12	221.7	206.64					
55.63	198.9	206.66					
56.02	212.3	176.99					
56.53	239.3	232.54				521.41	
57.06	213.8	197.3					
57.60	198.4	181.7					
58.11	174.5	177.4					
58.65	184.6	186.9				526.54	
59.05	196.7	150.6					
59.55	254.11	171.6					
60.06	197.3	174.8	ND	ND	ND		

Table AVI-18. APA Column Effluent Data from MFB Model Verification Experiment for Figures 4-68, 4-71, 4-74, and 4-77.

Bed Parameters	
Adsorbent	APA GAC
Particle Radius	0.42 cm
Particle Porosity	0.68
Apparent Density	0..674 g/ml
Bed Volume, ml	847.38
Bulk Density, g/ml	0.356
Wet Weight of Adsorbent, g	303
Dry Weight of Adsorbent, g	301.80
Total EBCT, min	17.7

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.51	ND	ND	ND	ND	ND		
0.67							10.03
1.51						33.64	10.19
3.16							9.78
4.52	ND	ND	ND	ND	ND		
7.55							9.22
10.82	ND	ND	ND	ND	ND		
12.55							7.09
13.82							6.59
15.73	ND	ND	ND	ND	ND		
18.03							7.4
21.52	ND	ND	ND	ND	ND		
23.08							7.6
25.53	ND	ND	ND	ND	ND		
27.99							7.4
29.56	ND	ND	ND	ND	ND		
32.48	ND	ND	ND	ND	ND		
32.96							7.65
38.08							7.83
40.53	ND	ND	ND	ND	ND		
42.61						56.67	
43.68	ND	ND	ND	ND	ND		
44.18	ND	ND	ND	ND	ND	67.29	
44.72	7.322	ND	ND	ND	ND	188.72	
45.10	41.86						
45.61	106.5					398.91	
46.13	199.6						
46.51	273	ND	ND	ND	ND	523.69	
47.04	388.1						
47.71	514.6					511.6	
48.13	561.9						
48.61	512.9					509.25	
49.00	582.2	ND	ND	ND	ND		
49.64	723.9	ND	ND	ND	ND	496.16	
50.04	670.6	0.1194					
50.63	650.4	0.7815				524.24	
51.09	576.6	3.98					
51.67	442.9	28.55				542.3	
52.08	371.9	69.42					
52.66	328.9	139.8					
53.08	271.7	148.1	ND	ND	ND		
53.61	275	180.4				649.35	
54.13	228.3	185.6					
54.54	216	190.1					
55.12	188.5	197.2					
55.63	200.8	223.6				623.18	
56.02	169.3	213.1					

Table AVI-18 Continued

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
56.53	178.5	199.8					
57.06	189.5	214.7					
57.60	177.2	227.5					
58.11	194.4	209.8				689.35	
58.65	193.6	216.2					
59.05	208.3	204.8					
59.55	213.7	208.7				754.9	
60.06	222.4	191.7					

Table AVI-19. XAD-4 Column Effluent Data from MFB Model Verification Experiment for Figures 4-69, 4-72, 4-75, and 4-78.

Bed Parameters	
Adsorbent	XAD-4 Resin
Particle Radius	0.060 cm
Particle Porosity	0.572
Apparent Density	0.443 g/ml
Bed Volume, ml	798.34
Bulk Density, g/ml	0.342
Wet Weight of Adsorbent, g	676
Dry Weight of Adsorbent, g	273.24
Total EBCT, min	16.7

Run Time (days)	TCE (mg/L)	Toluene (mg/L)	m-xylene (mg/L)	1,2,4-TCB (mg/L)	Naphthalene (mg/L)	TOC (mg/L)	pH
0.51	ND	ND	ND	ND	ND		
0.67							9.91
1.51						28.2	10.08
3.16							9.78
4.52	ND	ND	ND	ND	ND		
7.55							9.05
10.82	ND	ND	ND	ND	ND		
12.55							7.27
13.82							6.79
15.73	ND	ND	ND	ND	ND		
18.03							7.71
21.52	ND	ND	ND	ND	ND		
23.08							6.99
25.53	ND	ND	ND	ND	ND		
27.99							7.4
29.56	ND	ND	ND	ND	ND		
32.48	ND	ND	ND	ND	ND		
32.96							7.94
38.08							7.78
40.53	ND	ND	ND	ND	ND		
43.68						77.91	
44.72						76.56	
45.61						53.81	
46.51	ND	ND	ND	ND	ND	179.04	
47.04	ND	ND	ND	ND	ND		
47.71	ND	ND	ND	ND	ND	475.64	
48.13	ND	ND	ND	ND	ND		
48.61	0.2431	ND	ND	ND	ND	480.49	
49.00	6.346	ND	ND	ND	ND		
49.64	151.63	ND	ND	ND	ND		
50.04	257.3					480.48	
50.63	338.8					484.87	
51.09	380.7						
51.67	393.5					461.65	
52.08	477						
52.66	557.6					477.52	
53.08	571.4	0.0203					
53.61	671.3					491.29	
54.13	689.4						
54.54	652.3	0.0196	ND	ND	ND		
55.12		0.2068					
55.63	514.88	4.471					
56.02	447	16.46				523.28	
56.53	379.03	37.25					
57.06		86.57					
57.60		128.9					
58.11	233.7	136.8					
58.65	228.5	192.5				635.91	
59.05	236.6	180.8	ND	ND	ND		
59.55	164	193.4	ND	ND	ND		
60.06	226.8	209.4				693.47	

Volume II: Phase II

ABSTRACT

A mathematical model is presented for analysis and optimization of the adsorbents contained in the International Space Station (ISS) multifiltration bed (MFB) water processor. The fixed bed adsorption model includes multicomponent equilibrium using single solute isotherm parameters and fictitious components to predict the competitive adsorption interactions occurring during the adsorption process. Fictive Component Analysis (FCA) was used to describe the competitive adsorption interactions occurring in the unknown background matrices. Fictitious parameters were determined by fitting TOC and tracer isotherms using ideal adsorbed solution theory calculations. Multicomponent isotherms were conducted on waste water provided by NASA and were used to validate the multicomponent equilibrium description.

Fictive component analysis was able to describe the TOC adsorption potential for four waste streams: waste mixture, shower/handwash mixture, urine distillate and humidity condensate. The residual percent errors, which compare the model fit to the isotherm data, are less than 23 percent for the waste streams, with the exception of humidity condensate. Predicting known compounds in the waste and shower/handwash mixtures consistently overpredicted the adsorbent's reduction in capacity for weakly adsorbing compounds. The compounds were overpredicted because the fictive components were calibrated to give the greatest reduction in capacity based on the weakest adsorbing tracer compound. However, for the urine distillate and humidity condensate streams the reduction in capacity was accurately predicted for the weaker adsorbing compounds.

The adsorption potentials of the three MFB adsorbents: 580-26 GAC, APA GAC, and XAD-4 resin, were compared for the concentration range used in this study. It was found the adsorption potential of 580-26 and APA GAC are similar with APA GAC having a slightly lower nonadsorbing concentration. Over the studied concentration range, XAD-4 resin has a significantly lower adsorption potential than the two GACs this was strongly supported for the urine distillate and humidity condensate streams.

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ACRONYMS

DCM	Dichloromethane
EB	Ethylbenzene
FC	Fictive Component
FCs	Fictive Components
FCA	Fictive Component Analysis
GA	Genetic Algorithm
GAC	Granular Activated Carbon
IAST	Ideal Adsorbed Solution Theory
ISS	International Space Station
LLE	Liquid-Liquid Extraction
MC	Methylene Chloride
MFB	Multifiltration Bed
MFBs	Multifiltration Beds
PGAC	Powdered Granular Activated Carbon
RAHF	Research Animal Holding Facility
RPE	Relative Percent Error
SOC	Synthetic Organic Carbon
SOCs	Synthetic Organic Carbons
TCE	Trichloroethylene
TOC	Total organic Carbon
PCE	Perchloroethylene

1.0 INTRODUCTION

1.1 Multifiltration Bed Model Overview

A substantial amount of potable water is required for life support of the crew aboard the International Space Station (ISS). Water for drinking, food preparation, and personal hygiene accounts for over 90% by weight of the basic consumables (water, oxygen, and food) required for survival aboard the ISS. Life support of a four person crew would require transport of approximately 46,100 lbs of water per year to the ISS without onboard water recycling. The economic limitations of transporting water to the ISS necessitate onboard recovery and reuse of the aqueous waste streams (Carter *et al.*, 1992; Carter *et al.*, 1991)

The aqueous waste streams processed by the ISS water processor include: 1) urine distillate, 2) shower water, 3) handwash water, 4) humidity condensate, 5) oral hygiene and wet shave waste, 6) a mixture of humidity condensate and evaporated urine from the Research Animal Holding Facility (RAHF) and 7) equipment offgassing waste. These waste streams are complex mixtures of unknown composition. The waste streams are processed using four processes. One process is a combination of adsorption media and ion exchange resins which make up the Multifiltration Bed (MFB) system. A schematic of the MFB is shown in Figure 1-1. This MFB process is used to remove organic and inorganic compounds from the waste mixture. Appendix I lists the major waste streams including their identified inorganic and organic constituents and expected concentrations aboard the ISS (Carter *et al.*, 1992).

The MFBs require periodic replacement when capacity of the resins and adsorbents are exhausted. At the present time, the MFBs are considered to be consumable items requiring re-supply by space shuttle flights because the energy requirements for on-board regeneration are too high. The shuttle transport cost for a consumable item is approximately, $ 15,000 to $ 20,000 per lb. Consequently, it is important to design the MFBs to be as efficient as possible. Development of an efficient MFB process design using an experimental approach is very costly and time consuming. Therefore, a mathematical model which describes the MFB process is being developed to aid in its design and operation. The MFB model is an important design tool because it

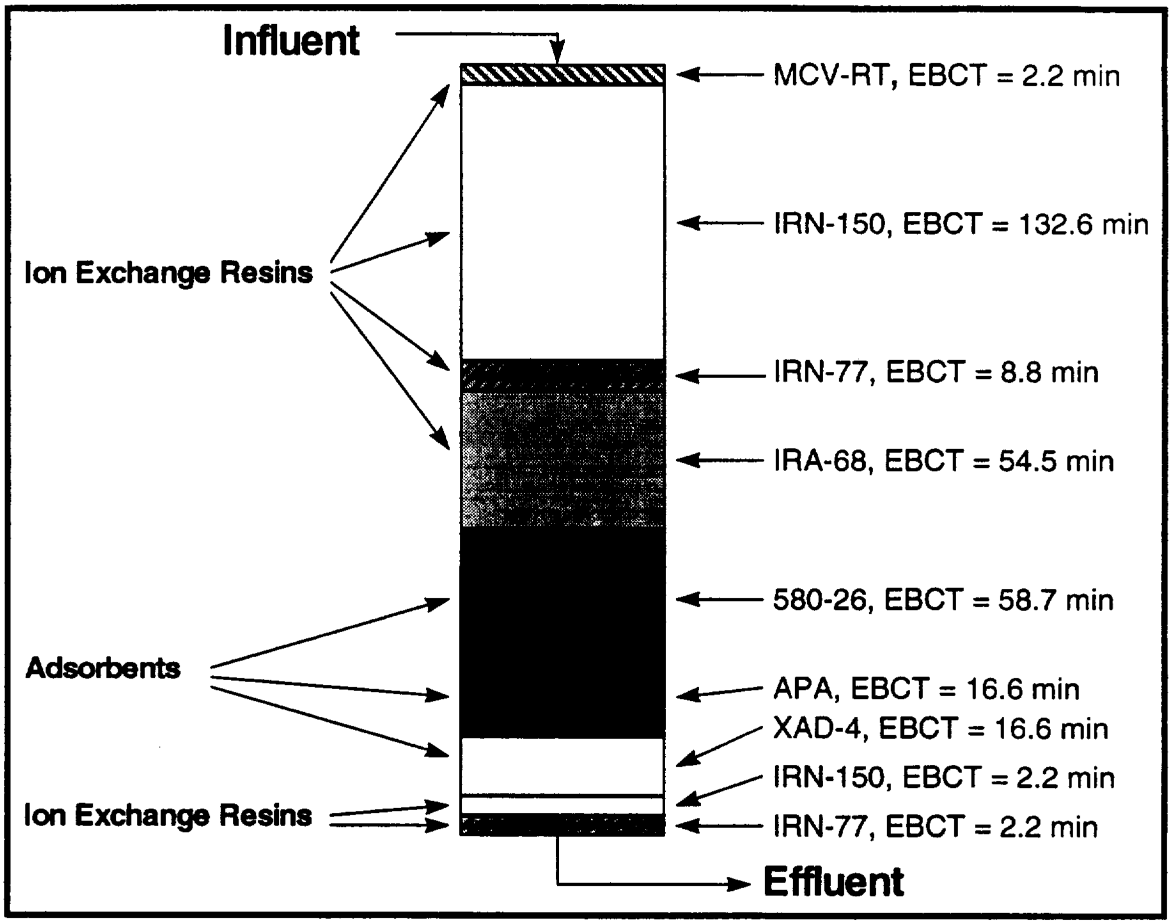

Figure 1-1. Multifiltration Bed Schematic

can be used to plan the scope of the pilot plant experiments by evaluating the impact of process variables on process performance and identify the most efficient design. The MFB model is also an important operational tool because it can be used to simulate MFB performance when unexpected changes in process feed streams occur.

Fictive Component Analysis (FCA) is used in the MFB model to describe the adsorption equilibrium of the total organic carbon (TOC) which makes up the waste water as well as the known compounds. Imaginary compounds are used as fictive components (FCs) to represent the distribution of unknown adsorbing compounds in the mixture which make up the overall total organic carbon (TOC) concentration. FCA is used because it allows adsorption modeling of the aqueous waste mixture without the requirement of knowing all the compounds in the solution. Hubele and Sontheimer (1983) and Frick and Sontheimer (1983) used the FCA to predict TOC adsorption isotherms for surface and groundwaters where each FC represented a portion of the total TOC, and the sum of the FC TOC concentrations and the nonadsorbing fraction equaled the overall TOC concentration. Crittenden *et al.* (1985) used FCA to predict the adsorption isotherms of tracer compounds using FCA in the presence of a known multicomponent background matrix.

In this study, FCA was used to model the TOC adsorption capacity of the waste water and the competitive adsorption effects on specific compounds. Determining fictive component parameters for the combined waste stream, as well as the shower/handwash, urine distillate and humidity condensate streams will be used to predict the overall performance of the MFBs. Predicting the performance will allow optimization of the MFB, to reduce the amount of consumables.

2.0 TOC ADSORPTION MODELING

2.1 TOC INTRODUCTION

The combined waste streams on-board the ISS are composed of several hundred organic compounds. At the present time, only about 85 to 90 percent of the waste mixture has been identified. Modeling all the known compounds would require determining single solute isotherm and kinetic information on each compound for each adsorbent. This would be a very costly and time consuming effort. In addition, numerically solving the fixed bed effluent profiles for several hundred compounds simultaneously would not be practical nor probable because of problems of convergence caused by the stiffness of the large number of ordinary differential equations. Consequently, TOC fictive component analysis is used for predicting the performance of organic contaminant removal in the MFB adsorption process. A total of 6 FCs were used to describe the TOC isotherms for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate stream on the three different adsorbents.

2.2 MATERIALS AND METHODS

2.2.1 Solution Preparation. Shower, handwash, humidity condensate, urine distillate, oral hygiene, wet shave, animal condensate and equipment off-gassing waste streams were generated in specially prepared facilities at Marshal Space Flight Center (MSFC) (Huntsville, AL). Samples of these waste waters were placed in glass containers with Teflon caps. The glass containers were placed in ice filled coolers and shipped overnight to laboratories at Michigan Technological University (MTU). Immediately after receiving the coolers, the waste waters were pumped through MCV resin (iodine releasing ion exchange resin) followed by filtration through a series of stainless steel filters and a Gelman 0.45 μm filter prior to mixing the waste streams. Prior to mixing, all the waters were stored in the same glass containers at 4°C. To minimize volatilization of the waste mixture (83.5 L), and shower/handwash (79.7 L) waters, they were pumped from the glass containers into Tedlar^{TM} bags.

The combined waste stream mixture was made up of 21.0 % shower water, 31.6 % handwash water, 18.8 % humidity condensate water, 13.9 % urine distillate water, 2.8 % L oral hygiene water, 3.2 % wet shave water, 6.9 % animal condensate water and 1.9

% equipment offgassing water. The shower/handwash waste stream was prepared by mixing 40.0 % shower water and 60.0 % handwash water. The humidity condensate and urine distillate waters were each MCV'd and stored in separate Tedlar™ bags. Waste stream dilutions were prepared by 50% dilution by volume using Milli-Q distilled-deionized water.

Distilled-deionized water was produced by distilling tap water and further purifying it with a Milli-Q UV Plus Water System (Millipore Corp., Bedford, MA). The Milli-Q™ system produces water with a background TOC concentration less than 0.1 mg/L. Milli-Q distilled-deionized water was used for waste stream dilutions and standard preparation.

2.2.2 Chemical Analysis. TOC was analyzed with a Sievers Model 800 Portable TOC Analyzer (Boulder, CO) utilizing UV-persulfate oxidation. The pH was determined using an Orion (Cambridge, MA) Model 501 pH meter.

2.2.3 Adsorbents. The following MFB adsorbents were used in this study:

- 580-26 coconut-shell based granular activated carbon (GAC), 18x25 USTM (Barneby and Sutcliffe Co., Columbus, OH)
- APA bituminous-coal based GAC, 12x40 USTM (Calgon Co., Pittsburgh, PA)
- XAD-4 polymeric adsorbent resin, 20x50 USTM (Rohm and Haas Co., Philadelphia, PA)

Representative adsorbent samples were obtained by mixing and splitting the samples of the adsorbents as received from the manufacturer. Powdered granular activated carbon (PGAC), USTM No. 200x400 sieve, was used in the isotherm studies. PGAC was obtained by crushing representative samples of the virgin GAC until a 100 percent passing size of USTM No. 200 mesh was achieved. The PGAC used for isotherms was the PGAC retained on a USTM No. 400 sieve which was washed with Milli-Q™ water and dried overnight at 105 °C. XAD-4 resin was rinsed with Milli-Q water and then used in its uncrushed form for isotherm studies.

2.2.4 Isotherm Procedure. A bottle point isotherm procedure was used for all adsorption isotherms (Crittenden *et al.*, 1983; Randtke and Snoeyink, 1983). A series of 250 mL screwcap bottles and 45 mL vials with Teflon septa each containing different dosages of adsorbent were filled with the same initial aqueous phase TOC concentration and allowed to equilibrate at room temperature. The waste and shower/handwash mixtures were allowed to equilibrate for 7 days, while the urine distillate and humidity condensate streams were given 10 days to reach equilibrium. During equilibration, the isotherm bottles were rotated in a tumbler at 18 revolutions per minute to provide good mixing of the adsorbents with the solution. The equilibrium liquid phase TOC concentrations in the isotherm bottles were then analyzed using the chemical analysis described in section 2.2.2. The equilibrium solid phase loading, $q_{e,i}$, for compound *i*, in each isotherm bottle was calculated from the equilibrium liquid phase concentrations, $C_{e,i}$, using the following mass balance on an isotherm bottle:

$$q_{e,i} = \frac{(C_{o,i} - C_{e,i})V}{M} \tag{2-1}$$

in which, $C_{o,i}$ is the initial liquid phase concentration of compound *i*; *V* is the volume of filling solution; and *M* is the mass of adsorbent in the isotherm bottle.

2.2.5 Scope of Experiments. The four waste streams: waste mixture, shower/handwash mixture, urine distillate and humidity condensate, each had TOC isotherms performed on three adsorbents, 580-26 GAC, APA GAC and XAD-4 resin.

2.3 FICTIVE COMPONENT ANALYSIS

Fictive components were used to represent the unknown background matrix estimating the adsorption strength of the four waste streams. TOC isotherms were used to estimate the adsorption strength of the waste streams. For each waste stream, physical parameters were assigned to the FCs and used in ideal adsorbed solution theory (IAST) calculations to model the adsorption potential.

2.3.1 Ideal Adsorbed Solution Theory. When all of the compounds present in a mixture have been identified, IAST can be used to predict the multicomponent adsorption equilibria of each compound (Crittenden *et al.* 1995; Fritz and Schlunder 1981; Jossens *et al.* 1978; Kuennen *et al.* 1989; Luft 1984; and Radke and Prausnitz 1992). IAST may be used to predict multicomponent equilibria based on the thermodynamics of adsorption using single solute isotherm parameters for the individual compounds and their respective initial concentrations. IAST development is discussed thoroughly by Radke and

Prausnitz (1972) and Crittenden *et al.* (1985). If the Freundlich isotherm equation is used to represent single solute behavior, IAST yields Equation 2-2 for the equilibrium condition of each adsorbate in a multicomponent isotherm (Crittenden *et al.*, 1985).

$$C_{oi} - \frac{M}{V} q_i - \frac{q_i}{\sum_{j=1}^{NC} q_j} \left[\frac{\sum_{j=1}^{NC} n_j q_j}{n_i K_i} \right]^{n_i} = F_i(q_1,\ldots,q_{NC}) = 0 \quad \text{for } i = 1,\ldots,NC \qquad (2\text{-}2)$$

in which, C_{oi} is the initial liquid phase concentration of compound i; q_i is the equilibrium solid phase concentration for compound i; V is the volume of filling solution; M is the mass of adsorbent in the isotherm bottle; and K_i is the Freundlich K parameter for the FC. n_i is the inverse of the Freundlich $1/n_i$ parameter for the FC. NC is the number of fictive components. q_j is the solid phase concentration for the corresponding fictive component. As shown in Equation 2-2, given the dosage of the adsorbent, initial concentrations, and Freundlich isotherm parameters of each adsorbate, the final equilibrium state may be determined by solving Equation 2-2 simultaneously for all components in the mixture. However, IAST requires all the compounds in the mixture to be identified to apply it in this manner. The wastewater generated on the ISS is a complex mixture of which complete characterization is not possible. Carter *et al.* (1992) identified over 250 organic compounds present in the waters and only accounted for approximately 85-90% of the wastewater TOC. In addition, the application of IAST with over 250 compounds is not practical. Consequently, fictive component analysis (FCA) was used to characterize the adsorption potential of the ISS waste streams.

2.3.2 Fictive Component Parameter Determination. In all these studies, the FCs are assigned physical properties and are used in IAST calculations to model the competitive adsorption strength of the unknown mixture. The parameters required for the FC multicomponent equilibrium calculations include: 1) molecular weight, 2) fraction of carbon, 3) Freundlich K, 4) Freundlich 1/n, and 5) initial concentration. Six fictive components were used to model the TOC and tracer isotherms. A sensitivity analysis to determine the optimum number of FCs is detailed in Appendix III.

The TOC fictive component parameters: molecular weight, fraction of carbon (FOC), and Freundlich K were determined by correlating the adsorption potential of the known compounds in the shower/handwash, urine distillate and humidity condensate streams (Appendix I). The known compounds were grouped by similar Freundlich K values as shown in Table 2-1. Table 2-1 shows the range of adsorption potentials for each group and the resulting Freundlich K calculated using weighted averages for 580-26 GAC. The compound's range of molecular weight and fraction of carbon along with their corresponding weighted averages are also summarized in Table 2-1.

Table 2-1. Groupings of the known compounds in the mixture.

	# of compounds	K range	K weighted average	MW range	MW weighted average	FOC range	FOC weighted average
Group 1	10	0.1 - 10	2.6	74-153	96.51	0.55-0.83	0.742
Group 2	6	10 - 70	42.3	92-130	123.2	0.62-0.92	0.710
Group 3	6	70 -200	97.6	87-357	95.3	0.60-0.90	0.753
Group 4	3	200 - 450	178.5	118-391	357.0	0.60-0.86	0.600
Group 5	18	450-3000	910.2	117-400	192.4	0.69-0.80	0.760
Group 6	5	> 3000	112231.9	214-400	270.7	0.73-0.95	0.800

*All K units: $(mg/g)(L/mg)^{1/n}$; All molecular weight units (MW): g/mol

Polanyi Potential Theory was used to determine the Freundlich parameters for the known compounds on 580-26 GAC. Weighted averages for molecular weight, fraction of carbon, and Freundlich K were calculated for each group using the relative concentration (C_i/C_{total}) of the contaminant, and its corresponding Freundlich K value. Equation 2-3 was used to calculate weighted averages:

$$P_{WA} = \sum_{i=1}^{N} P_i \left(\frac{C_i}{C_{total}} \right) \qquad \text{for } i=1,\ldots N \qquad (2\text{-}3)$$

in which, P_{WA} is the weighted average parameter; P_i is the parameter for compound i; C_i is the relative concentration of compound i; and N is the number of compounds in the group.

Once the FC Freundlich K values were determined, FC Freundlich 1/n values could also be determined. The Freundlich parameters for the known compounds in the mixture were graphed Freundlich 1/n vs. Freundlich K, on a semi-log graph for 580-26 GAC, APA GAC and XAD-4 resin. A linear correlation was determined relating the Freundlich parameters. Figures 2-1, 2-2, and 2-3 show the correlations for each adsorbent, 580-26 GAC, APA GAC and XAD-4 resin, respectively, and include the equation relating Freundlich 1/n to Freundlich K. These equations were used to determine all the Freundlich 1/n values based on the Freundlich K values.

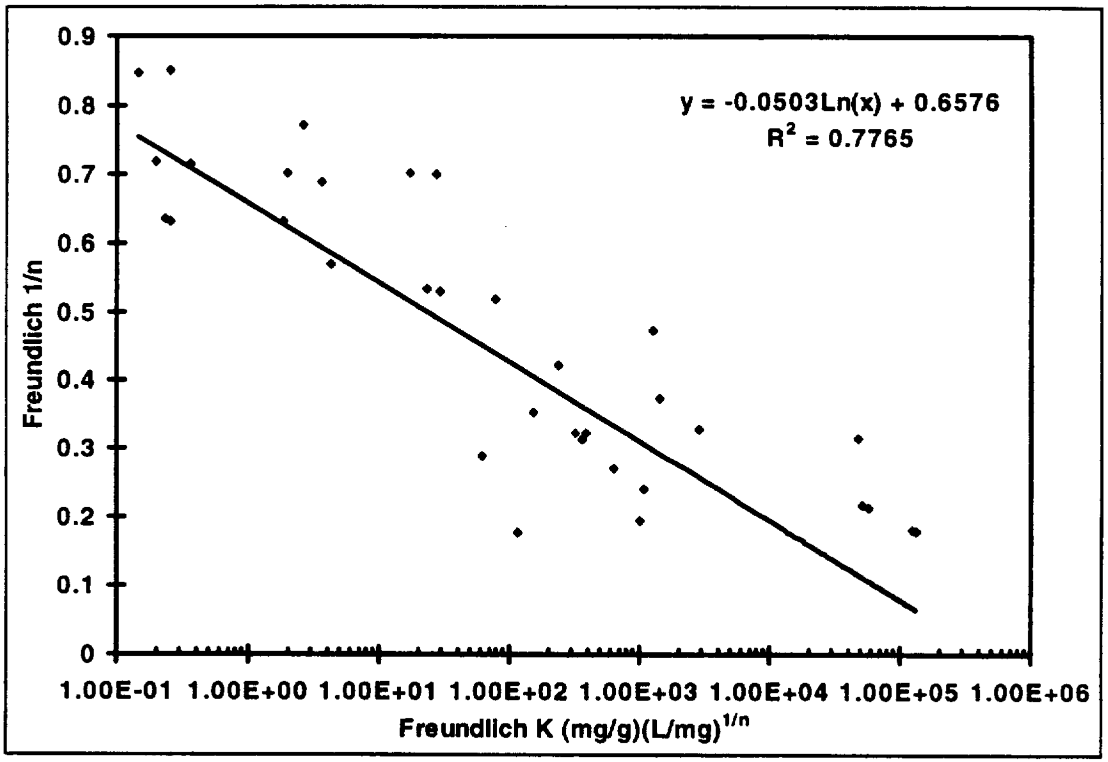

Figure 2-1. Correlation of Freundlich 1/n to Freundlich K for 580-26 GAC.

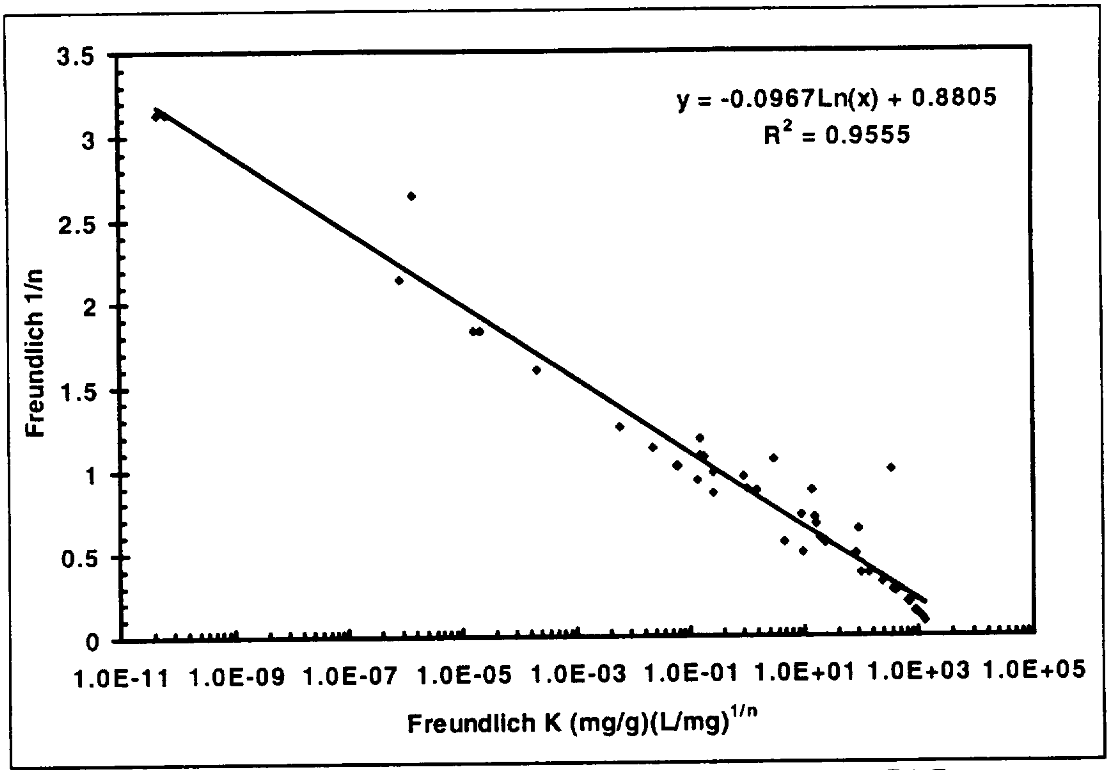

Figure 2-2. Correlation of Freundlich 1/n to Freundlich K for APA GAC.

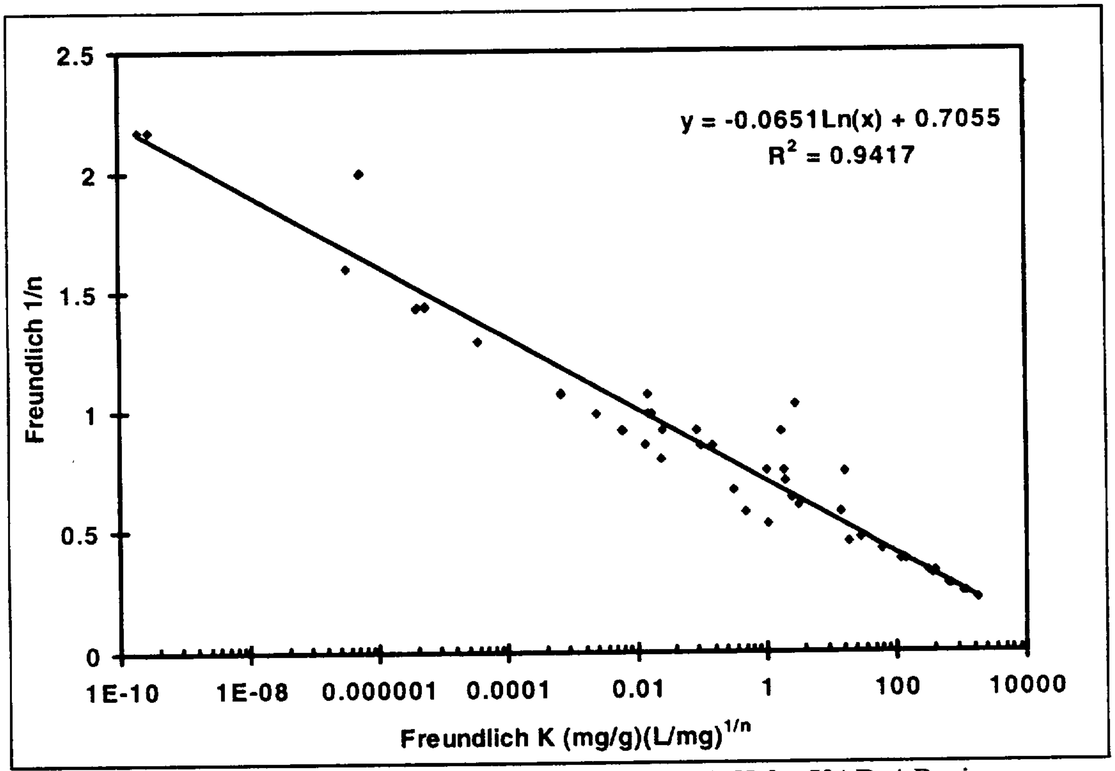

Figure 2-3. Correlation of Freundlich 1/n to Freundlich K for XAD-4 Resin.

The Fictive Component Analysis model requires a method to optimize the FC initial concentrations used in the IAST calculations, therefore the FCA model was combined with a genetic algorithm (GA) driver. (Carroll, 1996) The GA is a stochastic search/optimization technique which has been shown to be a robust optimization routine for solving complex nonlinear problems. (Gallagher and Sambridge 1994, Holland 1992, Forrest 1993) A fitness function is applied to compare the accuracy of the solutions and is maximized. (Gallagher and Sambridge 1994, Holland 1992, Forrest 1993) The fitness function, used in the FCA model for optimization, is calculated by Equation 2-4:

$$fitness = 100 - \frac{1}{2}\sum_{i=1}^{N}\left[\frac{\left|C_{e,i(\text{data})} - C_{e,i(\text{model})}\right|}{C_{e,i(\text{data})}} + \frac{\left|q_{e,i(\text{data})} - q_{e,i(\text{model})}\right|}{q_{e,i(\text{data})}}\right]^2 \quad \text{for i = 1,...N} \qquad (2\text{-}4)$$

in which, N is the total number of isotherm points being fit, $C_{e,i(data)}$ and $q_{e,i(data)}$ are the equilibrium liquid and solid phase TOC concentrations in each isotherm bottle, $C_{e,i(model)}$ and $q_{e,i(model)}$ are the IAST predicted equilibrium liquid and solid phase concentrations determined from the GA fitting routine. As the fitness increases, liquid and solid phase residual concentrations decrease, therefore fitting the model more accurately to the isotherm data. The optimized FC parameters were used in IAST equations to determine the adsorption strength of the unknown mixture.

The MFBs contain three adsorbents in series, therefore each adsorbent must be related to one another to model the unknown mixture as it passes through each adsorbent bed. The initial concentrations of the FCs for APA GAC and XAD-4 resin were held constant as determined from fitting the isotherm data for 580-26 GAC. Fitting the isotherm data for APA GAC and XAD-4 resin was accomplished using the FC concentrations from 580-26 GAC and optimizing the FC Freundlich Ks with the use of the GA. This method of holding FC concentrations constant for the APA GAC and XAD-4 resin FCs allows modeling of the beds in series operation by changing only the Freundlich K and 1/n.

2.3.3 TOC Isotherm Fitting. The TOC concentrations of the TOC isotherm fitting was made up of six TOC FCs and a nonadsorbing TOC fraction. The TOC isotherm fit using the FCA is based on the IAST solution with the FCs, and calculated by summing the TOC contribution of each individual TOC FC and the nonadsorbing concentration at each dosage. Six nonlinear IAST equations were solved simultaneously with the chosen FC parameters, optimizing the FC initial concentration using the genetic algorithm. Optimization was achieved by maximizing the fitness function, which minimized the error in both the liquid and solid phase. When fitting the nondilute and dilute TOC isotherms simultaneously, the dilute nonadsorbing concentration was calculated using the following equation.

$$C_{\text{nonadsorbing,dilute}} = \frac{C_{\text{nonadsorbing,nondilute}} C_{\text{total,dilute}}}{C_{\text{total,nondilute}}} \qquad (2\text{-}5)$$

in which, $C_{\text{nonadsorbing, dilute}}$ is the dilute nonadsorbing concentration calculated from the $C_{\text{nonadsorbing, nondilute}}$, the nondilute nonadsorbing concentration, $C_{\text{total, nondilute}}$, the total nondilute concentration and $C_{\text{total, dilute}}$, the total dilute concentration.

2.3.4 Relationship of FCs on Different Adsorbents. The MFB contains three adsorbents in series, therefore each adsorbent must be related to one another to model the unknown mixture as it passes through each adsorbent bed. The initial FC concentrations determined for 580-26 GAC were held constant and used as initial FC concentrations for APA GAC and XAD-4 resin. Fitting the isotherm data for APA GAC and XAD-4 resin was accomplished using the FC concentrations from 580-26 GAC and optimizing the FC Freundlich K values. The Freundlich 1/n parameter was correlated using the method described in section 2.3.2. This method of holding the FC concentrations constant for the APA GAC and XAD-4 resin allows modeling of the beds in series operation by changing only the FC Freundlich parameters representing the unknown background matrix.

2.3.5 TOC Equilibrium on 580-26 GAC, APA GAC, and XAD-4 resin. The adsorption capacity of the three adsorbents was compared for each of the four waste streams. Figures 2-4 through 2-6 show the adsorption capacity of the waste mixture, shower/handwash mixture, and urine distillate, respectively. The comparison indicates the adsorption capacity for 580-26 and APA GAC are similar, with the adsorption capacity of TOC on XAD-4 resin to be significantly lower. 580-26 GAC is a microporous adsorbent with a high surface area where, APA GAC has a larger pore size distribution in the meso-porous range than the 580-26 GAC. XAD-4 resin is mostly mesoporous in pore size and has the lowest surface area of the three adsorbents which is the most likely reason for the lower adsorption capacity. The adsorption capacity of TOC for urine distillate on XAD-4 appears to be weakly adsorbing.

Humidity condensate TOC isotherms (nondilute) on 580-26 GAC, APA GAC and XAD-4 resin are presented in Figure 2-7. Humidity condensate TOC is mostly nonadsorbing on all three adsorbents. The adsorption capacity on 580-26 GAC and APA GAC are slightly higher than XAD-4 resin at very low concentrations.

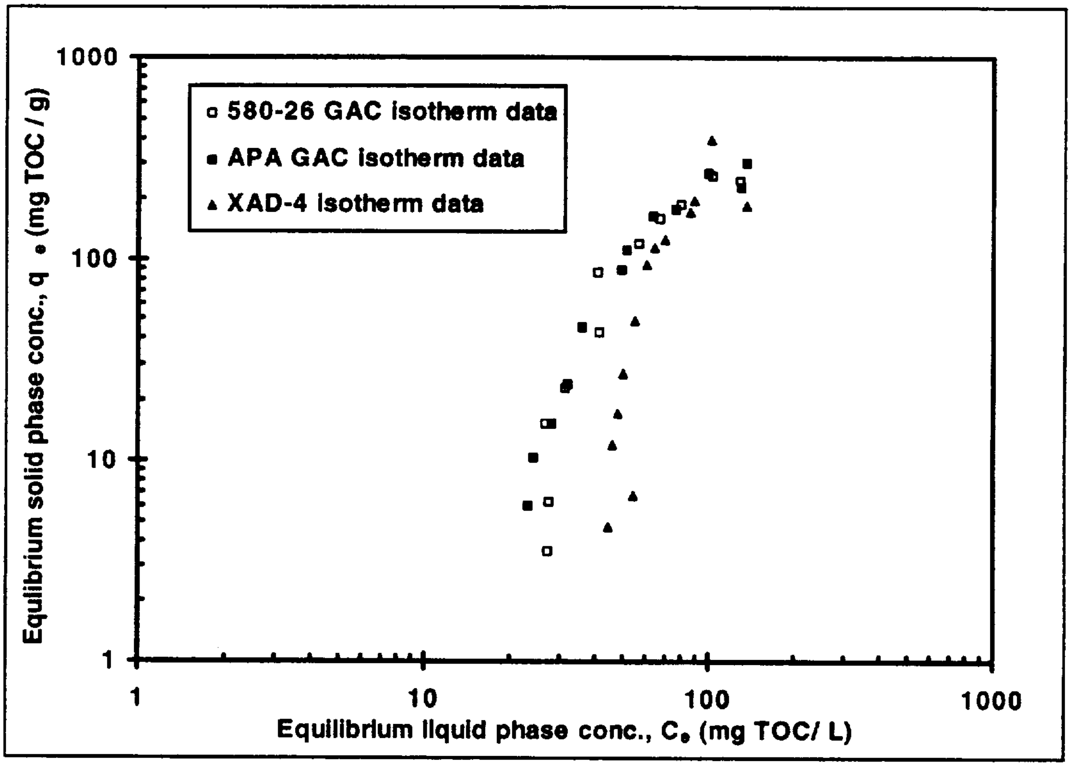

Figure 2-4. Waste mixture TOC isotherms on 580-26 GAC, APA GAC and XAD-4 resin.

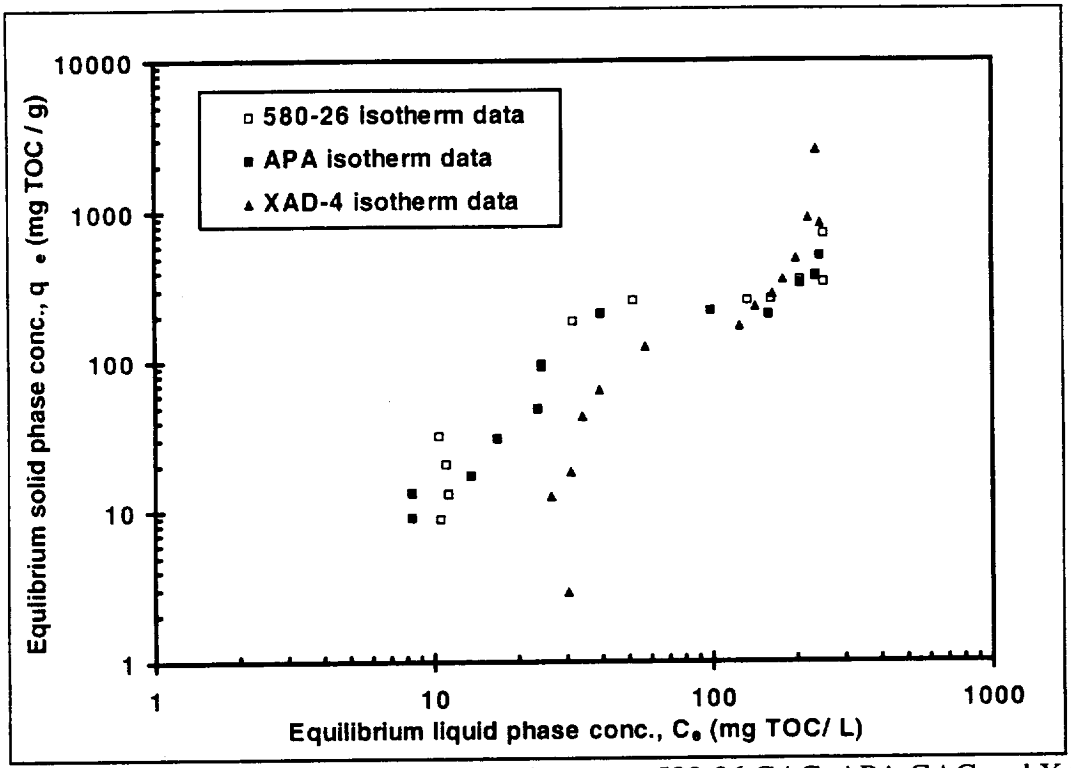

Figure 2-5. Shower/handwash TOC isotherms on 580-26 GAC, APA GAC and XAD-4 resin.

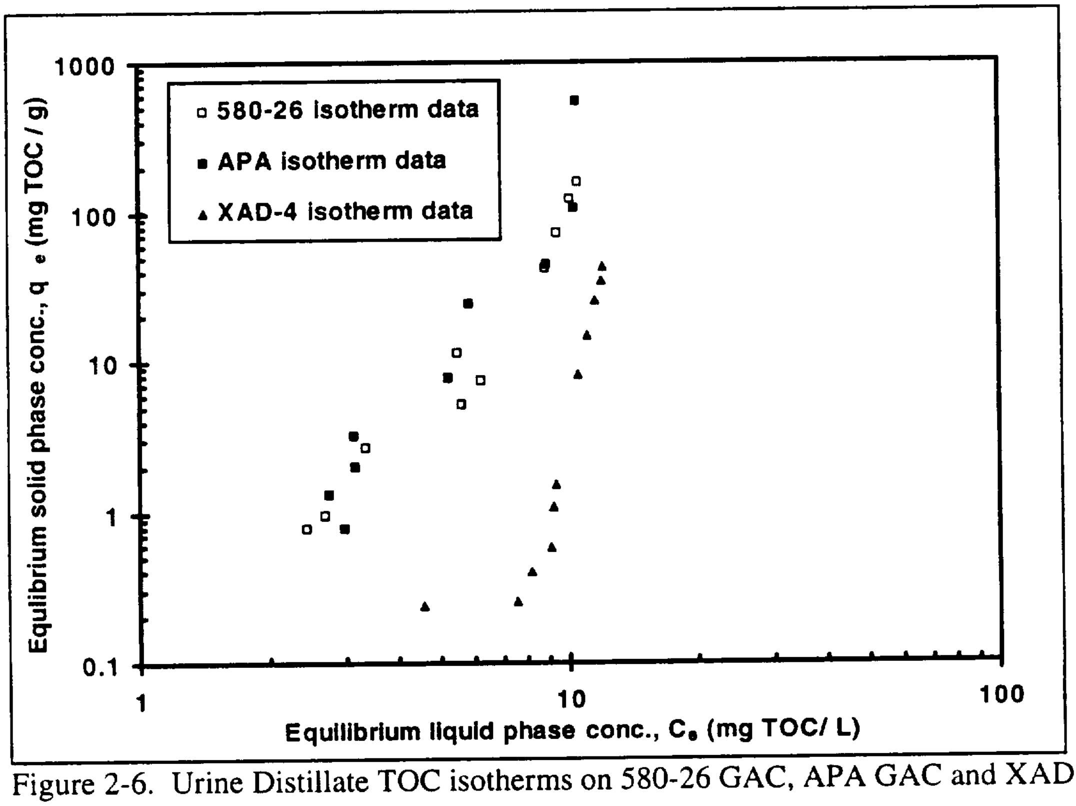

Figure 2-6. Urine Distillate TOC isotherms on 580-26 GAC, APA GAC and XAD-4 resin.

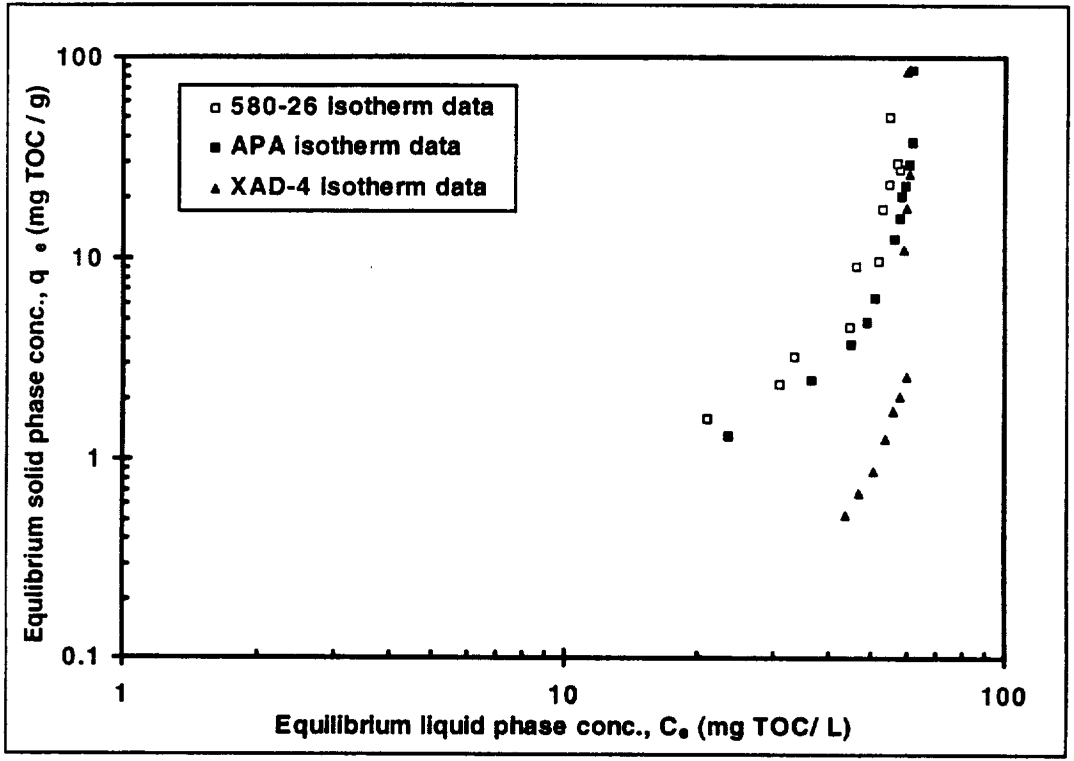

Figure 2-7. Humidity condensate TOC isotherms on 580-26 GAC, APA GAC and XAD-4 resin.

2.4 FCA TOC RESULTS

2.4.1 WASTE MIXTURE

The TOC FC results for the waste mixture were determined by fitting the nondilute and dilute TOC isotherms simultaneously, on each respective adsorbent. TOC bottle point isotherms were conducted using the waste mixture on 580-26 GAC, APA GAC, and XAD-4 resin.

2.4.1.1 TOC FC Results on 580-26 GAC. The TOC FC initial concentrations were determined by fitting the waste mixture nondilute and dilute TOC isotherms simultaneously, on 580-26 GAC. Table 2-2 contains the TOC FC parameters determined on 580-26 GAC for each waste stream. Molecular weight, fraction of carbon and Freundlich K and 1/n for 580-26 GAC are based on the known compounds in the waste mixture. The FC concentrations for 580-26 GAC were determined by comparing this with the TOC isotherm data.

The results of the waste mixture nondilute and dilute TOC FCA isotherm fit on 580-26 GAC are presented in Figure 2-8. Included in these isotherm plots are the experimental nondilute isotherm data (hollow squares), the nondilute FCA isotherm fit (solid squares connected by a solid line), the dilute isotherm data (hollow triangles) and the dilute FCA isotherm fit (solid triangles connected by a solid line). The solid squares correspond to the same isotherm dosages as the experimental data. The results show that the TOC capacity of the waste mixture on 580-26 GAC, based on the FCs in IAST calculations, is close to the observed experimental isotherm. Again, the TOC FCA isotherm fit is compared to the isotherm data. It is observed there is a slight discrepancy in the nonadsorbing TOC concentration between the model and the data. This is because, as mentioned previously, the nonadsorbing concentration for the dilute TOC isotherm is calculated in the FCA model based on the overall TOC concentrations for the nondilute and dilute isotherms and the nonadsorbing concentration of the nondilute isotherm. Other than the nonadsorbing concentration the model closely fits the isotherm data using the TOC FCs. This shows the FCs are able to account for changes in the initial concentration due to dilution of the waste mixture.

Relative percent error (RPE) is calculated for the liquid and solid phase concentrations for the nondilute and dilute TOC isotherms and are displayed on the isotherm figures. RPE is defined as:

$$RPE = \frac{100}{N}\sum\left[\frac{\left|X_{\text{experimental}} - X_{\text{model}}\right|}{X_{\text{experimental}}}\right] \qquad (2\text{-}6)$$

in which, X is C_e if the RPE in the liquid phase is being determined, and q_e if RPE in the solid phase is being determined. Table 2-3 summarizes the RPE results for fitting the TOC isotherms on 580-26 GAC, APA GAC, and XAD-4 resin. The RPEs for the TOC isotherms on 580-26 GAC show the model can predict the TOC isotherms over a range of TOC concentrations. The purpose of the RPE is to compare the overall residual concentrations in the liquid and solid phase.

Table 2-2. TOC FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on 580-26 GAC determined from fitting the TOC isotherms simultaneously

Component	Molecular Weight	Fraction of Carbon	Freundlich K	Freundlich 1/n	Waste Mixture		Shower/handwash		Urine Distillate		Humidity Condensate	
					Co	% Co	Co	% Co	Co	% Co	Co	% Co
TOC FC 1	96.51	0.742	2.6	0.73	13.68	11.55	7.40	2.96	3.58	33.93	19.32	51.55
TOC FC 2	123.2	0.710	42.3	0.47	27.85	23.51	58.50	23.52	3.76	35.64	12.66	33.78
TOC FC 3	95.3	0.753	97.6	0.43	41.18	34.76	91.61	36.65	0.51	4.83	0.47	1.25
TOC FC 4	357.0	0.600	178.5	0.17	29.77	25.13	78.73	31.50	0.51	4.83	2.47	6.59
TOC FC 5	192.4	0.760	910.2	0.31	0.24	0.20	1.33	0.53	1.47	13.93	0.68	1.81
TOC FC 6	270.7	0.800	112231.9	0.07	5.76	4.86	12.39	4.96	0.52	4.93	1.88	5.02
nonads. conc.					26.6		10.5		2.4		21.0	
total conc.					145.08		260.46		12.75		58.48	

Table 2-3. RPEs for the waste mixture TOC isotherm fits on 580-26 GAC, APA GAC, and XAD-4 resin.

	Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
Compound	**Relative % error**		**# of Data points**	**Relative % error**		**# of Data points**
	C	**q**		**C**	**q**	
580-26 GAC	6.15	6.76	12	15.76	8.94	13
APA GAC	10.62	15.02	12	21.09	5.32	11
XAD-4 resin	6.25	9.42	13	17.00	18.27	12

Table 2-4. TOC FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on APA GAC determined from fitting the TOC isotherms simultaneously

Component	Waste Mixture			Shower/handwash Mixture			Urine Distillate			Humidity Condensate		
	K	1/n	Co	K	1/n	Co	K	1/n	Co	K	1/n	Co
TOC FC 1	27.86	0.56	14.07	39.27	0.53	7.47	5.81	0.71	3.41	0.44	0.96	18.29
TOC FC 2	110.18	0.66	28.65	31.73	0.55	59.01	31.55	0.55	3.58	13.17	0.63	11.99
TOC FC 3	34.08	0.54	42.36	40.76	0.52	92.42	26.69	0.56	0.49	184.87	0.38	0.44
TOC FC 4	78.46	0.46	30.62	64.53	0.48	79.42	58.06	0.49	0.48	244.68	0.35	2.34
TOC FC 5	930.85	0.22	0.25	887.23	0.22	1.34	981.44	0.21	1.40	788.37	0.24	0.65
TOC FC 6	75.75	0.46	5.93	103.59	0.43	12.5	736.69	0.24	0.50	58.35	0.49	1.77
nonads. conc.			23.2			8.3			2.9			23.0
total conc.			145.08			260.46			12.75			58.48

* All K units: (mg/g)(L/mg)$^{1/n}$; All C_o units: mg TOC/L

Table 2-5. TOC FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on APA GAC determined from fitting the TOC isotherms simultaneously

Component	Waste Mixture			Shower/handwash Mixture			Urine Distillate			Humidity Condensate		
	K	1/n	Co	K	1/n	Co	K	1/n	Co	K	1/n	Co
TOC FC 1	11.08	0.55	11.64	27.90	0.49	6.93	0.54	0.75	2.58	0.44	0.76	7.98
TOC FC 2	49.15	0.45	23.69	10.26	0.55	54.78	10.88	0.55	2.71	10.62	0.55	5.23
TOC FC 3	20.88	0.51	35.03	27.39	0.49	85.78	63.28	0.44	0.37	43.58	0.46	0.19
TOC FC 4	52.32	0.45	25.32	52.08	0.45	73.72	144.04	0.38	0.37	75.16	0.42	1.02
TOC FC 5	466.29	0.31	0.20	703.81	0.28	1.25	51.86	0.45	1.06	115.44	0.40	0.28
TOC FC 6	68.33	0.43	4.90	616.75	0.29	11.60	294.05	0.34	0.38	890.97	0.26	0.77
nonads. conc.			44.3			26.4			5.5			48.43
total conc.			145.08			260.46			12.75			58.48

* All K units: (mg/g)(L/mg)$^{1/n}$; All C_o units: mg TOC/L

2.4.1.2 TOC FC Results on APA GAC. The TOC isotherms on APA GAC were fit simultaneously using the FC parameters in Table 2-4. FC initial concentrations were held constant from fitting 580-26 TOC isotherms, however the adsorbing TOC concentration on APA GAC is slightly larger than the adsorbing TOC concentration on 580-26 GAC. To adjust for this difference, the FC concentrations from 580-26 GAC were scaled to equal the adsorbing TOC concentration on APA GAC. The TOC isotherm parameters were fit by adjusting the Freundlich K values of the FCs and the Freundlich 1/n was correlated based on the known compounds in the waste mixture (Figure 2-2).

The results of the nondilute and dilute TOC isotherms are shown in Figure 2-9. The results of this fit appear similar to the results produced for the 580-26 GAC TOC isotherms. The RPE results for the APA TOC isotherm fits are summarized in Table 2-3. The RPEs for APA GAC are slightly higher than the RPEs for the 580-26 GAC TOC isotherms. These results indicate the method used to accommodate different adsorbent beds in series, by holding each FC initial concentration constant and fitting each FC Freundlich K, is able to fit the TOC isotherms on APA GAC.

2.4.1.3 TOC FC Results on XAD-4 resin. The nondilute and dilute TOC isotherms for the waste mixture on XAD-4 resin were fit using the same method as was used for the APA TOC isotherm fitting. The XAD-4 TOC adsorbing concentration was lower than the 580-26 TOC adsorbing concentration, therefore the same procedure to scale the FC concentrations was used for the XAD-4 TOC FCs. The Freundlich K values were optimized using the FCA and the Freundlich 1/n values were correlated using the method described in section 2.3.2. The XAD-4 TOC FCs are summarized in Table 2-5. The results of fitting the waste mixture nondilute and dilute TOC isotherms simultaneously on XAD-4 resin are shown in Figures 2-10. The results of the nondilute TOC FCA isotherm fit were slightly better than the other two adsorbents. The dilute TOC FCA isotherm model results slightly overpredict the adsorption capacity of XAD-4 resin, however it appears this is attributed to the slight difference in the model calculated nonadsorbing concentration. The RPE values for the TOC isotherms on XAD-4 resin are summarized in Table 2-3. The RPE nondilute results are similar to the other adsorbents and the RPE results for the dilute TOC isotherm are slightly higher.

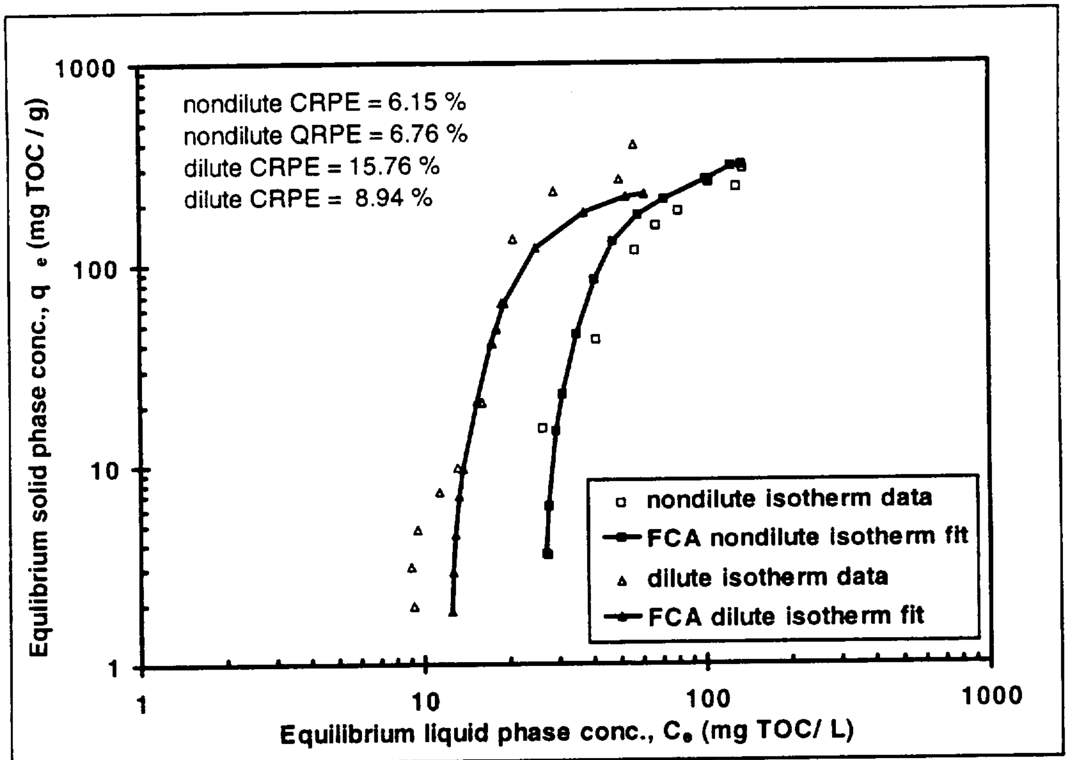

Figure 2-8. Nondilute and dilute TOC isotherms fit simultaneously on 580-26 for the waste mixture.

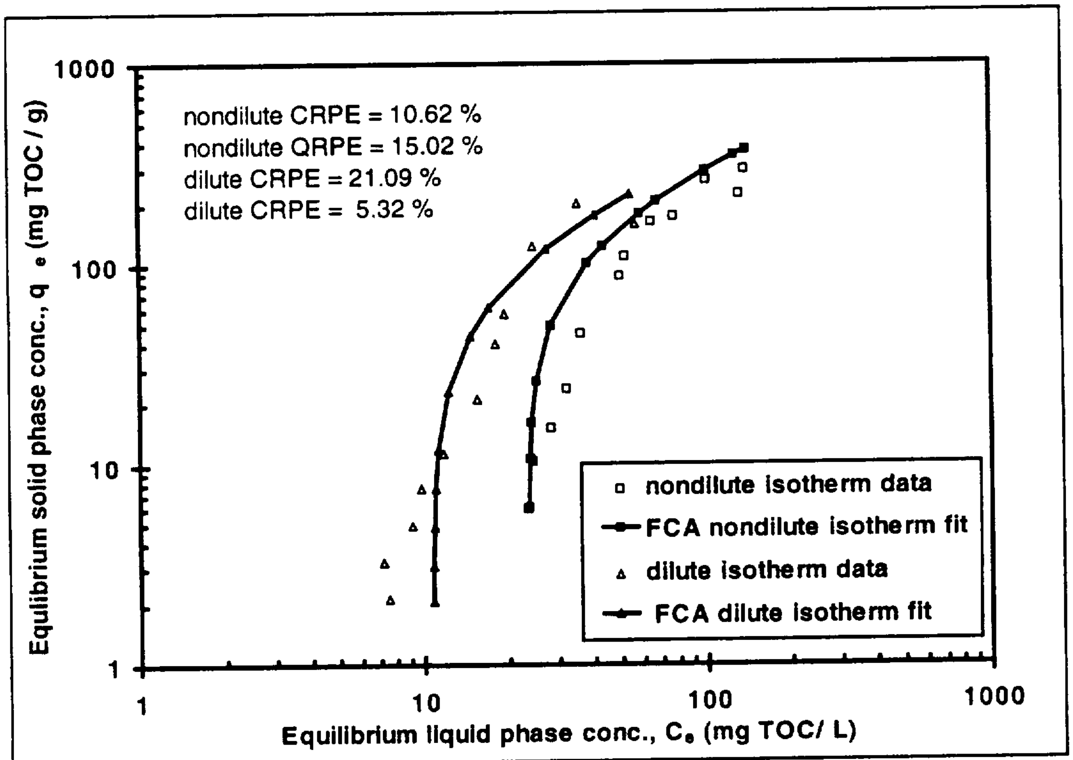

Figure 2-9. Nondilute and dilute TOC isotherms fit simultaneously on APA GAC for the waste mixture.

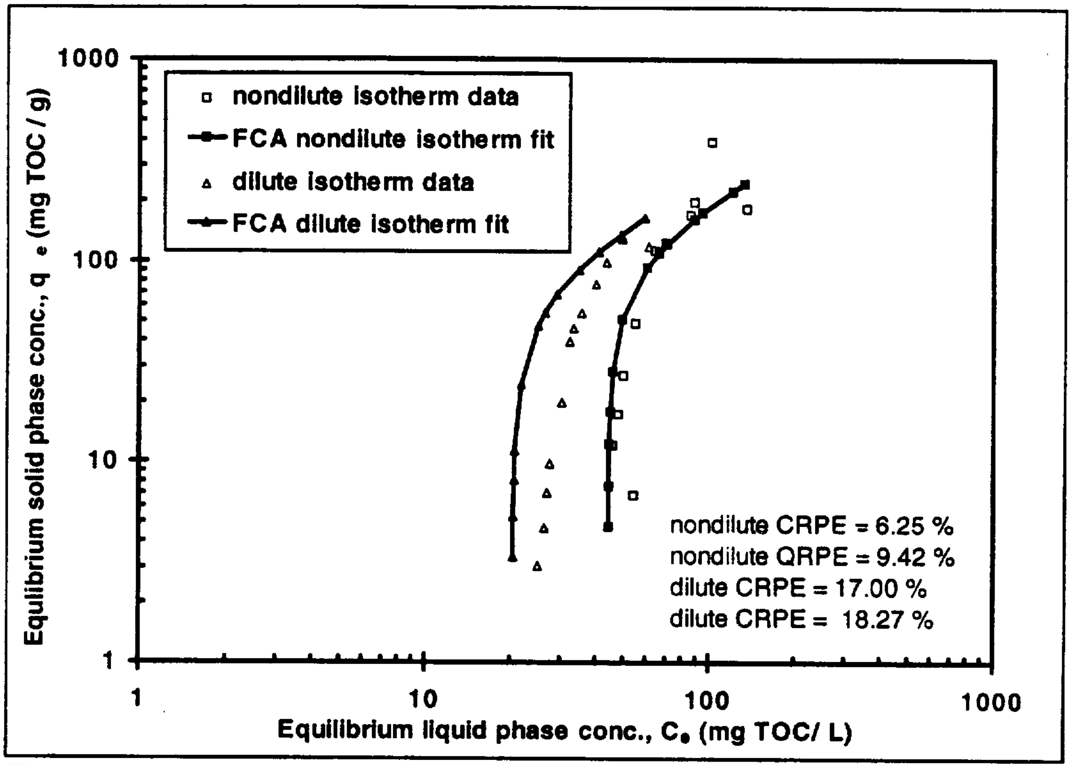

Figure 2-10. Nondilute and dilute TOC isotherms fit simultaneously on XAD-4 resin for the waste mixture.

2.4.2 SHOWER/HANDWASH RESULTS

The TOC FC results for the shower/handwash mixture were determined using the same method described in section 2.4.1 for the waste mixture. TOC bottle point isotherms were conducted using the shower/handwash mixture on 580-26 GAC, APA GAC, and XAD-4 resin. These isotherms were used to determine TOC FC parameters for the shower/handwash mixture.

2.4.2.1 TOC FC Results on 580-26 GAC. The TOC FC initial concentrations were determined by fitting the nondilute and dilute TOC isotherms for the shower/handwash mixture simultaneously for each respective adsorbent. Table 2-2 contains the TOC FC parameters determined for 580-26 GAC, APA GAC and XAD-4 resin in the shower/handwash mixture. Molecular weight, fraction of carbon and Freundlich K and 1/n for 580-26 are based on the known compounds in the mixtures. These four parameters for 580-26 GAC are the same for the shower/handwash mixture as for the waste mixture. The FC concentrations for 580-26 GAC were determined using FCA by fitting the TOC isotherm data.

The results of the shower/handwash nondilute and dilute TOC FCA isotherm fit on 580-26 GAC are presented in Figure 2-11. The results show that the shower/handwash TOC adsorption capacity on 580-26 GAC is close to the observed experimental isotherm. It is observed there is a slight discrepancy in the nonadsorbing TOC concentration between the model and the data. This was also observed in the waste mixture modeling. Theoretically the nonadsorbing concentration for the dilute TOC isotherm can be calculated, as explained previously, which is the value used for the dilute nonadsorbing concentration. Other than the nonadsorbing concentration the model closely fits the isotherm data using the TOC FCs. This shows the FCs are able to account for changes in the initial concentration due to dilution of the shower/handwash mixture. Table 2-6 contains the RPE values of the TOC isotherms on the shower/handwash mixture.

Table 2-6. RPEs for the shower/handwash mixture TOC isotherm fits on 580-26 GAC, APA GAC, and XAD-4 resin.

	Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
Compound	**Relative % error**		**# of Data points**	**Relative % error**		**# of Data points**
	C	**q**		**C**	**q**	
580-26 GAC	10.58	15.50	13	22.23	16.04	12
APA GAC	22.98	18.82	12	18.18	8.12	10
XAD-4 resin	5.81	11.01	14	8.83	7.64	13

2.4.3.2 TOC FC Results on APA GAC. The shower/handwash TOC isotherms on APA GAC were fit simultaneously using the FC parameters in Table 2-4. FC initial concentrations were held constant from fitting the 580-26 TOC isotherms and scaled to equal the adsorbing TOC concentration for APA GAC. Freundlich K was used as the fitting parameter to fit these TOC isotherms and Freundlich 1/n was correlated based on the known compounds in the waste streams. This is the same method used to fit the TOC isotherms on APA GAC for the waste mixture.

The results of the shower/handwash nondilute and dilute TOC FCA isotherm fits are shown in Figure 2-12. The nondilute TOC FCA isotherm fit slightly overpredicts adsorption capacity. The dilute TOC FCA isotherm fits the isotherm data very well, with the nonadsorbing concentration calculated in the model to be very accurate. The RPE results, presented in Table 2-6, show the dilute isotherm fits more accurately than the nondilute TOC isotherm.

2.4.3.3 TOC FC Results on XAD-4 resin. The shower/handwash nondilute and dilute TOC isotherms on XAD-4 resin were fit using the same method as was used for the APA TOC isotherm fitting. The XAD-4 TOC adsorbing concentration was scaled using the method previously described. The Freundlich K values were optimized using the FCA and the Freundlich 1/n values were correlated using the method described in section 2.3.2. The XAD-4 TOC FC parameters are summarized in Table 2-5. The results of fitting the shower/handwash nondilute and dilute TOC isotherms simultaneously on XAD -4 resin are presented in Figure 2-13. The results of the nondilute TOC FCA isotherm fit on XAD-4 resin are better than the other two adsorbents; this is supported by comparing the RPE values in Table 2-6. Both the nondilute and dilute TOC FCA isotherm fits follow the trend of the data, predicting the adsorption capacity of the shower/handwash mixture.

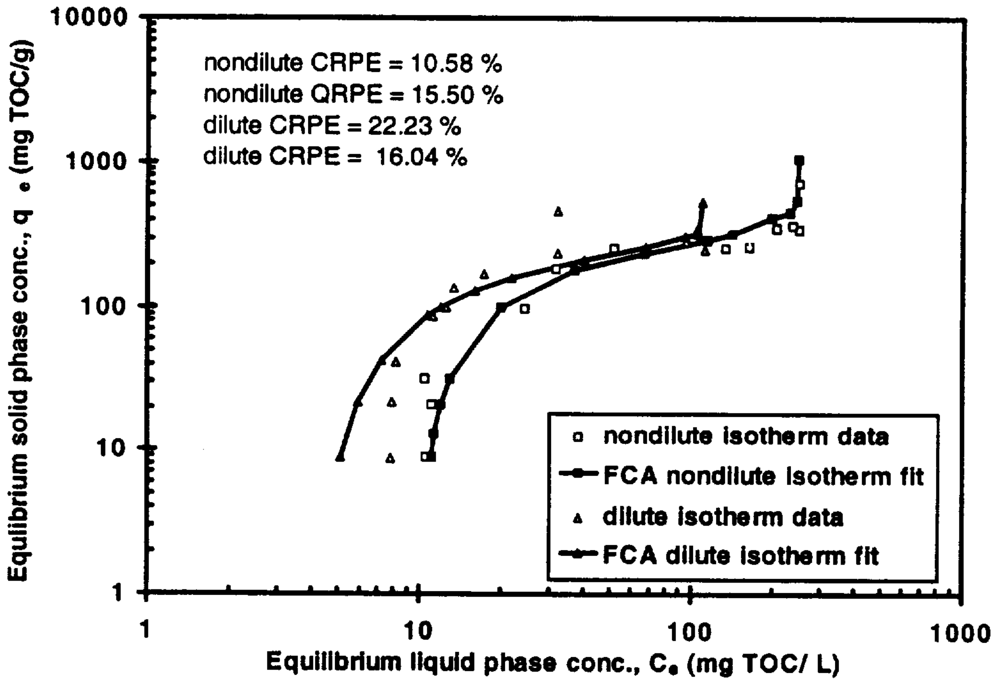

Figure 2-11. Nondilute and dilute TOC isotherms fit simultaneously on 580-26 GAC for the shower/handwash mixture.

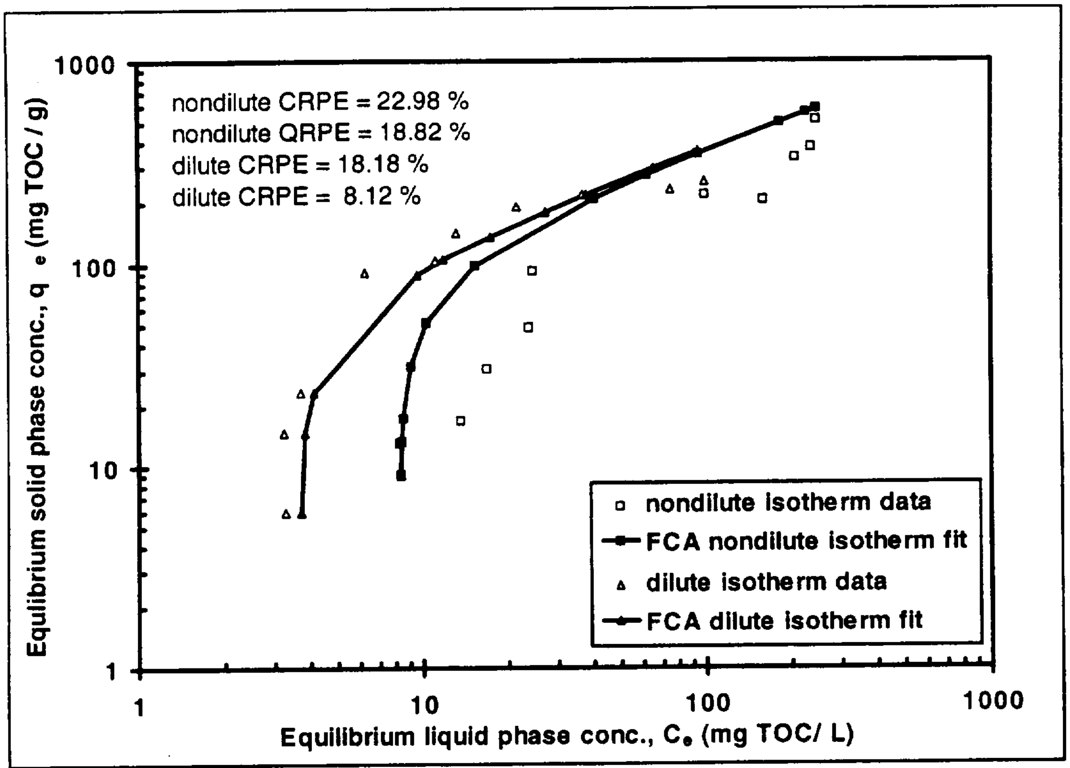

Figure 2-12. Nondilute and dilute TOC isotherms fit simultaneously on APA GAC for the shower/handwash mixture.

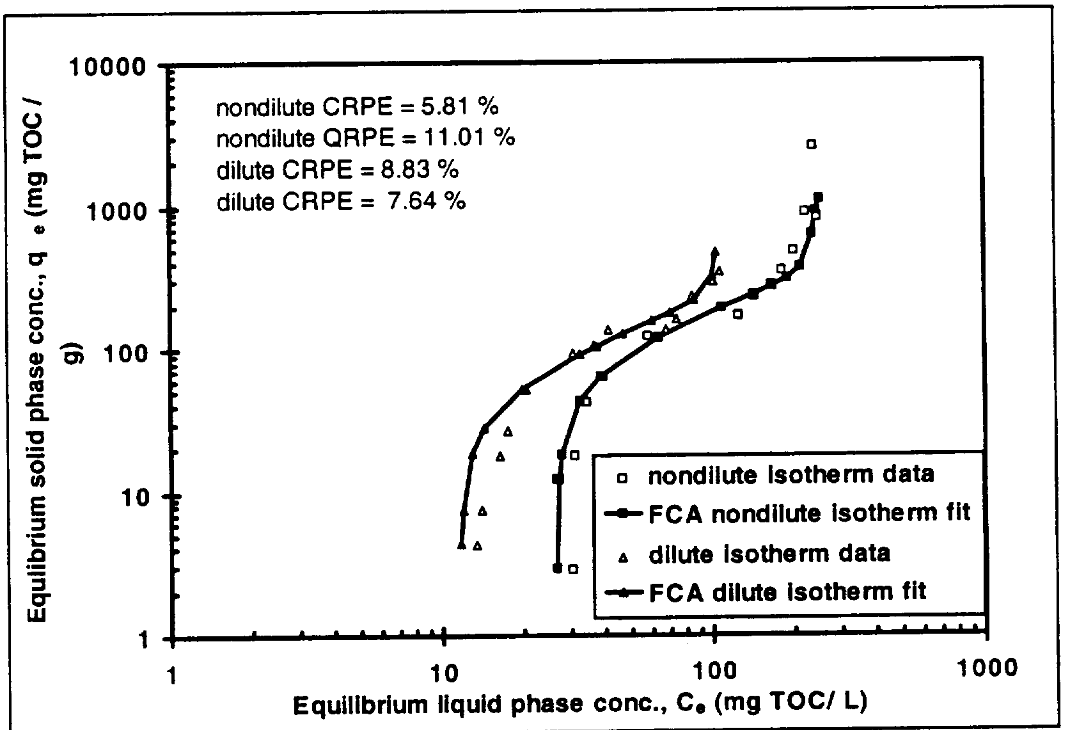

Figure 2-13. Nondilute and dilute TOC isotherm fit simultaneously on XAD-4 resin for the shower/handwash mixture. Fit simultaneously with the dilute TOC isotherm.

2.4.3 URINE DISTILLATE RESULTS

The TOC FC results for the urine distillate stream were determined using the same method described in section 2.4.1 for the waste mixture. TOC bottle point isotherms were conducted using the urine distillate stream on 580-26 GAC, APA GAC, and XAD-4 resin. These isotherms were used to determine TOC and tracer FC parameters.

2.4.3.1 TOC FC Results on 580-26 GAC. The TOC FC initial concentrations were determined by fitting the urine distillate nondilute and dilute TOC isotherms simultaneously for each respective adsorbent. Table 2-2 contains the urine distillate TOC FC parameters determined for 580-26 GAC, APA GAC, and XAD-4 resin. Molecular weight, fraction of carbon and Freundlich K and 1/n for 580-26 are based on the known compounds in the waste streams. These four parameters for 580-26 GAC are the same as the waste mixture. The FC concentrations for 580-26 were determined using FCA by fitting the TOC isotherm data.

The results of the urine distillate nondilute and dilute TOC FCA isotherm fit on 580-26 GAC are presented in Figure 2-14. The results show that the TOC capacity of urine distillate on 580-26 GAC, based on the FCs in IAST calculations, is slightly overpredicted. The RPEs for the TOC isotherms on 580-26 GAC, APA GAC, and XAD-4 resin are summarized in Table 2-7. The RPE values for the nondilute TOC isotherm show similar error of residuals in the liquid and solid phase. The dilute TOC FCA isotherm fit slightly underpredicts the adsorption capacity of the adsorbent. The overprediction of the nondilute and the underprediction of the dilute TOC isotherm may be because the model is attempting to fit both isotherms simultaneously.

Table 2-7. RPEs for urine distillate TOC isotherm fits on 580-26 GAC, APA GAC, and XAD-4 resin.

	Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
Compound	**Relative % error**		**# of Data points**	**Relative % error**		**# of Data points**
	C	**q**		**C**	**q**	
580-26 GAC	11.27	10.80	10	16.33	8.96	6
APA GAC	6.00	6.92	8	10.69	5.97	7
XAD-4 resin	18.10	62.22	11	16.17	44.81	6

2.4.3.2 TOC FC Results on APA GAC. The TOC isotherms on APA GAC were fit simultaneously using the FC parameters in Table 2-4. FC initial concentrations were held constant from fitting TOC isotherms on 580-26 GAC. The adsorbing TOC concentration of the FCs was scaled to equal the adsorbing TOC concentration on APA GAC. Freundlich K was the fitting parameter used to fit these TOC isotherms and Freundlich 1/n was correlated based on the known compounds in the waste streams. This is the same method used to fit the TOC isotherms on APA for the waste mixture.

The results of the nondilute and dilute TOC isotherms on APA GAC are shown in Figure 2-15. The results of this fit show the nondilute TOC FCA isotherm fit models the isotherm data accurately with low RPE values in both the liquid and solid phases. RPE results are summarized in Table 2-7. The dilute TOC FCA isotherm fit represents the data, however there appears to be scatter within the isotherm data. RPE values for dilute TOC are also fairly low with error in the solid phase to be slightly higher than the error in the liquid phase.

2.4.3.3 TOC FC Results on XAD-4 resin. The nondilute and dilute TOC isotherms for urine distillate on XAD-4 resin were fit using the same method as was used for the APA TOC isotherm fitting. The TOC adsorbing FC concentrations from fitting the TOC isotherms on 580-26 GAC, were scaled using the method previously described to equal the adsorbing TOC concentration on XAD-4 resin. The FC Freundlich K values were optimized using the FCA, and Freundlich 1/n was correlated using the method described in section 2.3.2. The TOC FCs for XAD-4 resin are summarized in Table 2-5. The results of fitting the urine distillate nondilute and dilute TOC isotherms simultaneously on XAD-4 resin are shown in Figure 2-16. The results of the nondilute TOC FCA isotherm fit show the model overpredicts the adsorption capacity. However urine distillate on XAD-4 resin appears to be almost nonadsorbing, which may explain this difference. The dilute TOC isotherm also appears to be nonadsorbing, causing difficulty when attempting the model the adsorption capacity.

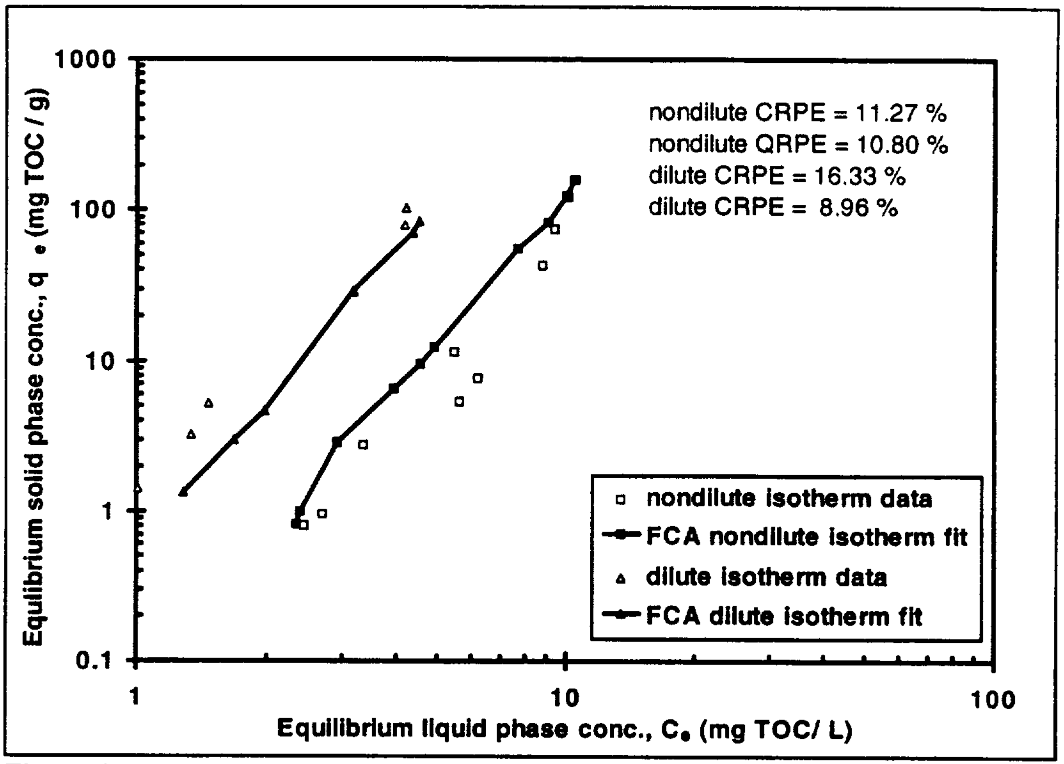

Figure 2-14. Nondilute and dilute TOC isotherms fit simultaneously on 580-26 for urine distillate.

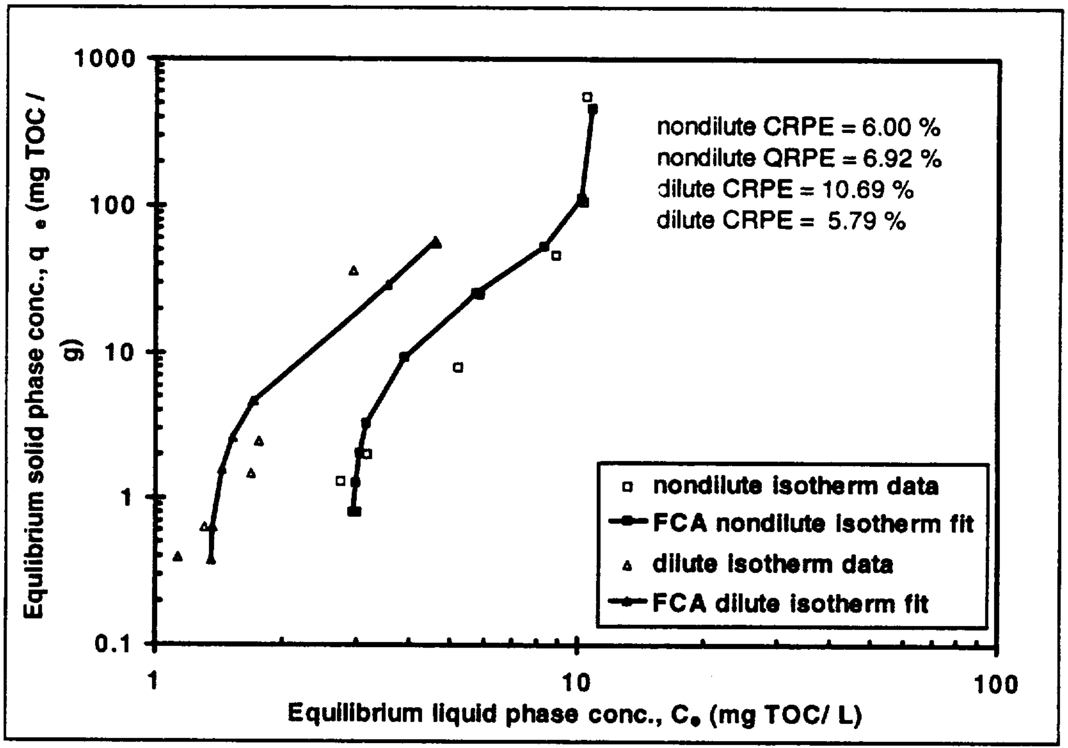

Figure 2-15. Nondilute and dilute TOC isotherms fit simultaneously on APA GAC for urine distillate. Fit simultaneously with the dilute TOC isotherm.

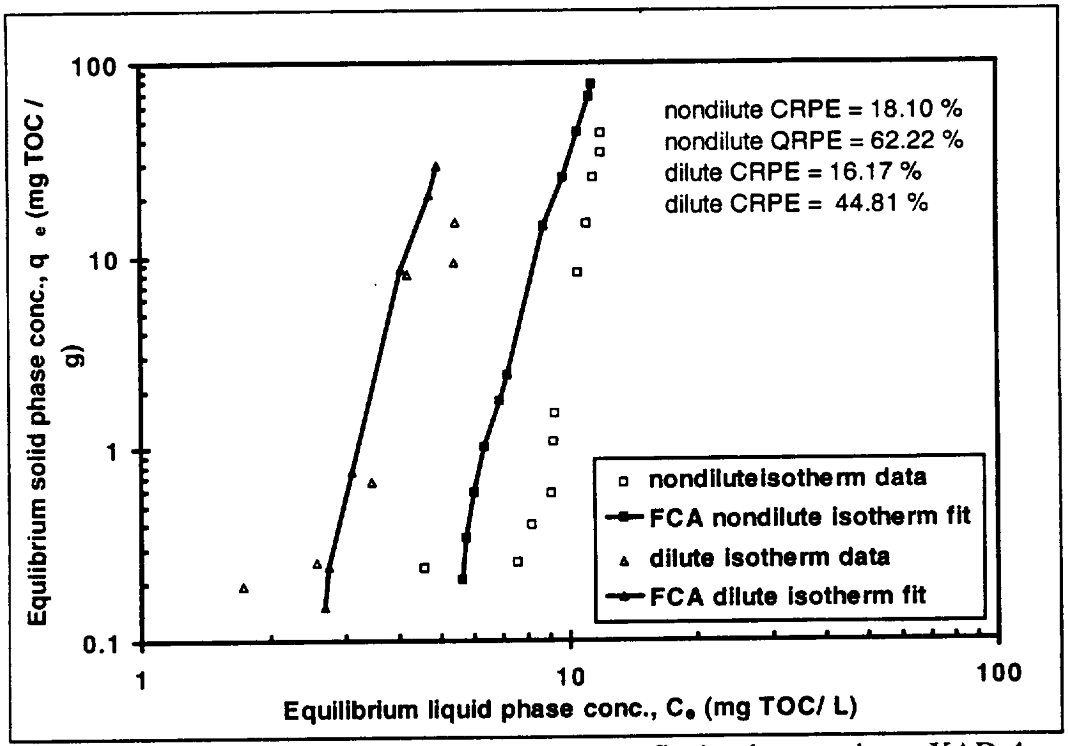

Figure 2-16. Nondilute and dilute TOC isotherms fit simultaneously on XAD-4 resin for urine distillate. Fit simultaneously with the dilute TOC isotherm.

2.4.4 HUMIDITY CONDENSATE RESULTS

The TOC FC results for humidity condensate were determined using the same method described in section 2.4.1 for the waste mixture. TOC and tracer bottle point isotherms were conducted using humidity condensate on 580-26 GAC, APA GAC and XAD-4 resin. These isotherms were used to determine TOC and tracer FC parameters for humidity condensate.

2.4.4.1 TOC FC Results on 580-26 GAC. The TOC FC initial concentrations for humidity condensate were determined by fitting the nondilute and dilute TOC isotherms simultaneously for each respective adsorbent. Table 2-2 contains the humidity condensate TOC FC parameters determined for 580-26 GAC, APA GAC and XAD-4 resin. Molecular weight, fraction of carbon and Freundlich K and 1/n for 580-26 GAC are based on the known compounds in the mixtures. These four parameters for 580-26 GAC are the same for the humidity condensate stream as for the waste mixture. The FC concentrations for 580-26 GAC were determined using FCA by fitting the TOC isotherm data.

The results of the humidity condensate nondilute and dilute TOC FCA isotherm fits on 580-26 GAC are presented in Figure 2-17. The results show that the TOC adsorption capacity of humidity condensate on 580-26 GAC, based on the FCs in IAST calculations, overpredicts the adsorption capacity. The TOC isotherms show humidity condensate is weakly adsorbing on 580-26 GAC, which explains why FCA overpredicts the adsorption capacity. RPE results for the TOC isotherms on all three adsorbents are summarized in Table 2-8. The results indicate the error in the liquid phase concentration to be considerably less than the error in the solid phase concentration. This is again due to the nonadsorbing nature of humidity condensate.

Table 2-8. RPEs for humidity condensate TOC isotherm fits on 580-26 GAC, APA GAC, and XAD-4 resin.

	Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
Compound	**Relative % error**		**# of Data points**	**Relative % error**		**# of Data points**
	C	**q**		**C**	**q**	
580-26 GAC	19.76	159.76	12	19.73	92.31	9
APA GAC	15.29	161.72	12	15.53	106.31	12
XAD-4 resin	6.75	102.34	12	6.75	102.34	12

2.4.4.2 TOC FC Results on APA GAC. The TOC isotherms on APA GAC were fit simultaneously with the FC parameters in Table 2-4. FC initial concentrations were held constant from fitting the humidity condensate TOC isotherms on 580-26 GAC, and scaled to equal the adsorbing TOC concentration for APA GAC. Freundlich K was used as the fitting parameter to fit these TOC isotherms and Freundlich 1/n was correlated based on the known compounds in the waste streams. This is the same method used to fit the TOC isotherms on APA GAC for the waste mixture.

The results of the humidity condensate nondilute and dilute TOC isotherms on APA GAC are shown in Figures 2-18. The results of the TOC FCA isotherm fits show the model slightly overpredicts the adsorption capacity of the adsorbent for both isotherms. Again this is due to the weakly adsorbing nature of humidity condensate on the APA GAC. The RPE results presented in Table 2-8 are similar to the 580-26 results.

2.4.4.3 TOC FC Results on XAD-4 resin. The nondilute and dilute TOC isotherms for humidity condensate on XAD-4 resin were fit using the same method as was used for the APA TOC isotherm fitting. The XAD-4 TOC adsorbing concentration was scaled using the method previously described. The Freundlich K values were optimized using the

FCA and the Freundlich 1/n values were correlated using the method described in section 2.3.2. The humidity condensate TOC FCs on XAD-4 resin are summarized in Table 2-5. The results of fitting the humidity condensate nondilute and dilute TOC isotherms on XAD-4 resin simultaneously are presented in Figure 2-19. The results of the nondilute and dilute TOC FCA isotherm fits on XAD-4 resin are again similar to the results obtained for 580-26 and APA GAC. Humidity condensate on XAD-4 resin appears to be nonadsorbing, which causes the FCA model to overpredict the adsorption capacity.

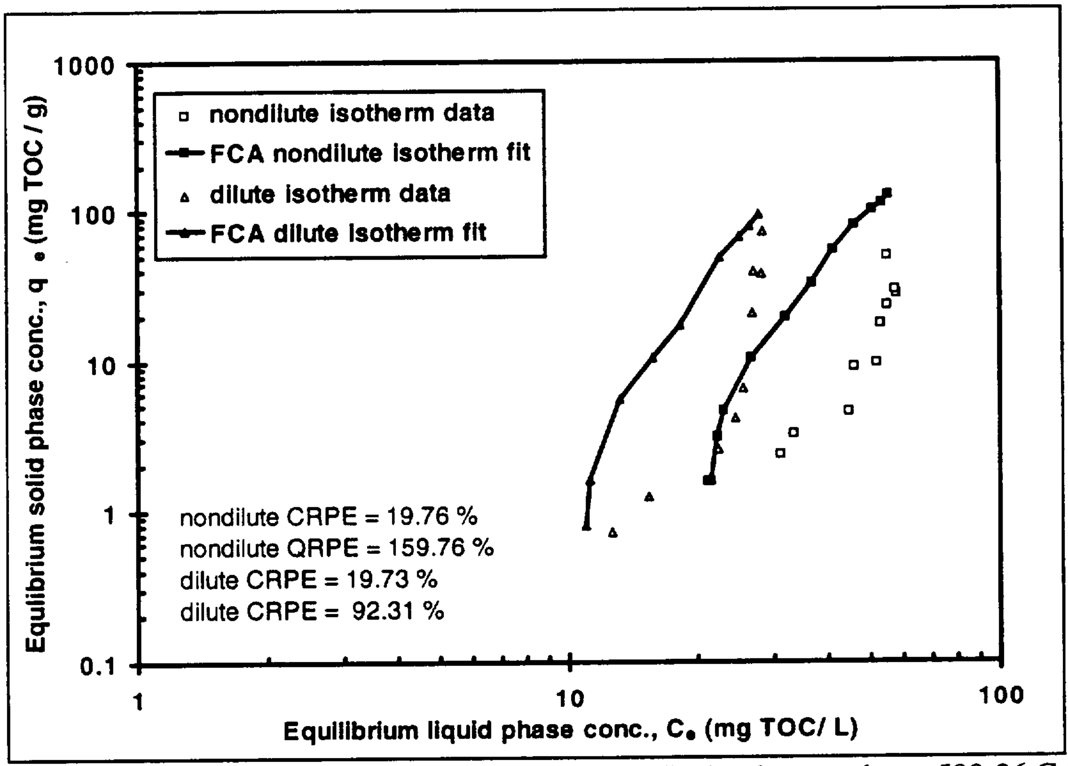

Figure 2-17. Nondilute and dilute TOC isotherms fit simultaneously on 580-26 GAC for humidity condensate.

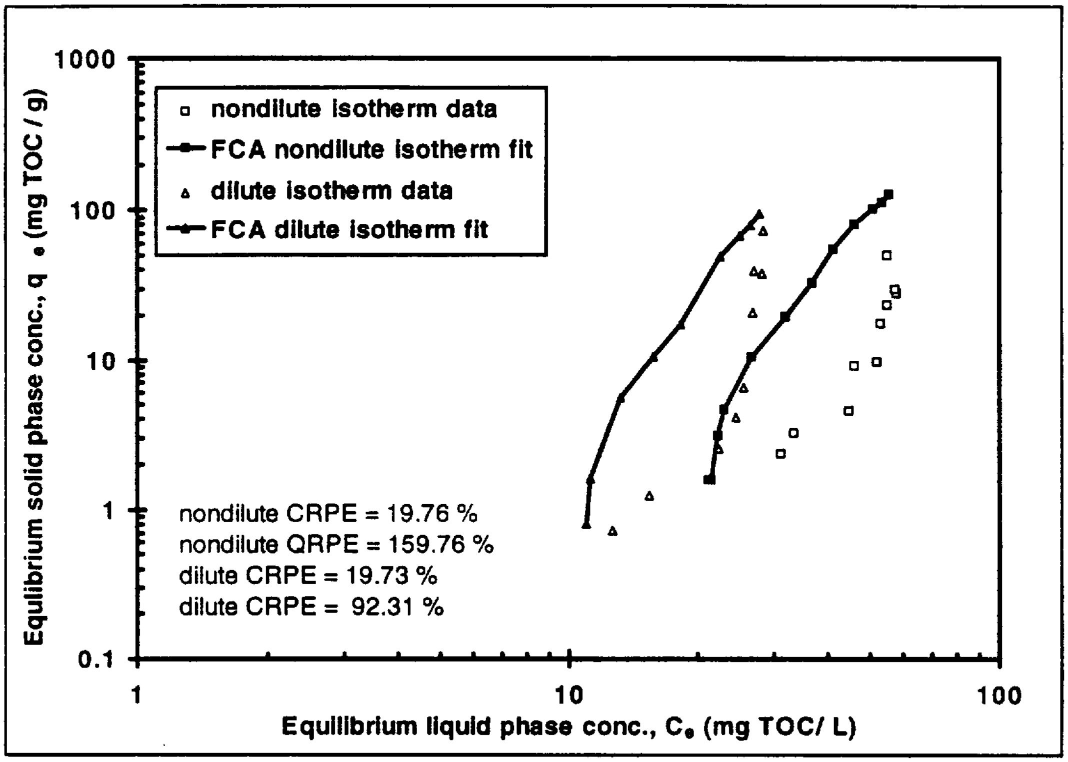

Figure 2-18. Nondilute and dilute TOC isotherms fit simultaneously on APA GAC for humidity condensate.

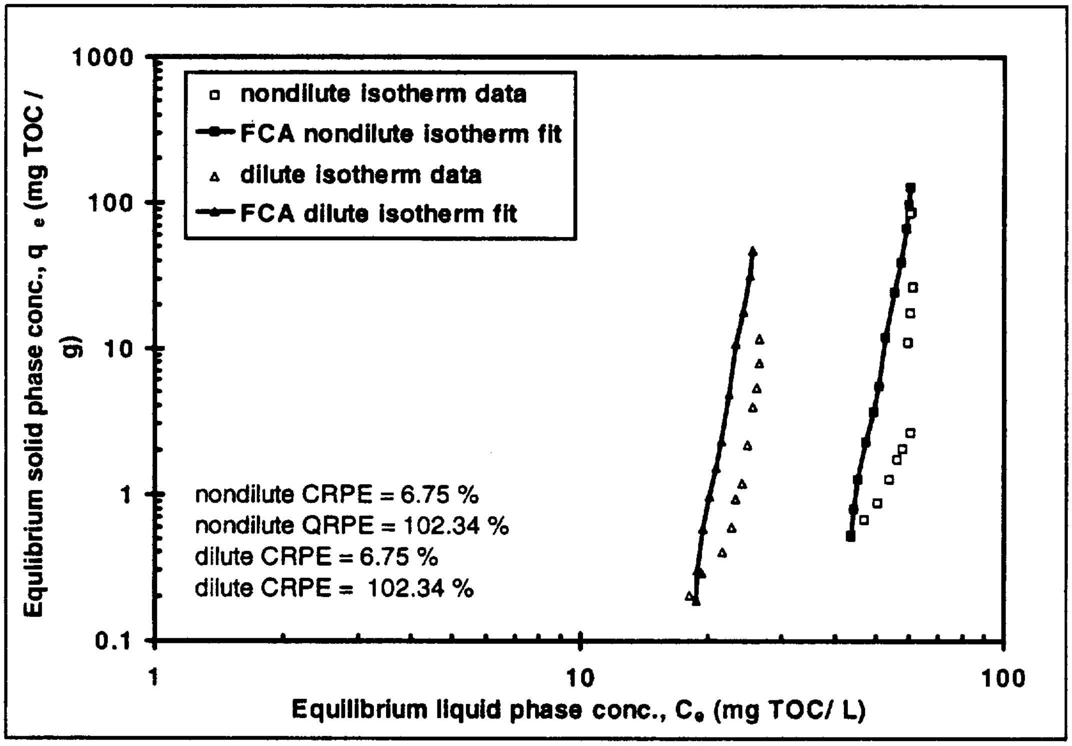

Figure 2-19. Nondilute and dilute TOC isotherms fit simultaneously on XAD-4 resin for humidity condensate.

3.0 TRACER ADSORPTION MODELING

3.1 TRACER INTRODUCTION

Predicting the reduction in capacity of tracer compounds due to competitive adsorption is required to determine how much of a known compound is being removed in the MFB. Tracer FC parameters were determined for the waste streams on each adsorbent. This was accomplished by fitting the tracer isotherms conducted on the different waste streams. The FCs account for the reduction in capacity of the known compound from its single solute due to the competitive interactions of the background TOC concentration.

3.2 MATERIALS AND METHODS

3.2.1 Chemicals. All chemicals used were reagent grade or better. Chloroform, dichloromethane (DCM), ethylbenzene (EB), methylene chloride (MC), naphthalene, perchloroethylene (PCE), toluene, and trichloroethylene (TCE) were obtained from Aldrich Chemical Co. (Milwaukee, WI). All the compounds listed were used for spiking the tracer isotherms except DCM and EB which were used for chemical analysis. PCE was used for both purposes.

3.2.2 Solution Preparation. The waste mixture, shower/handwash mixture, urine distillate stream and humidity condensate stream were prepared as described in section 2.2.1.

3.2.3 Chemical Analysis. Synthetic organic chemicals (SOCs) spiked into the waste mixture and shower/handwash were analyzed with a Hewlett-Packard (Wilmington, DE) Model 5880 gas chromatograph using direct aqueous injection. SOCs for the urine distillate and humidity condensate streams were analyzed with a Hewlett-Packard (Wilmington, DE) Model 5890 II gas chromatograph using a modified EPA Method 625 liquid-liquid extraction (LLE) and a Hewlett-Packard 5970B mass selective detector. The pH was determined using an Orion (Cambridge, MA) Model 501 pH meter.

3.2.4 Adsorbents. The adsorbents for the tracer isotherms were prepared as described in section 2.2.3.

3.2.5 Isotherm Procedure. The tracer isotherm procedure is the same as described in section 2.2.3. The tracer compounds were spiked into the nondilute waste waters and allowed to equilibrate. The tracer concentrations were then analyzed using the chemical analysis described in section 2.3.2. The tracer solid phase loading was calculated using equation 2-1.

3.2.6 Single Solute Equilibrium. Single solute experiments were conducted to determine the single solute Freundlich K and 1/n values for the following tracer compounds: methylene chloride, chloroform, TCE, toluene, naphthalene, and PCE. Milli-Q water was spiked with the tracer compound to a known concentration and the solution was added to several isotherm bottles that contained various dosages of the adsorbent. The single solute isotherms were conducted on 580-26 GAC, APA GAC and XAD-4 resin. The bottle point isotherm procedure detailed in section 2.2.4 was also used to conduct these experiments. The initial and final equilibrium liquid phase concentrations of the tracer compounds were determined by gas chromatography and the solids phase concentrations determined using Equation 2-1.

The Freundlich equation was chosen to describe single solute equilibrium for this work:

$$q_i = K_i C_i^{1/n_i} \tag{3-1}$$

in which, K_i is the Freundlich capacity constant and $1/n_i$ is the Freundlich intensity parameter for compound i. To determine the Freundlich K and 1/n values for each compound, the isotherm is plotted as, solid phase concentration versus liquid phase concentration on a log-log scale. The resulting plot is linear and can be represented by the following equation:

$$\log q_i = \log K_i + \frac{1}{n_i} \log C_i \tag{3-2}$$

Equation 3-2 is in the form of y = mx + b. The slope of the isotherm represents Freundlich $1/n_i$ and the y-intercept represents Freundlich K_i. The single solute parameters for the tracer compounds: MC, chloroform, TCE, toluene, naphthalene, and PCE are listed in Table 3-1.

Table 3-1. Single solute Freundlich parameters for the tracer compounds used in the waste mixtures.

	580-26 GAC		APA GAC		XAD-4 resin	
	K	1/n	K	1/n	K	1/n
MC	0.83	0.71	1.04	0.79	0.5	0.98
Chloroform	6.06	0.80	7.07	0.78	2.77	0.96
TCE	45.71	0.49	31.62	0.49	21.25	0.55
Toluene	61.09	0.40	61.09	0.40	26.09	0.58
PCE	180.31	0.71	163.29	0.46	61.89	0.8
Naphthalene	276.5	0.47	181.26	0.38	73.18	0.46

3.2.7 Scope of Experiments. The four waste streams: waste mixture, shower/handwash mixture, urine distillate and humidity condensate, each had tracer isotherm performed on three adsorbents, 580-26 GAC, APA GAC, and XAD-4 resin. Table 3-2 summarizes the tracer isotherms performed.

Table 3-2. Tracer initial concentrations for the waste streams on each adsorbent.

	580-26 GAC		APA GAC		XAD-4 resin	
	nondil.	dilute	nondil.	dilute	nondil.	dilute
Waste Mixture						
MC	8.225	1.370	7.453	1.272	7.514	1.250
Chloroform	9.480	0.882	9.480	0.882	9.480	0.882
PCE		0.888		0.851		0.898
Shower/handwash mixture						
MC	8.112	1.144	8.103	1.044	7.619	0.982
Chloroform	8.979	0.813	8.979	0.813	8.979	0.813
Urine Distillate						
TCE	6.3	0.365	7.065	0.394	5.365	0.255
Toluene	7.116	0.425	7.065	0.389	5.365	0.488
Naphthalene	0.926	0.104	0.928	0.106	0.949	0.107
Humidity Condensate						
TCE	9.942	0.552	9.940	0.558	8.394	0.561
Toluene	9.447	0.489	8.957	0.433	9.497	0.465
Naphthalene	1.067	0.1024	1.047	0.099	0.990	0.010

units: concentration mg/L

3.3 FICTIVE COMPONENT ANALYSIS

3.3.1 Ideal Adsorbed Solution Theory. IAST is described in section 2.3.1. When a tracer is present, Equation 2-2 is applied for the FCs and the tracer compound.

3.3.2 Fictive component Parameter Determination. Tracer fictive component parameters were determined to describe the tracer isotherm data obtained from the wastewaters. Tracer isotherms were used to verify if a specific compound's equilibrium concentration could be predicted through the adsorbent bed. The known compounds in the waste streams were grouped using Freundlich K values equal and less than 500 $(mg/g)(L/mg)^{1/n}$. FC Freundlich K values were determined from the distribution range with the weakest FC Freundlich K value being less than the weakest adsorbing tracer compound which has a Freundlich K of 0.83 $(mg/g)(L/mg)^{1/n}$. Within this range 0.4 to 500 $(mg/g)(L/mg)^{1/n}$, FC Freundlich K values were chosen. The known compounds in the mixture were grouped according to these values and the groups were used to determine weighted averages for the FC molecular weight and fraction of carbon. The corresponding 1/n values for the Freundlich K values were correlated from the known compounds in the waste waters as described in section 2.3.2. The FC initial concentrations for 580-26 GAC were determined using the same method as the TOC FC initial concentrations. The same method was used to model the adsorbent beds in series as was used for the TOC isotherms.

3.3.3 Tracer Isotherm Fitting. The tracer isotherms were fit using six tracer FCs to represent the unknown background matrix and the single solute parameters for the tracer compound. The FC initial concentrations for 580-26 were optimized applying the same method used for the TOC isotherms. IAST calculations were made with the tracer FCs and the tracer parameters; the results were compared to the tracer isotherm data. Equation 2-4 was used for optimization of the FC concentration, comparing the liquid and solid phase residual concentrations for the tracer compound. There are nondilute and dilute tracer isotherms with the nondilute spike concentration being greater than the dilute spike concentration. Tracer isotherms were conducted on the nondilute aqueous waste streams.

3.3.4 Relationship of FCs on Different Adsorbents. The relationship of the different adsorbents in series is described in section 2.3.4.

3.4 FCA TRACER RESULTS

Predicting the adsorption of known compounds through the MFB can provide valuable information related to MFB operation and control. For example if a spill of a known compound occurs onboard the ISS or an astronaut is on medication, the model can be used to evaluate the effectiveness of the MFB to remove the compound. Decisions can then be taken ahead of time as to whether changes in the MFB operation need to be made.

FCA was used to predict the fate of known or tracer compounds through the MFB. Tracer isotherms were performed in the presence and absence of the various waste waters. The tracer compounds (methylene chloride, chloroform, trichloroethene, toluene, tetrachloroethene, and naphthalene) were chosen such that they represent a wide range of adsorption potentials. The tracer FC parameters were determined for each waste stream on each adsorbent. This was accomplished by fitting each tracer isotherm performed in the presence of the waste water. The FC parameters were adjusted until the best fit of the tracer isotherm was obtained. The FCs represent the adsorption strength of the waste water which caused the reduction in capacity of the tracer isotherm from its single solute isotherm.

3.4.1 WASTE MIXTURE

3.4.1.1 Tracer FC Results on 580-26 GAC. The waste mixture nondilute and dilute methylene chloride (MC) tracer isotherms on 580-26 GAC were fit simultaneously to determine the tracer FC concentrations. MC was chosen as a tracer because it is a weakly adsorbing compound. Fitting a weak adsorbing compound will yield FC concentrations that will predict the maximum equilibrium displacement of a tracer compound from its single solute. Determining the FC concentrations from a weak adsorbing compound will better define the adsorption strength of the background mixture. The tracer FC parameters were used to predict the chloroform and PCE tracer isotherms.

The tracer FCs determined for the four waste streams on 580-26 GAC are included in Table 3-3. The tracer isotherm fits and data are compared for the 580-26 nondilute and dilute MC tracer isotherms in Figures 3-1 and 3-2, respectively. Included in these plots are the isotherm data (hollow squares), the FCA isotherm fit (solid squares linked with a solid line), and the single solute isotherm (solid line). The solid squares of the FCA isotherm fit correspond to the same dosages as the isotherm data. The single solute line is compared to the FCA isotherm fit and the data to show the reduction in capacity of the tracer from its single solute level. This reduction in capacity is due to competitive adsorption of the unknown background mixture and tracer. Note the concentration scales on the figures vary due to the range of concentrations used for the tracer isotherms. The FCA isotherm fit overpredicts the competitive adsorption of MC when compared to the experimental data. However, the overprediction is conservative when compared to the isotherm data. Table 3-4 contains the RPE results for the tracer isotherm fit and predictions for the waste mixture on 580-26 GAC, APA GAC and XAD-4 resin. The error in the liquid phase generally is larger than the error in the solid phase.

Table 3-3. Tracer FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on 580-26 GAC determined from fitting the MC tracer isotherms simultaneously

Component	Molecular Weight	Fraction of Carbon	Freundlich K	Freundlich 1/n	Waste Mixture		Shower/handwash		Urine Distillate		Humidity Condensate	
					Co	% Co	Co	% Co	Co	% Co	Co	% Co
TOC FC 1	106.0	0.703	0.4	0.70	47.51	40.10	124.97	50.00	1.13	10.91	27.54	73.47
TOC FC 2	96.5	0.742	2.5	0.61	3.25	2.74	17.09	6.84	0.99	9.58	0.67	1.79
TOC FC 3	100.0	0.730	10.0	0.54	2.30	1.94	0.20	0.08	0.54	5.25	1.54	4.10
TOC FC 4	355.0	0.711	50.0	0.46	57.78	48.77	69.57	27.83	0.63	6.04	6.44	17.18
TOC FC 5	217.6	0.735	100.0	0.43	0.58	0.49	24.96	9.98	6.99	67.52	0.17	0.45
TOC FC 6	257.5	0.757	500.0	0.34	7.06	5.96	13.17	5.27	0.07	0.71	1.12	3.00
nonads. conc.					26.6		10.5		2.4		21.0	
total conc.					145.08		260.46		12.75		58.48	

Table 3-4. RPEs for the waste mixture tracer isotherm fits on 580-26 GAC, APA GAC, and XAD-4 resin.

	Compound	**Nondilute waste mixture TOC isotherm**			**Dilute waste mixture TOC isotherm**		
		Relative % error		**# of Data points**	**Relative % error**		**# of Data points**
		C	**q**		**C**	**q**	
580-26	MC	80.41	28.11	7	36.86	13.25	7
	Chloroform	31.62	6.25	9	97.68	29.73	9
	PCE				77.51	33.86	4
APA	MC	19.86	13.35	5	16.44	8.67	7
	Chloroform	43.55	10.75	8	58.00	11.08	8
	PCE				85.74	130.72	5
XAD-4	MC	11.03	4.73	6	17.27	17.61	6
	Chloroform	34.99	6.63	8	52.99	7.92	8
	PCE				0.03	0.40	10

Table 3-5. Tracer FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on APA GAC determined from fitting the MC tracer isotherms simultaneously

Component	Waste Mixture			Shower/handwash Mixture			Urine Distillate			Humidity Condensate		
	K	1/n	Co	K	1/n	Co	K	1/n	Co	K	1/n	Co
TOC FC 1	0.15	1.0	48.87	0.44	0.96	126.07	48.59	0.51	1.08	1.61	0.83	26.07
TOC FC 2	20.12	0.59	3.34	13.96	0.63	17.24	13.26	0.63	0.94	29.62	0.55	0.64
TOC FC 3	99.53	0.44	2.37	41.29	0.52	0.20	21.41	0.58	0.52	143.17	0.40	1.46
TOC FC 4	201.93	0.37	59.44	68.69	0.47	70.19	72.72	0.47	0.60	66.61	0.47	6.10
TOC FC 5	184.59	0.38	0.60	125.65	0.41	25.18	220.79	0.36	6.66	131.68	0.41	0.16
TOC FC 6	437.89	0.29	7.26	383.60	0.31	13.28	336.97	0.32	0.07	399.15	0.30	1.06
nonads. conc.			23.2			8.3			2.9			23.0
total conc.			145.08			260.46			12.75			58.48

* All K units: $(mg/g)(L/mg)^{1/n}$; All C_o units: mg TOC/L

Table 3-6. Tracer FCs for the waste mixture, shower/handwash mixture, urine distillate and humidity condensate streams on XAD-4 resin determined from fitting the MC tracer isotherms simultaneously

Component	Waste Mixture			Shower/handwash Mixture			Urine Distillate			Humidity Condensate		
	K	1/n	Co	K	1/n	Co	K	1/n	Co	K	1/n	Co
TOC FC 1	0.10	1.00	40.41	0.15	1.00	117.02	12.34	0.54	0.81	2.83	0.64	11.37
TOC FC 2	98.07	0.44	2.76	14.58	0.62	16.00	15.10	0.29	0.71	11.23	0.55	0.28
TOC FC 3	99.71	0.44	1.96	118.18	0.42	0.19	22.82	0.50	0.39	32.32	0.48	0.64
TOC FC 4	75.77	0.46	49.15	142.21	0.40	65.15	81.02	0.42	0.45	245.16	0.35	2.66
TOC FC 5	583.71	0.27	0.49	156.74	0.39	23.37	389.72	0.32	5.03	750.78	0.27	0.07
TOC FC 6	773.11	0.24	6.00	143.74	0.40	12.33	543.91	0.30	0.53	294.75	0.34	0.46
nonads. conc.			44.3			26.4			5.5			48.43
total conc.			145.08			260.46			12.75			58.48

* All K units: $(mg/g)(L/mg)^{1/n}$; All C_o units: mg TOC/L

The 580-26 GAC tracer FCs were used in IAST calculations to predict a nondilute and dilute chloroform tracer and a PCE tracer isotherm on 580-26 GAC. These predictions were made to determine if the tracer FCs from fitting the MC tracer isotherms could predict equilibrium for other compounds in the mixture. Figures 3-3 and 3-4 show the predicted isotherms for nondilute and dilute chloroform using IAST calculations. The chloroform predictions overpredict the reduction in capacity at higher adsorbent dosages. Figure 3-5 compares the predicted PCE tracer isotherm to the isotherm data. The tracer FCs underestimate the competitive adsorption of PCE. Perhaps this is because PCE is the strongest adsorbing tracer compound used in the waste mixture and the FCs do not account enough for the strongly adsorbing compounds.

The reduction in capacity of MC, chloroform and PCE from their single solute is different for each compound. MC is the weakest adsorbing compound and therefore, it would theoretically be expected to have the greatest reduction in capacity compared to the other two compounds. However this is not observed on 580-26 GAC. MC appears to have the least reduction in capacity. This may be explained by the differences in the intraparticle diffusion rates between MC and the background mixture. A major component of the background waste mixture is the soap component called sodium coconut acid-n-methyl taurate (SCMT). SCMT accounts for over 60 % of the waste mixture TOC. SCMT is a large molecule relative to MC and the other compounds which make-up the background. SCMT is a more strongly adsorbing compound and has a slower diffusion rate then MC. Consequently, the intraparticle flux of SCMT is much slower then MC. In the isotherm bottle, MC is able to diffuse into the adsorbent particles ahead of the SCMT. SCMT will eventually displace the MC causing it to counter diffuse out of the adsorbent particle. However, because SCMT is a large molecule and 580-26 GAC is microporous, diffusion interactions between the SCMT and the MC will cause the MC to very slowly counter diffuse out of the adsorbent particle to reach equilibrium. If it was possible to equilibrate the isotherm bottles for a longer period of time, the displacement effects of MC from its single solute would be greater. However, SCMT may also trap the MC in the adsorbent by blocking the small pores within the adsorbent, preventing the MC from counter diffusing.

3.4.1.2 Tracer FC Results on APA GAC. The tracer FC concentrations determined when fitting 580-26 MC tracer isotherms were held constant as the waste stream passes through the other adsorbents in series. The tracer FC concentrations were scaled to account for differences in the adsorbing concentration of the three adsorbents. Scaling of the FC concentrations was accomplished using the same method as was used for the TOC FC concentrations. The APA MC nondilute and dilute tracer isotherms for the waste mixture were fit simultaneously optimizing the FC Freundlich K value. FC Freundlich 1/n was correlated to the FC Freundlich K value using the equation presented in Figure 2-3. The FC parameters for APA GAC on the waste mixture are presented in Table 3-5. Figures 3-6 and 3-7 show the nondilute and dilute MC FCA tracer isotherm fits. The results indicate the FCA isotherm fit underpredicts the adsorption capacity at low dosages for the MC nondilute isotherm. This may also be because the flux for MC entering the adsorbent particle is greater than SCMT, as described for the 580-26 GAC. The RPE's for the fits and predictions on APA GAC for the waste mixture are presented in Table 3-4. The RPE results show MC fit better on APA GAC compared to 580-26 GAC. The APA FC results when fitting MC tracer isotherms simultaneously were used to determine if other tracer compounds on APA GAC could be predicted.

A nondilute and dilute chloroform tracer and a PCE tracer isotherm were predicted using the APA FC parameters in IAST calculations. The nondilute and dilute chloroform tracer isotherms are shown in Figures 3-8 and 3-9, respectively, and the PCE tracer isotherm is presented in Figure 3-10. The nondilute and dilute chloroform tracer isotherms slightly underpredicts adsorption capacity at low adsorbent dosages and overpredicts adsorption capacity at the higher adsorbent dosages. The RPE's show the prediction estimates the solid phase concentration more accurately than the liquid phase concentration. The prediction of the PCE isotherm overpredicts the adsorption capacity of APA GAC. This may be because PCE is a strongly adsorbing compound which is underrepresented by the tracer FCs. The RPE values for PCE are noticeably higher than the other isotherms.

3.4.1.3 Tracer FC results on XAD-4 resin. Tracer FCs were determined for XAD-4 resin using the same procedure used to determine the tracer FCs for APA GAC. Table 3-

6 includes the tracer FC results for XAD-4 resin. XAD-4 MC nondilute and dilute tracer isotherms were fit simultaneously to determine FC Freundlich K values. The results of the MC nondilute and dilute fits are shown in Figures 3-11 and 3-12, respectively. The nondilute MC tracer isotherm fit well, with fairly low RPE values. RPE values for XAD-4 resin fit and predictions are listed in Table 3-4. The dilute MC tracer isotherm overpredicts adsorption capacity at high liquid phase concentrations and slightly underpredicts adsorption capacity at low concentrations. The RPE in the liquid and solid phase are equal, showing the same error in both phases.

Figures 3-13 and 3-14 show the predictions for the XAD-4 nondilute and dilute chloroform tracer isotherms. The chloroform tracers are predicted fairly well, the adsorption capacity as the concentration decreases is slightly underpredicted. For both, the nondilute and dilute chloroform tracer isotherms, the RPEs show the liquid phase concentration is slightly off, but the solid phase concentrations are fairly accurate. The XAD-4 PCE tracer isotherm prediction is shown in Figure 3-15. This prediction was very accurate with RPE values less than 1. The tracer FCs were able to accurately predict the competitive adsorption of PCE in the unknown background matrix.

The reduction in capacity trend of the three tracer compounds on XAD-4 resin is significantly different than on 580-26 GAC. The reduction in capacity of MC, chloroform and PCE on XAD-4 resin are as expected, with MC having the greatest displacement and PCE the least displacement from their single solute. Diffusion interactions between MC and SCMT are decreased on XAD-4 resin compared to 580-26 GAC. XAD-4 resin is a macroporous adsorbent, therefore the large SCMT molecules create less of a hindrance as MC counter diffuses into the liquid.

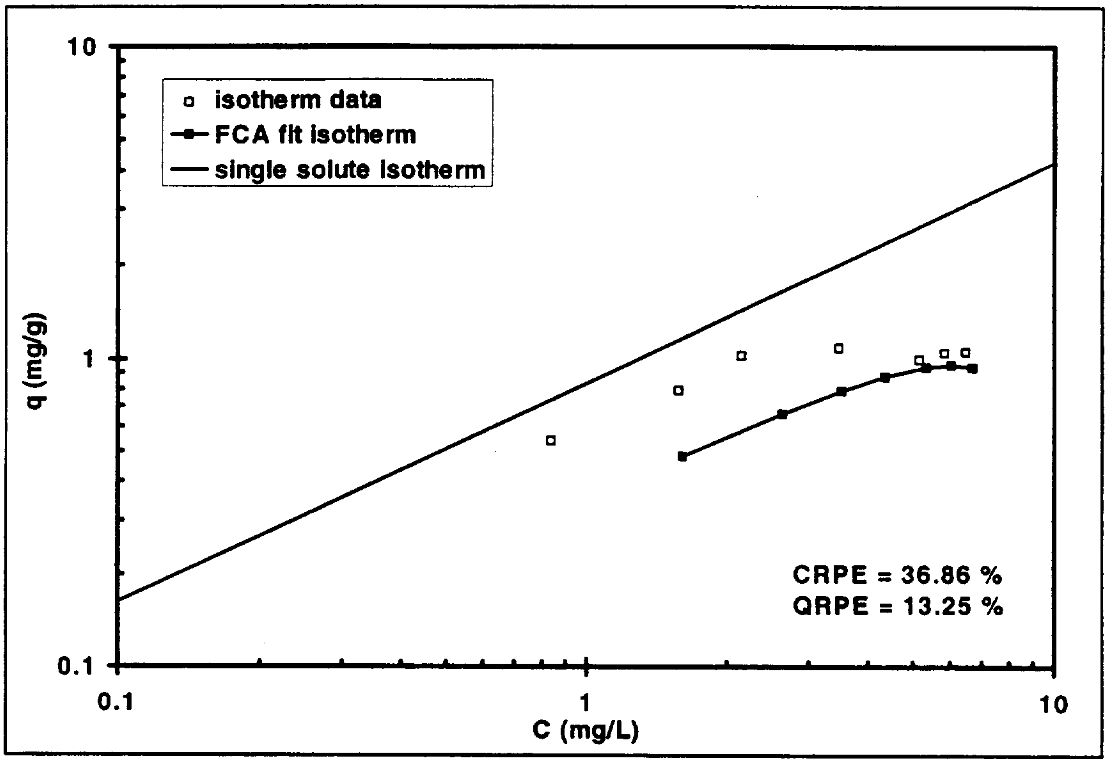

Figure 3-1. Methylene chloride tracer isotherm fit on 580-26 GAC for the waste mixture. Fit simultaneously with the dilute methylene chloride tracer isotherm.

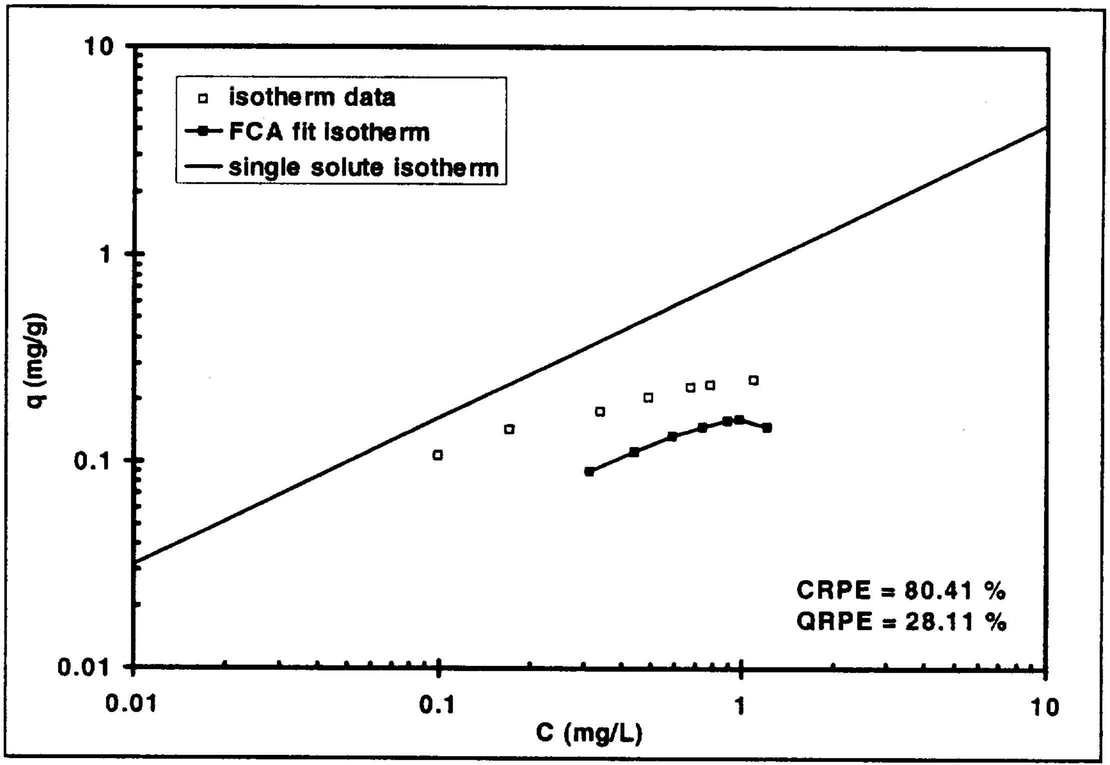

Figure 3-2. Dilute methylene chloride tracer isotherm fit on 580-26 GAC for the waste mixture. Fit simultaneously with the methylene chloride tracer isotherm.

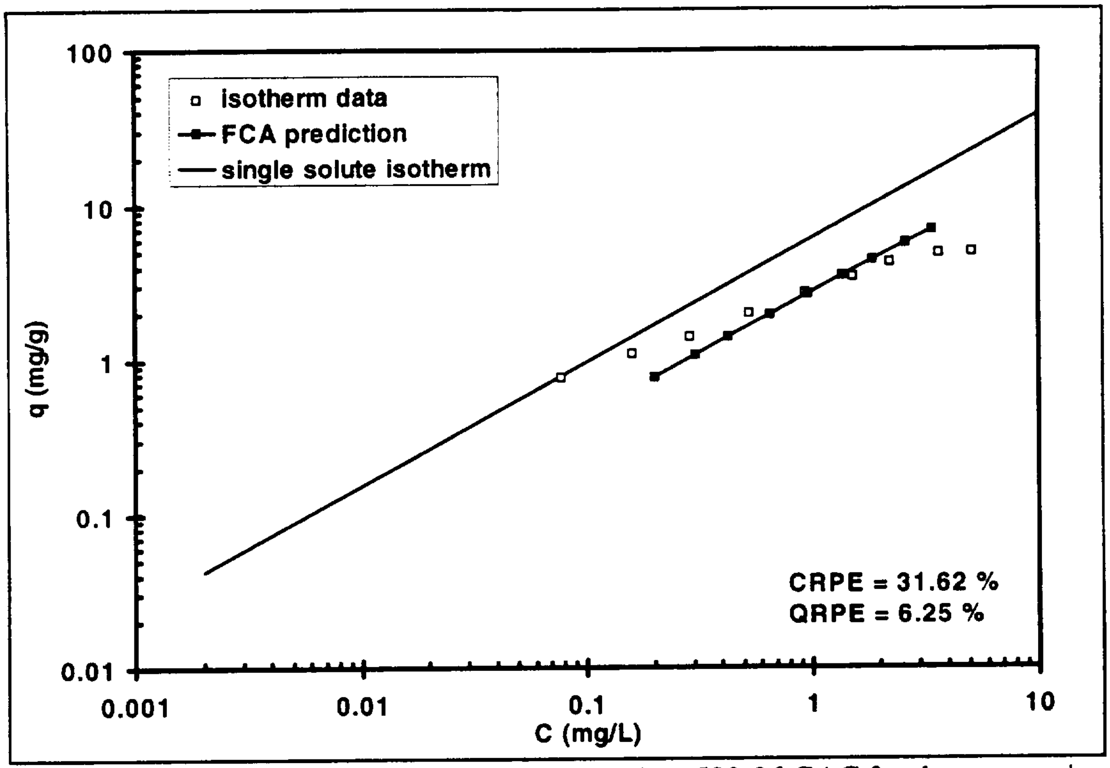

Figure 3-3. Chloroform tracer isotherm predicted on 580-26 GAC for the waste mixture.

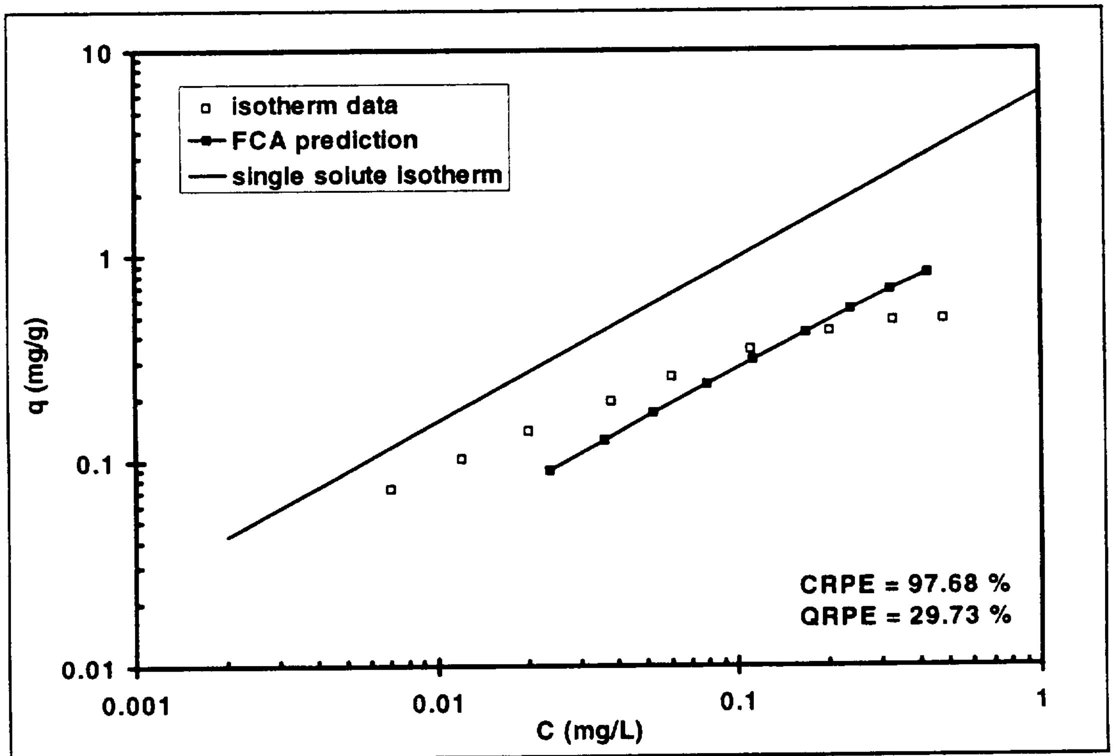

Figure 3-4. Dilute chloroform tracer isotherm predicted on 580-26 GAC for the waste mixture.

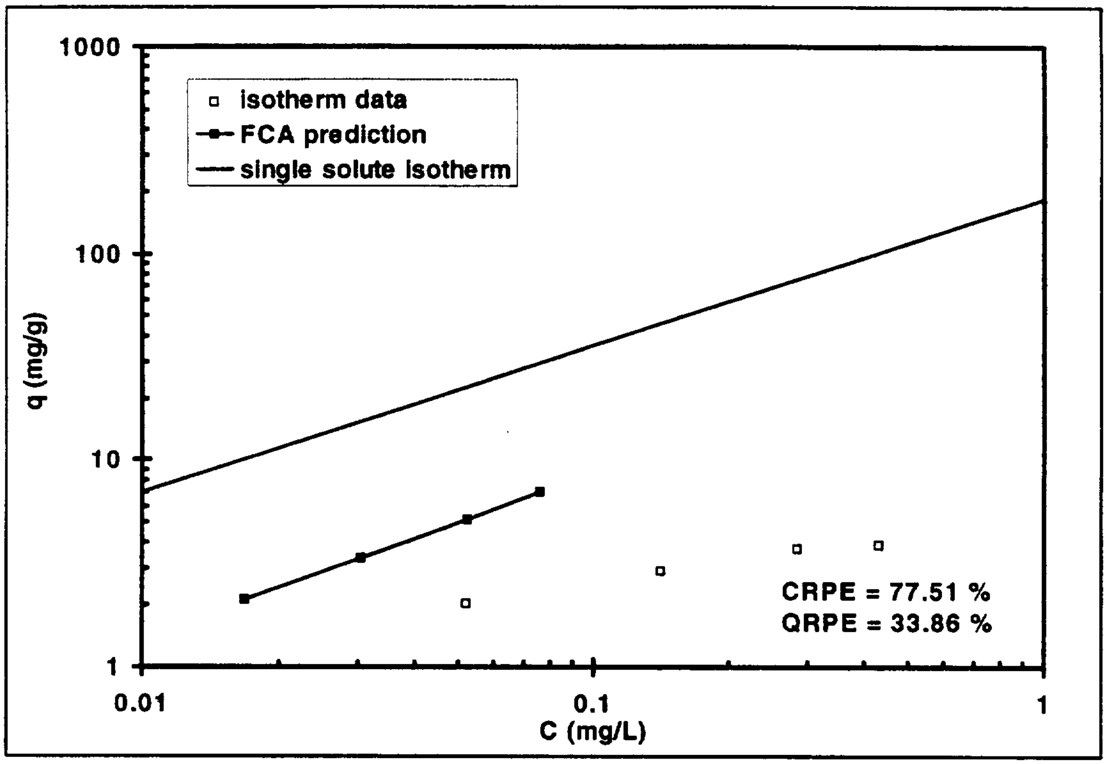

Figure 3-5. PCE tracer isotherm predicted on 580-26 GAC for the waste mixture.

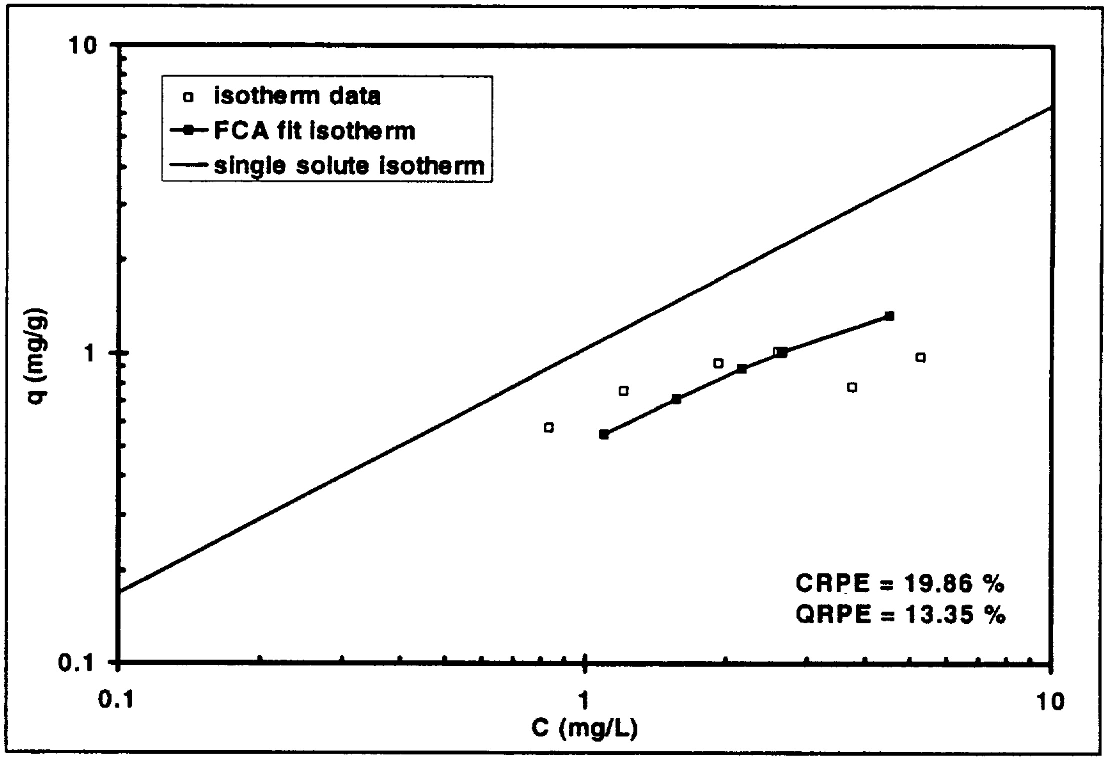

Figure 3-6. Methylene chloride tracer isotherm fit on APA GAC for the waste mixture. Fit simultaneously with the dilute methylene chloride tracer isotherm.

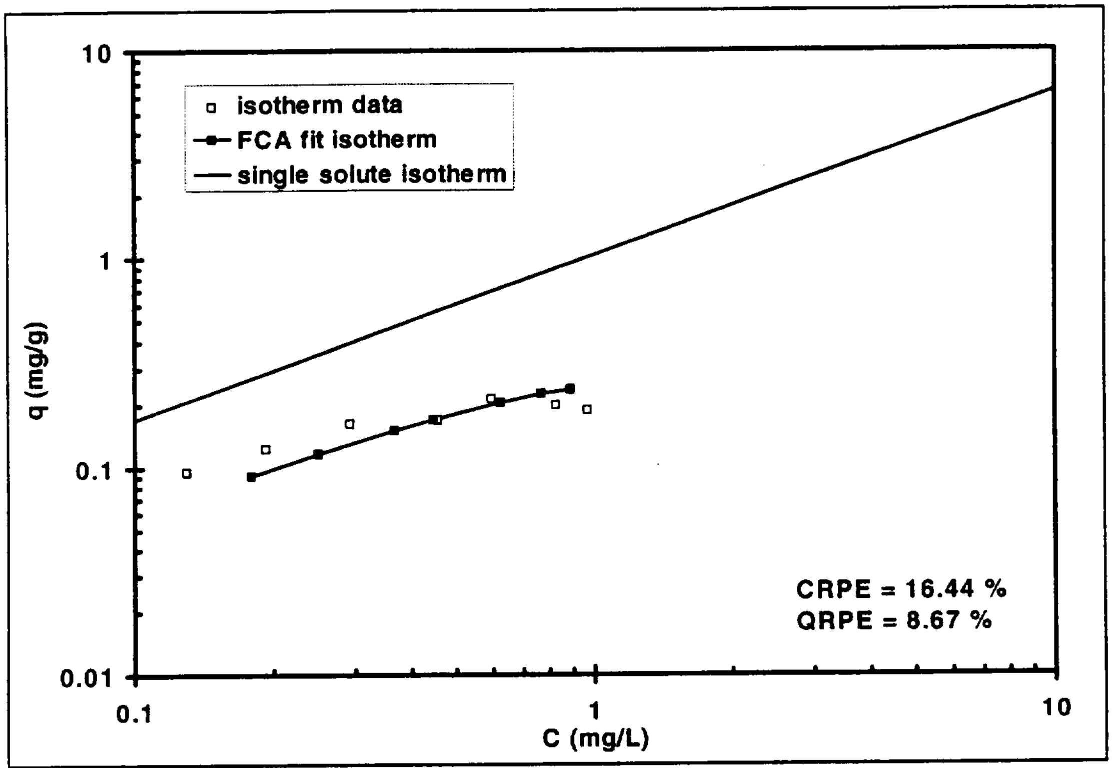

Figure 3-7. Dilute methylene chloride tracer isotherm fit on APA GAC for the waste mixture. Fit simultaneously with the methylene chloride tracer isotherm.

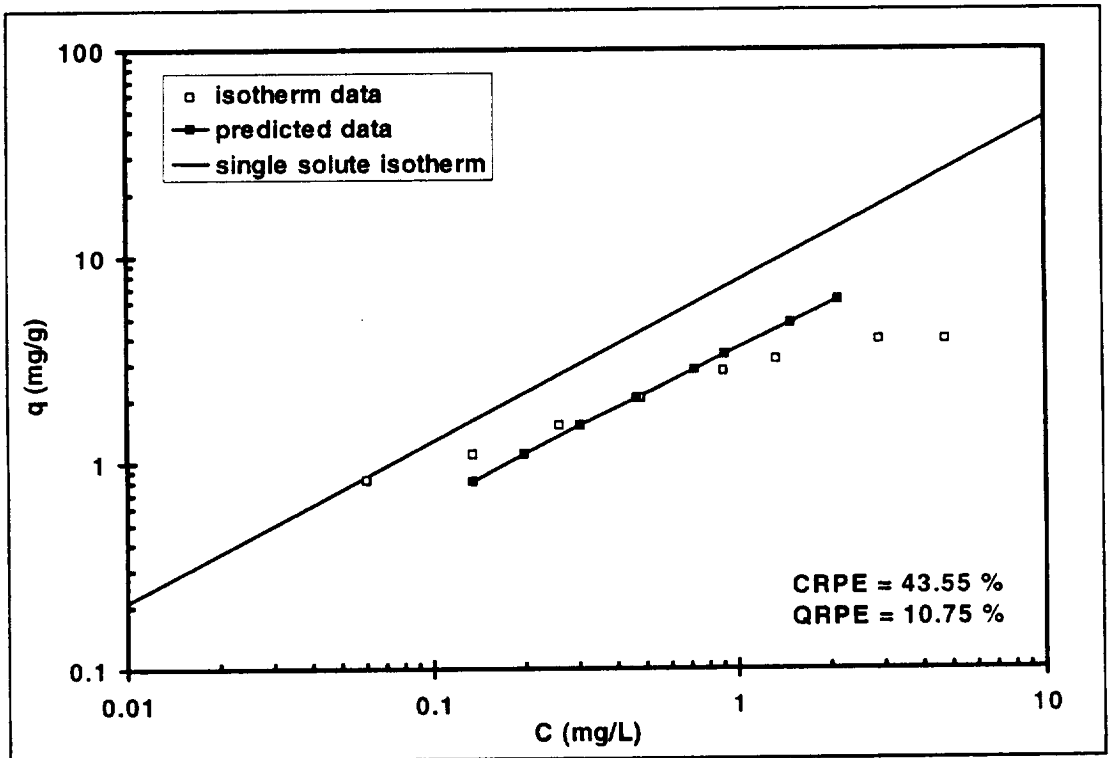

Figure 3-8. Chloroform tracer isotherm predicted on APA GAC for the waste mixture.

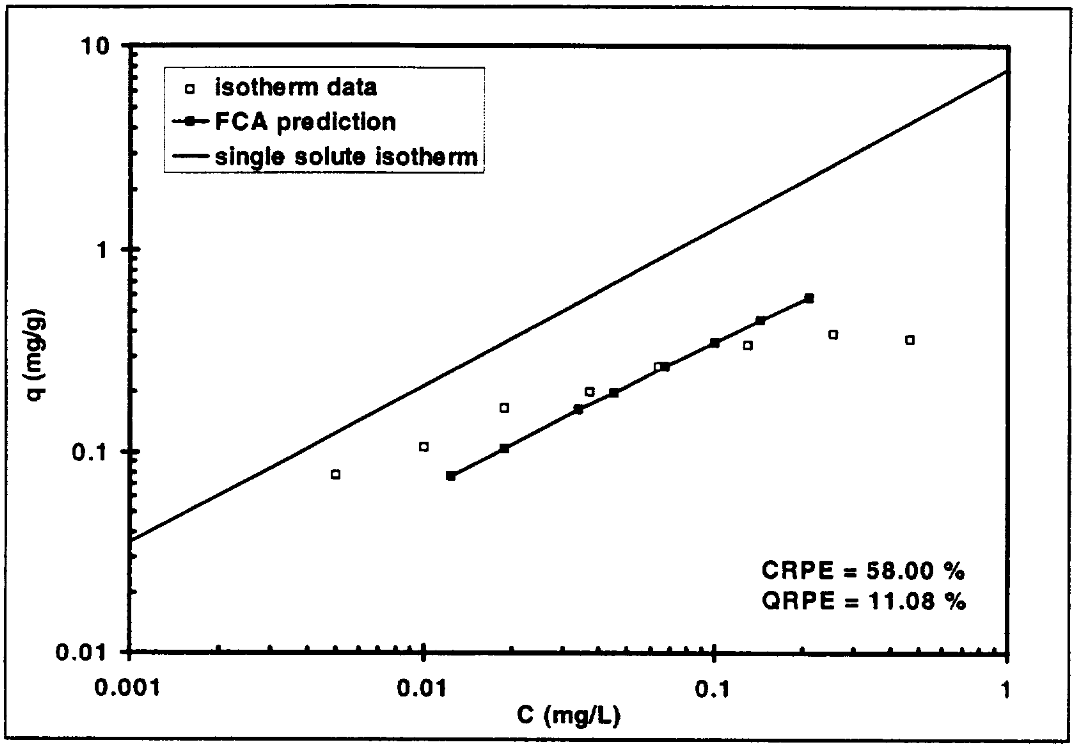

Figure 3-9. Dilute chloroform tracer isotherm predicted on APA GAC for the waste mixture.

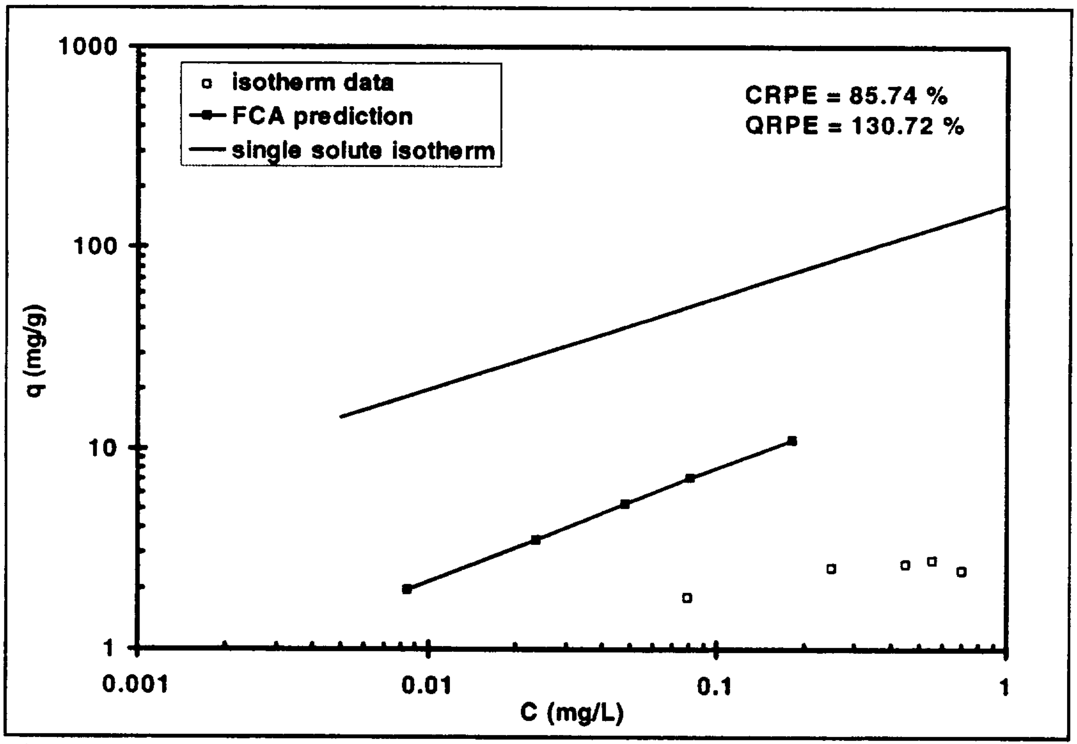

Figure 3-10. PCE tracer isotherm predicted on APA GAC for the waste mixture.

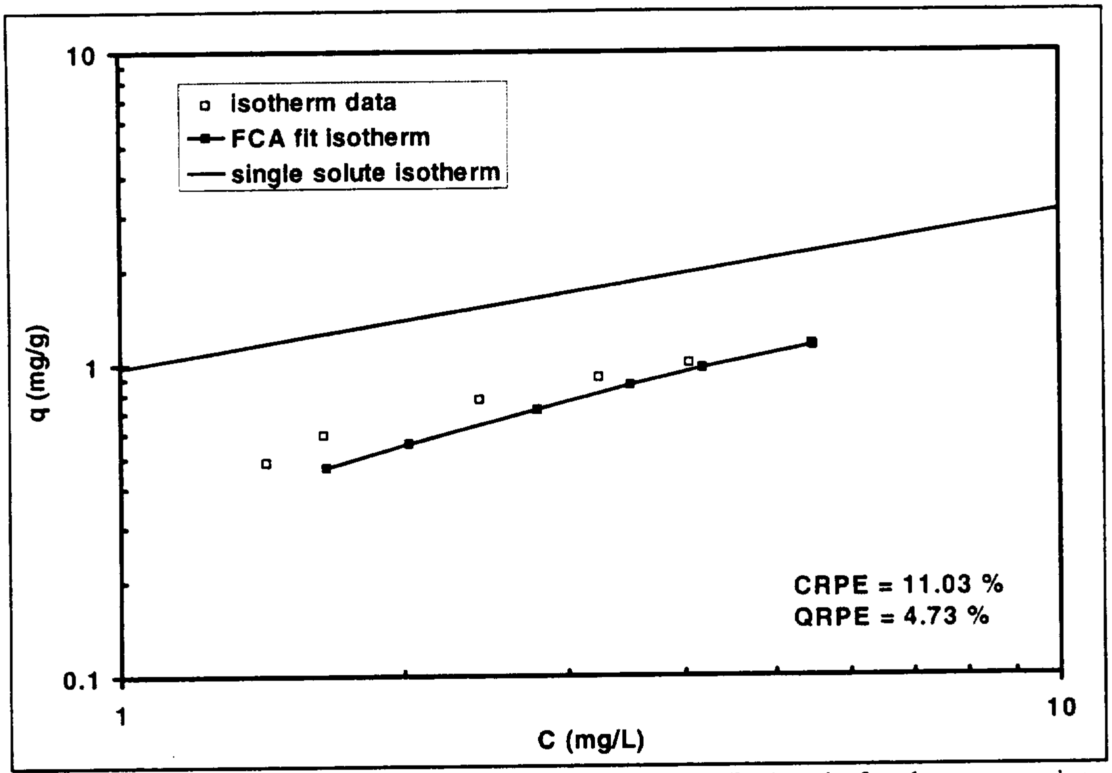

Figure 3-11. Methylene chloride tracer isotherm on XAD-4 resin for the waste mixture. Fit simultaneously with dilute methylene chloride tracer isotherm.

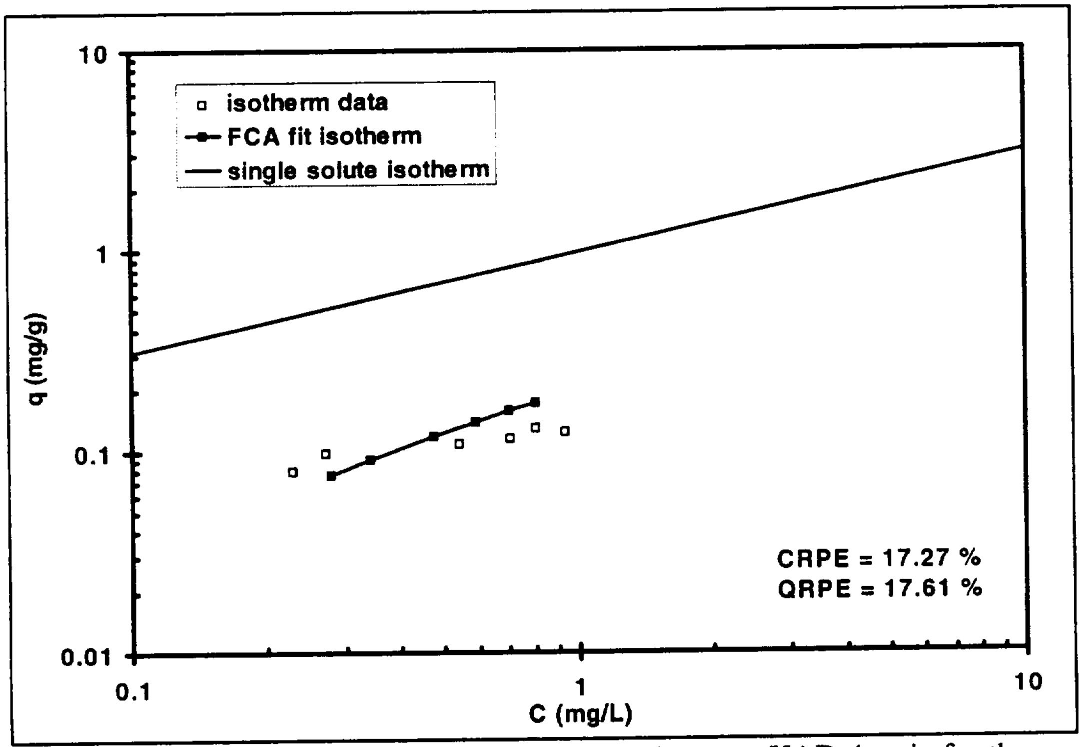

Figure 3-12. Dilute methylene chloride tracer isotherm on XAD-4 resin for the waste mixture. Fit simultaneously with methylene chloride tracer isotherm.

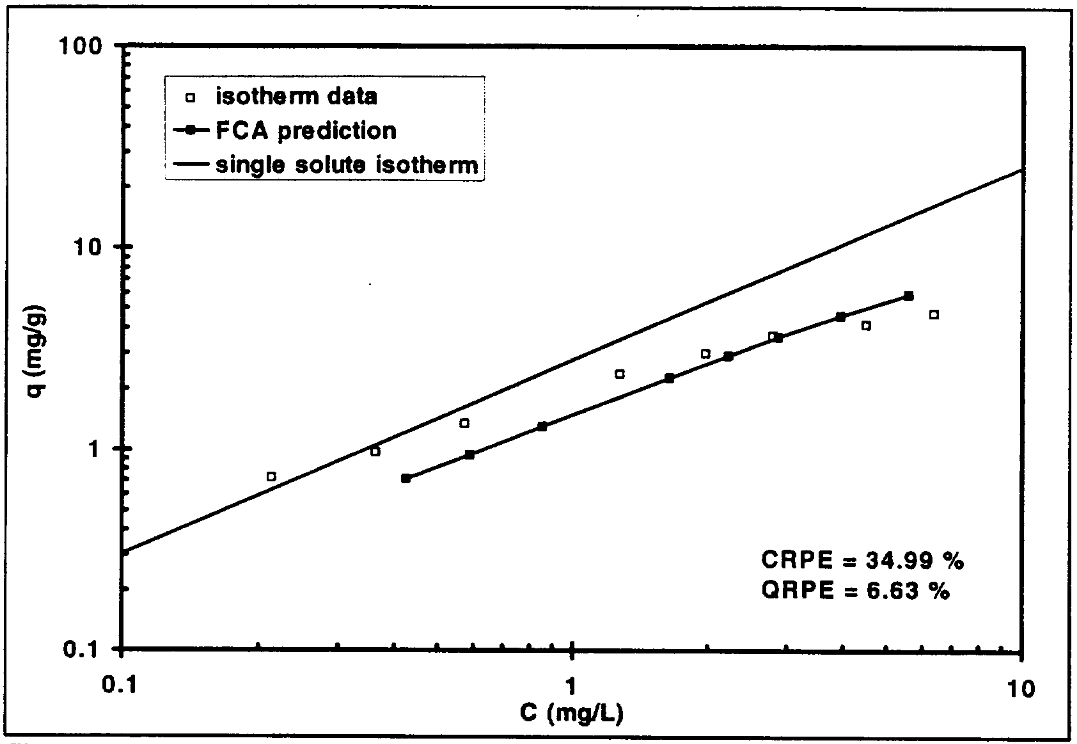

Figure 3-13. Chloroform tracer isotherm predicted on XAD-4 resin for the waste mixture.

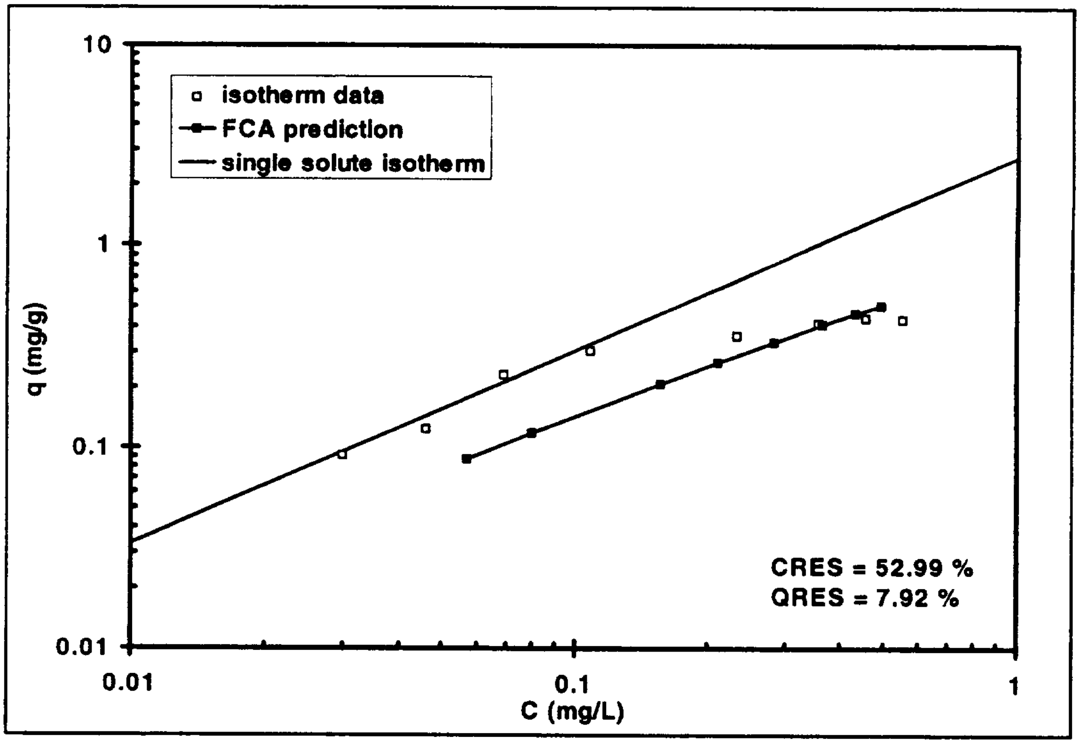

Figure 3-14. Dilute chloroform tracer isotherm predicted on XAD-4 resin for the waste mixture.

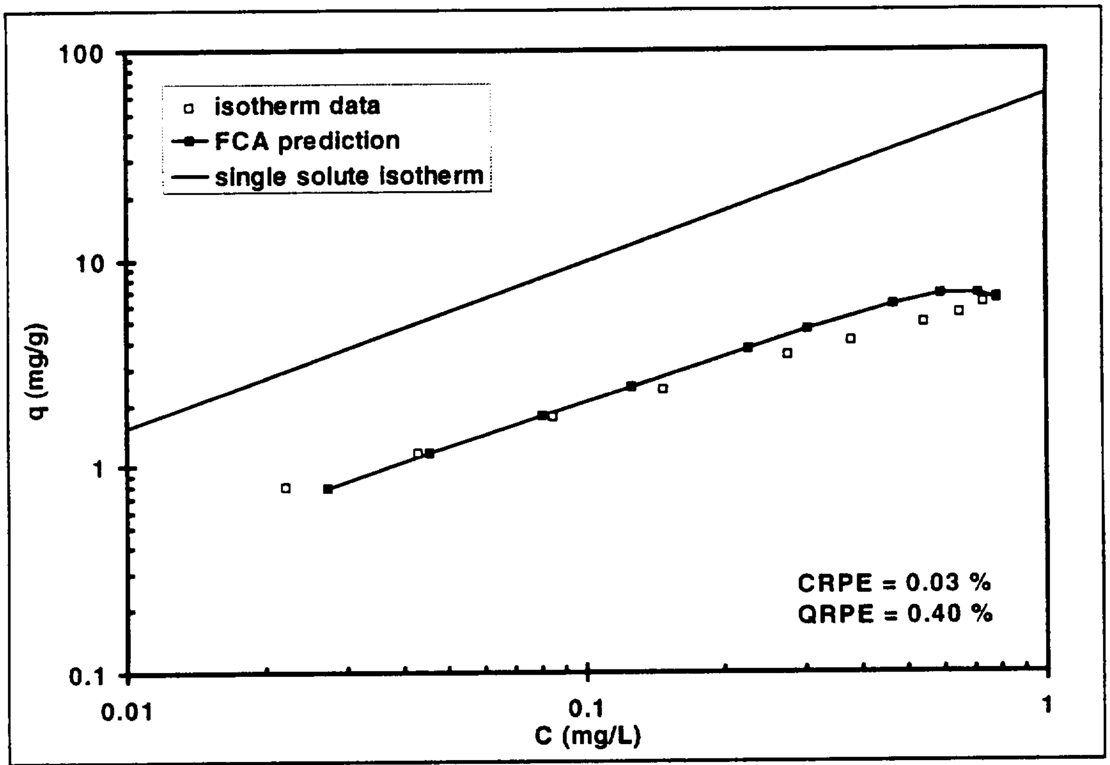

Figure 3-15. PCE tracer isotherm predicted on XAD-4 resin for the waste mixture.

3.4.2 SHOWER/HANDWASH MIXTURE

3.4.2.1 Tracer FC Results on 580-26 GAC. The 580-26 nondilute and dilute methylene chloride (MC) tracer isotherms on the shower/handwash mixture were fit simultaneously to determine the tracer FC concentrations. The approach used to fit and predict the tracer isotherms for the shower/handwash mixture is the same as the waste mixture. MC is the weakest adsorbing tracer compound spiked in the shower/handwash mixture, therefore the MC tracer isotherms were fit simultaneously to determine the tracer FC concentrations. The tracer FC concentrations were then used in IAST calculations to predict the chloroform tracer isotherms.

The shower/handwash tracer FCs determined on 580-26 GAC are included in Table 3-3. The tracer isotherm fits and data are compared for the 580-26 nondilute and dilute MC tracer isotherms in Figure 3-16 and 3-17, respectively. The MC FCA isotherm fits overpredict the reduction in capacity from its single solute, when compared to the experimental data. This is similar to the MC tracer isotherm results for the waste mixture. Table 3-7 contains the RPE results for the tracer isotherm fit and predictions for the shower/handwash mixture on 580-26 GAC, APA GAC, and XAD-4 resin. The RPEs show the error in the liquid phase is much larger than the solid phase.

Table 3-7. RPEs for the shower/handwash mixture tracer isotherm fits and predictions on 580-26 GAC, APA GAC, and XAD-4 resin.

		Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
	Compound	**Relative % error C**	**q**	**# of Data points**	**Relative % error C**	**q**	**# of Data points**
580-26	MC	91.10	32.50	6	152.43	37.86	5
	Chloroform	48.00	5.78	7	88.96	8.23	8
APA	MC	35.33	9.40	5	71.15	10.54	5
	Chloroform	78.47	12.37	7	135.96	16.77	8
XAD-4	MC	12.44	8.98	7	14.78	9.95	6
	Chloroform	46.06	9.72	10	29.81	54.77	9

The tracer FCs from fitting MC tracer isotherms on 580-26 GAC were used in IAST calculations to predict nondilute and dilute chloroform tracer isotherms on 580-26 GAC. These predictions were made to determine if the tracer FCs from fitting the MC tracer isotherms could predict equilibrium for other compounds in the shower/handwash mixture. Figures 3-18 and 3-19 present the predicted nondilute and dilute chloroform tracer isotherms. The chloroform predictions overpredict the reduction in capacity of the adsorbent at higher adsorbent dosages. This is similar to the results when predicting chloroform tracer isotherms for the waste mixture.

The reduction in capacity for the tracer compounds shown by the isotherm data is similar to the trends shown for the waste mixture. This is described by diffusion of the compounds with SCMT present in the water as described for the waste mixture.

3.4.2.2 Tracer FC Results for APA GAC. The tracer FC concentrations determined when fitting 580-26 MC tracer isotherms were held constant as the shower/handwash mixture passes through the other adsorbents in series. The tracer FC concentrations were scaled to equal the adsorbing TOC concentration on APA GAC. The shower/handwash MC nondilute and dilute tracer isotherms on APA GAC were fit simultaneously optimizing FC Freundlich K's. FC Freundlich 1/n was correlated to the FC Freundlich K for APA GAC. The shower/handwash tracer FC parameters for APA GAC are presented in Table 3-5. The nondilute and dilute MC FCA tracer isotherm fits are presented in Figures 3-20 and 3-21. The results indicate the FCA isotherm fits overpredict the competitive adsorption in the shower/handwash water. This is consistent with the shower/handwash MC results on 580-26 GAC, and also results from the waste mixture. The RPE's for the shower/handwash tracer isotherm fits and predictions on APA GAC are presented in Table 3-7.

The APA FC results when fitting MC tracer isotherms simultaneously were used to determine if the reduction in capacity of other compounds in the shower/handwash mixture could be predicted on APA GAC. A nondilute and dilute chloroform tracer isotherm were predicted using the APA FC parameters in IAST calculations. The nondilute and dilute chloroform tracer isotherms are presented in Figures 3-22 and 3-23, respectively. Again the results are similar to what was observed in the waste mixture. The nondilute and dilute chloroform tracer isotherms slightly underpredict reduction in capacity at low adsorbent dosages and overpredict reduction in capacity of the adsorbent at the higher adsorbent dosages. RPE values show high error in the liquid phase and low errors in the solid phase.

3.4.2.3 Tracer FC results for XAD-4 resin. The tracer FCs were determined for XAD-4 resin using the same procedure used to determine the tracer FCs for APA GAC. Table 3-6 includes the tracer FC results for XAD-4 resin. Shower/handwash MC nondilute and dilute tracer isotherms on XAD-4 resin were fit simultaneously to determine FC Freundlich K values. FC Freundlich 1/n values were correlated from the known compounds in the waste streams. The results of the MC nondilute and dilute fits are shown in Figures 3-24 and 3-25, respectively. The nondilute MC tracer isotherm fit overpredicts the effect of competitive adsorption at high adsorbent dosages. Figures 3-26 and 3-27 show the shower/handwash nondilute and dilute chloroform tracer isotherm predictions on XAD-4 resin. The chloroform predictions overpredict the reduction in capacity of the adsorbent at high adsorbent dosages. The RPE results for the fit and predicted shower/handwash tracer isotherms on XAD-4 resin are summarized in Table 3-7.

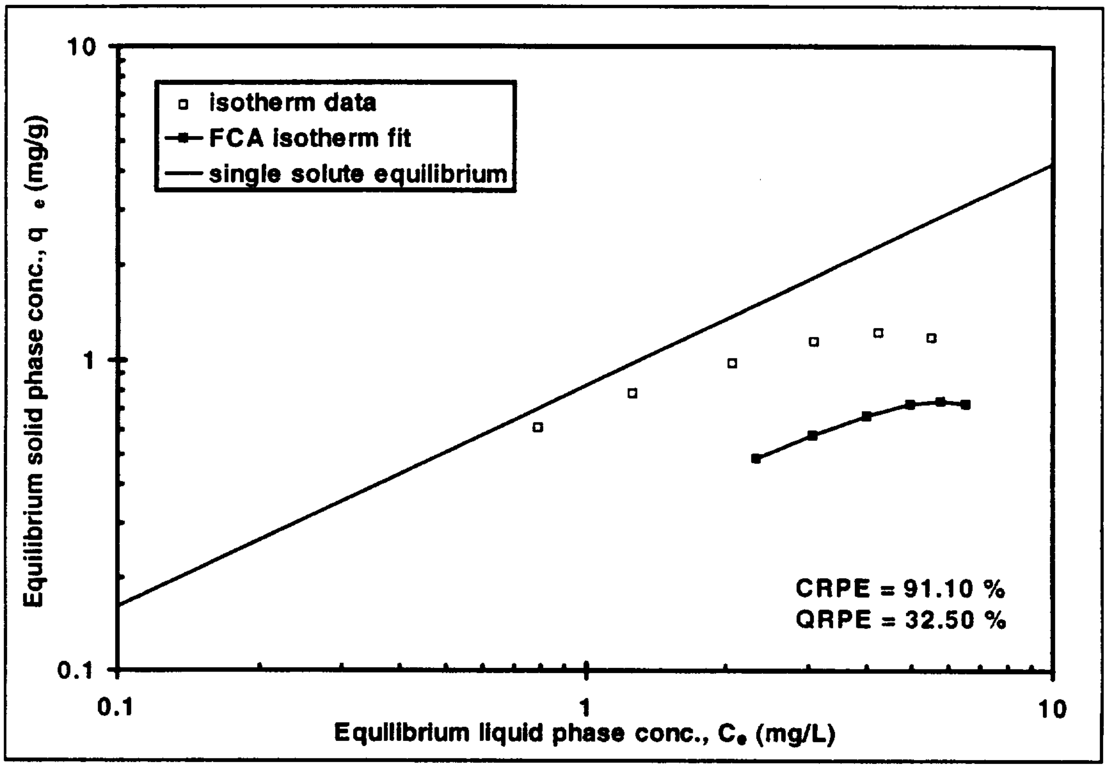

Figure 3-16. Nondilute MC tracer isotherm on 580 GAC for the shower/handwash mixture. Fit simultaneously with the dilute MC tracer isotherm.

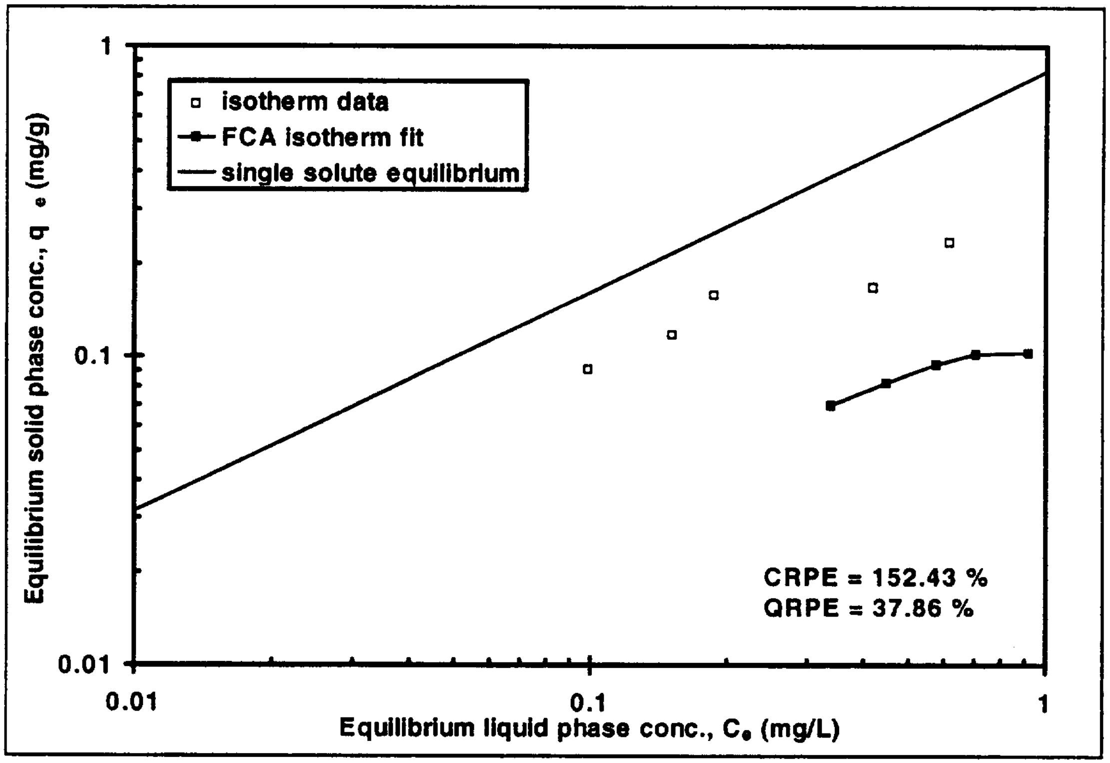

Figure 3-17. Dilute MC tracer isotherm on 580-26 GAC for the shower/handwash mixture. Fit simultaneously with the nondilute MC tracer isotherm.

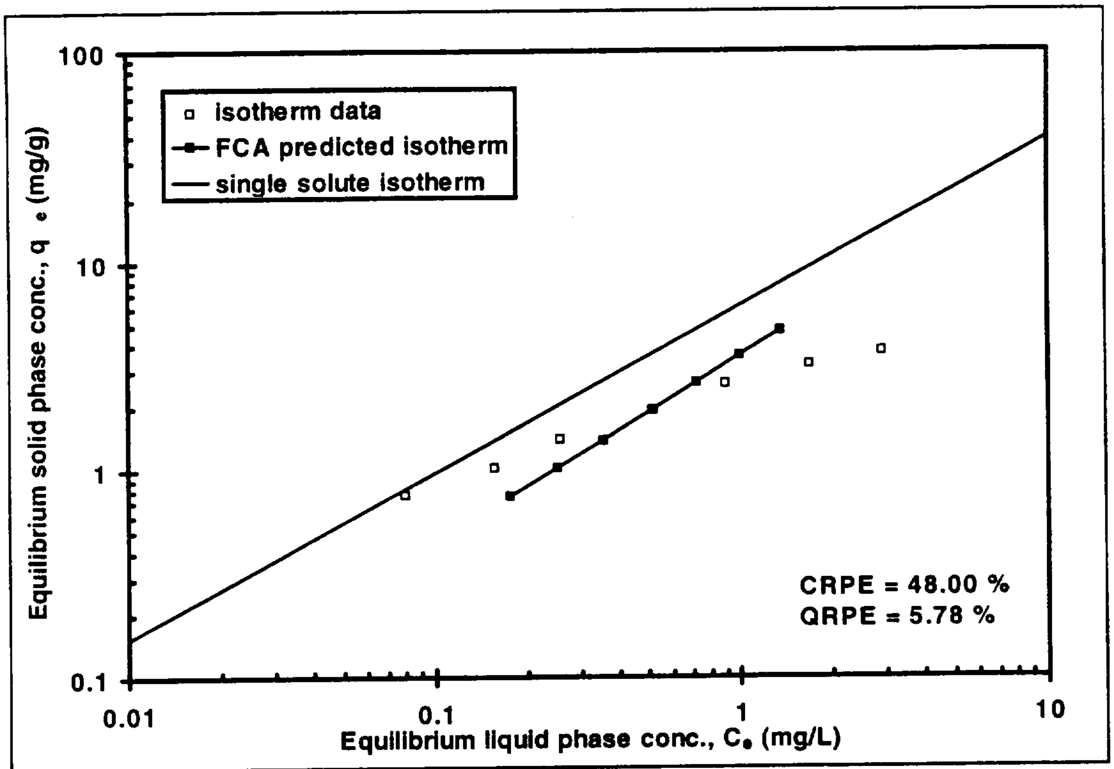

Figure 3-18. Nondilute chloroform tracer isotherm predicted on 580 GAC for the shower/handwash mixture.

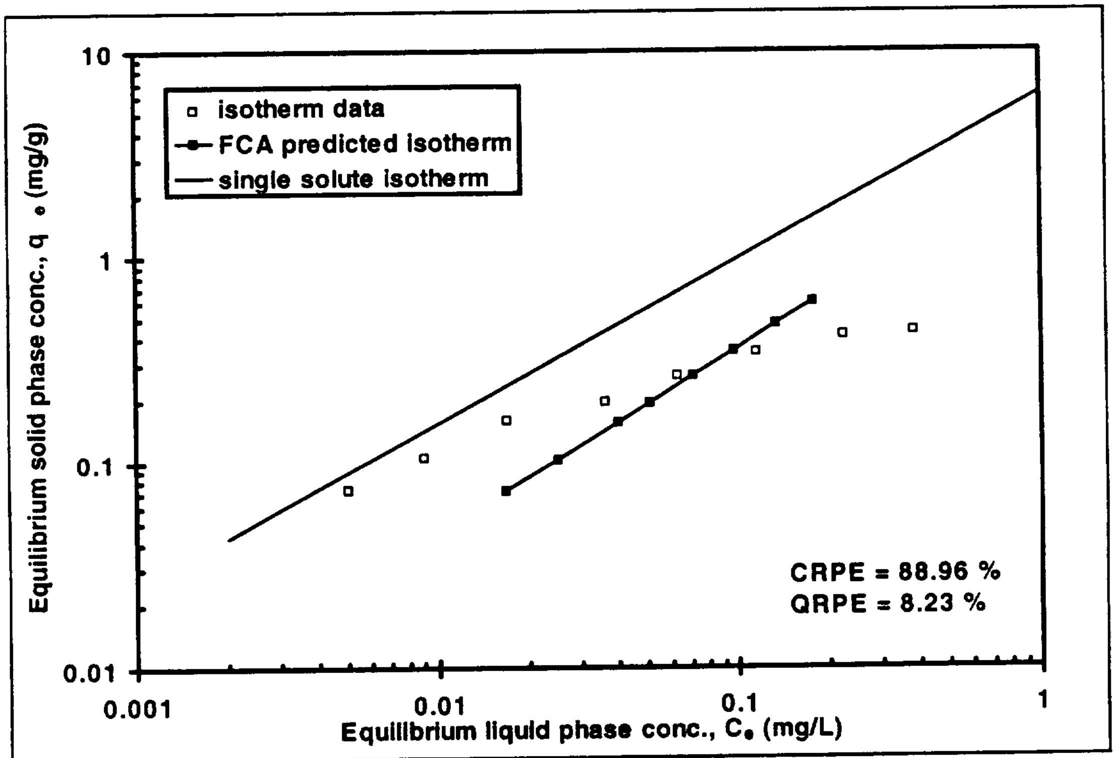

Figure 3-19. Dilute chloroform tracer isotherm predicted on 580 GAC for the shower/handwash mixture.

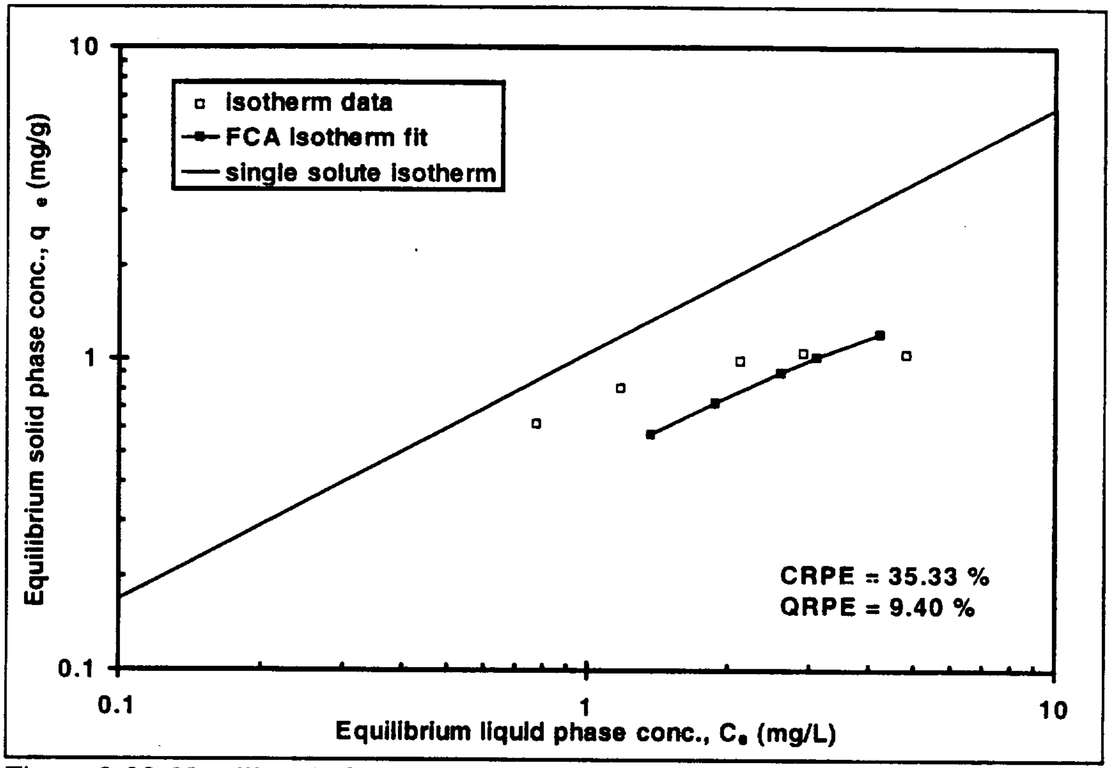

Figure 3-20. Nondilute MC tracer isotherm on APA GAC for the shower/handwash mixture. Fit simultaneously with the dilute MC isotherm.

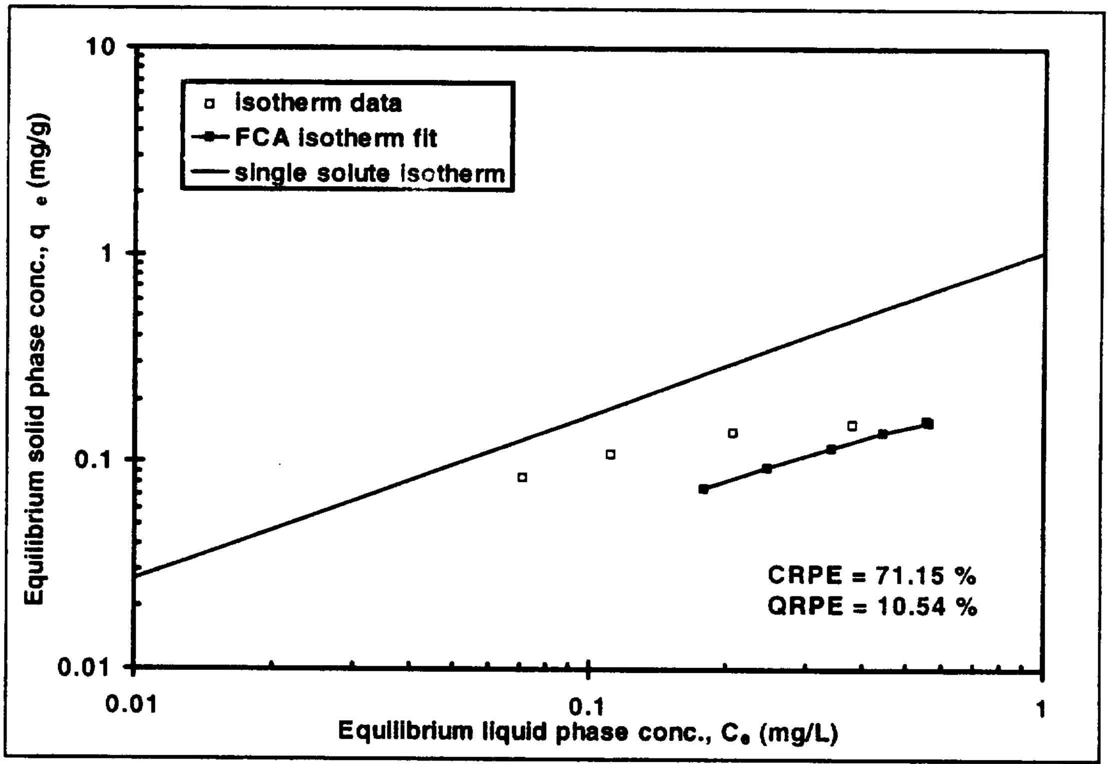

Figure 3-21. Dilute MC tracer isotherm on APA GAC for the shower/handwash mixture. Fit simultaneously with the nondilute MC isotherm.

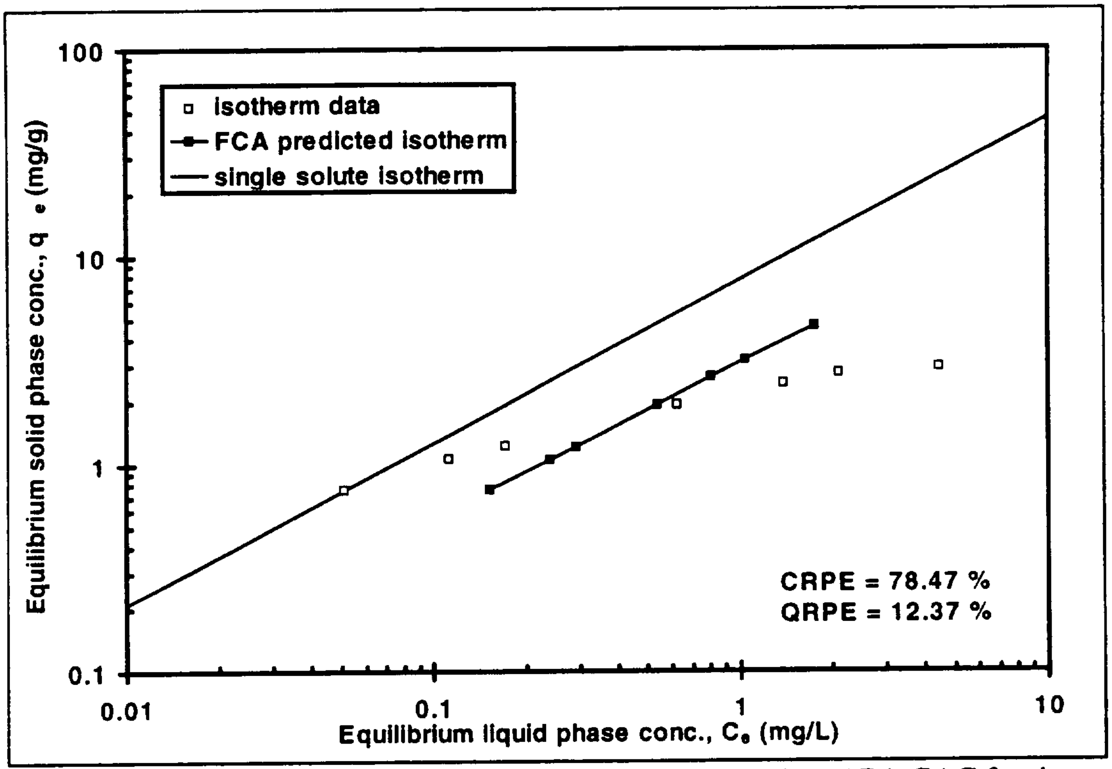

Figure 3-22. Nondilute chloroform tracer isotherm predicted on APA GAC for the shower/handwash mixture.

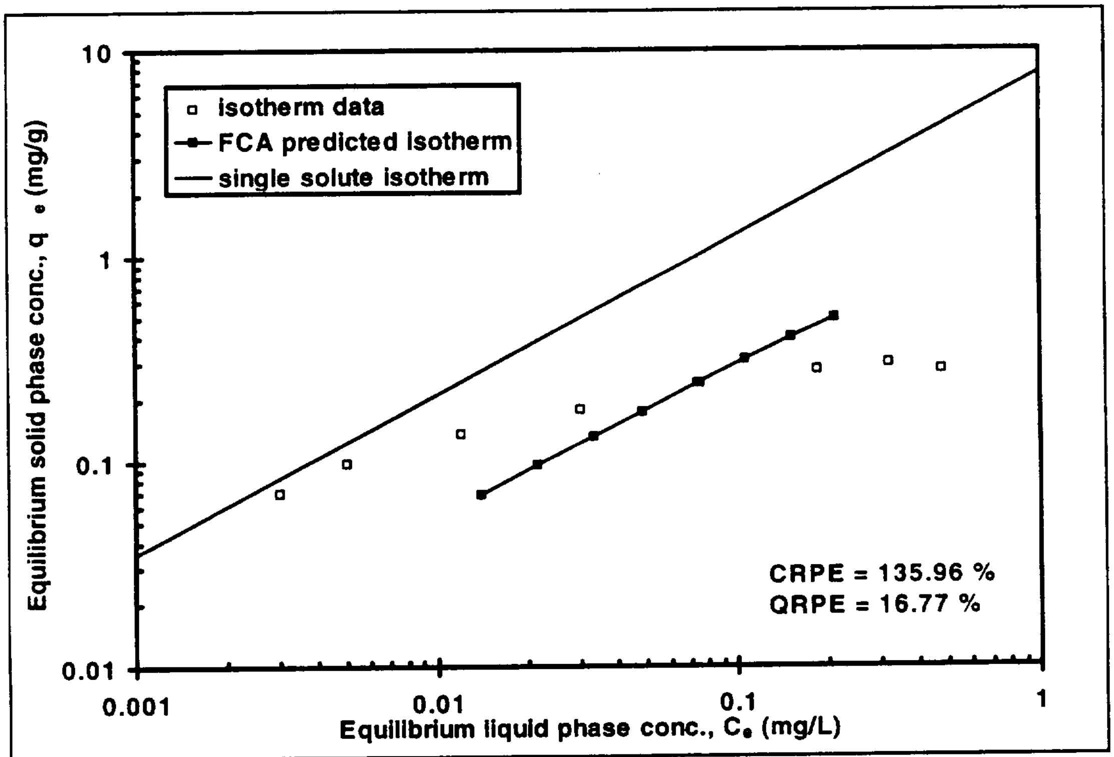

Figure 3-23. Dilute chloroform tracer isotherm predicted on APA GAC for the shower/handwash mixture.

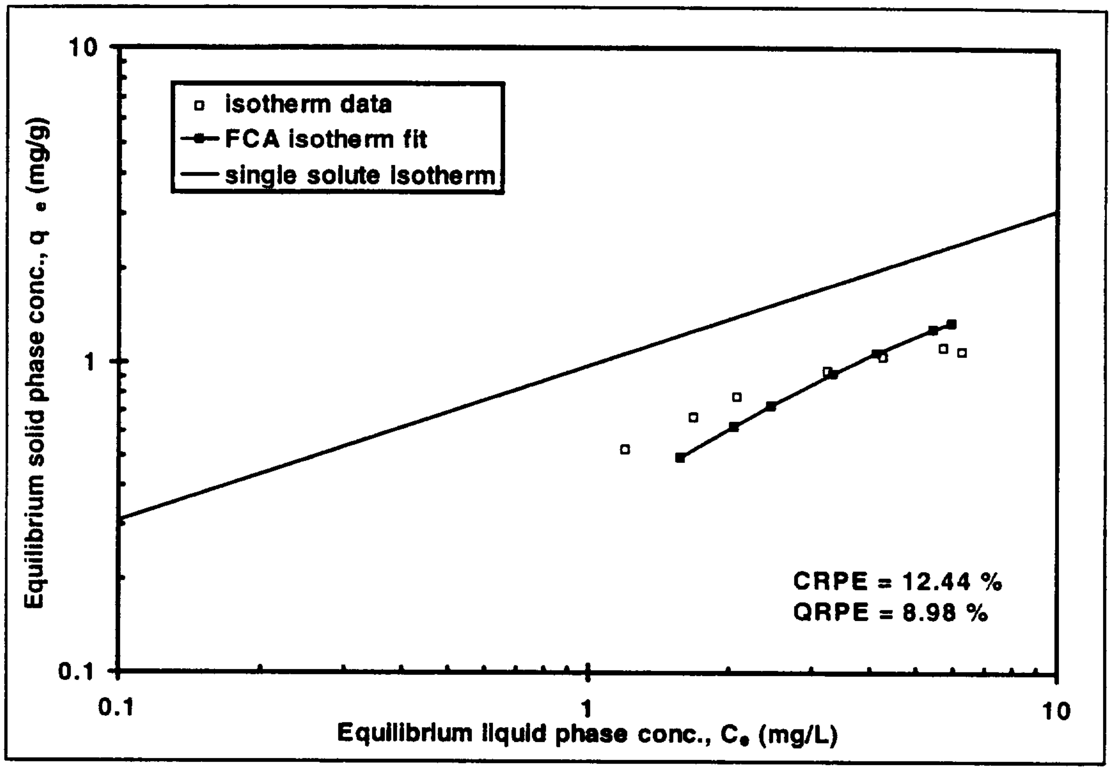

Figure 3-24. Nondilute MC tracer isotherm on XAD resin for the shower/handwash mixture. Fit simultaneously with the dilute MC tracer isotherm.

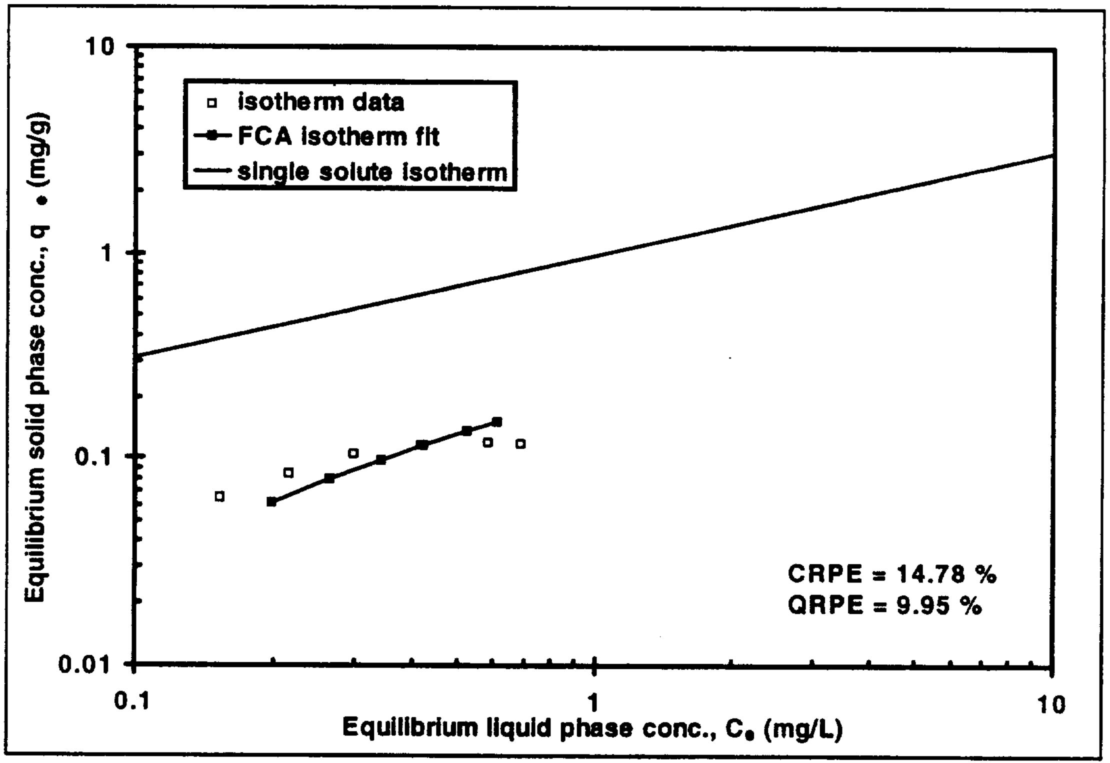

Figure 3-25. Dilute MC tracer isotherm on XAD-4 resin for the shower/handwash mixture. Fit simultaneously with the nondilute MC tracer isotherm.

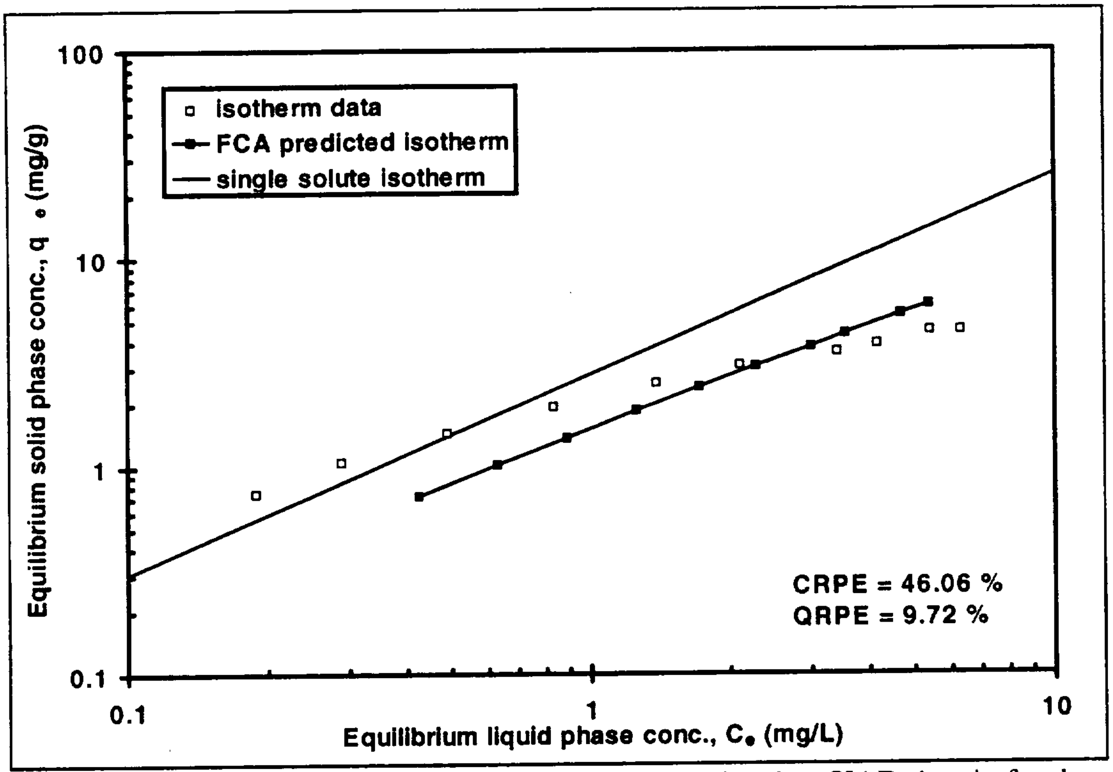

Figure 3-26. Nondilute chloroform tracer isotherm predicted on XAD-4 resin for the shower/handwash mixture.

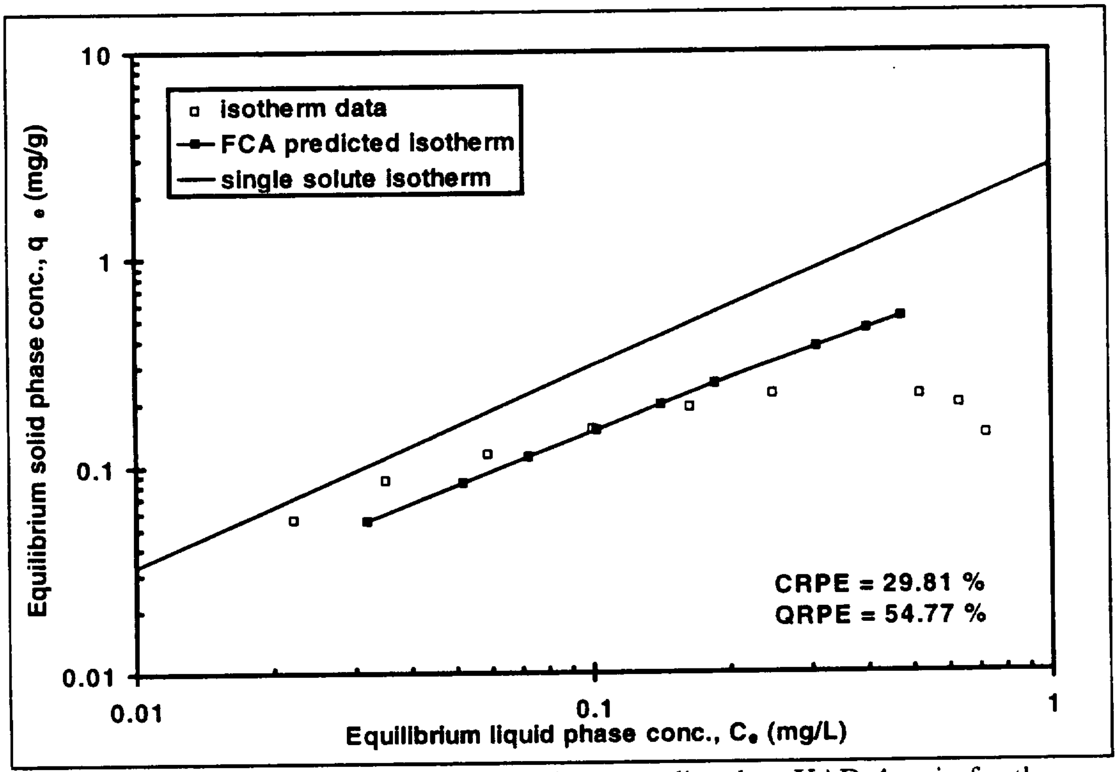

Figure 3-27. Dilute chloroform tracer isotherm predicted on XAD-4 resin for the shower/handwash mixture.

3.4.3 URINE DISTILLATE STREAM

3.4.3.1 Tracer FC Results for 580-26 GAC. The urine distillate nondilute and dilute TCE tracer isotherms on 580-26 GAC were fit simultaneously to determine the tracer FC concentrations. The same approach was used to fit and predict the tracer isotherms for urine distillate as was used for the waste mixture. The weakest adsorbing tracer compound spiked in urine distillate was TCE, therefore the TCE tracer isotherms were fit simultaneously to determine the tracer FC concentrations. The tracer FC concentrations were then used to predict the toluene and naphthalene tracer isotherms.

The tracer FCs determined for urine distillate on 580-26 GAC are included in Table 3-3. The nondilute and dilute TCE tracer isotherm fits and data are compared in Figure 3-28 and 3-29, respectively. The TCE FCA isotherm fits for both the nondilute and dilute isotherms closely follow the isotherm data. The fit accurately represents the reduction in capacity of the adsorbent due to competitive adsorption interactions of the background matrix. Table 3-8 contains the RPE results for the tracer isotherm fit and predictions for urine distillate on 580-26 GAC, APA GAC, and XAD-4 resin. The RPEs for the TCE isotherms show similar results for the nondilute and dilute isotherms with the liquid phase error slightly higher than the solid phase.

Table 3-8. RPEs for urine distillate tracer isotherm fits and predictions on 580-26 GAC, APA GAC, and XAD-4 resin.

	Compound	**Nondilute waste mixture TOC isotherm**			**Dilute waste mixture TOC isotherm**		
		Relative % error C	**q**	**# of Data points**	**Relative % error C**	**q**	**# of Data points**
580-26	TCE	14.19	7.01	8	16.74	4.43	4
	toluene	146.63	2.18	9	306.51	13.06	7
	naphthalene	321.71	9.89	4	11.03	4.73	4
APA	TCE	16.38	6.46	6	8.73	4.32	8
	toluene	12.80	1.15	11	105.00	10.90	7
	naphthalene	1054.34	28.82	6	563.36	59.10	3
XAD-4	TCE	31.52	10.91	11	37.58	25.33	6
	toluene	51.60	6.46	10	35.59	2.45	5
	naphthalene	146.26	31.25	10	166.66	42.35	9

The 580-26 GAC tracer FCs were used in IAST calculations to predict nondilute and dilute toluene and naphthalene tracer isotherms on 580-26 GAC. These predictions were to determine if the tracer FCs from fitting the TCE tracer isotherms could predict

equilibrium for other compounds in urine distillate. Figures 3-30 and 3-31 show the predicted nondilute and dilute toluene tracer isotherms on 580-26 GAC. The nondilute toluene prediction slightly overpredicts competitive adsorption, however the isotherm data indicates virtually no reduction in capacity from the single solute isotherm. The dilute toluene isotherm overpredicts the reduction in capacity due to competitive adsorption. The RPE results indicate the overpredictions of the two isotherms. Figures 3-32 and 3-33 show the predicted nondilute and dilute naphthalene tracer isotherms on 580-26 GAC. The naphthalene predictions also overpredict the reduction in capacity.

The trends of the reduction in capacity for the tracer compounds are as expected. The weaker adsorbing compound (TCE) has a greater reduction in capacity than the strongly adsorbing compound (naphthalene). The phenomenon observed in the waste mixture and the shower/handwash mixture are not seen in the urine distillate, this is most likely because SCMT is not present in the urine distillate waste stream. The tracer isotherms also follow the trend that the dilute tracer isotherms have a greater reduction in capacity than the nondilute tracer isotherms. This is because the background TOC concentration has a greater impact at lower tracer concentrations. The stronger adsorbing tracer compounds show at higher concentrations there is no competition with the background water this is shown in the isotherm data for the nondilute toluene and naphthalene tracers.

3.4.3.2 Tracer FC Results for APA GAC. The tracer FC concentrations determined when fitting 580-26 TCE tracer isotherms were held constant as urine distillate passes through the other adsorbents in series. The tracer FC concentrations were scaled to equal the adsorbing TOC concentration on APA GAC. The urine distillate TCE nondilute and dilute tracer isotherms on APA GAC were fit simultaneously optimizing FC Freundlich K. FC Freundlich 1/n was correlated to FC Freundlich K for APA GAC. The urine distillate tracer FC parameters for APA GAC are presented in Table 3-5. Figures 3-34 and 3-35 show the urine distillate nondilute and dilute TCE FCA tracer isotherm fits, respectively, on APA GAC. The results indicate the FC parameters accurately describe the reduction in capacity of the competition in the background water. The RPEs for the fits and predictions for the urine distillate tracer isotherms on APA GAC are presented in Table 3-8. The RPE results for TCE show are relatively low indicating a good overall fit.

The FC results for APA GAC when fitting the TCE tracer isotherms simultaneously were used to determine if other compounds on APA GAC could be predicted. Nondilute and dilute toluene and naphthalene tracer isotherms were predicted using the APA FC parameters in IAST calculations. The nondilute and dilute toluene tracer isotherms are shown in Figures 3-36 and 3-37, respectively. The nondilute toluene tracer isotherm prediction is very accurate when compared to the isotherm data, this is supported by the low RPEs. The dilute toluene tracer isotherm prediction slightly overpredicts the reduction in adsorption capacity. The nondilute and dilute naphthalene tracer isotherms are shown in Figures 3-38 and 3-39. The nondilute and dilute naphthalene tracer isotherm predictions overpredict the reduction in capacity on APA GAC. The RPEs indicate there is a large error in the solid phase residuals.

3.4.3.3 Tracer FC results for XAD-4 resin. The tracer FCs for XAD-4 resin were determined using the same procedure used to determine the tracer FCs for APA GAC. Table 3-6 includes the urine distillate tracer FC results for XAD-4 resin. TCE nondilute and dilute tracer isotherms on XAD-4 resin were fit simultaneously to determine FC Freundlich K values. FC Freundlich 1/n was correlated to the FC Freundlich Ks. The results of the TCE nondilute and dilute fits are shown in Figures 3-40 and 3-41, respectively. The TCE FCA isotherm fits tend to underpredict the reduction in capacity at high adsorbent dosages. Figures 3-42 and 3-43 show the nondilute and dilute toluene tracer isotherms predicted on XAD-4 resin for urine distillate. The nondilute toluene tracer isotherm prediction underpredicts the reduction in capacity at high adsorbent dosages. The dilute toluene tracer isotherm prediction overpredicts the reduction in capacity at low adsorbent dosages and underpredicts the reduction in capacity at high adsorbent dosages. Figures 3-44 and 3-45 show the nondilute and dilute naphthalene tracer isotherms predicted on XAD-4 resin for urine distillate. The nondilute and dilute naphthalene tracer isotherm predictions both overpredict the reduction in capacity of the adsorbent. The RPE values for the fits and predictions on XAD-4 resin are presented in Table 3-8.

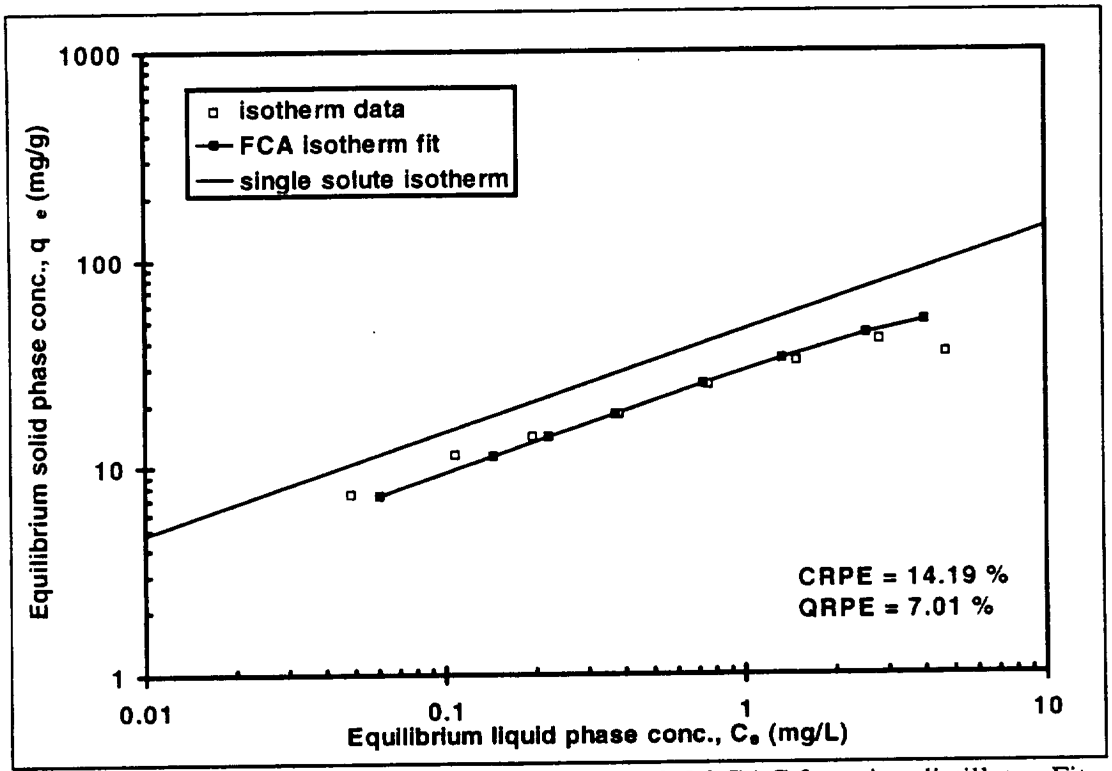

Figure 3-28. Nondilute TCE tracer isotherm on 580-26 GAC for urine distillate. Fit simultaneously with the dilute TCE isotherm.

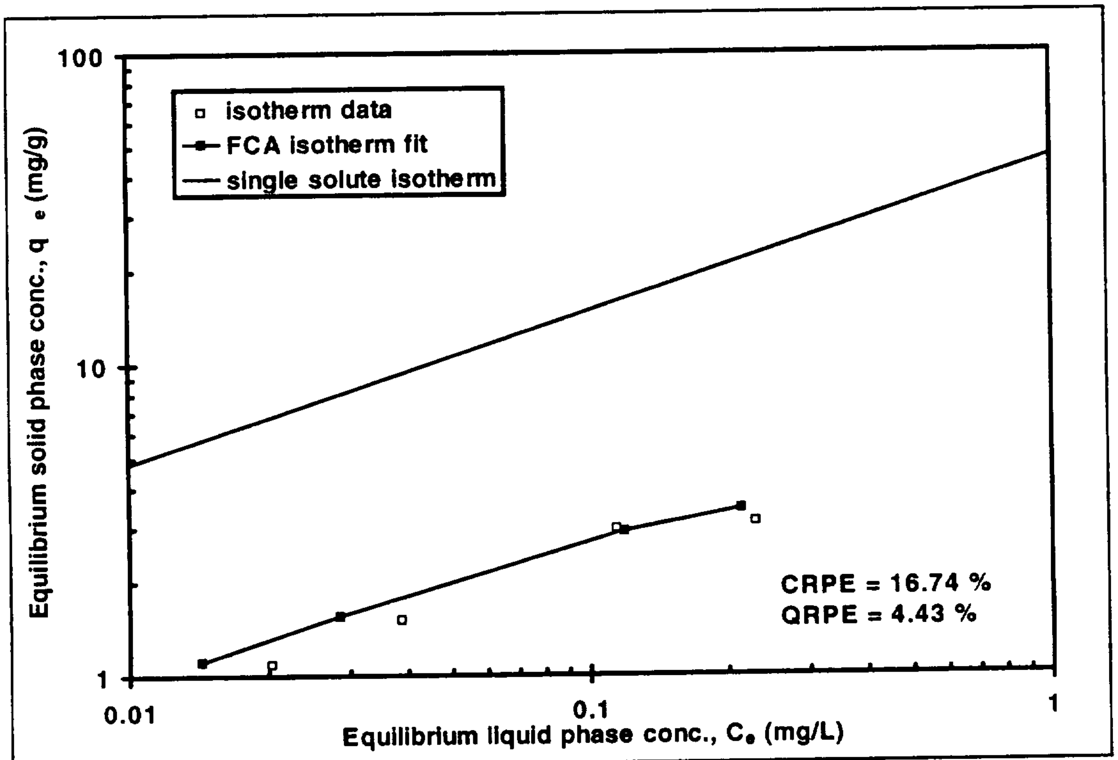

Figure 3-29. Dilute TCE tracer isotherm on 580-26 GAC for urine distillate. Fit simultaneously with the nondilute TCE isotherm.

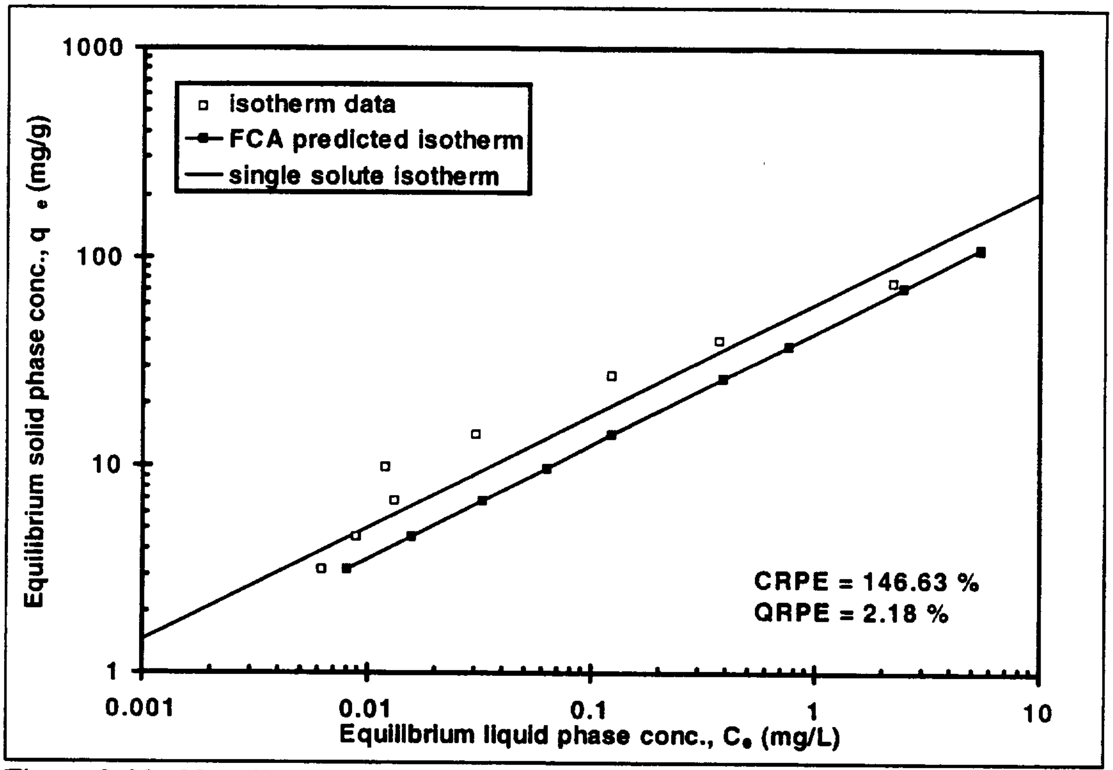

Figure 3-30. Nondilute toluene tracer isotherm predicted on 580-26 GAC for urine distillate.

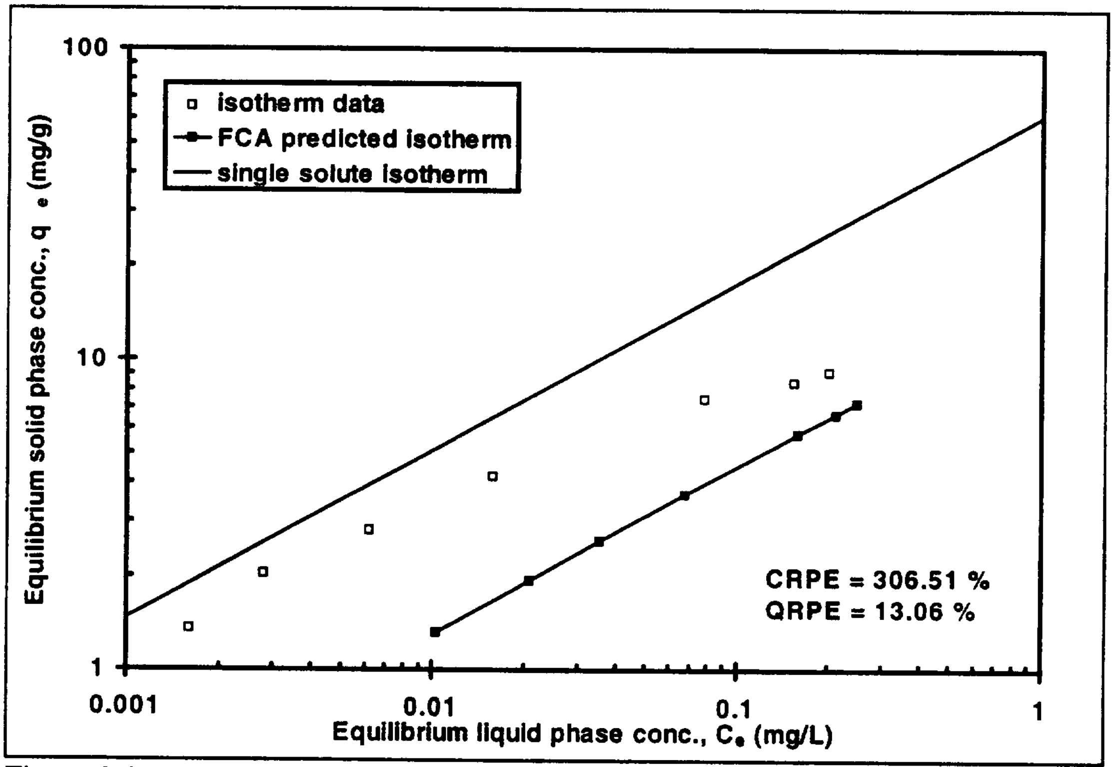

Figure 3-31. Dilute toluene tracer isotherm predicted on 580-26 GAC for urine distillate.

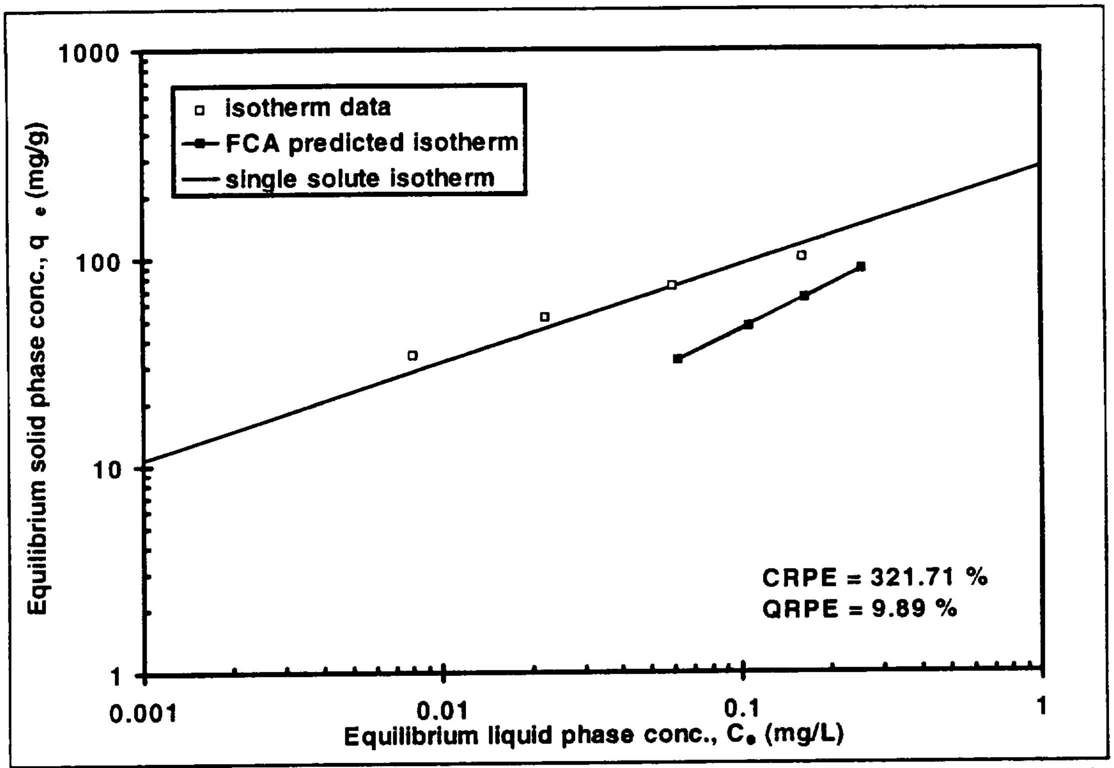

Figure 3-32. Nondilute naphthalene tracer isotherm predicted on 580-26 GAC for urine distillate.

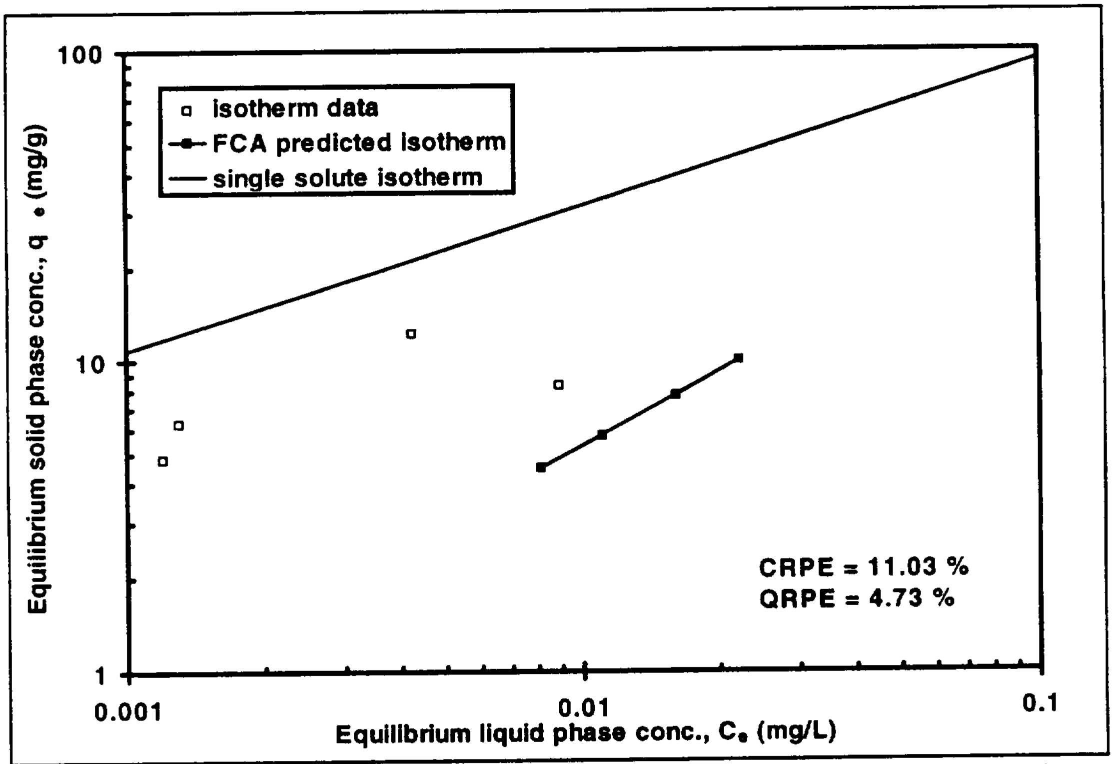

Figure 3-33. Dilute naphthalene tracer isotherm predicted on 580-26 GAC for urine distillate.

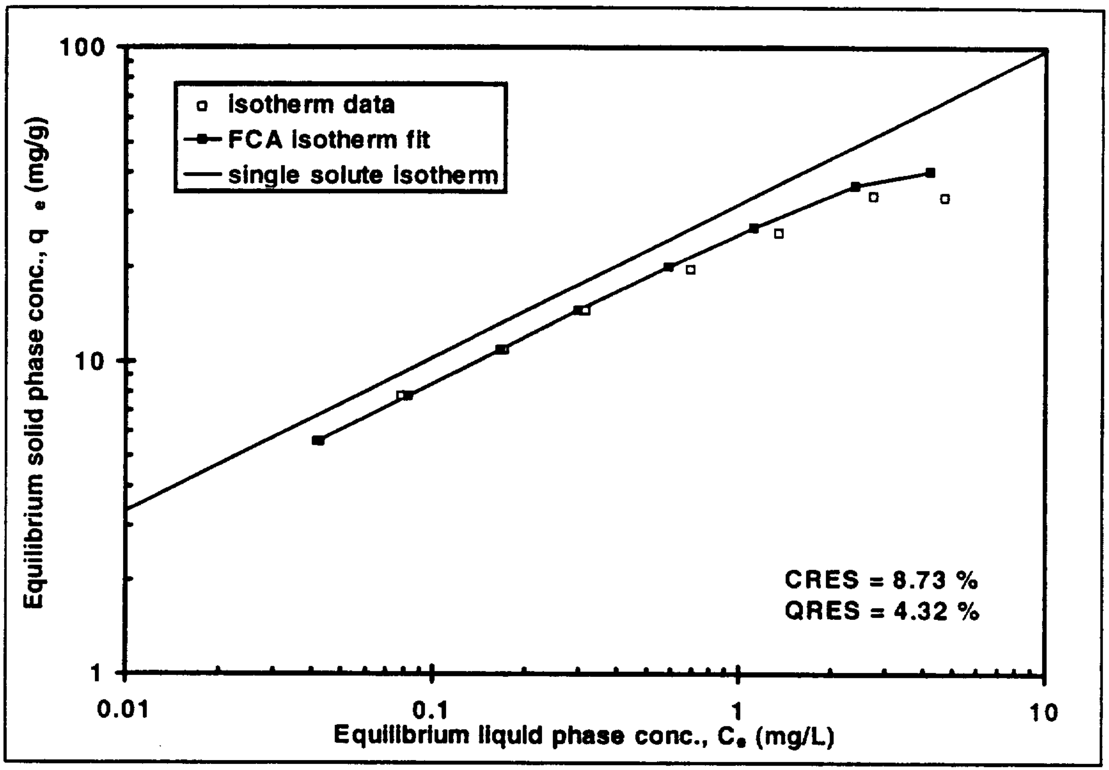

Figure 3-34. Nondilute TCE tracer isotherm on APA GAC for urine distillate. Fit simultaneously with the dilute TCE tracer isotherm.

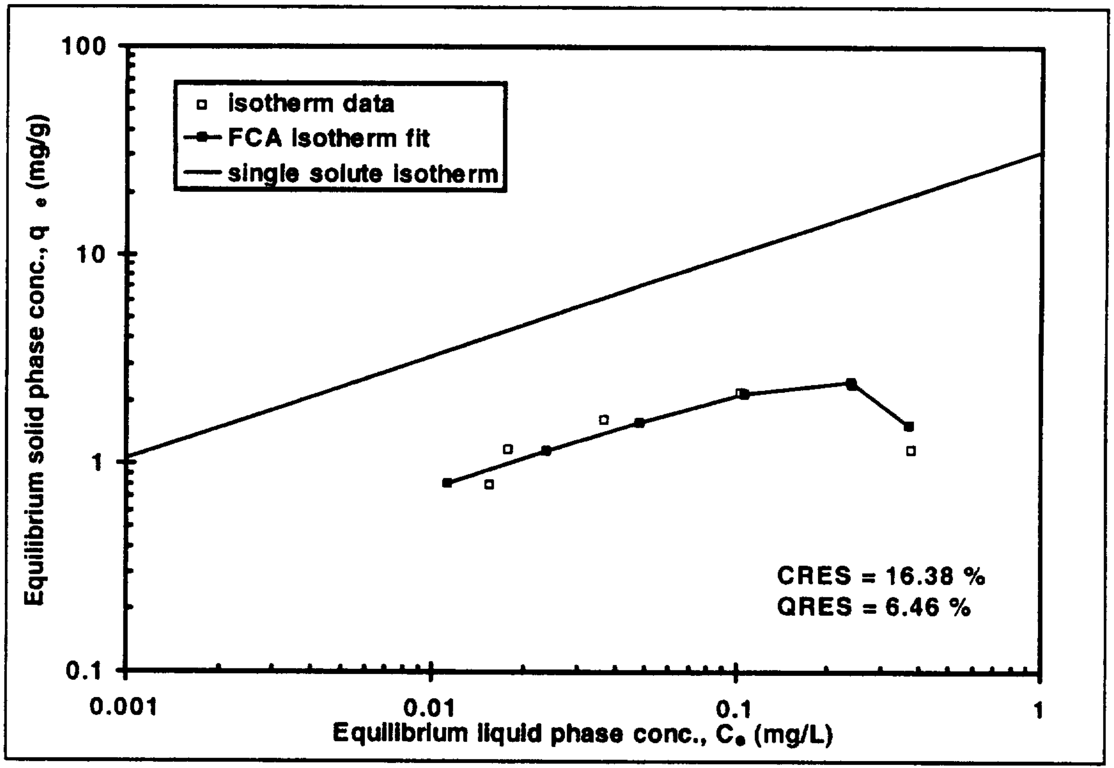

Figure 3-35. Dilute TCE tracer isotherm on APA GAC for urine distillate. Fit simultaneously with the nondilute TCE tracer isotherm.

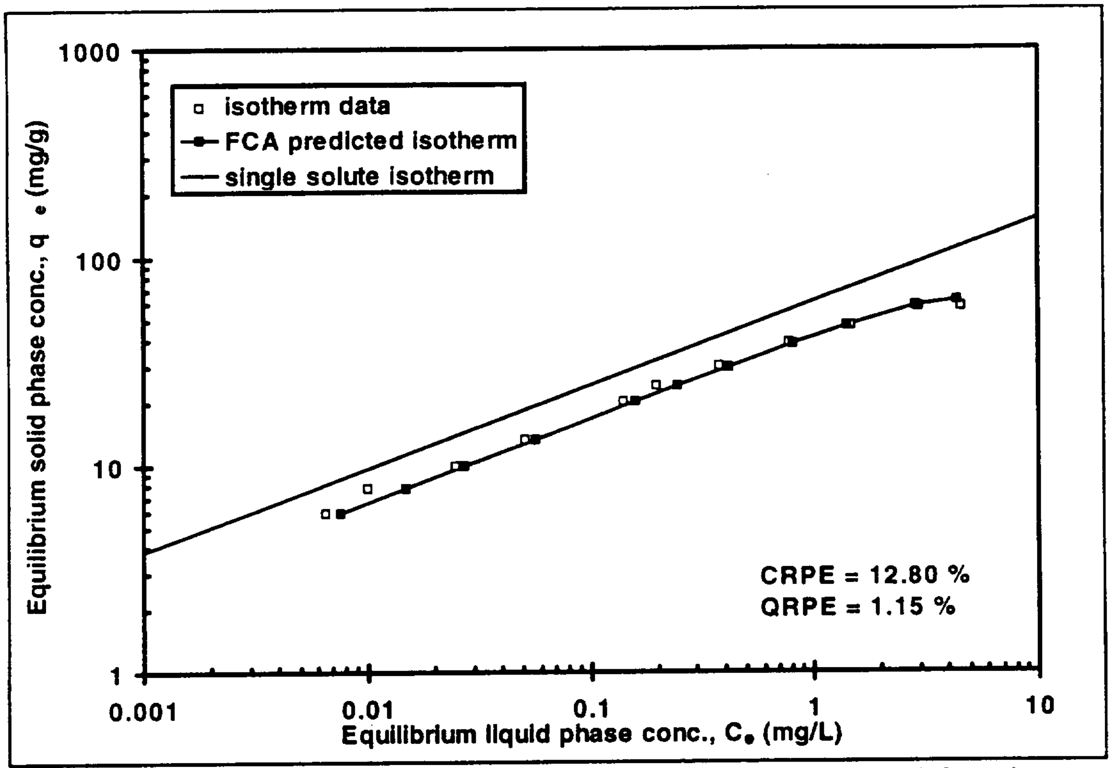

Figure 3-36. Nondilute toluene tracer isotherm predicted on APA GAC for urine distillate.

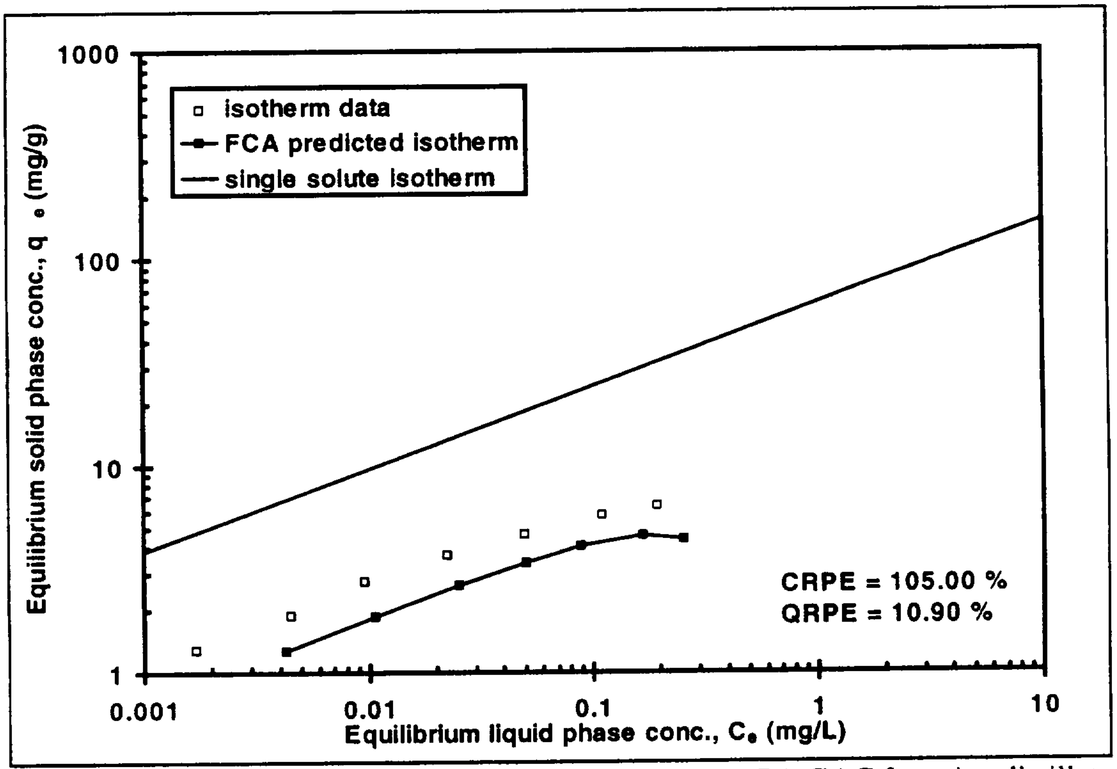

Figure 3-37. Dilute toluene tracer isotherm predicted on APA GAC for urine distillate.

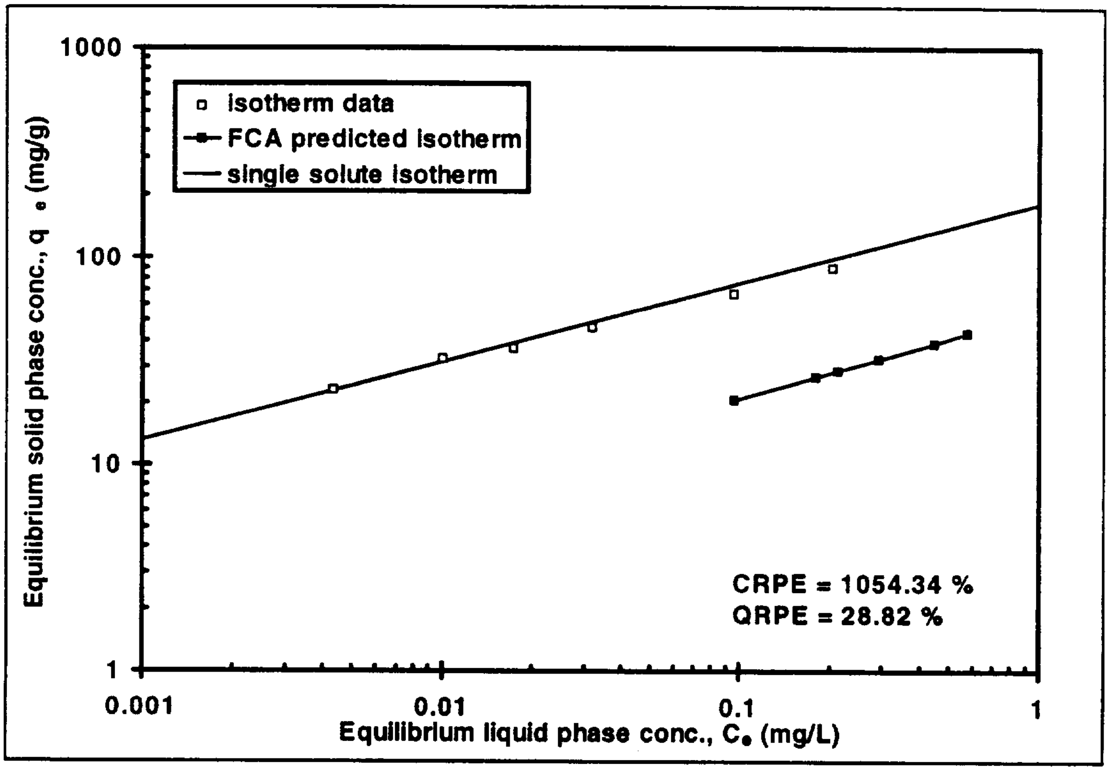

Figure 3-38. Nondilute naphthalene tracer isotherm predicted on APA GAC for urine distillate.

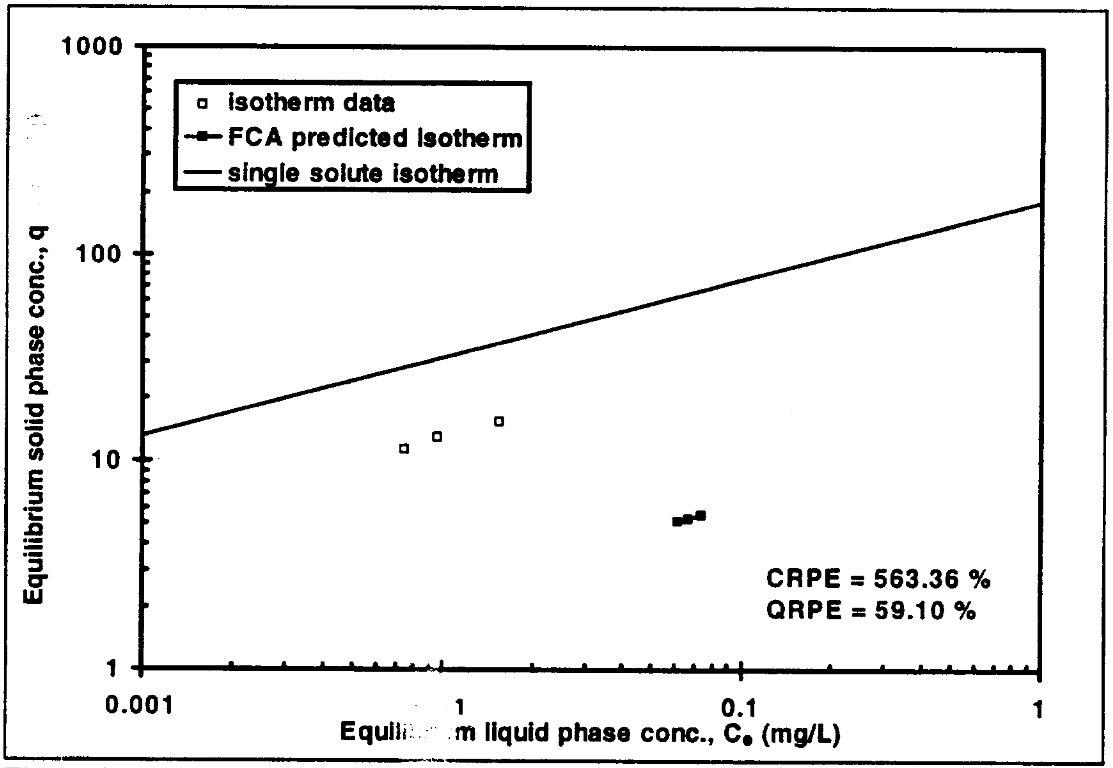

Figure 3-39. Dilute naphthalene tracer isotherm predicted on APA GAC for urine distillate.

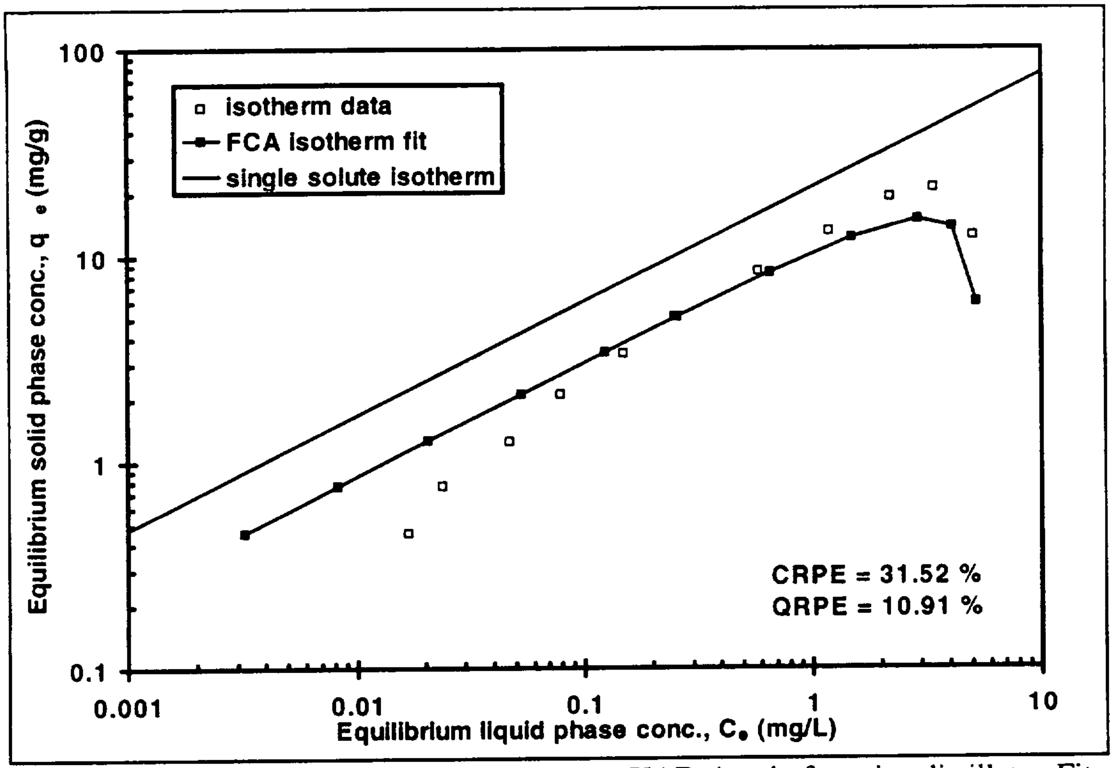

Figure 3-40. Nondilute TCE tracer isotherm on XAD-4 resin for urine distillate. Fit simultaneously with the dilute TCE tracer isotherm.

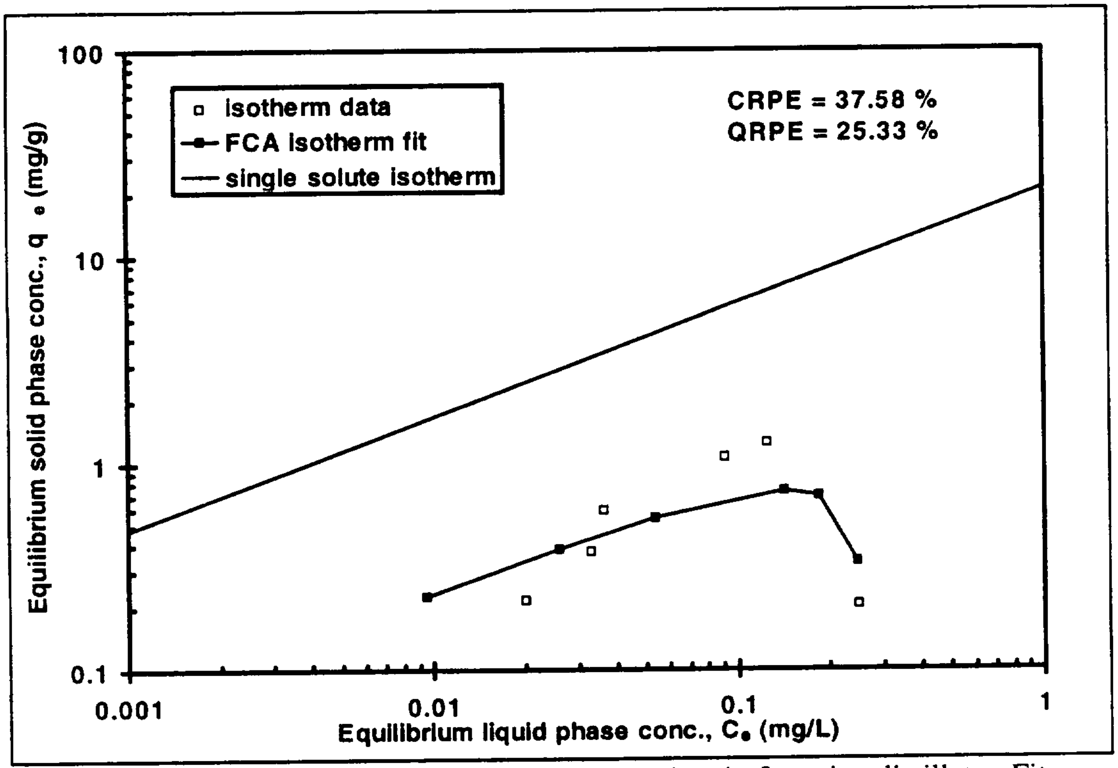

Figure 3-41. Dilute TCE tracer isotherm on XAD-4 resin for urine distillate. Fit simultaneously with the nondilute TCE tracer isotherm.

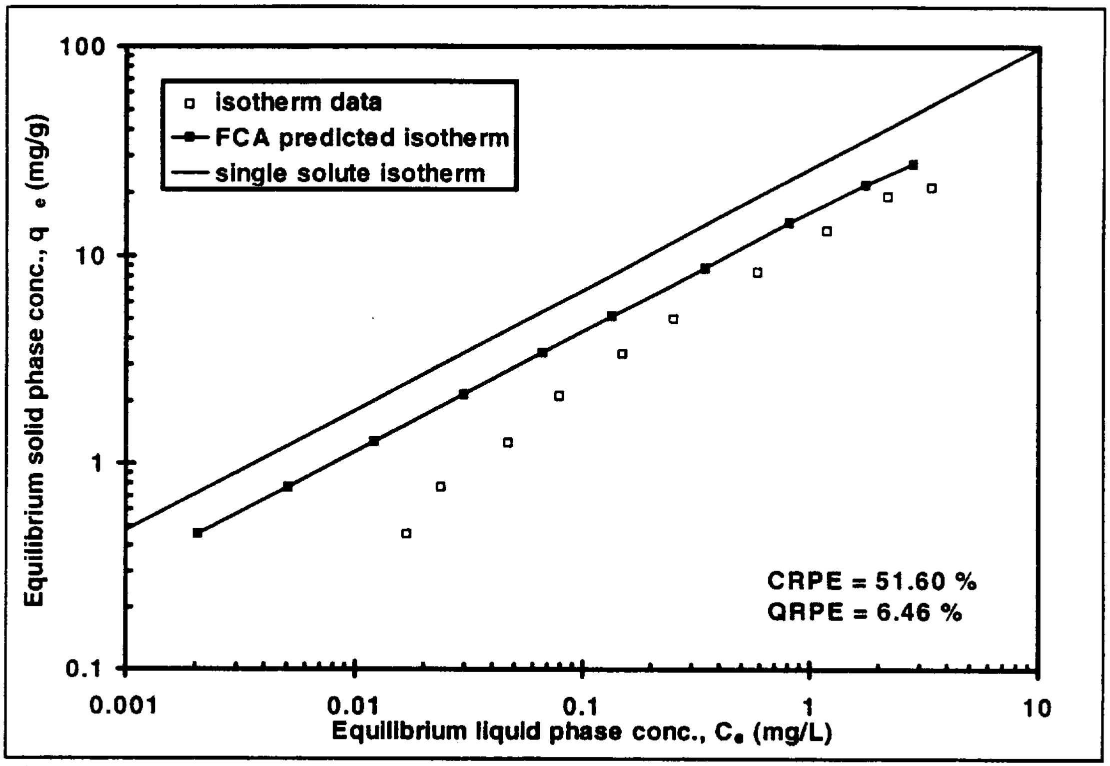

Figure 3-42. Nondilute toluene tracer isotherm predicted on XAD-4 resin for urine distillate.

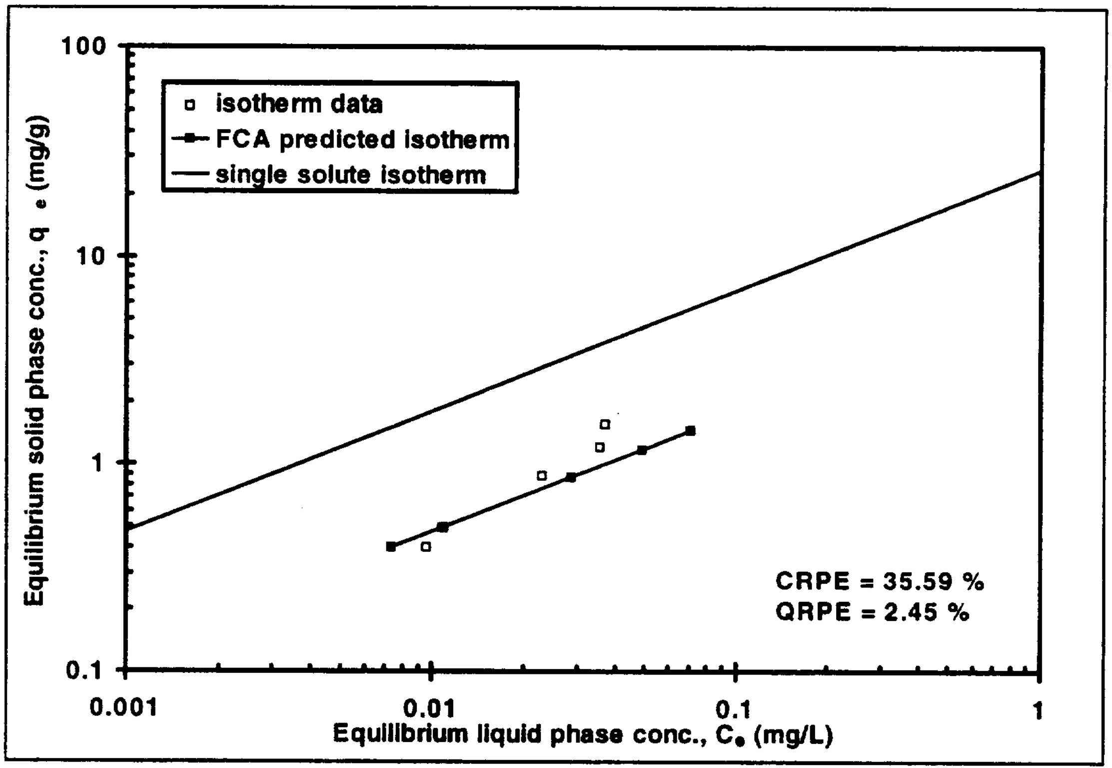

Figure 3-43. Dilute toluene tracer isotherm predicted on XAD-4 resin for urine distillate.

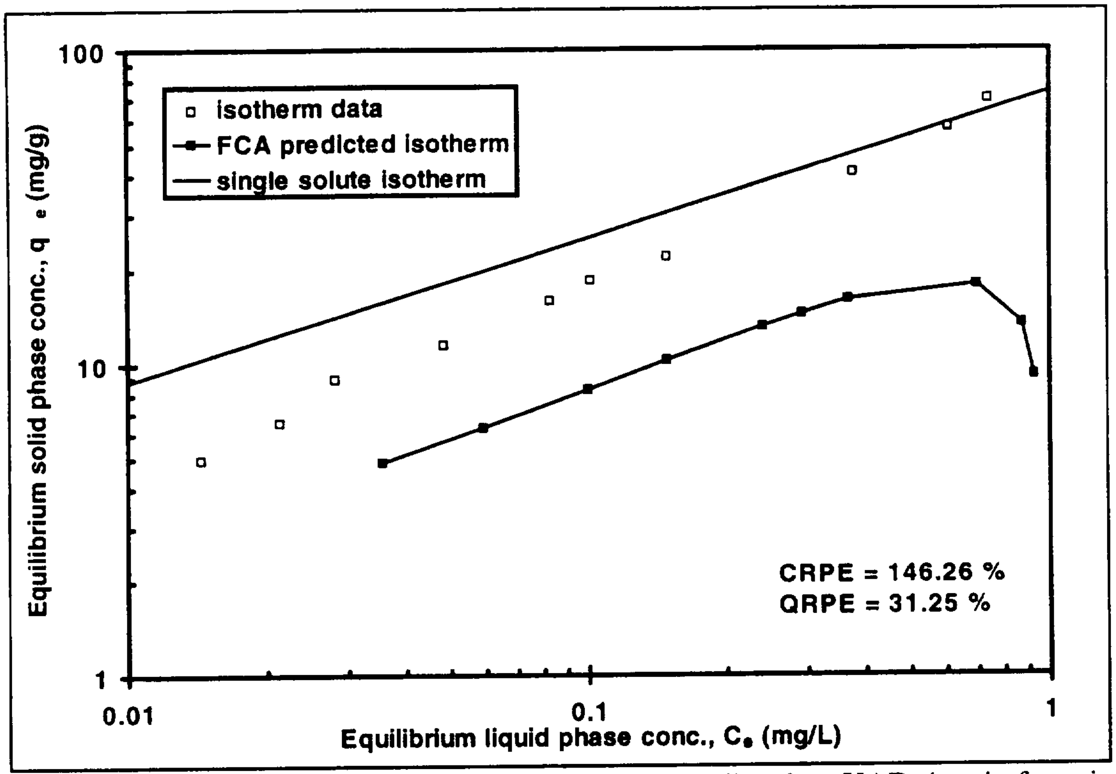

Figure 3-44. Nondilute naphthalene tracer isotherm predicted on XAD-4 resin for urine distillate.

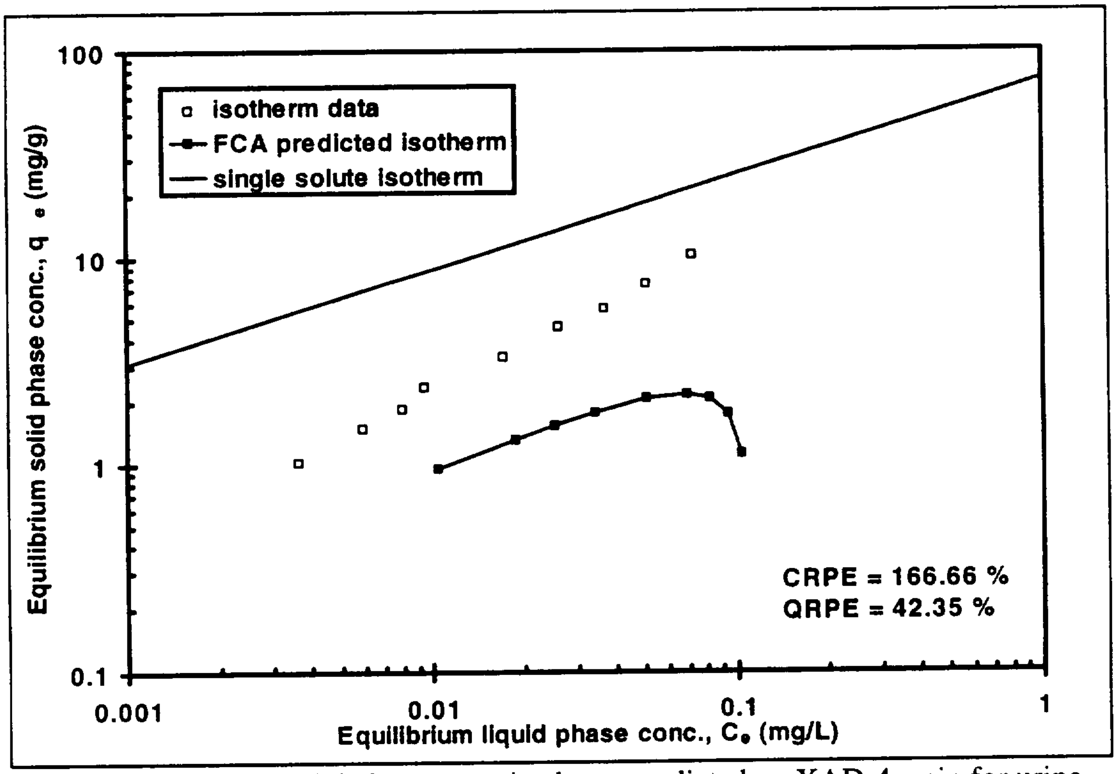

Figure 3-45. Dilute naphthalene tracer isotherm predicted on XAD-4 resin for urine distillate.

3.4.4 HUMIDITY CONDENSATE STREAM

3.4.4.1 Tracer FC Results for 580-26 GAC. The humidity condensate nondilute and dilute TCE tracer isotherms on 580-26 GAC were fit simultaneously to determine the tracer FC concentrations. The approach used to fit and predict the tracer isotherms for humidity condensate is the same as was used for the waste mixture. The weakest adsorbing tracer compound spiked in humidity condensate was TCE, therefore the TCE tracer isotherms were fit simultaneously to determine the tracer FC concentrations. The tracer FC concentrations were then used to predict the toluene and naphthalene tracer isotherms.

The tracer FCs determined for humidity condensate on 580-26 GAC are included in Table 3-3. The tracer FCA isotherm fits and data are compared for the 580-26 nondilute and dilute TCE tracer isotherms in Figures 3-46 and 3-47, respectively. The TCE FCA isotherm fits for both the nondilute and dilute isotherms closely follow the isotherm data, accurately representing the reduction in capacity of the adsorbent due to competitive adsorption interactions of the unknown background matrix. Table 3-9 contains the RPE results for the tracer isotherm fits and predictions for humidity condensate on 580-26 GAC, APA GAC, and XAD-4 resin. The RPEs for the TCE isotherms show similar results with the error in the solid phase lower than the liquid phase.

Table 3-9. RPEs for humidity condensate tracer isotherm fits and predictions on 580-26 GAC, APA GAC, and XAD-4 resin.

		Nondilute waste mixture TOC isotherm			**Dilute waste mixture TOC isotherm**		
	Compound	**Relative % error**		**# of Data points**	**Relative % error**		**# of Data points**
		C	**q**		**C**	**q**	
580-26	TCE	11.13	6.56	9	24.59	6.13	7
	toluene	71.20	2.24	11	162.77	10.93	8
	naphthalene	112.72	15.48	10	195.78	48.27	10
APA	TCE	27.8	4.94	11	20.32	4.24	7
	toluene	8.00	1.65	12	92.35	5.20	10
	naphthalene	162.77	10.93	8	464.12	66.13	8
XAD-4	TCE	26.82	17.29	12	33.07	7.37	12
	toluene	28.45	11.81	10	72.42	25.94	12
	naphthalene	353.32	40.36	11	462.79	64.71	10

The 580-26 GAC tracer FCs were used in IAST calculations to predict nondilute and dilute toluene and naphthalene tracer isotherms on 580-26 GAC. These predictions were to determine if the tracer FCs from fitting the TCE tracer isotherms could predict equilibrium for other compounds in the stream. Figures 3-48 and 3-49 show the predicted nondilute and dilute toluene tracer isotherms on 580-26 GAC. The nondilute toluene prediction slightly overpredicts competitive adsorption in the water. The isotherm data indicates virtually no reduction in capacity relative to the single solute isotherm. The dilute toluene isotherm shows a slight reduction in capacity due to competitive adsorption. The dilute FCA predicted isotherm overestimates the reduction in capacity when compared to the isotherm data. This is a conservative prediction because the tracer FCs are determined to describe the maximum competition for the weakest adsorbing tracer compound. When stronger adsorbing tracer compounds are predicted using the tracer FCs, the competition is overestimated because the FCs have been calibrated to show the competition based on the weakest adsorbing tracer compound. The nondilute and dilute naphthalene tracer isotherm predictions are presented in Figures 3-50 and 3-51, respectively. Both cases show the FCA predicted isotherm overpredicts competitive adsorption in humidity condensate. The RPEs indicate much larger error in the liquid phase than the solid phase.

The TOC isotherms show humidity condensate is weakly adsorbing. Due to the weakly adsorbing nature of humidity condensate, the tracer isotherms overall fit very well. The comparison of the reduction in capacity of the tracer compounds shows theoretical trends are followed, with the reduction in capacity of the weaker adsorbing tracers to be greater than the strongly adsorbing tracer compounds.

3.4.4.2 Tracer FC Results for APA GAC. The tracer FC concentrations determined when fitting TCE tracer isotherms on 580-26 GAC were held constant as humidity condensate passes through the other adsorbents in series. The tracer FC concentrations were scaled to equal the adsorbing TOC concentration for APA GAC. The humidity condensate TCE nondilute and dilute tracer isotherms on APA GAC were fit simultaneously optimizing FC Freundlich Ks. FC Freundlich 1/n was correlated to FC Freundlich K for APA GAC. The tracer FC parameters for APA GAC on humidity condensate are presented in Table 3-5. Figures 3-52 and 3-53 show the humidity condensate nondilute and dilute TCE FCA tracer isotherm fits on APA GAC, respectively. The results indicate the FC parameters accurately describe the competitive adsorption in humidity condensate. The nondilute TCE FCA tracer isotherm fit slightly underpredicts competitive adsorption, and the dilute TCE FCA tracer isotherm fit slightly overpredicts competitive adsorption. This occurs because the isotherms are fit simultaneously to fit a range of TCE concentrations. The RPE results are summarized in Table 3-9 for the tracer fits and predictions. The RPEs for the TCE isotherms are similar.

The APA FC results when fitting TCE tracer isotherms simultaneously were used to determine if other compounds on APA GAC could be predicted. Nondilute and dilute toluene and naphthalene tracer isotherms were predicted using the APA FC parameters in IAST calculations. The nondilute and dilute toluene tracer isotherms are shown in Figures 3-54 and 3-55, respectively. The nondilute toluene tracer isotherm prediction accurately predicts the competitive adsorption in the unknown background matrix, with RPEs below 10 percent. The dilute toluene tracer isotherm prediction overpredicts the competitive adsorption, relative to the toluene single solute isotherm. The nondilute and dilute naphthalene tracer isotherms are shown in Figures 3-56 and 3-57. The nondilute and dilute naphthalene tracer isotherm predictions both overpredict the competitive adsorption in the humidity condensate stream. RPEs for the naphthalene predictions indicate a large amount of error in the solid phase concentrations.

3.4.4.3 Tracer FC Results for XAD-4 resin. The tracer FCs for XAD-4 resin were determined by applying the same procedure used to determine the tracer FCs for APA GAC. Table 3-6 includes the humidity condensate tracer FC results for XAD-4 resin. TCE nondilute and dilute tracer isotherms were fit simultaneously to determine FC Freundlich K values. The results of the TCE nondilute and dilute isotherm fits are presented in Figures 3-58 and 3-59. The nondilute TCE tracer isotherm prediction overpredicts competitive adsorption at lower adsorbent dosages and slightly underpredicts competitive adsorption at the high adsorbent dosages. The dilute TCE tracer isotherm prediction underestimates the competitive adsorption in the stream at high adsorbent dosages. Figures 3-60 and 3-61 show the humidity condensate nondilute and dilute toluene tracer isotherm predictions on XAD-4 resin. The nondilute toluene tracer isotherm prediction is similar to the nondilute TCE tracer isotherm fit. The dilute toluene tracer isotherm overpredicts competitive adsorption at the low dosages and slightly underpredicts the competition at high dosages. Figures 3-62 and 3-63 are the nondilute and dilute naphthalene tracer isotherm predictions using the XAD-4 FC parameters in IAST calculations. The naphthalene tracer isotherm predictions overpredict competitive adsorption in the unknown background matrix, for both the nondilute and dilute isotherms. The RPEs for the fits and predictions are summarized in Table 3-9.

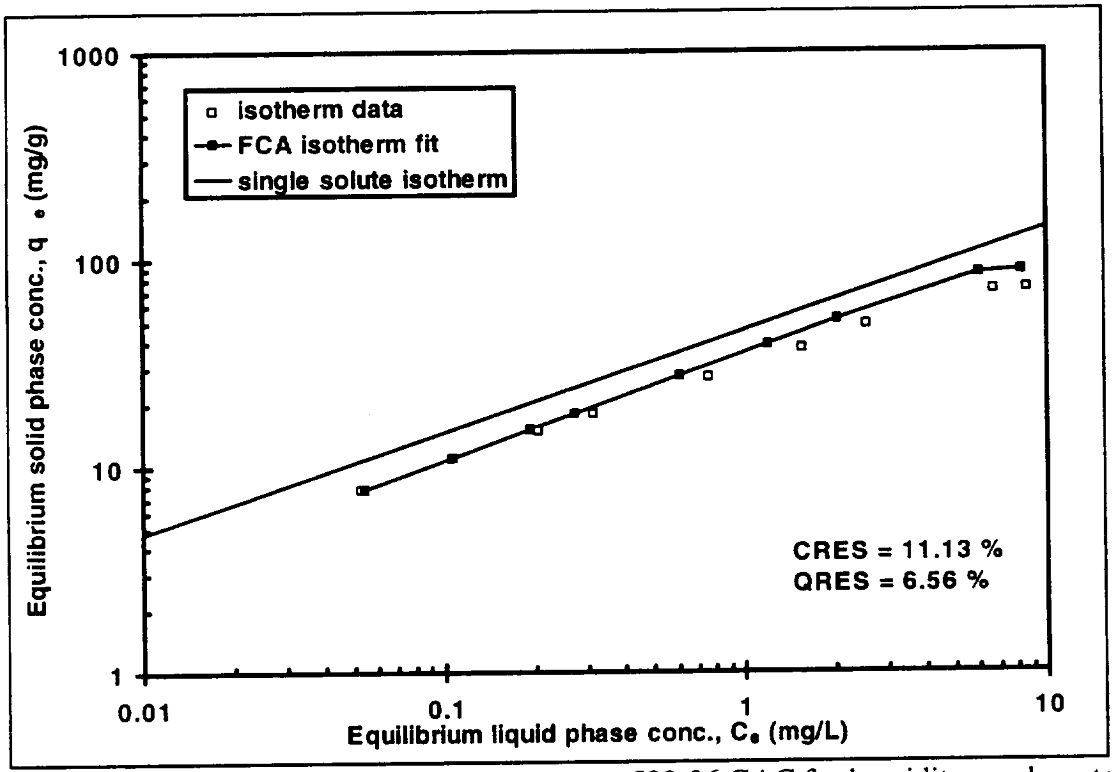

Figure 3-46. Nondilute TCE tracer isotherm on 580-26 GAC for humidity condensate. Fit simultaneously with the dilute TCE tracer isotherm.

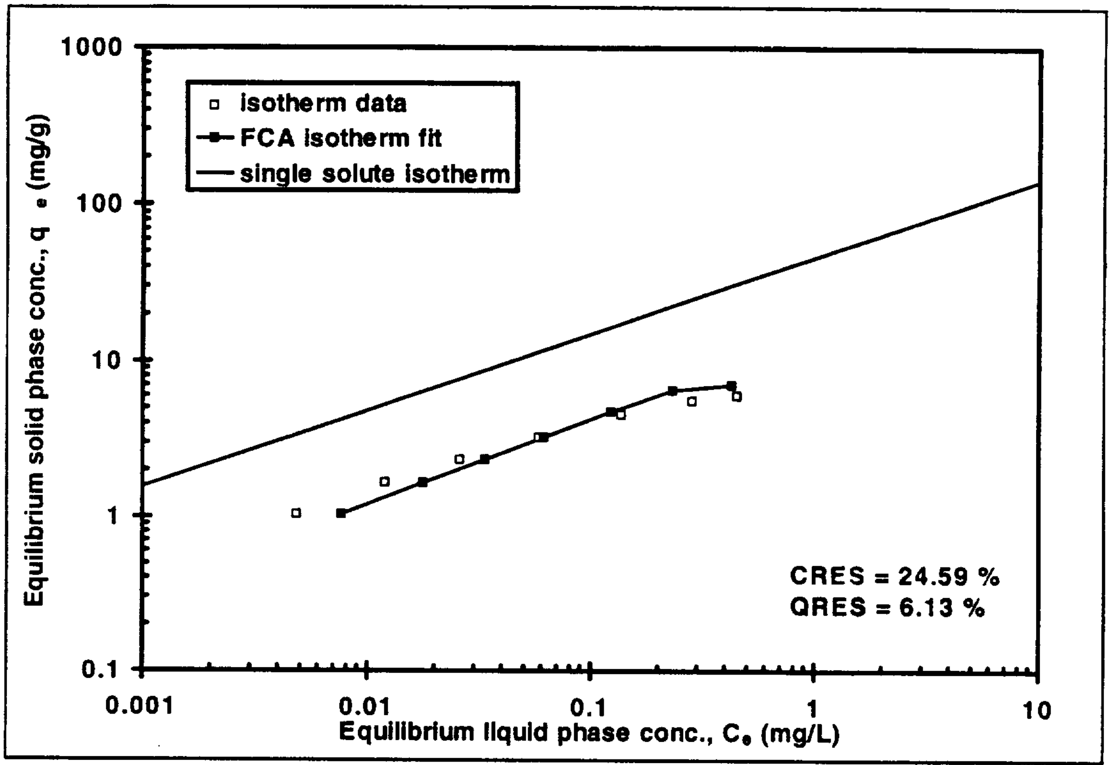

Figure 3-47. Dilute TCE tracer isotherm on 580-26 GAC for humidity condensate. Fit simultaneously with the nondilute TCE tracer isotherm.

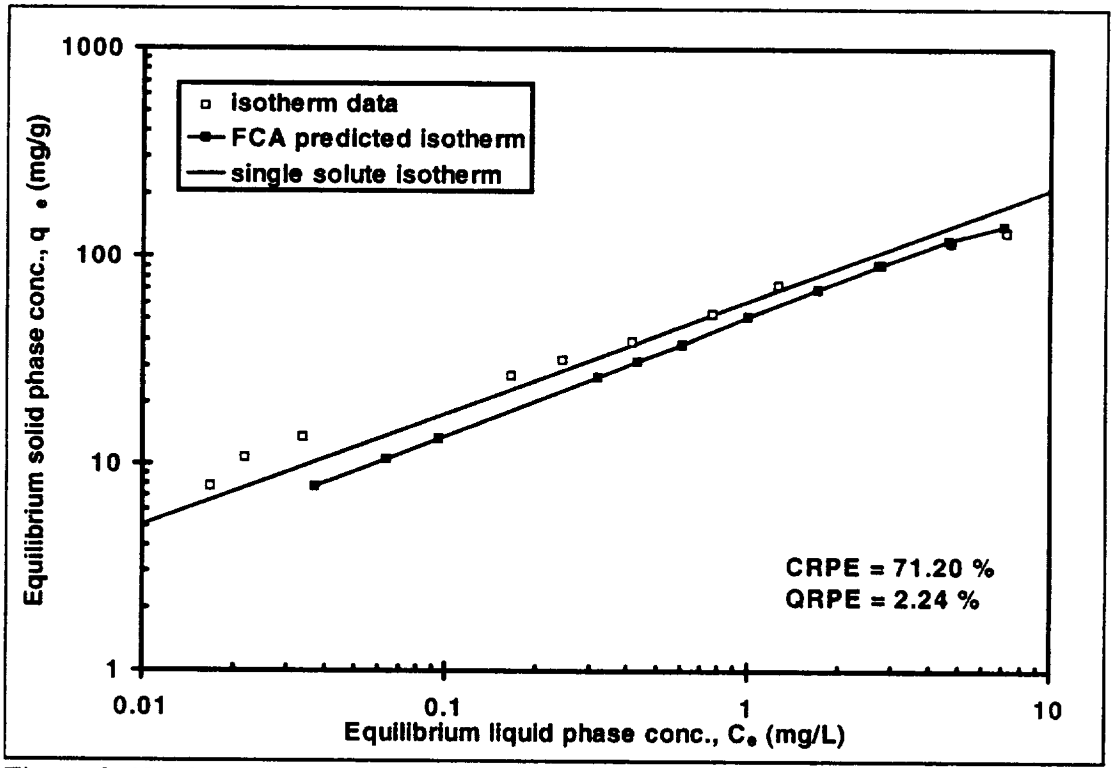

Figure 3-48. Nondilute toluene tracer isotherm predicted on 580-26 GAC for humidity condensate.

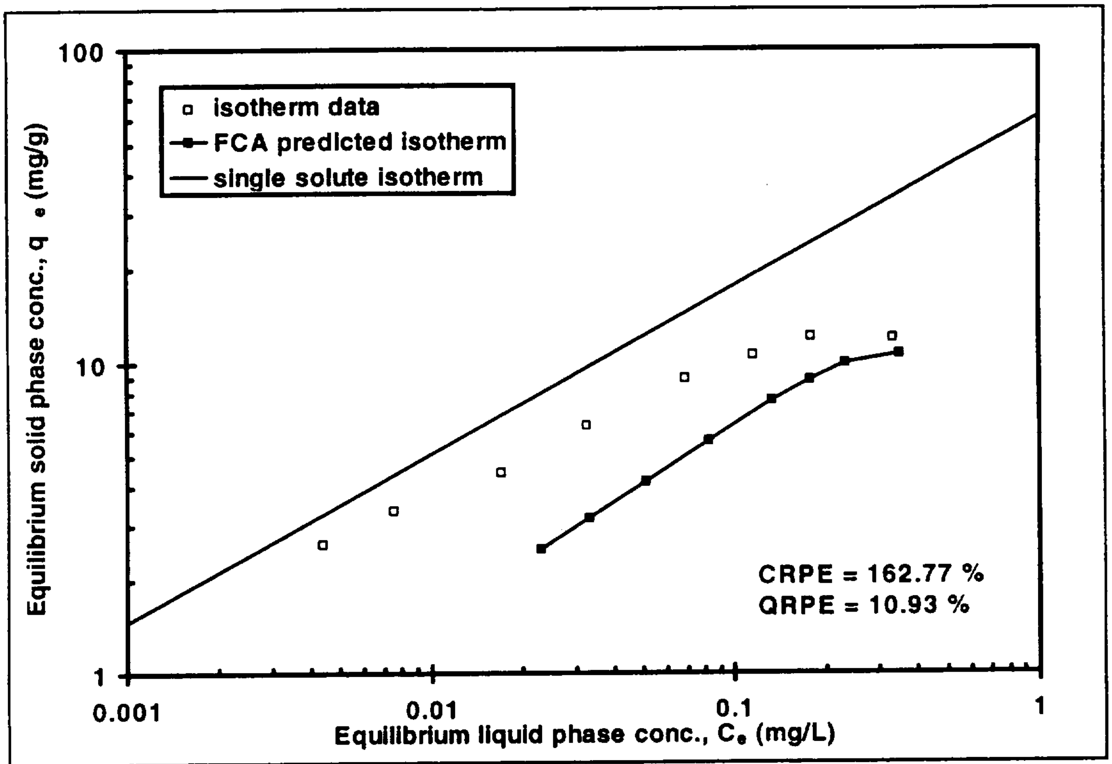

Figure 3-49. Dilute toluene tracer isotherm predicted on 580-26 GAC for humidity condensate.

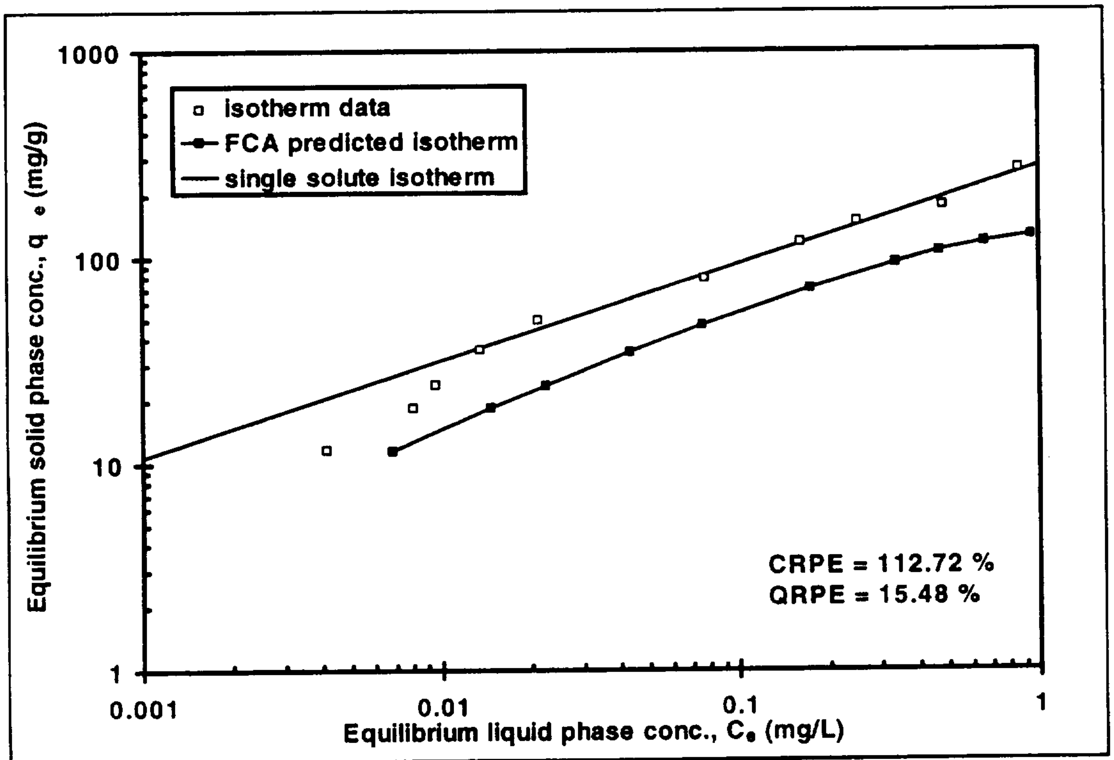

Figure 3-50. Nondilute naphthalene tracer isotherm predicted on 580-26 GAC for humidity condensate.

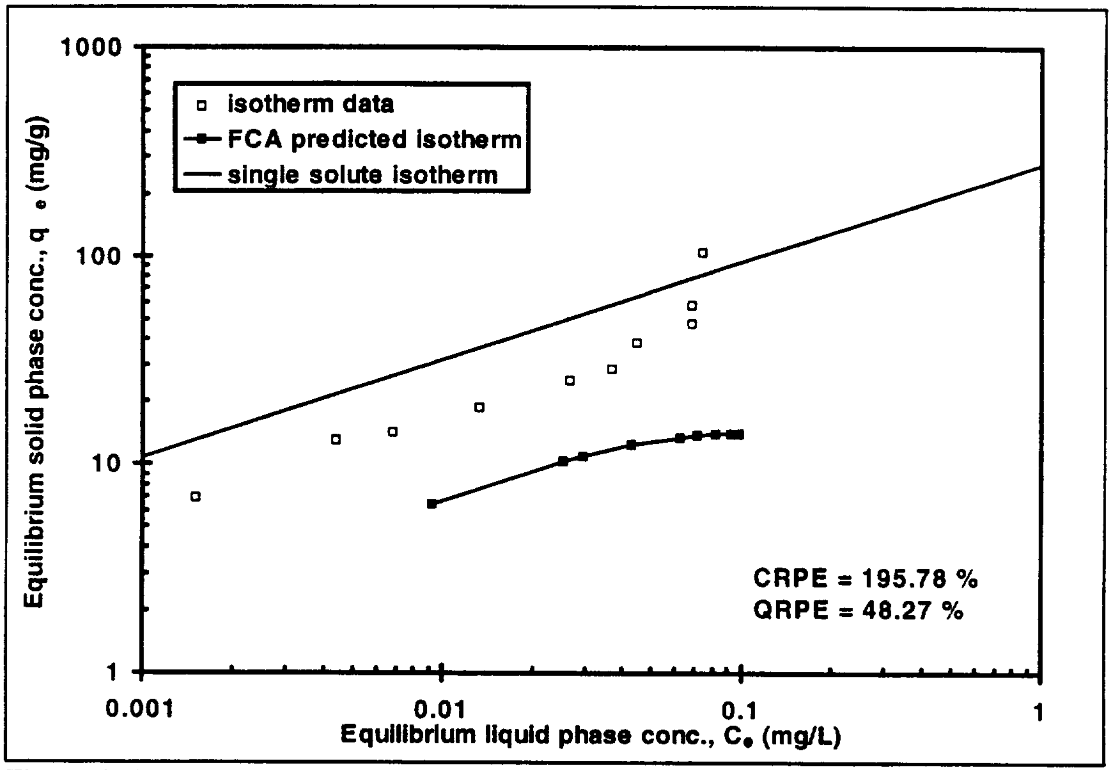

Figure 3-51. Dilute naphthalene tracer isotherm predicted on 580-26 GAC for humidity condensate.

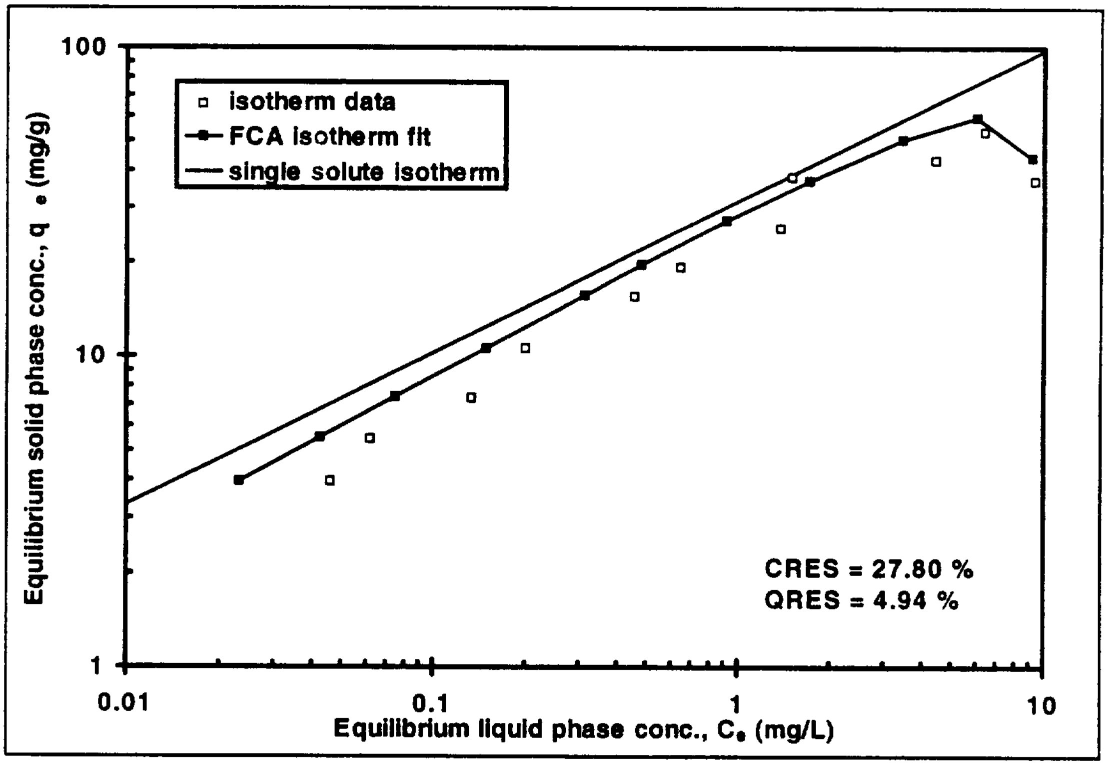

Figure 3-52. Nondilute TCE tracer isotherm fit on APA GAC for humidity condensate. Fit simultaneously with the dilute TCE tracer isotherm.

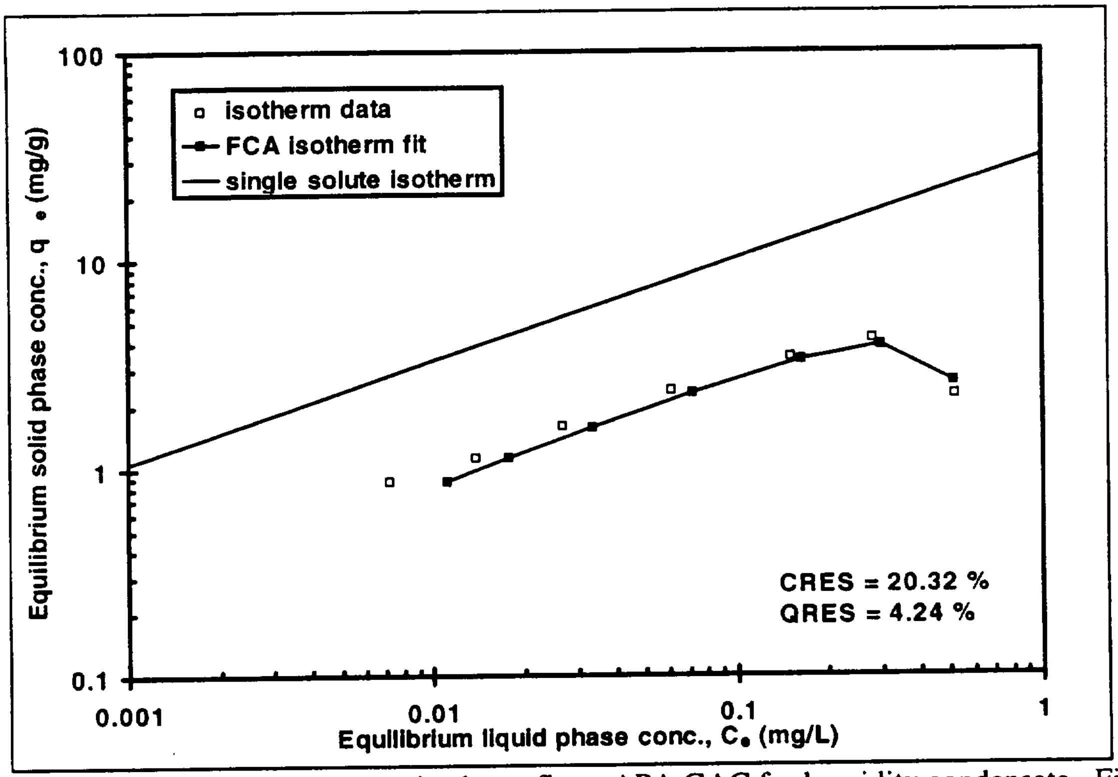

Figure 3-53. Dilute TCE tracer isotherm fit on APA GAC for humidity condensate. Fit simultaneously with the nondilute TCE tracer isotherm fit.

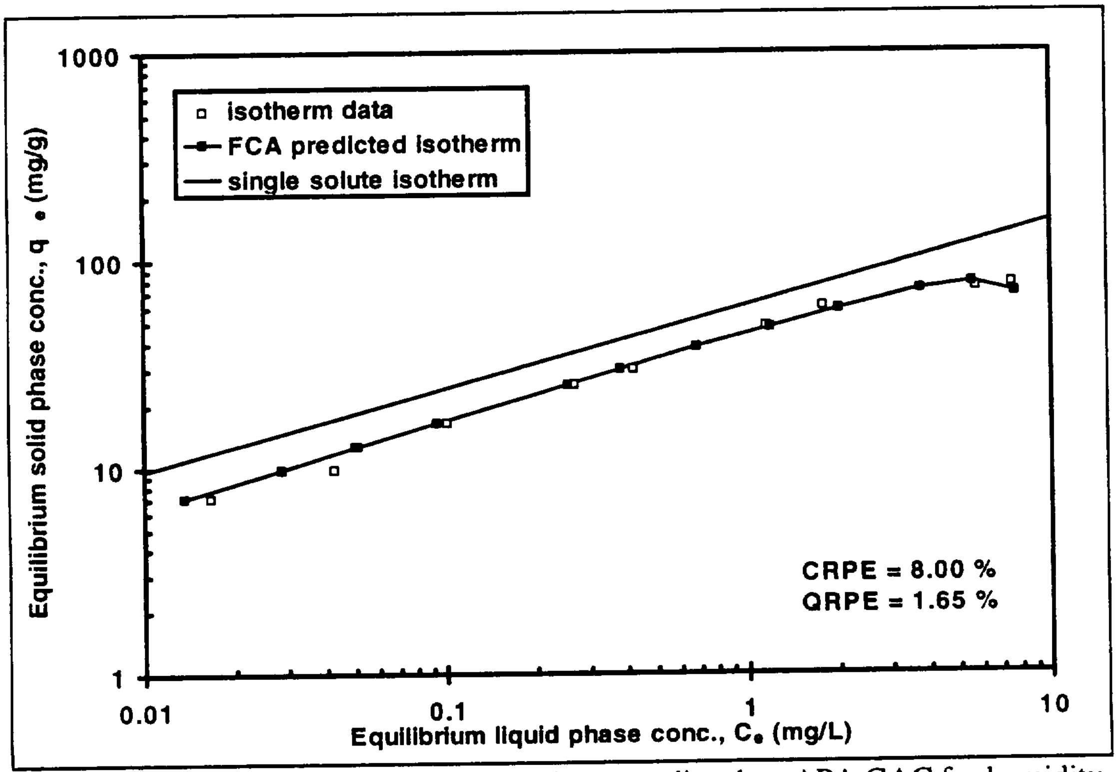

Figure 3-54. Nondilute toluene tracer isotherm predicted on APA GAC for humidity condensate.

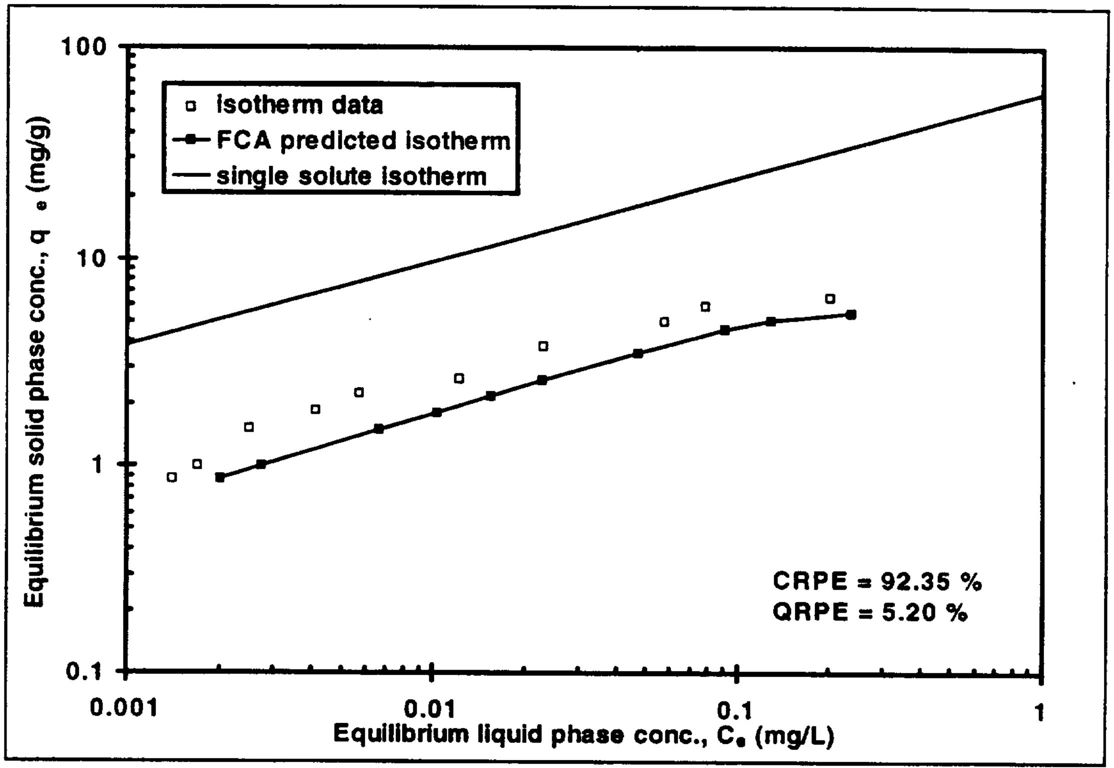

Figure 3-55. Dilute toluene tracer isotherm predicted on APA GAC for humidity condensate.

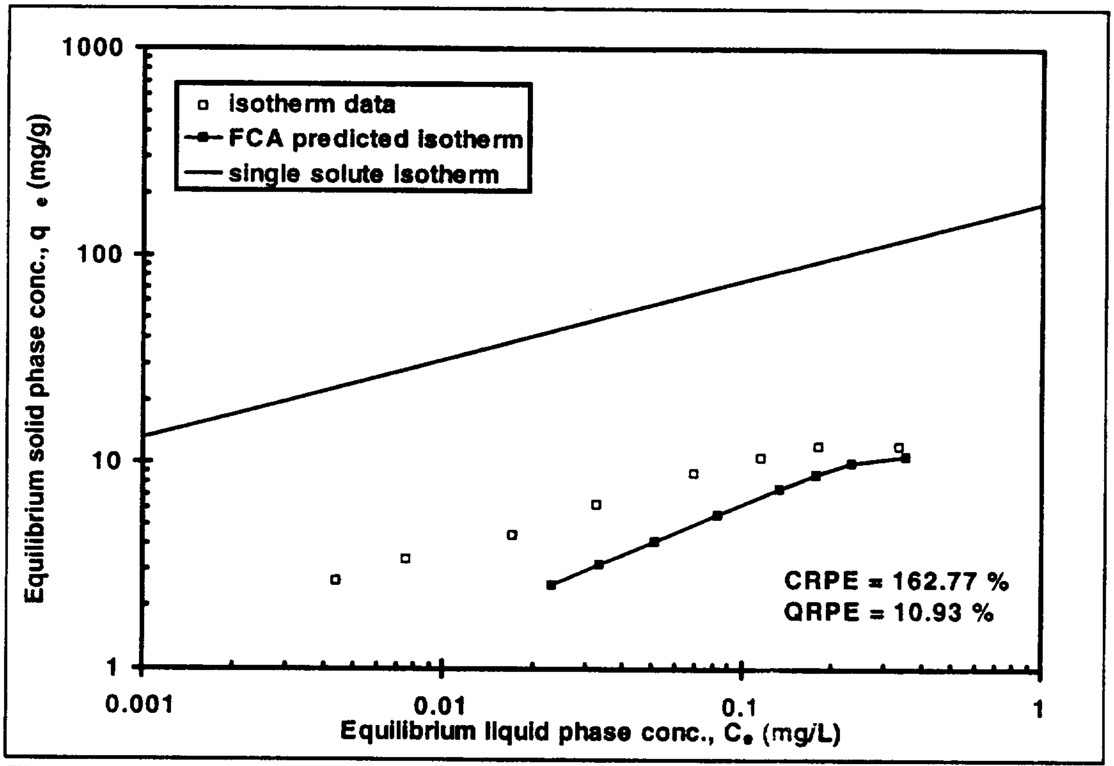

Figure 3-56. Nondilute naphthalene tracer isotherm predicted on APA GAC for humidity condensate.

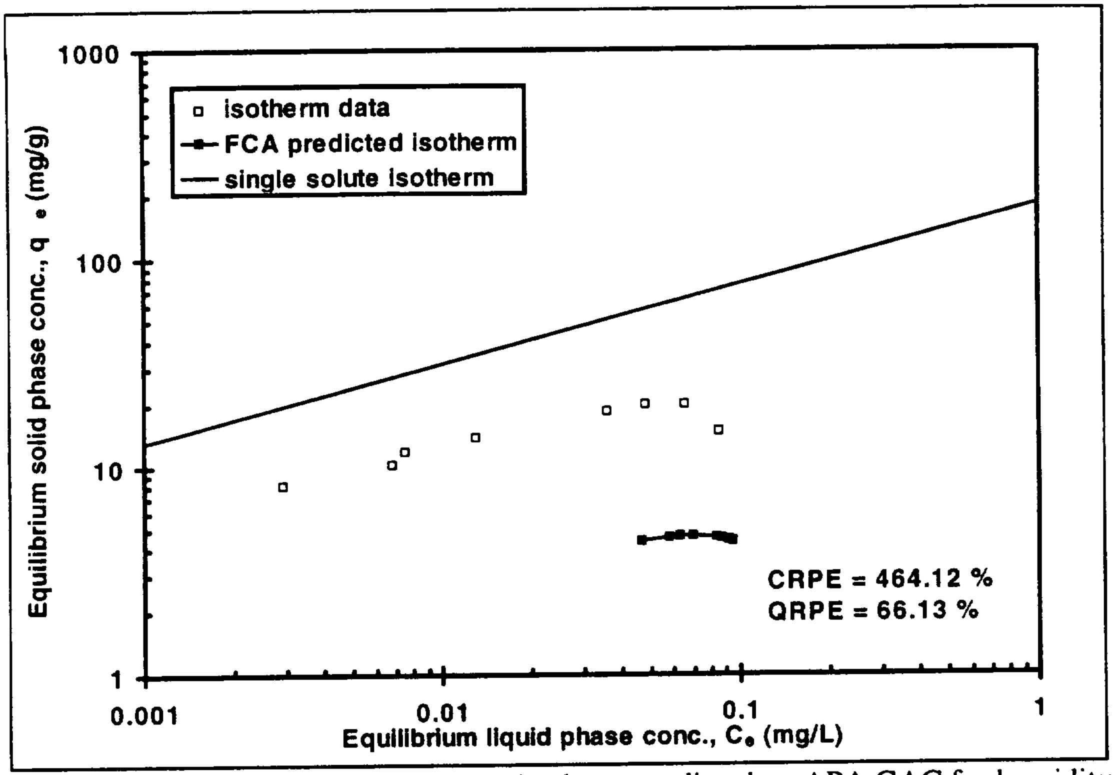

Figure 3-57. Dilute naphthalene tracer isotherm predicted on APA GAC for humidity condensate.

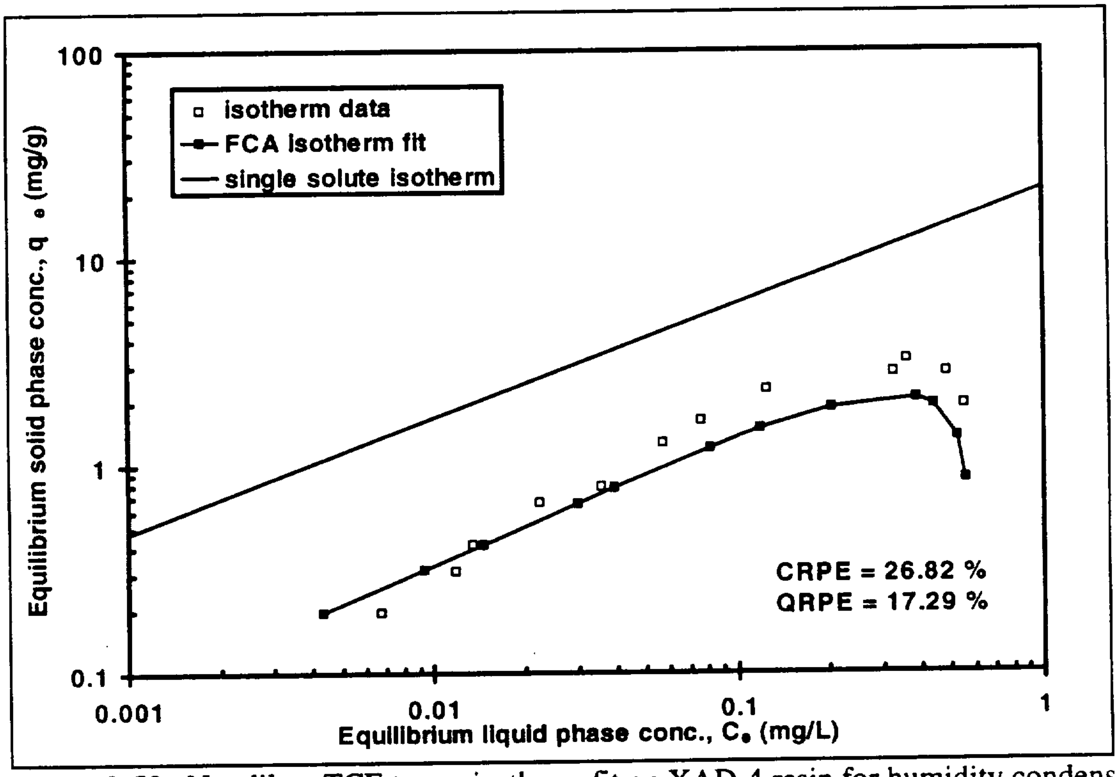

Figure 3-58. Nondilute TCE tracer isotherm fit on XAD-4 resin for humidity condensate. Fit simultaneously with the dilute TCE tracer isotherm.

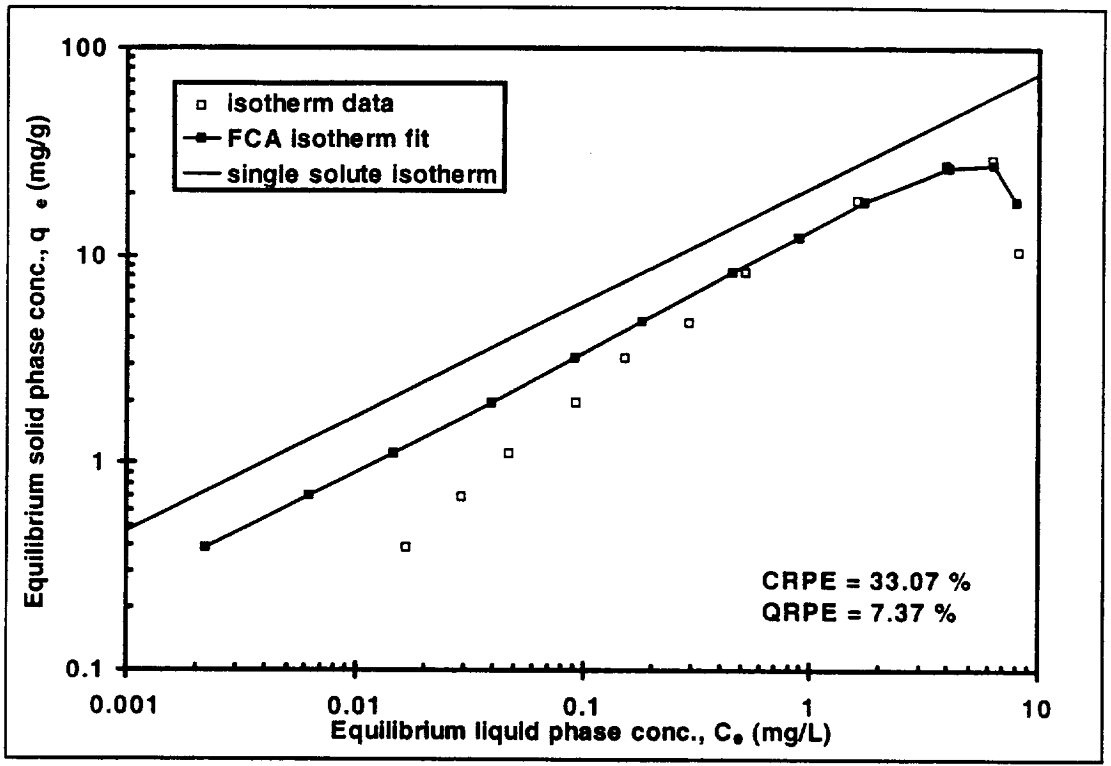

Figure 3-59. Dilute TCE tracer isotherm fit on XAD-4 resin for humidity condensate. Fit simultaneously with the nondilute TCE tracer isotherm.

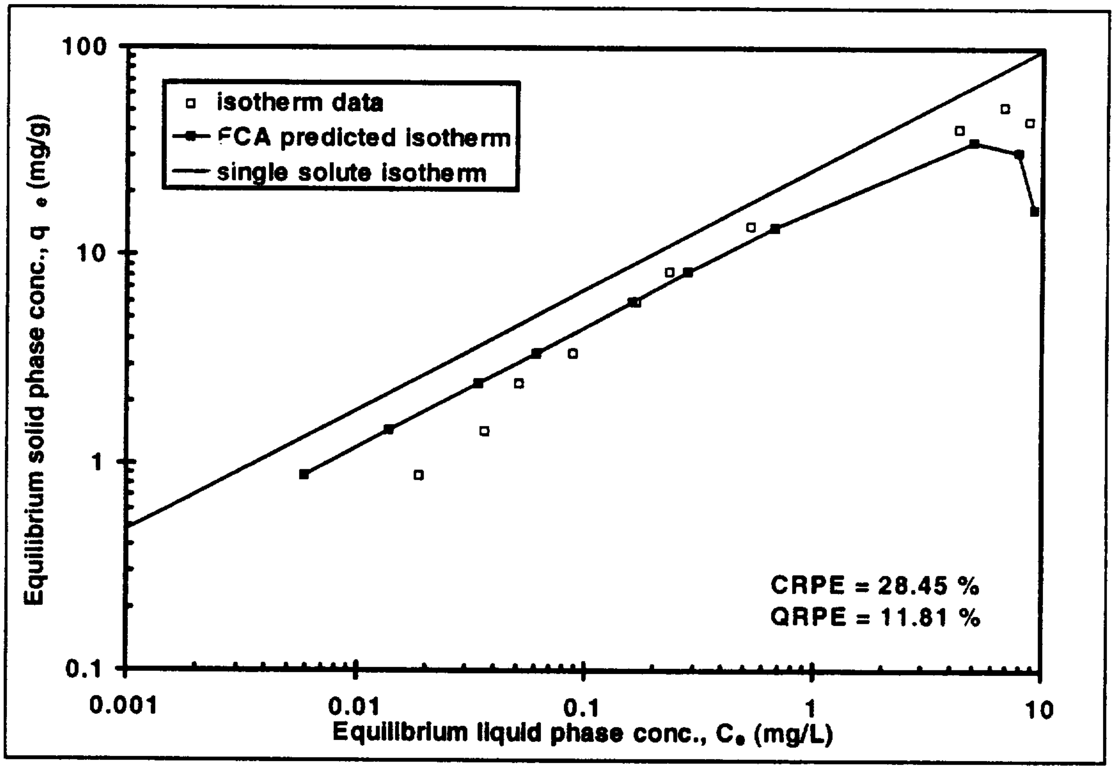

Figure 3-60. Nondilute toluene tracer isotherm predicted on XAD-4 resin for humidity condensate.

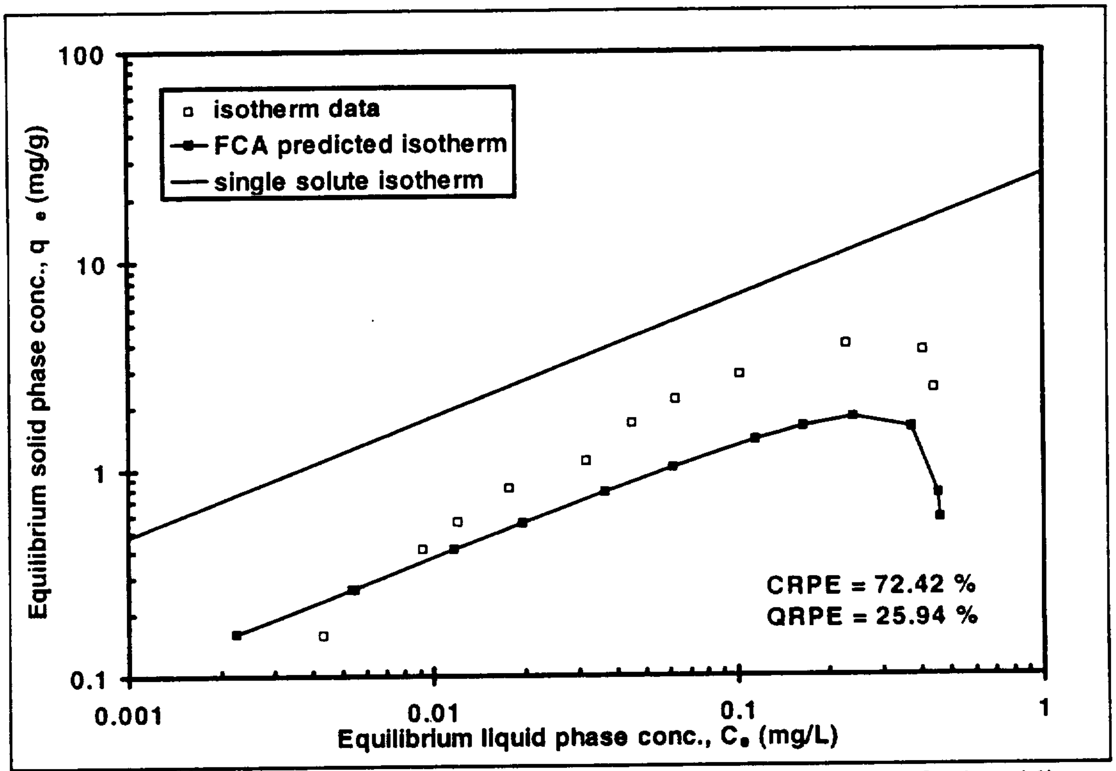

Figure 3-61. Dilute toluene tracer isotherm predicted on XAD-4 resin for humidity condensate.

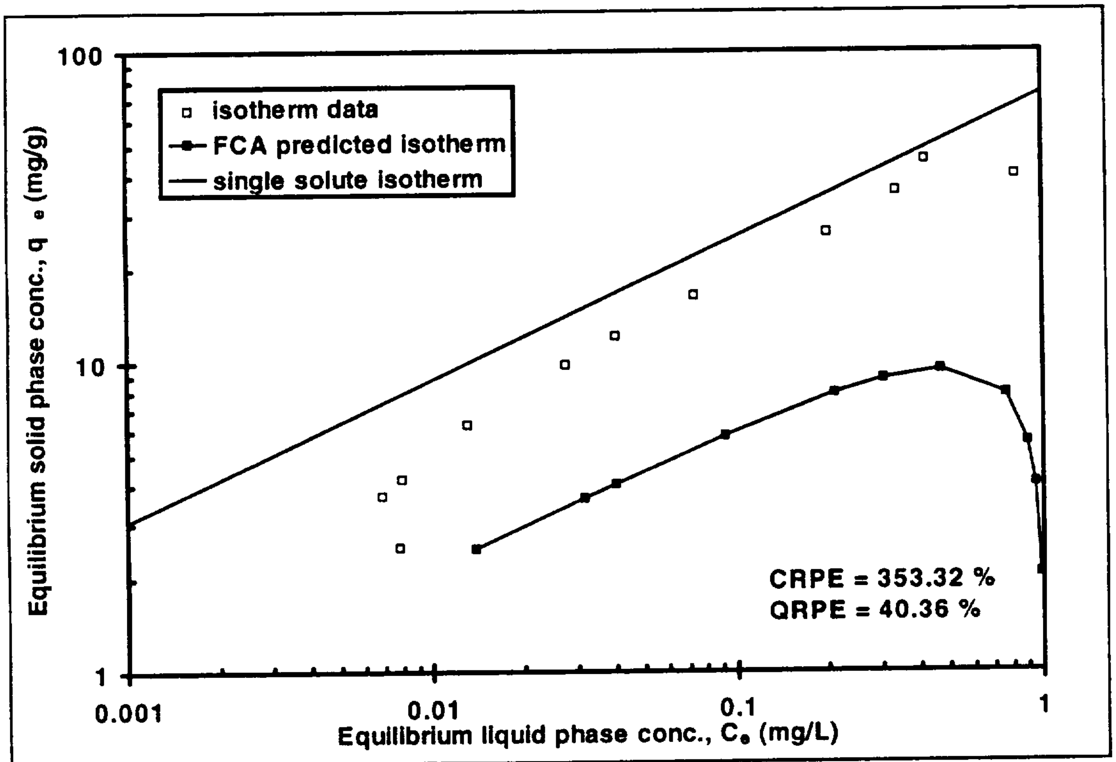

Figure 3-62. Nondilute naphthalene tracer isotherm predicted on XAD-4 resin for humidity condensate.

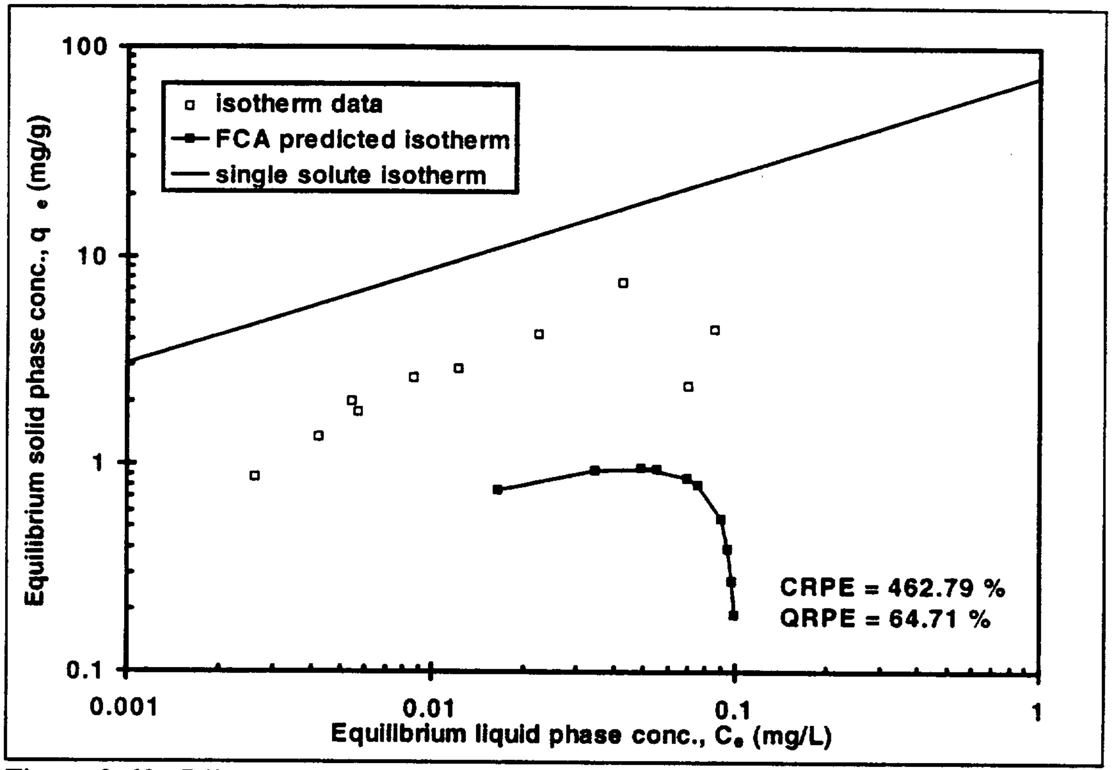

Figure 3-63. Dilute naphthalene tracer isotherm on XAD-4 resin for humidity condensate.

4.0 CONCLUSIONS AND FUTURE WORK

Multicomponent adsorption equilibrium was investigated on 580-26 GAC, APA GAC and XAD-4 resin using four different waste streams: waste mixture, shower/handwash mixture, urine distillate and humidity condensate. The waste streams represent the wastewater generated on the ISS. Fictive component analysis was used to describe the competitive interactions occurring in the unknown background waters. TOC and tracer fictive component parameters including molecular weight, fraction of carbon, Freundlich K and 1/n, and initial concentration were determined for each adsorbent on each waste stream. TOC and tracer isotherms were performed on each of the adsorbents using the four waste waters. The isotherms were fit to determine the FC parameters using a method that would facilitate modeling the adsorbent beds in series.

TOC FC parameters were determined by fitting a nondilute and dilute TOC isotherm simultaneously using FCA. FC concentrations were optimized on 580-26 GAC and held constant through the bed. FC Freundlich K was the fitting parameter for APA GAC and XAD-4 resin. The TOC FC parameters for the waste, shower/handwash and urine distillate mixtures accurately describe the competitive adsorption occurring in the unknown background matrices of these mixtures. The TOC FC parameters for the humidity condensate stream were less accurate because of the weakly adsorbing nature of the compounds in this stream. A set of fictive components with lower K values could be used to better describe the humidity condensate and urine distillate TOC isotherms because they contain weaker adsorbing compounds than the waste and shower/handwash mixtures.

The tracer FC parameters were determined by fitting the weakest adsorbing tracer compound and then using the FC parameters to predict other tracer compounds in the waters. The tracer FC parameters were optimized similar to the TOC FC parameters. FC concentration was optimized on 580-26 GAC and FC Freundlich K was fit for APA GAC and XAD-4 resin. The tracer FC parameters for the waste and shower/handwash mixtures were determined by fitting the MC tracer isotherms simultaneously on each adsorbent. The FC parameters overestimated the reduction in capacity of MC on 580-26 and APA GACs. The FC parameters were then used to predict chloroform in both mixtures and PCE in the waste mixture. The predictions for chloroform accurately determined the displacement of the isotherm from its single solute. The reduction in capacity of PCE in the waste mixture was underestimated using the tracer FCs. The urine distillate tracer FCs were determined by fitting the TCE tracer isotherms simultaneously on each adsorbent. TCE's reduction in capacity from its single solute was accurately determined in most cases. The FC parameters were then used to predict toluene and naphthalene tracer isotherms. Toluene was also accurately described on each adsorbent where naphthalene's reduction in capacity was overpredicted. The humidity condensate FC parameters determined by fitting the TCE tracer isotherms and the toluene and naphthalene tracer isotherms were then predicted. The tracer FCs were able to describe the reduction in capacity of TCE and toluene. The reduction in capacity of the naphthalene tracer isotherms was overpredicted using the tracer FCs.

The fictive component parameters determined in this work describe the competitive adsorption in the waste streams. Combining these FC parameters in the MFB model will allow column predictions of different waste streams as they pass through both the ion exchange resins and the adsorbents. The tracer fictive components allow the prediction of known compounds in the waste streams. The tracer FCs can be used to predict a known compound through the MFB if the FC parameters: Freundlich K and 1/n, molecular weight, fraction of carbon and concentration of the known compound can be determined. The ability to predict the MFB performance will aid in designing pilot plant studies as well as determining the most efficient MFB design. The MFB model will also be used to simulate MFB performance when unexpected changes in the feed stream occur.

This research was conducted on four different waste streams. Further work should be conducted to determine the effect of changing major components and their concentration in the waste water. It should be verified if the FC parameters determined in this work describe the waste streams with these changes in components and concentrations. A second aspect of this research which should be further investigated is the assumption that the waste stream is an ideal solution. IAST assumes the solution is ideal, if this is an invalid assumption how can IAST be applied to a non-ideal solution.

The urine distillate and humidity condensate waste streams do not contain SCMT and it is observed the weakly adsorbing tracer compounds exhibit a greater reduction in capacity from their single solute as is expected. The waste and shower/handwash mixtures which do contain SCMT show less of a reduction in capacity from the single solute for the weakly adsorbing tracer compounds. This may be explained by the kinetics and the competition the weakly adsorbing compounds have with the SCMT. More accurate tracer isotherm data should be obtained to more accurately describe the tracer equilibrium data.

5.0 NOMENCLATURE

$C_{e,i}$ = equilibrium liquid phase concentration of compound i
$C_{o,i}$ = initial liquid phase concentration of compound i
C_i/C_{total} = relative concentration of compound in the waste streams
K_i = Freundlich isotherm capacity constant $[(M/L^3)(L^3/M)^{1/n}]$
M = mass of adsorbent added to isotherm bottle (M)
$1/n_i$ = Freundlich isotherm intensity constant (dimensionless)
N = number of compounds in each group or number of isotherm points fit
NC = number of fictive components
P_{WA} = weighted average parameter
P_i = parameter for compound i
$q_{e,i}$ = equilibrium solid phase concentration (M/M)
V = volume of isotherm bottle (L^3)

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APPENDIX I. Multifiltration Bed Influent Wastewaters

Compound	Carbon Fraction	Humidity Condensate	Shower Handwash	Clothes Wash	Urine Distillate
		ug/L	ug/L	ug/L	ug/L
Total Organic Carbon (TOC)		50000	704000	101600	11100
Acenapthylene	0.947		10	8	
Acetaldehyde	0.545	170		26	330
Acetic Acid	0.4	8000	10800	11000	990
Acetone	0.621	500	60	98	353
Acetophenone	0.8				2.2
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	0.837			47	
4-Acetyl morpholine	0.558	2100			
Acetyloxyoctadecenoic acid, Methyl ester	0.704			5	
Adipate	0.493				22
Alphahydroxybenzeneneacetic acid ester	0.651				33
Amine(unknown)	0.6	170			
2-Amino benzoic acid methyl ester	0.636				1
Benzaldehyde	0.792	10			9
Benzene	0.923	1		1	
Benzeneacetic acid	0.706	4	64		24
Benzene ethanol	0.787	50		8	
Benzene methanol	0.778	380			
Benzoic Acid	0.689	150	50	60	660
Benzophenone	0.857	5			
2H-1-Benzopyran-2-one	0.74	4			
Benzothiazole	0.622	40		8	
Benzyl alcohol	0.778	200		5	33
1,1-Biphenyl-2-ol	0.847	10			
Bis(2-ethylhexyl)phthalate	0.738	10	150	15	33
Bis(1-methylethyl)ester hexadecanoic acid	0.626	30			
Bis(2-methypropyl)phthalate	0.691	6			
1,3-Butanedoid	0.533	14			6
Butanoic acid	0.545	70	44800	3040	1320
2-Butanol	0.649	1000	1600		
2-Butanone	0.667	50			34
2-Butoxyethanol	0.61	900	8	23	9
2-Butoxyethoxyethanol	0.593	500		18	
Butylated hydroxy anisole	0.733	60		14	
Butylbenzylphthalate	0.731	4			9
(1-Butylheptl) benzene	0.879			23	
(1-Butyloctyl) benzene	0.878			40	
Butyraldehyde	0.666	25			
Butyrolactone	0.558				22
C12 Alcohol	0.774			20	
C12+Aldehyde-methyloxime	0.723		20		
C11+ Alkylsubstituted benzene	0.878			75	
C4-Substituted cyclohexanol	0.784	20			
C5-7 Ketone	0.697				11
Caffeine	0.495		50	25	
Caprolactam	0.637	12000	1700	17	110
Carbon Disulfide	0.273	500			
4-Chloro aniline	0.565		10		
Chlorobenzene	0.352			14	
2-Chloroethanol phosphate	0.135	160			
Chloroform	0.101				18
1-Chloro-4-isocyanato benzene	0.549		9		
Chloromethylphenol	0.59				21
Chlorophenol	0.561	7			30
Cholesterol	0.839		1400	310	
Cis-p-menth-2-ene-1,8-diol	0.706				5
Cotinine	0.682		10		
Crotonaldehyde	0.685	10			

Cyclohexanone	0.734	100			
2-Cyclohexen-1-ol	0.72	1			
2-Cyclohexen-1-one	0.734	5			
1-(1-Cyclohexen-1-yl)ethanone	0.774				25
Cyclopentanone	0.714				5
Decanoic acid	0.69	100	40	23	12
Decanoic acid, Methyl ester	0.71		10		
1-Decanol	0.759		100		
1,4-diacetylbenzene	0.741	12			
Butyl amine	0.744	1000			51
di-n-Butylphthalate	0.691	100	5	7	
2,4-Dichloroaniline	0.445		5		
Dichlorobenzoic acid	0.44	20			
2,4-Dichlorophenol	0.442				15
Diethylene glycol	0.453	3			
Diethylene glycol diecetate	0.505	400			
Diethylphthalate	0.649	320	12	10	22
Dihydroacetic acid	0.387	4			
2,3-Dihydrobenzofuran	0.8				34
Dihydro-5,5-dimethyl-2(3H)-furanone	0.632				97
Dihydro-5-ethenyl-5-methyl-2H-furanone	0.667				72
Dihydro-5-ethyl-2H-furanone	0.632	28			121
1,3-Dihydro-2H-indol-2-one	0.722				9
Dihydro-5-methyl-2(3H)-furanone	0.612	33	30		212
2,3-Dihydro-4-methyl-1H-indole	0.812				10
1-(Dimethylamino)-2-propanol	0.588	85			
a,a-Dimethyl benzenemethanol	0.787	150			
Dimethylbenzyl alcohol	0.794	100			7
(3,3-Dimethyldecyl) benzene	0.878			28	
Dimethyl disulfate	0.255				14
4-(1,1-Dimethylethyl)-benzoic acid	0.741	16			
3-(1,1-Dimethylethyl)-phenol	0.8	50			
2,2-Dimethyl-1-(2-hydroxy-1-methylethyl) -propyl ester propanoic acid	0.667	73			
3,7-Dimethyl-1,5-octadien-3-ol	0.779	10			11
Dimethylphthalate	0.619	40			39
2,2-dimethyl propanoic acid	0.448	50			
2,3-Dimethylpyrazine	0.667				11
Dimethyl sulfide	0.387		25		
Dimethyl sulfone	0.255	140	76	75	75
Dimethylsulfoxide	0.307		10	9	
Dimethyltetrahydropyranone	0.656				8
2,6-Dinitrotoluene	0.454	80			
1,6-Dioxacyclododecane-7,12-dione	0.631	450			
Dipropyleneglycol methyl ether	0.568	50		12	
Docosane	0.852	10			
Docosanoic acid	0.776		80		
Docosanoic acid, methyl ester	0.78		190		
Dodecanal, o-methyloxime	0.732		440		
Dodecanoic acid	0.72	50	2250	160	78
Dodecanoic acid, methyl ester	0.729		900		
Dodecanol	0.774	6	160	43	
Eicosane	0.851	21			
Eicosanoic acid	0.769		180	41	
Eicosanoic acid, methyl ester	0.773		250		
2,2-[1,2-Ethaneoxybis(oxy)] bis-ethanoldiacetate	0.513	200			
Ethanol	0.522	7000	2400	500	3850
Substituted ethanone	0.65	40			
2-Ethoxyethanol	0.533	200			
Ethoxyethanol acetate	0.545	100			
Ethoxyethoxy ethanol	0.537	500		15	
Ethoxyethoxy ethanol acetate	0.539	25			
1-(2-Ethoxypropoxy)-2-propanol	0.592	130			

Ethylacetate	0.545				3
Ethyl benzene	0.905			8	
2-Ethyl-1-butanol	0.706				110
(1-Ethyldecyl) benzene	0.878			28	
Ethelene glycol	0.386	3000	790	310	
2-Ethyl hexanoic acid	0.667	500	4	21	5
2-Ethylhexanol	0.738	40	10	6	11
2-Ethylhexylphthalate	0.738			63	
4-Ethyl-2-methoxyphenol	0.71				5
4-ethyl morpholine	0.73	6600	910		187
1-Ethylnonyl) benzene	0.879			25	
1-Ethylpiperidine	0.743	26			
Formaldehyde	0.4	6000	120	120	127
Formic Acid	0.261	3000	3500		4400
Freon 113	0.141				
2-Furan methanol	0.612				65
2-(3H)-furanone	0.571	7		7	
Furanone, alkyl substituted	0.714				17
Glycerol	0.391	1400	110		
Glycol ether	0.3	420			
Glycolic acid	0.316	4000	3000		220
Hendecanoic acid	0.702		90		22
Heneicosanoic acid, methyl ester	0.776		40		
Heptacosane	0.853			46	
Heptadecane	0.85		5		
Heptadecanoic acid	0.755		130	48	
Heptadecanoic acid, methyl ester	0.761		50		
Heptanoic acid	0.646	200	3	6	11
4-Heptanol	0.724				6
4-Heptanone	0.737				41
Hexacosane	0.852	3		23	
Hexadecanoic acid	0.75	5	2450	340	3
9-Hexadecanoic acid, eicosyl ester	0.809		75	53	
Hexadecanoic acid, hexadectyl ester	0.799		90		
Hexadecanoic acid, methyl ethyl ester	0.626	26	600	9	
Hexadecanoic acid, octadectyl ester	0.803		50		
Hexadecanol	0.793		46	53	24
Hexadecenoic acid	0.756		230	190	11
Hexadecenoic acid, methyl ester	0.761	11	200		
2,4-Hexadienedioic acid	0.507	9			
Hexanal, o-methoxime	0.651		1360		
Hexanedioic acid, bis(1-metyhylethyl) ester	0.939	20			
2,5-Hexanedione	0.632				5
Hexanoic acid	0.621	200	13	10	18
Hexanoic acid, methyl ester	0.646		5		0
2-Hexanol	0.706		95	110	114
3-Hexanone	0.72				5
Hexenal	0.61	13			
1-Hexen-3-ol	0.7195	3			
4-Hydroxybenzoic acid	0.609	2			
Hydroxybenzoic acid, methyl ester	0.568	13	305	10	
3-Hydroxy-2-butanone	0.545	20			
Hydroxybutyric acid	0.462			180	488
Hydroxymethoxybenzaldehyde	0.632	9			21
1-(4-Hydroxy-3-methoxyphenol)ethanone	0.651				13
4-Hydroxy-4-methyl-2-pentanone	0.621	200	130	36	5
1-(2-Hydroxy-5-methylphenyl)ethanone	0.8	14			100
Hydroxyphenylacetic acid, choroethyl ester	0.56				30
Hydroxyphenylethanone	0.706				8
3-(2-Hydroxyphenyl)-2-propenoic acid	0.663				10
1-Hydroxy-2-propanone	0.486	30			46
Hydroxypropoxy propanol	0.537	400			0
Substituted hydroxyquinoline	0.755	40			0

Indole	0.821		210		11
Iodoacetic acid	0.129			21	14
1-(3H)Isobenzofuranone	0.716	20			5
Isobutyric acid	0.545	640			
Isocitric acid	0.375	575			
Isophorone	0.783	18			
Isoketoglutaric acid	0.411		80		
Lactic acid	0.4	3250	30000	15000	154
Methacrylic acid	0.558	5			
Methanol	0.375	1000	1400	434	1900
2-Methoxyethanol	0.474	100			
2-(2-Methoxyethoxy) ethanol	0.5	50			
1-(2-Methoxy-1-methylethoxy)-2-propanol	0.564	100			
Methoxymethylpropanol	0.582	100			
Methoxy phenol	0.677	150			32
1-(4-Methoxyphenol)-ethanone	0.72				58
3-Methoxy-1,2-propanediol	0.453	70			
2-Methoxy-4-(1-propenyl)-phenol	0.732				13
1-(2-Methoxypropoxy)-2-propanol	0.568	100		11	
2-Methyl benzaldehyde	0.8				7
Methylbenzoic acid	0.706	22			
3-Methyl butanoic acid	0.588	25			190
3-Methyl-2-butanone	0.697				3
3-Methylcyclopentanone	0.735				8
(1-Methyldecyl) benzene	0.879			40	7
2-Methyl-2,2-dimethyl-1-(2-hydroxy propyl) - propionic acid	0.667	25			
2-Methyl-2,2-dimethyl-1-(2-hydroxy,1methylethyl) - propyl esterpropionic acid	0.667	24		12	
2-Methyl-2,2-dimethyl-1-(2-hydroxy,1-methyl) - propionic acid	0.667	50			
2-Methyl, 1-(1,1,-dimethyl)-2-methyl -1,3-propanediyl ester propionic acid	0.667	25			
Methylene chloride	0.141	5			17
Methyl-2-heptanol	0.76		20		
2-Methyl-3-hydroxy-2,2,4-trimethylpentyl -ester propionic acid	0.556	50		13	
Methylisopropylcyclohexanol	0.769	37			
Methyl methacrylate	0.6				11
Methyl-(methylethenyl)-2-cyclohexen-1-one	0.81	10			12
5-methyl-2-(1-methylethyl)-phenol	0.8	200			110
Methyloxime	0.261		42		
14-Methyl-pentadecanoic acid,methyl ester	0.756		8		
2-Methyl-2,4-pentanediol	0.61	425			
4-Methyl pentanoic acid	0.62	6			
2-Methyl-3-pentanone	0.719				18
4-Methyl-3-penten-2-one	0.735			8	
Methyl phenol	0.778	300			268
2-Methyl propanoic acid	0.545	25	7	6	105
2-Methyl-2-propenoic acid	0.558	50			
Methyl pyrazine	0.638				12
1-Methyl-2-pyrrolidinone	0.606	100	550		
12-Methyl-tetradecanoic acid	0.744		30		
(1-Methylundecyl) benzene	0.877			3	
Morpholine	0.551	500			
Substituted Morpholine	0.6	220			
Morpholine ethanamine	0.549	130			
N,N-di-n-butylformamide	0.688	250		10	
N,N-diethyl-3-methylbenzamide	0.754	20			
N,N-diethyl-m-toluamide	0.754	23			
N,N-dimethylacetamide	0.552	40		4	
N,N-dimethylbenzylamine	0.8	40			3
N,N-dimethylthioformamide	0.493	400	4	13	

N,N-dimethylthioformamide	0.404	40			
n-Butyl ether	0.738	5			
N-Butylbenzenesulfonamide	0.563	20			
N-Methyl-2-pyrrolidinone	0.605	1200	4	18	
N-Nitrosodimethyl amine	0.324	30			
N-Nitrosomorpholine	0.414	6			
Nicotine	0.74		17		
Nitrophenol (ortho)	0.518	6			57
Nonacosane	0.853			25	
Nonadecanoic acid, methyl ester	0.769		47		
Nonanoic acid	0.683	30	16	21	
Octacosane	0.853	20		35	
9,12-Octadecadienoic acid, methyl ester	0.775		47		
Octadecanoic acid	0.76		410	330	
Octadecanoic acid, methyl ester	0.765		2450	153	
Octadecanol	0.799		100	116	
Octadecenoic acid	0.765		2800	1100	
Octadecenoic acid, methyl ester	0.77		360	12	
9-Octadecen-1-ol	0.857		39		
Octanoic acid	0.667	300	35	14	7
1-octanol	0.738			41	
Octenoic acid	0.676				142
Oxalic acid	0.267	200	80	310	880
4-Oxo-pentanoic acid	0.517	20			
1,1-Oxybis (2-ethoxy) ethane	0.592	100		8	
1,1-Oxybis-2-propanol	0.537	50			
Pantolactone	0.554				36
Pentachlorophenol	0.271	4			
Pentacosane	0.852	20		14	
Pentadecanoic acid	0.744		230	75	
Pentadecanoic acid, methyl ester	0.75		185		
Pentadecanol	0.714		53	306	
Pentadecenoic acid	0.75		30	58	
2,4-Pentanedione	0.6				11
Pentanoic acid	0.588	100	2	2	13
2-Pentanone	0.698				5
2,5,8,11,14-Pentaoxapentadecane	0.541	50	12		
Phenol	0.766	300	410	7	103
2-Phenoxyethanol	0.696	50		4	
2-Phenoxy-1-propanol	0.711	22			
Phenyl acetic acid, alpha methyl-4-isobutyl	0.757				40
Phenylacetonitrile	0.82		140		171
1,1-(phenylene)bis ethanone	0.714	27			
2-phenylethanol	0.787	100			13
1-Phenylethanone	0.806	120			7
Phenyl propanoic acid	0.72				7
Phosphoric acid triethyl ester	0.396	35			
Phthalate ester	0.65	120	240		
1,2-Propanediol	0.473	5000	440	3400	396
1-Propanol	0.6		260	200	
2-Propanol	0.6	300		200	275
Propionic acid	0.486	12000	17800	13000	2530
2-Propoxyethanol	0.577	300			
Pyrene	0.95				2
2-Pyridinamine	0.638				15
1H-pyrrole	0.896				7
Pyruvic acid	0.409		180		220
Sodium coconut acid-n-methyl taurate (SCMT)	0.525		425200		
Sodium dodecyl benzene sulfonate	0.621			98000	
Squalene	0.877		7700	2040	3
4-(tert-butyl) benzoic acid	0.741	6			
3-tertbutyl phenol	0.8	60			5
Tetrachloroethene	0.145		4	11	

Tetracosane	0.852	20		18	
Tetracosanoic acid, methyl ester	0.785		140		
Tetradecanal, o-methyloxime	0.747		100		
Tetradecanoic acid	0.736	7	1570	120	1
Tetradecanoic acid, 3 hydroxy-methyl ester	0.698		4		
Tetradecanoic acid, methyl ester	0.744		750	10	
Tetradecanol	0.784		85	206	5
Tetradecene	0.857			5	
Tetradecenoic acid	0.743			90	
Tetraethylene glycol diacetate	0.518	2			
Tetraethylene glycol monoacetate	0.508		4		
Tetrahydro-5,6-dimethyl-2H-pyran-2-one	0.656				106
Tetrahydro-6-methyl-2H-pyran-2-one	0.632	45			75
Tetrahydrothiophene-1,1-dioxide (sulfolane)	0.4	28			
4-(2,2,3,3) Tetramethylbutyl phenol	0.816				7
Tetramethylurea	0.517	31			
Tetraoxadodecane	0.539				
Toluene	0.913	1	1000	5	
Total Amino Acids	0.442		275	320	374
Total Protein	0.5	1300	23000	19700	1100
Tri(2-chlorethoxy)phosphate	0.254	120			
Triacontane	0.853			96	
Triacotanoic acid	0.773		95		
Triacosane	0.852	16		5	
Tri(2-chloroethoxy)phosphate	0.254	150			
Trichloropropene	0.25		3	21	
Tricosanoic acid, methyl ester	0.783		37		
Tridecanoic acid	0.729		12	16	
Tridecanoic acid, methyl ester	0.737		42		
Triethoxyphosphate	0.396	26			
Triethylene glycol	0.5	5			
Triethylene glycol diacetate	0.513	46	3		
Trimethylbenzylalcohol	0.8				9
Triumethylcyclohexenemethanol	0.779	41			14
Trimethyl-2-cyclopenten-1-one	0.787				8
2,2,4-Trimethyl-1,3-pentanediol	0.738	60			
1-(2,4,6-trimethylphenyl)ethanone	0.761	8			
Trimethylpyrazine	0.688				8
1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6-trione	0.578	12			
Undecanoic acid	0.709	10			
1-Undecene	0.851		9		
Urea	0.2	1000	15000	19600	3300
Vanillin	0.632	7			13
Vinyl benzylalcohol	0.806			16	
Aluminum	NA	25			25
Ammonium	NA	14000	6723	2630	1400
Arsenic	NA		10.8	20	3
Barium	NA		10.8	10	12
Bicarbonate	NA	30000	17604	22760	1700
Bromide	NA	50	54	100	
calcium	NA	55	3574.8		100
Carbon dioxide	NA				
Chloride	NA	200	125280	91880	1100
Chromium	NA				8
Copper	NA		75.6		10
Cyanide	NA				280
Fluoride	NA	220	2376	75	160
Iodide	NA				110
Iodine	NA				
Iron	NA		129.6	110	45
Lead	NA	10			3
Magnesium	NA		421.2	430	28

Manganese	NA		10.8		3
Mercury	NA	3			
Nickel	NA		21.6		16
Nitrate	NA	150	270	140	110
Nitrite	NA	190		100	120
Phosphate	NA		3375	660	480
Potassium	NA	95	18122.4	9450	450
Selenium	NA				3
Sodium	NA	665	135000	78720	1070
Sulfate	NA	240	17820	6810	1240
Zinc	NA	3		30	8
Volume (l/day)		9.25	27.22	49.9	8.13
note: all values are in ppb unless noted					

Appendix II. Equilibrium Isotherm Procedure

Equilibrium isotherms are used to determine the liquid and solid phase concentrations of adsorbates at equilibrium with an adsorbent. The liquid phase concentration (C_e) is measured directly, and the solid phase concentration (q_e) is determined by a mass balance on the isotherm bottle:

$$q_e = \frac{V}{M}(C_0 - C_e)$$

where V is the isotherm bottle volume and M is the adsorbent mass.

1.0) **Cleaning procedure for isotherm equipment**

All equipment used in the experiments was cleaned with the following procedure or that set forth by Sievers Co. (Boulder, CO) for ultra low level TOC analysis.

A.) All equipment is washed with Micro, a phosphate free laboratory cleaner.

B.) The equipment is rinsed with Milli-Q water several times and then air dried.

The Milli-Q UV system consists of:

1.) Activated carbon cartridges to remove dissolved organics.

2.) Ion exchange cartridges to remove ionic species.

3.) 185 nm and 254 nm UV lamp for disinfection and organic oxidation.

4.) A membrane filter to remove particulates greater than 0.22 μm.

C.) The equipment is rinsed with ethanol and air dried.

D.) All glassware is baked in a 250° C forced air oven for one hour. All Teflon and stainless steel apparatus was dried at 105° C in a forced air oven for one hour.

2.0) **Preparation of adsorbents for isotherms**

2.1) **Powdered adsorbent preparation (580-26 and APA GAC)**

A.) Separate an adequate amount of adsorbent from the cleaned adsorbent to perform all the necessary isotherms.

B.) Completely crush all the adsorbent to be used for the isotherm experiments to a 200 by 400 (USTM) sieve size using a mortar and pestle for crushing.

C.) Place the powdered adsorbent in isotherm bottles so that they are approximately 1/3 full. Fill the remaining volume with Milli-Q water and shake for a few minutes, then centrifuge each bottle for at least ½ hour at 2300 rpm.

D.) Pour off supernatant. This will remove the fine suspended particles that may interfere with the final isotherm procedure.

E.) Place the isotherm bottles containing the adsorbent in the oven at 105° C overnight (16-20 hours). Cool in a desiccator.

F.) Store adsorbent in airtight, borosilicate, dark glass bottles in the dark until ready to use.

2.2) XAD-4 resin preparation

A.) XAD-4 resin was used in its uncrushed form for isotherm experiments. XAD-4 resin was rinsed with Milli-Q water until the effluent rinse water exhibited nondetectable carbonate concentrations to remove sodium carbonate added to the adsorbent to inhibit biological growth in shipping and storage.

3.0) Weighting procedure

3.1) XAD-4 adsorbent resin weighting procedure

A.) Prior to weighing, the resin was transferred to an absorbent pad to remove excess water.

B.) The weight of the resin was found by first weighting a piece of weighing paper, adding the approximate resin dosage, and re-weighing the weighing paper subsequent to resin placement in the bottle.

C.) To determine the percent solids of the resin, three solids samples were taken during the weighing procedure (beginning, middle, and end). The solids determination consisted of:

1.) Solids samples were weighed directly from the adsorbent pad (as were the isotherm samples).

2.) Samples were dried at 110° C for 8 hours and cooled in a desiccator.

3.) Dry samples were weighted to determine the difference in weight due to water.

3.2) Powdered adsorbent weighing procedure

A.) The powdered adsorbents were weighed out using procedure 3.1 except step 3.1 A was omitted.

4.0) **Solution Preparation and Handling**

4.1) **Waste mixture**

A.) Water samples were transported from NASA/ION in glass jars with Teflon caps and shipped overnight in coolers with ice packs.

B.) The samples were pumped through MCV resin, to limit microbial growth, and restored in glass jars at 4° C.

C.) The samples were passed through a series of stainless steel mesh filters, followed by a Gelman 0.45 μm filter prior to mixing of the waste streams.

D.) The waste streams making up the waste mixture were pumped into 100 L Tedlar bags. The waste mixture consisted of 21.0% shower water, 31.6% handwash water, 18.8% humidity condensate water, 13.9% urine distillate water, 2.8% oral hygiene water, 3.2% wet shave water, 6.9 % animal condensate water and 1.9% equipment offgassing water.

E.) Waste stream dilutions were prepared by 50% dilution by volume using Milli-Q water.

4.2) **Shower/handwash water**

A.) The shower/handwash water was prepared following the same procedure given in 4.1 except 4.1 D including the content of the mixture. The shower/handwash mixture consisted of 40% shower water and 60% handwash water.

4.3) Urine Distillate and Humidity Condensate waters

A.) The urine distillate and humidity condensate waters were prepared following the procedure given in 4.1 except 4.1 D including the content of the mixture. These streams consisted of 100% urine distillate and 100% humidity condensate.

5.0) Isotherm bottle filling

A.) The resin or powdered adsorbent dosages were added to the isotherm bottles.

B.) The bottles plus the resin or adsorbent were weighed then filled with solution and capped with Teflon septa. A procedure is used to fill the bottles that causes the least amount of solution agitation. The Teflon tube from the Tedlar gas bag is not allowed to come into contact with the solution in the isotherm bottle since adsorbent or ion exchange resin can cling to the Teflon tube and change the dosage. To prevent loss of adsorbent resin from the isotherm bottle when they are capped, approximately 1 ml of headspace is left in the bottle. Two isotherm bottles containing only the filling solution were taken at the start and end of all isotherms as blanks to determine initial concentration. Two additional bottles containing only the filling solution were taken in the middle of the isotherms to determine if volatilization of adsorbate was occurring during the filling process. The blanks were all taken in duplicate and one was analyzed at the beginning of the equilibrium period and one was analyzed at the end as controls to monitor volatilization or microbial degradation of the solutes during equilibrium.

C.) The filled bottles were re-weighed to determine the exact volume of the solution added.

6.0) Equilibrium and Sampling

A.) The isotherm bottles were tumbled at 18 rpm at room temperature for a minimum time period of 7 to 10 days.

B.) The isotherm bottles were then removed from the tumbler and centrifuged to settle all adsorbent to the bottom of the isotherm bottle. The supernatant was then sampled and analyzed for pH and the adsorbates of interest.

Appendix III. Sensitivity Analysis on Number of Fictive Components

Sensitivity analysis was completed to determine if the use of six fictive components was sufficient, or if increasing the number of FCs produced significantly improved results. Three methods were attempted to address this concern 1) Varying the number of fictive components from 3 to 10, with Freundlich K values ranging from 0.4 to 1200 (mg/g)(L/mg)$^{1/n}$; 2) Optimizing FC Freundlich K and FC concentration values simultaneously, defining the range of Freundlich K to be between 0.5 and 100,000 (mg/g)(L/mg)$^{1/n}$; and 3) Optimizing only FC concentration using chosen FC Freundlich K values in the range of 0.2 to 80,000 (mg/g)(L/mg)$^{1/n}$. The results of these three methods were compared to the modeling results using weighted averages (section 3.2). All results presented for the sensitivity analysis are for the case where waste mixture, non-dilute and dilute TOC isotherms, on 580-26 GAC are fit simultaneously.

1.0 Six fictive components using weighted averages

The original approach for determining FC parameters for six fictive components was determined using weighted averages as described in section 3.2. The FC concentration was then optimized using the genetic algorithm. The fitness value, used for optimization, is calculated by the following equation:

$$fitness = 100 - \frac{1}{2}\sum_{i=1}^{N}\left[\frac{\left|C_{e,i(\text{data})} - C_{e,i(\text{model})}\right|}{C_{e,i(\text{data})}} + \frac{\left|q_{e,i(\text{data})} - q_{e,i(\text{model})}\right|}{q_{e,i(\text{data})}}\right]^2 \quad \text{for } i = 1,\ldots N$$

The fitness value compares the model data with the isotherm data. As the fitness increases, liquid- and solid- phase residual concentrations decrease. Fitting the two TOC isotherms in this manner results in a fitness of 95.64. The FC parameters and fit concentrations for this case are presented in Table AIII-1.

Table AIII-1 - FC parameters and fit concentration for TOC isotherms, using parameters calculated from weighted averages.

	Freundlich K $(mg/g)(L/mg)^{1/n}$	Freundlich 1/n	Molecular Weight	Fraction of Carbon	Concentration (mg TOC/L)
FC 1	2.6	0.73	96.5	0.742	13.682
FC 2	42.3	0.47	123.2	0.710	27.853
FC 3	97.6	0.43	95.3	0.753	41.175
FC 4	178.5	0.17	357.0	0.6	29.774
FC 5	910.2	0.31	192.4	0.760	0.239
FC 6	112231.9	0.07	270.7	0.800	5.756

Figures AIII-1 and AIII-2 compare the model fit to the isotherm data. Figure AIII-1 shows the non-dilute TOC isotherm model fit describes the isotherm data very well. Figure AIII-2, the dilute TOC isotherm, also describes the isotherm data trend fairly well. The model slightly overpredicts the non-adsorbing concentration for the dilute TOC isotherm. This occurs because the non-adsorbing concentration for the model is calculated based on the non-adsorbing concentration of the non-dilute TOC isotherm and the total TOC concentrations of the dilute and non-dilute isotherms.

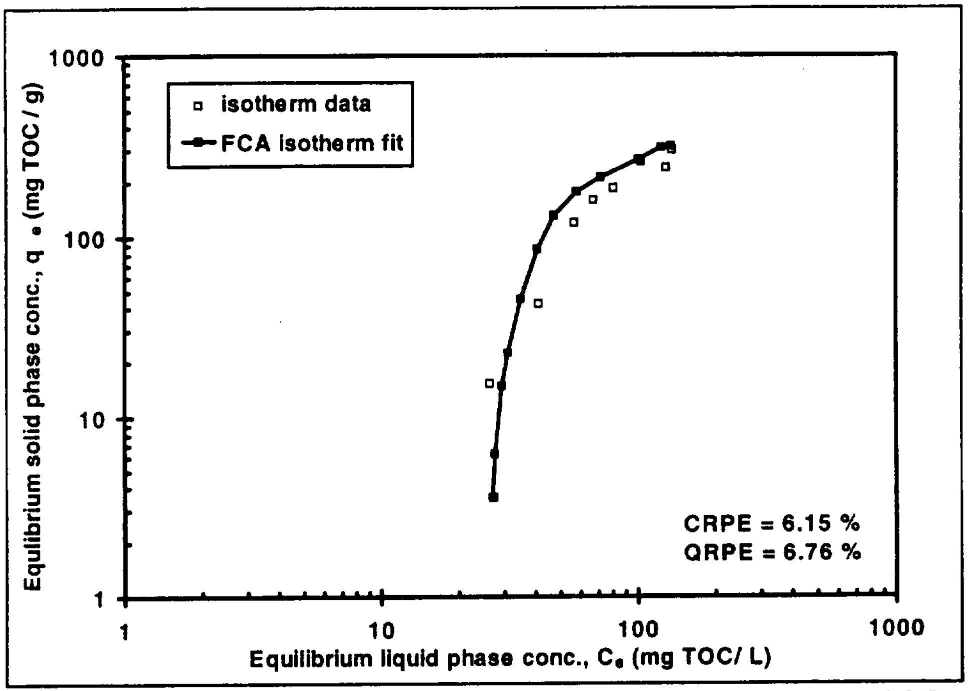

Figure AIII-1 - Non-dilute TOC isotherm on the waste mixture on 580-26 GAC, fit simultaneously with the dilute TOC isotherm, using the FC parameters in Table 3.

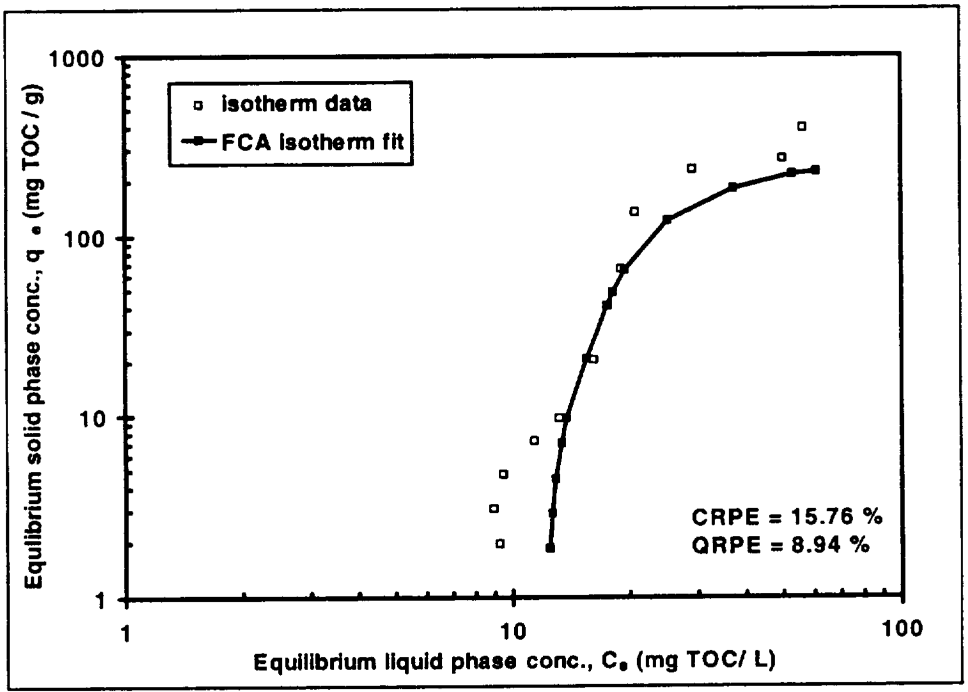

Figure AIII-2 -Dilute TOC isotherm on the waste mixture on 580-26 GAC, fit simultaneously with the non-dilute TOC isotherm, using the FC parameters in Table 3.

2.0 Varying the Number of Fictive Components

2.1 Optimizing FC concentration with Freundlich K ranging from 0.4 to 1200 (mg/g)(L/mg)$^{1/n}$

The first method used to vary the number of fictive components included specifying the Freundlich K values and optimizing the FC concentration using the genetic algorithm. Table AIII-2 contains the FC Freundlich K and fitness values used as the number of fictive components varied.

Table AIII-2. Freundlich K values used for each simulation varying the number of fictive components (mg/g)(L/mg)$^{1/n}$.

	3 FCs	4 FCs	5 FCs	6 FCs	7 FCs	8 FCs	9 FCs	10 FCs
FC 1	1	1	1	0.4	0.4	0.4	0.4	0.4
FC 2	200	200	200	2.5	2.5	2.5	2.5	2.5
FC 3	350	350	350	10	10	10	10	10
FC 4		500	500	50	50	50	50	50
FC 5			750	100	100	100	100	100
FC 6				500	250	250	250	250
FC 7					500	500	500	500
FC 8						750	750	750
FC 9							900	900
FC 10								1200
fitness	84.22	88.75	88.07	94.63	94.36	92.69	92.75	92.72

The fitness results in Table AIII-2 show the fitness decreases as the number of fictive components is increased and that the highest fitness value is achieved when six fictive components are used. Figures AIII-3 and AIII-4 compare the model results as the number of fictive components are varied for the non-dilute and dilute TOC isotherms, respectively. It is evident from Figures AIII-3 and AIII-4 the model results do not consistently describe the isotherm data. There are two problems associated with this method of varying the number of FCs: 1) As the number of FCs was varied, the range of the adsorption potentials was not held constant and 2) the whole range of adsorption potential found in the waste mixture was not represented by the Freundlich K's used in this set of model fits. To rectify these problems, the following two methods were tried.

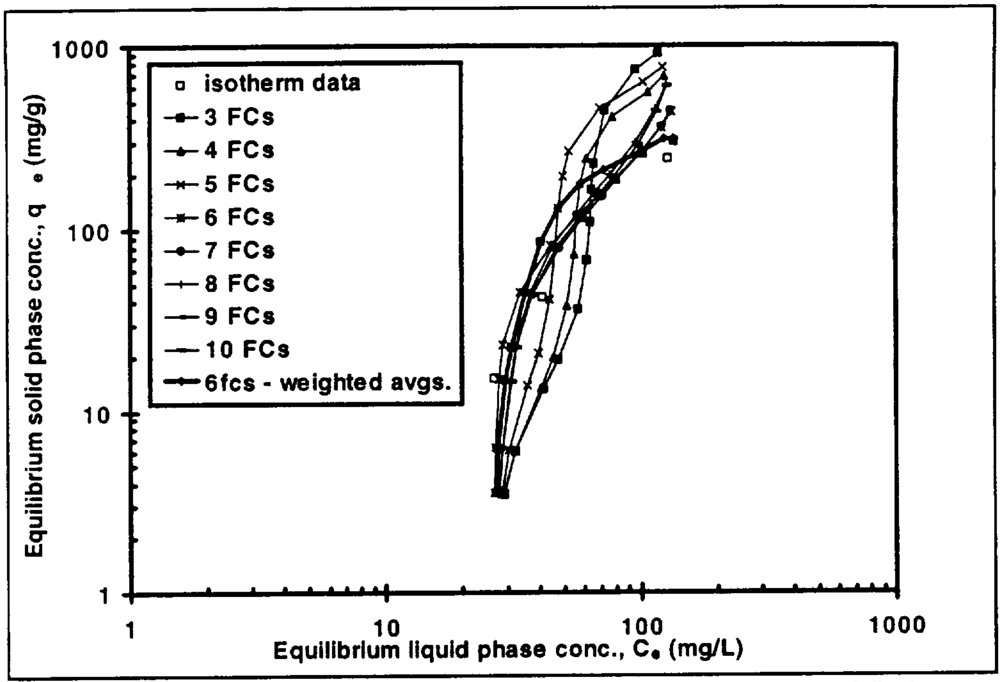

Figure AIII-3 - Non-dilute TOC isotherm - Varying the number of fictive components with Freundlich K ranging from 0.4 to 1200 (mg/g)(L/mg)$^{1/n}$, fitting parameter: FC concentration.

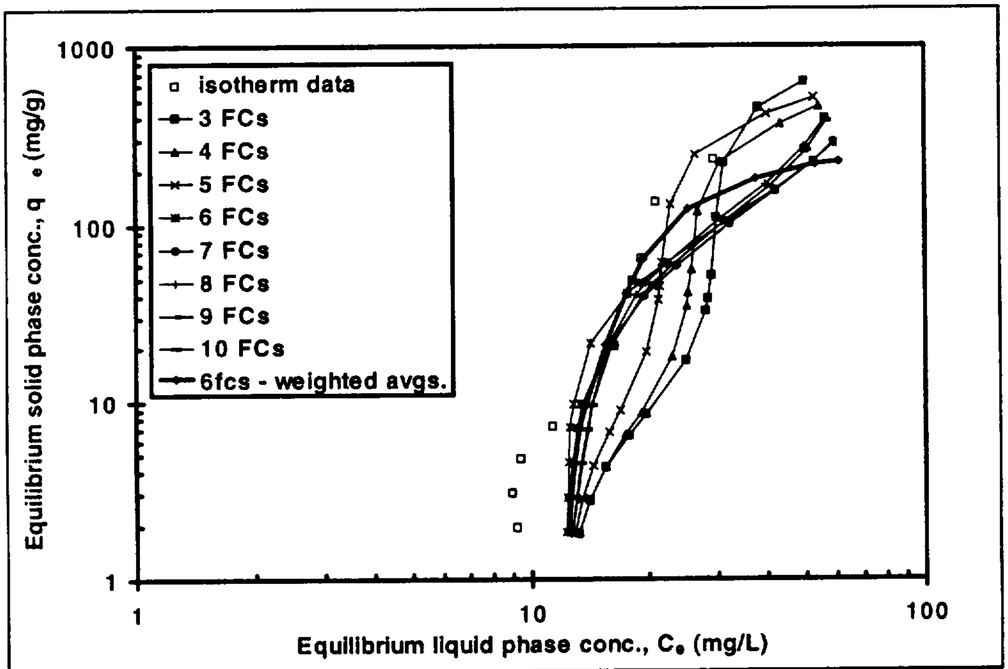

Figure AIII-4 - Dilute TOC isotherm - Varying the number of fictive components with Freundlich K ranging from 0.4 to 1200 (mg/g)(L/mg)$^{1/n}$, fitting parameter: FC concentration.

2.2 Optimizing FC Freundlich K and FC concentration simultaneously

The FCA model was programmed with the genetic algorithm to optimize the FC Freundlich K and concentration values simultaneously. The Freundlich K's were constrained to the range of 0.5 to 100,000 (mg/g)(L/mg)$^{1/n}$. This range of Freundlich K values was chosen because it represented the adsorption potential of the waste mixture. Freundlich 1/n values were calculated using the 580-26 GAC Freundlich K vs. 1/n correlation determined from the known compounds in the waste mixture. The average molecular weight and fraction of carbon were calculated from the known compounds in the waste mixture to be 173.08 g/mol and 0.73, respectively. These values were held constant for each fictive component. Holding molecular weight and fraction of carbon constant takes out any dependence of Freundlich K on these parameters. The two TOC (non-dilute and dilute) isotherms for the waste mixture were fit simultaneously using the parameters specified. Table AIII-3 summarizes the fit FC Freundlich K, fit FC concentration, and fitness values determined when varying the number of FCs from 3 to 9.

Table AIII-3 - Varying number of FCs, fitting Freundlich K and concentration simultaneously for TOC isotherms on 580-26 GAC.

Freundlich K (mg/g)(L/mg)$^{1/n}$							
	3 FCs	**4 FCs**	**5 FCs**	**6 FCs**	**7 FCs**	**8 FCs**	**9 FCs**
FC 1	818.463	54472.63	75.554	48887.65	48843.5	86672.93	73.811
FC 2	66.017	99.396	70035.2	77236.94	739.785	7174.867	88485.0
FC 3	34059.41	17967.46	97600.18	671.598	38.933	195.43	51520.45
FC 4		71379.87	1133.556	33092.1	28331.76	40020.14	680183.23
FC 5			12450.1	15.377	89563.41	22.721	110.554
FC 6				10987.26	67693.08	35734.06	56595.12
FC 7					78850.07	28945.64	58654.95
FC 8						69813.28	55547.89
FC 9							73190.04
Concentration (mg TOC/L)							
FC 1	13.384	16.164	53.387	7.578	5.379	4.602	33.059
FC 2	94.372	100.252	5.227	15.073	32.113	23.505	1.391
FC 3	10.725	0.875	27.834	49.753	30.673	20.068	2.281
FC 4		1.19	25.815	16.133	13.74	11.979	1.49
FC 5			6.217	22.108	11.008	25.657	30.786
FC 6				7.835	20.046	16.813	17.284
FC 7					5.503	12.761	24.717
FC 8						3.097	3.091
FC 9							4.381
fitness	91.64	92.708	78.91	73.76	72.01	65.00	75.34

When optimizing Freundlich K and concentration simultaneously, the Freundlich K values determined by the genetic algorithm do not well represent the whole range of adsorption potential in the waste mixture. Although the genetic algorithm is a robust fitting routine, as the number of fitting parameters are increased and more non-linear IAST equations are solved simultaneously, the system becomes very complex. It appears that as the number of fitting parameters increases, the genetic algorithm has difficulty finding the best solution and may possibly be finding a local minimum. Therefore, the model is able to fit the isotherms more accurately when fitting less parameters, such as by specifying the Freundlich K values and only fitting the concentrations.

Figures AIII-5 and AIII-6 graphically compare the model results to the isotherm data for each simulation (varying the number of FCs from 3 to 9, and fitting Freundlich K and concentration simultaneously), and the model fit using weighted averages (Table AIII-1), for the non-dilute and dilute TOC isotherms, respectively. It is apparent from Figures AIII-5 and AIII-6 that the best model fit resulted when the FC parameters were determined from weighted averages of the known compounds in the mixture, and FC concentration was used as a fitting parameter (Table AIII-1).

2.3 Optimizing FC concentration - Freundlich K ranging from 0.2 to 80,000 (mg/g)(L/mg)$^{1/n}$

The optimized Freundlich K values (Table AIII-3) were unrealistic, therefore, FC Freundlich K values were specified based on the representative waste mixture and the FC concentrations were fit using the genetic algorithm. The chosen Freundlich K values, fit concentrations and fitnesses for this case are listed in Table AIII-4. The range of Freundlich K values (0.2 to 80,000 (mg/g)(L/mg)$^{1/n}$) was chosen directly from Figure AIII-7 (corresponding Freundlich K values given in Table AIII-4). The Freundlich K values were chosen such that the exact same range of adsorption potentials was covered for fictive components ranging from 3 to 9. This range falls slightly below the previously specified range in order to allow more of the weakly adsorbing group of compounds to be represented.

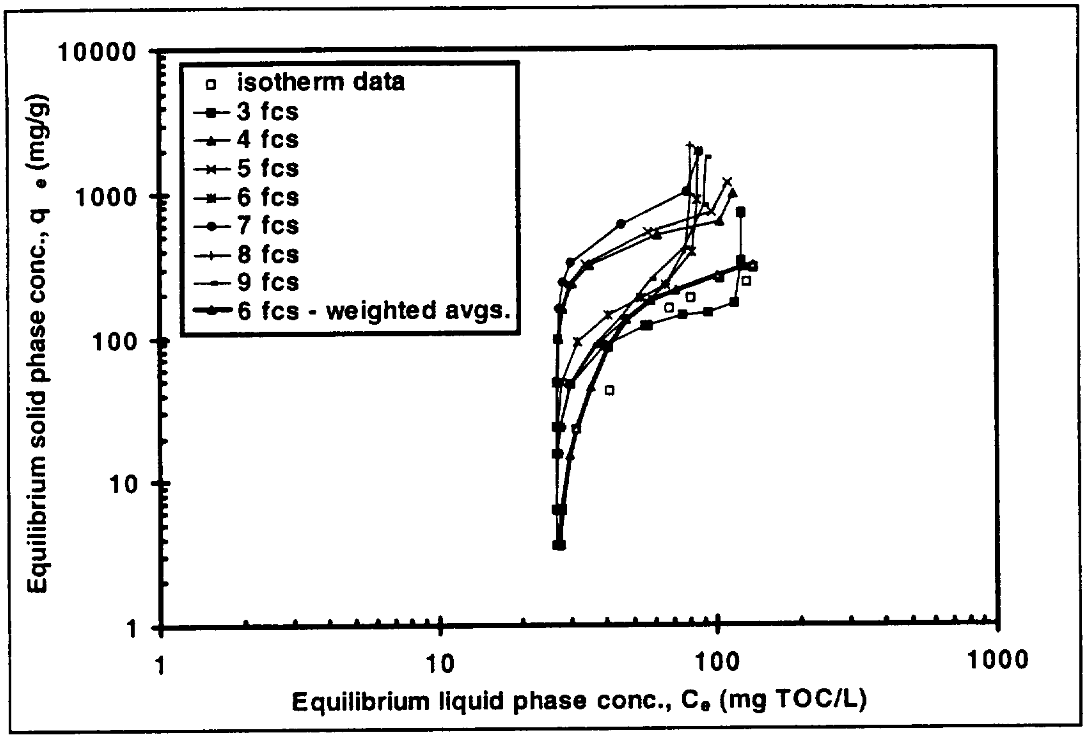

Figure AIII-5 - Non-dilute TOC isotherm - Varying the number of fictive components, fitting parameter: FC Freundlich K and FC concentration.

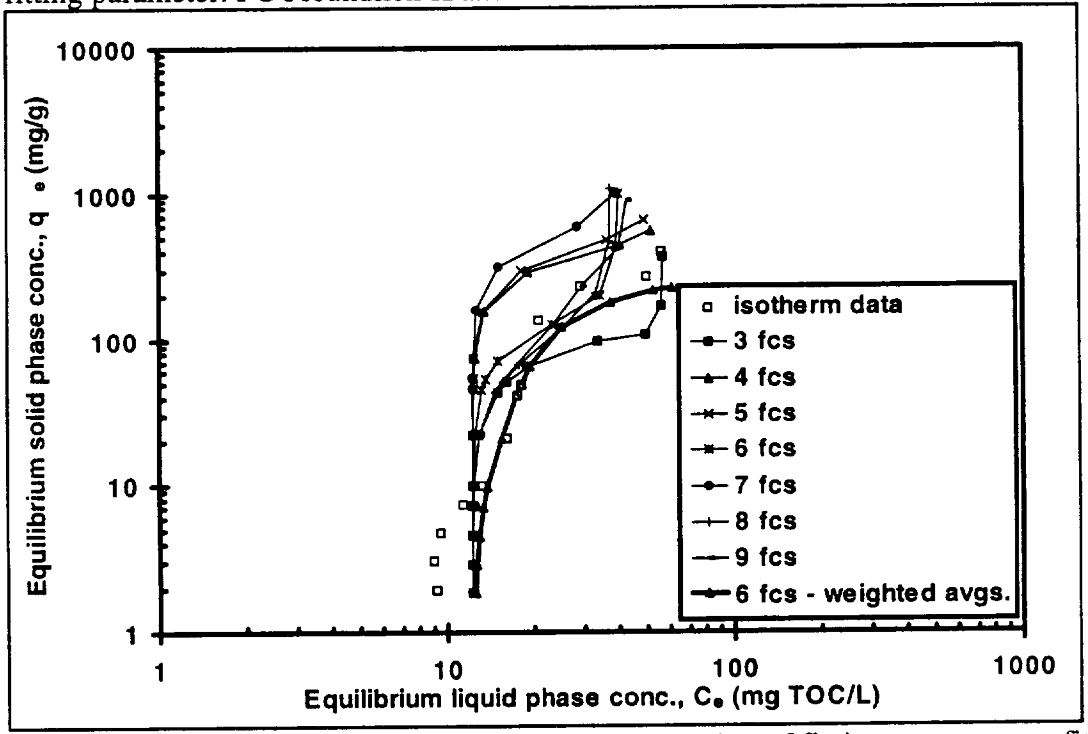

Figure AIII-6 - Dilute TOC isotherm - varying the number of fictive components, fitting parameter: FC Freundlich K and FC concentration

Table AIII-4 - Varying number of FCs, fitting only FC concentration for TOC isotherms.

	Freundlich K (mg/g)(L/mg)$^{1/n}$						
	3 FCs	**4 FCs**	**5 FCs**	**6 FCs**	**7 FCs**	**8 FCs**	**9 FCs**
FC 1 (a)	0.2	0.2	0.2	0.2	0.2	0.2	0.2
FC 2 (b)	60	20	3	3	3	3	3
FC 3 (c)	80000	600	100	20	20	20	20
FC 4 (d)		80000	1000	250	100	100	60
FC 5 (e)			80000	1000	250	250	100
FC 6 (f)				80000	1000	600	250
FC 7 (g)					80000	1000	600
FC 8 (h)						80000	1000
FC 9 (i)							80000
	Concentration (mg TOC/L)						
FC 1	5.065	5.963	1.171	0.608	1.974	1.682	1.909
FC 2	102.2	95.611	9.457	8.055	4.782	9.917	8.815
FC 3	11.215	15.647	94.014	42.436	29.121	19.786	20.523
FC 4		1.259	0.273	55.59	48.428	63.183	45.952
FC 5			13.565	3.531	26.663	1.682	5.247
FC 6				8.26	0.569	11.42	29.121
FC 7					6.944	3.054	1.406
FC 8						7.757	0.079
FC 9							5.428
fitness	93.52	91.31	94.72	92.48	94.80	93.57	94.61

Table AIII-4 shows the chosen Freundlich K values for each simulation. The range of Freundlich K values was held constant from 0.2 to 80,000 (mg/g)(L/mg)$^{1/n}$ for each number of FCs that was used. The Freundlich K values were chosen for each number of FCs based on the known distribution of compounds in the waste mixture as shown in Figure AIII-7. The FCs labeled in Figure AIII-7 are labeled with numbers and letters. The number corresponds to the number of FCs (3-9) fit simultaneously. The corresponding letter refers to the number FC (1-9), as listed in Table AIII-4.

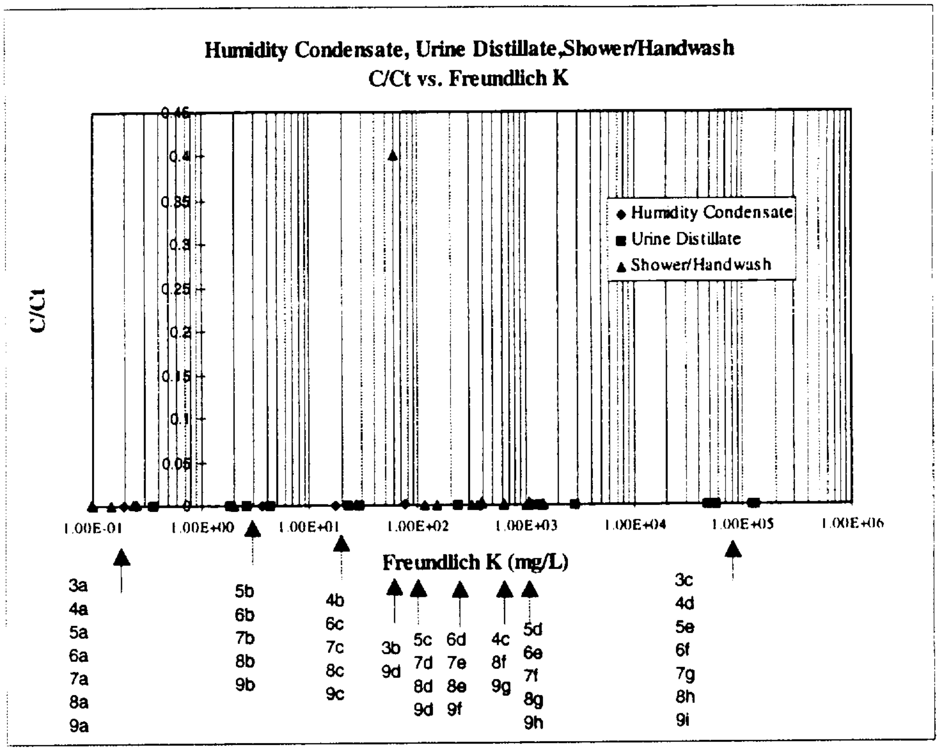

Figure AIII-7 - Distribution of Freundlich K values used when varying the number of fictive components and fitting only the FC concentrations.

Table AIII-4 shows the fitness values range from 91.3 to 94.8 when varying the number of fictive components and fitting concentrations. These fitness values are significantly higher than the fitness values determined when optimizing both Freundlich K and concentration simultaneously.

Figures AIII-8 and AIII-9 graphically compare the model results when varying the number of fictive components, choosing Freundlich K values from the range of known adsorption potentials and using FC concentration as a fitting parameter. Figure AIII-8 shows the non-dilute TOC isotherm and Figure AIII-9 presents the dilute TOC isotherm for the waste mixture on 580-26 GAC. Also shown on Figures AIII-8 and AIII-9 are the results when fitting TOC isotherms simultaneously using FC parameters calculated from weighted averages.

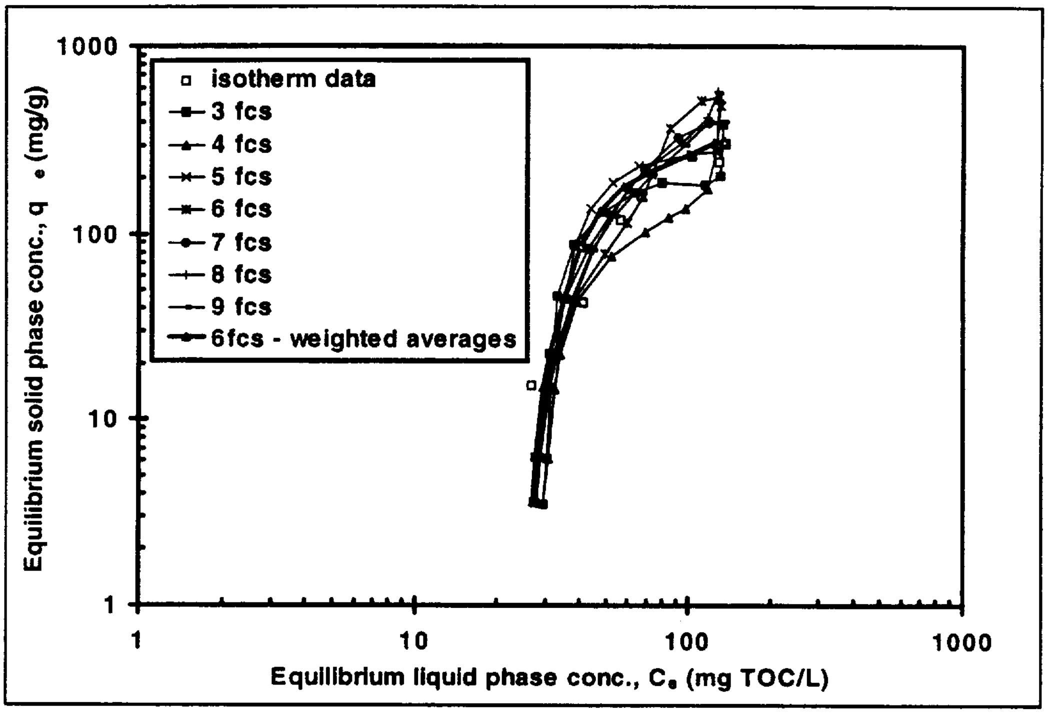

Figure AIII-8 - Non-dilute TOC isotherm - Varying the number of fictive components, fitting parameter: FC concentration

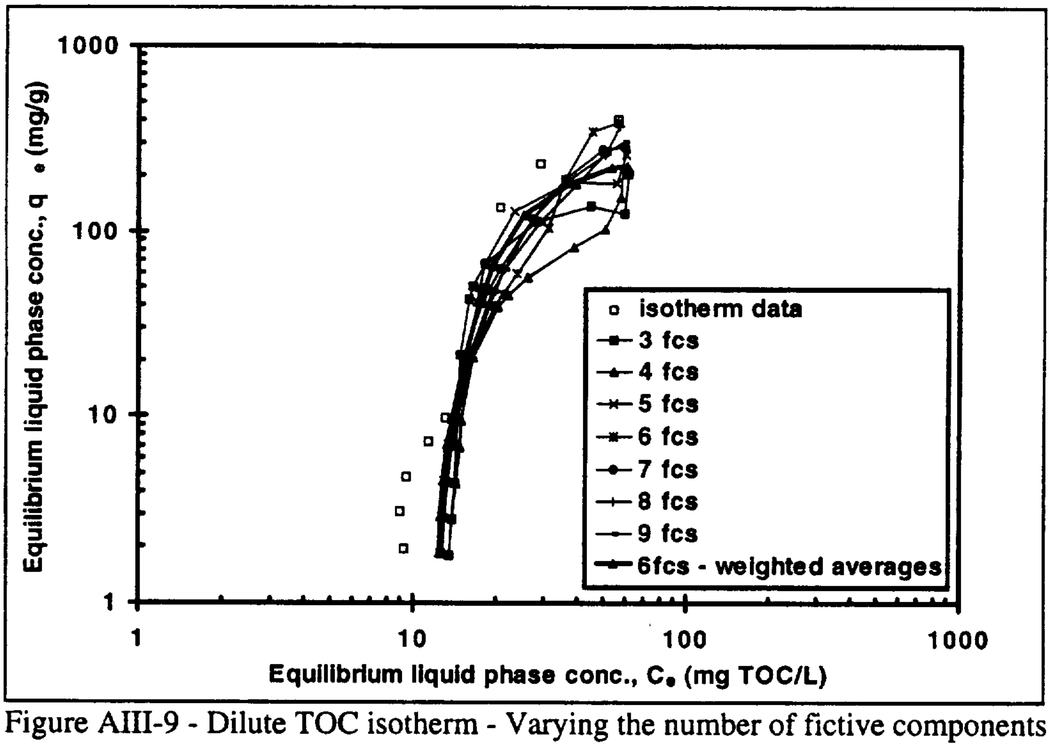

Figure AIII-9 - Dilute TOC isotherm - Varying the number of fictive components, fitting parameter: FC concentration

3.0 Conclusion of Sensitivity Analysis

The method using six fictive components and weighted averages resulted in the best fit of the TOC isotherms. When attempting to optimize the FC Freundlich K and FC concentration values simultaneously, the FC Freundlich K parameter values become unrealistic and do not represent the K values for the known components in the waste mixture. By constraining the Freundlich K values to realistic values representative of the known compounds in the waste mixture, increasing the number of fictive components does not improve the fitness beyond a certain point. This is because the complexity of the non-linear system of IAST equations increases dramatically as the number of fictive components is increased. The model results using six FC parameters determined from weighted averages, represent the best fit of the isotherm data. Even Figure AIII-7 shows 5-6 distinct groups of adsorption potentials. Because of limitations in the accuracy of the experimental measurement techniques, it is not possible to obtain a best fit greater than 96 percent. The most appropriate method for varying the number of FCs, entailed using a range of Freundlich K values from 0.2 to 80,000 $(mg/g)(L/mg)^{1/n}$ and optimizing the FC concentration. These results show there is not a significant advantage in using large numbers of fictive components. Six FCs were chosen because they can represent the distribution of adsorbing compounds in the waste streams and can minimize the time required for fixed-bed computations.

APPENDIX IV. Waste Mixture Isotherm Data

TABLE IV-1. 580-26 GAC TOC ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-8.9
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2503	0.0034	145.06	143.90	85.78
0.2499	0.0075	145.06	136.05	301.60
0.2483	0.0165	145.06	128.98	241.62
0.0427	0.0070	145.06	102.77	259.01
0.0434	0.0150	145.06	80.36	186.70
0.0427	0.0209	145.06	67.35	158.81
0.0433	0.0321	145.06	56.58	119.63
0.0420	0.0431	145.06	57.27	85.54
0.0428	0.0522	145.06	40.84	85.46
0.0436	0.1061	145.06	41.14	42.73
0.0420	0.2098	145.06	31.13	22.80
0.0422	0.3269	145.06	26.62	15.30
0.0420	0.5080	145.06	24.35	9.97
0.0427	0.7978	145.06	27.64	6.29
0.0361	1.1965	145.06	27.32	3.56
BLANK 1			141.47	
BLANK 2		218.29		
BLANK 3			143.57	
BLANK 4		214.33		
BLANK 5			156	
BLANK 6		214.02		

TABLE IV-2. 580-26 GAC TOC ISOTHERM, DILUTE WASTE MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-8.0
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Dilute Waste Stream Mixture

	Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
	0.2513	0.0030	67.00	66.85	12.63
	0.2506	0.0069	67.00	56.14	396.46
	0.2506	0.0161	67.00	49.88	266.20
	0.0424	0.0069	67.00	29.24	233.33
	0.0430	0.0147	67.00	20.86	134.78
	0.0437	0.0210	67.00	21.58	94.49
	0.0431	0.0316	67.00	19.07	65.35
	0.0421	0.0424	67.00	18.17	48.50
	0.0427	0.0513	67.00	17.60	41.08
	0.0437	0.1073	67.00	16.25	20.65
	0.0378	0.2088	67.00	13.15	9.76
	0.0426	0.3230	67.00	11.38	7.33
	0.0424	0.5091	67.00	9.43	4.80
	0.0424	0.7972	67.00	8.95	3.09
	0.0404	1.1918	67.00	9.22	1.96
BLANK 1				63.18	
BLANK 2			104.85		
BLANK 3				65.59	
BLANK 4			103.41		
BLANK 6			103.85		

TABLE IV-3. 580-26 GAC METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.3
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0395	0.0073	1.370	1.339	0.167
0.0425	0.0137	1.370	1.303	0.208
0.0433	0.0243	1.370	1.305	0.116
0.0433	0.0487	1.370	1.088	0.251
0.0388	0.0955	1.370	0.785	0.237
0.0434	0.1318	1.370	0.675	0.229
0.0426	0.1821	1.370	0.492	0.205
0.0430	0.2548	1.370	0.339	0.174
0.0417	0.3489	1.370	0.170	0.143
0.0415	0.4896	1.370	0.099	0.108
BLANK 1			1.393	
BLANK 5			1.347	

TABLE IV-4. 580-26 GAC METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.3
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0426	0.0265	8.225	7.627	0.963
0.0428	0.0485	8.225	7.871	0.312
0.0425	0.0696	8.225	6.492	1.057
0.0424	0.0964	8.225	5.852	1.043
0.0424	0.1302	8.225	5.169	0.995
0.0419	0.1842	8.225	3.474	1.080
0.0427	0.2539	8.225	2.149	1.021
0.0414	0.3488	8.225	1.571	0.790
0.0363	0.4975	8.225	0.841	0.538
BLANK 1			8.381	
BLANK 5			8.069	

TABLE IV-5. 580-26 GAC CHLOROFORM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.1
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0439	0.0051	0.882	0.870	0.104
0.0435	0.0109	0.882	0.819	0.251
0.0382	0.0131	0.882	0.784	0.286
0.0427	0.0199	0.882	0.710	0.369
0.0426	0.0350	0.882	0.481	0.488
0.0431	0.0500	0.882	0.328	0.478
0.0430	0.0683	0.882	0.202	0.428
0.0434	0.0968	0.882	0.110	0.346
0.0426	0.1359	0.882	0.060	0.258
0.0429	0.1861	0.882	0.038	0.195
0.0413	0.2542	0.882	0.020	0.140
0.0428	0.3619	0.882	0.012	0.103
0.0420	0.5036	0.882	0.007	0.073
BLANK 1			0.920	
BLANK 3			0.914	
BLANK 5			0.914	

TABLE IV-6. 580-26 GAC CHLOROFROM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.2-7.3
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0392	0.0054	9.480	9.256	1.638
0.0434	0.0074	9.480	9.283	1.149
0.0424	0.0129	9.480	8.603	2.885
0.0427	0.0184	9.480	7.910	3.654
0.0431	0.0374	9.480	5.153	4.979
0.0426	0.0508	9.480	3.651	4.891
0.0422	0.0719	9.480	2.227	4.256
0.0427	0.0977	9.480	1.535	3.473
0.0424	0.1329	9.480	0.936	2.728
0.0424	0.1880	9.480	0.526	2.017
0.0422	0.2708	9.480	0.289	1.431
0.0421	0.3568	9.480	0.161	1.100
0.0425	0.5102	9.480	0.077	0.783
BLANK 1			9.849	
BLANK 3			9.636	
BLANK 5			9.764	

TABLE IV-7. 580-26 GAC PCE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	PCE
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	21
pH	5.9-7.0
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2501	0.0038	0.888	0.867	1.391
0.2500	0.0062	0.888	0.845	1.745
0.2505	0.0095	0.888	0.802	2.258
0.2486	0.0156	0.888	0.685	3.235
0.0430	0.0050	0.888	0.432	3.947
0.0428	0.0069	0.888	0.284	3.774
0.0424	0.0108	0.888	0.141	2.922
0.0432	0.0177	0.888	0.052	2.042
BLANK 1			0.891	
BLANK 5			0.884	

TABLE IV-8. APA GAC TOC ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND...	TOC
ADSORBENT TYPE..	APA
ISOTHERM TYPE...	Virgin
PARTICLE SIZE...	200x400 mesh
TEMPERATURE, Deg C..	23
pH...	5.9-7.0
EQUILIBRATION TIME, days.......................................	7
BACKGROUND WATER MATRIX...........................	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2494	0.0038	145.06	143.63	93.07
0.2504	0.0069	145.06	136.85	299.00
0.2491	0.0158	145.06	130.87	223.53
0.0433	0.0073	145.06	100.25	266.62
0.0385	0.0150	145.06	76.77	174.89
0.0426	0.0212	145.06	63.75	163.39
0.0373	0.0316	145.06	51.60	110.09
0.0391	0.0425	145.06	49.38	87.95
0.0430	0.0518	145.06	36.35	90.38
0.0433	0.1038	145.06	35.93	45.49
0.0438	[illegible]	145.06	31.87	23.98
0.0419	[illegible]	145.06	28.23	15.26
0.0429	[illegible]	145.06	24.13	10.35
0.0384	0.7349	145.06	23.17	5.96
0.0420	1.1822	145.06	28.99	4.13

BLANK 1			134.29
BLANK 2		220.02	
BLANK 3			132.02
BLANK 4		220.4	
BLANK 5			143.2
BLANK 6		221.62	

TABLE IV-9. APA GAC TOC ISOTHERM, DILUTE WASTE MIXTURE

CHEMICAL COMPOUND.. TOC
ADSORBENT TYPE.. APA
ISOTHERM TYPE.. Virgin
PARTICLE SIZE.. 200x400 mesh
TEMPERATURE, Deg C... 23
pH.. 5.9-7.1
EQUILIBRATION TIME, days... 7
BACKGROUND WATER MATRIX... Dilute Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2478	0.0162	67.00	56.55	159.46
0.0421	0.0066	67.00	35.36	203.27
0.0425	0.0147	67.00	24.41	123.47
0.0421	0.0202	67.00	17.37	103.74
0.0380	0.0318	67.00	19.28	57.10
0.0432	0.0427	67.00	20.13	47.44
0.0421	0.0513	67.00	17.87	40.33
0.0435	0.1045	67.00	15.51	21.42
0.0428	0.2066	67.00	11.75	11.45
0.0426	0.3198	67.00	9.73	7.63
0.0424	0.4993	67.00	9.02	4.92
0.0423	0.7830	67.00	7.13	3.23
0.0423	1.1814	67.00	7.44	2.13
BLANK 1			65.35	
BLANK 2		101.21		
BLANK 3			66.89	
BLANK 4		98.26		
BLANK 5			65.51	
BLANK 6		93.91		

TABLE IV-10. APA GAC METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0427	0.0356	1.272	1.188	0.101
0.0431	0.0486	1.272	1.111	0.143
0.0428	0.0700	1.272	0.965	0.188
0.0426	0.0956	1.272	0.826	0.199
0.0424	0.1333	1.272	0.599	0.214
0.0381	0.1835	1.272	0.455	0.170
0.0427	0.2563	1.272	0.294	0.163
0.0405	0.3544	1.272	0.192	0.123
0.0417	0.4974	1.272	0.129	0.096
BLANK 1			1.281	
BLANK 5			1.262	

TABLE IV-11. APA GAC METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0426	0.0261	7.453	7.369	0.137
0.0406	0.0351	7.453	7.441	0.014
0.0432	0.0488	7.453	6.817	0.562
0.0428	0.0955	7.453	5.269	0.978
0.0381	0.1299	7.453	3.740	1.088
0.0379	0.1809	7.453	2.590	1.019
0.0423	0.2509	7.453	1.926	0.933
0.0425	0.3515	7.453	1.207	0.756
0.0427	0.4906	7.453	0.834	0.576
BLANK 1			7.382	
BLANK 5			7.523	

Table IV-12. APA GAC CHLOROFORM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND... Chloroform
ADSORBENT TYPE.. APA
ISOTHERM TYPE... Virgin
PARTICLE SIZE.. 200x400 mesh
TEMPERATURE, Deg C.. 23
pH.. 6.0-6.5
EQUILIBRATION TIME, days.. 7
BACKGROUND WATER MATRIX................................. Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0437	0.0102	0.882	0.872	0.043
0.0424	0.0188	0.882	0.826	0.126
0.0435	0.0263	0.882	0.761	0.200
0.0435	0.0495	0.882	0.467	0.365
0.0431	0.0704	0.882	0.253	0.385
0.0433	0.0961	0.882	0.130	0.339
0.0429	0.1320	0.882	0.064	0.266
0.0430	0.1822	0.882	0.037	0.199
0.0430	0.2551	0.882	0.019	0.146
0.0426	0.3506	0.882	0.010	0.106
0.0431	0.4907	0.882	0.005	0.077

BLANK 1			0.915	
BLANK 3			0.909	
BLANK 5			0.910	

TABLE IV-13. APA GAC CHLOROFORM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.6
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0430	0.0107	9.480	9.381	0.398
0.0431	0.0138	9.480	9.220	0.815
0.0437	0.0181	9.480	8.987	1.190
0.0424	0.0257	9.480	8.149	2.195
0.0422	0.0504	9.480	4.737	3.973
0.0428	0.0712	9.480	2.897	3.957
0.0377	0.0961	9.480	1.335	3.199
0.0430	0.1318	9.480	0.901	2.795
0.0422	0.1840	9.480	0.480	2.064
0.0424	0.2560	9.480	0.259	1.528
0.0421	0.3538	9.480	0.135	1.112
0.0426	0.4852	9.480	0.060	0.827
BLANK 1			9.830	
BLANK 3			9.750	
BLANK 5			9.810	

TABLE IV-14. APA GAC PCE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	PCE
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	21
pH	6.0-7.0
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2495	0.0044	0.851	0.834	0.971
0.2493	0.0064	0.851	0.788	2.471
0.2490	0.0095	0.851	0.754	2.534
0.2519	0.0154	0.851	0.702	2.439
0.0424	0.0046	0.851	0.552	2.777
0.0431	0.0066	0.851	0.450	2.639
0.0431	0.0103	0.851	0.248	2.517
0.0422	0.0180	0.851	0.079	1.813
BLANK 1			0.869	
BLANK 5			0.833	

TABLE IV-15. XAD-4 RESIN TOC ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.2
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0435	0.0048	145.06	102.20	389.96
0.0427	0.0123	145.06	89.01	194.54
0.0429	0.0150	145.06	85.76	169.30
0.0381	0.0231	145.06	70.12	123.55
0.0432	0.0308	145.06	64.53	112.85
0.0430	0.0389	145.06	60.63	93.30
0.0427	0.0794	145.06	55.01	48.43
0.0433	0.1527	145.06	50.26	26.87
0.0421	0.2392	145.06	47.78	17.11
0.0442	0.3677	145.06	45.83	11.94
0.0439	0.5884	145.06	45.34	7.44
0.0434	0.9215	145.06	44.52	4.74
BLANK 1			149.06	
BLANK 2		187.80		
BLANK 3			150.55	
BLANK 4		191.24		
BLANK 5			154.85	

TABLE IV-16. XAD-4 RESIN TOC ISOTHERM, DILUTE WASTE MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.0
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Dilute Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2486	0.0122	67.00	61.23	117.33
0.0414	0.0056	67.00	49.68	128.69
0.0432	0.0103	67.00	43.40	98.65
0.0414	0.0147	67.00	39.90	76.20
0.0423	0.0239	67.00	35.72	55.43
0.0415	0.0305	67.00	33.20	46.11
0.0426	0.0377	67.00	32.14	39.31
0.0420	0.0787	67.00	30.45	19.48
0.0386	0.1578	67.00	27.50	9.66
0.0431	0.2458	67.00	26.98	7.02
0.0428	0.3737	67.00	26.44	4.65
0.0422	0.5834	67.00	25.00	3.04
0.0443	0.9294	67.00	23.24	2.09
BLANK 2		87.57		
BLANK 4		85.20		

TABLE IV-17. XAD-4 RESIN METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	5.9-7.8
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0434	0.0404	1.250	1.207	0.046
0.0385	0.0548	1.250	1.118	0.093
0.0425	0.1094	1.250	0.932	0.124
0.0429	0.1498	1.250	0.802	0.128
0.0434	0.2051	1.250	0.703	0.116
0.0437	0.2865	1.250	0.541	0.108
0.0398	0.3987	1.250	0.270	0.098
0.0441	0.5617	1.250	0.228	0.080
BLANK 1			1.243	
BLANK 5			1.256	

TABLE IV-18. XAD-4 RESIN METHYLENE CHLORIDE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.2
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0380	0.0106	7.514	7.432	0.293
0.0427	0.0145	7.514	7.254	0.765
0.0432	0.0289	7.514	6.881	0.947
0.0431	0.0767	7.514	5.461	1.153
0.0438	0.1506	7.514	4.049	1.008
0.0434	0.2039	7.514	3.235	0.911
0.0434	0.2864	7.514	2.415	0.772
0.0396	0.3926	7.514	1.645	0.593
0.0440	0.5528	7.514	1.426	0.484
BLANK 1			7.485	
BLANK 5			7.542	

TABLE IV-19. XAD-4 RESIN CHLOROFORM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND.. Chloroform
ADSORBENT TYPE.. XAD-4
ISOTHERM TYPE.. Virgin
PARTICLE SIZE.. 200x400 mesh
TEMPERATURE, Deg C... 23
pH.. 6.0-6.3
EQUILIBRATION TIME, days.................................... 7
BACKGROUND WATER MATRIX............................. Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0434	0.0056	0.882	0.875	0.055
0.0435	0.0083	0.882	0.848	0.179
0.0437	0.0115	0.882	0.802	0.303
0.0425	0.0151	0.882	0.753	0.362
0.0388	0.0293	0.882	0.555	0.433
0.0436	0.0422	0.882	0.455	0.441
0.0442	0.0561	0.882	0.357	0.414
0.0434	0.0778	0.882	0.243	0.357
0.0422	0.1073	0.882	0.109	0.304
0.0429	0.1506	0.882	0.069	0.232
0.0434	0.2954	0.882	0.046	0.123
0.0427	0.3999	0.882	0.030	0.091
0.0434	0.5815	0.882	0.019	0.064
BLANK 1			0.918	
BLANK 3			0.928	

TABLE IV-20. XAD-4 RESIN CHLOROFORM TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.3
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0383	0.0109	9.480	8.611	3.058
0.0432	0.0158	9.480	8.278	3.279
0.0377	0.0207	9.480	7.247	4.062
0.0432	0.0284	9.480	6.381	4.714
0.0447	0.0537	9.480	4.489	4.150
0.0426	0.0785	9.480	2.789	3.634
0.0429	0.1074	9.480	1.975	2.997
0.0427	0.1479	9.480	1.276	2.369
0.0442	0.2926	9.480	0.573	1.345
0.0432	0.4061	9.480	0.362	0.970
0.0439	0.5599	9.480	0.213	0.726
BLANK 1			10.190	
BLANK 3			10.110	

TABLE IV-21. XAD-4 RESIN PCE TRACER ISOTHERM, WASTE MIXTURE

CHEMICAL COMPOUND	PCE
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	21
pH	5.8-7.1
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Waste Stream Mixture filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2498	0.0045	0.898	0.781	6.493
0.2504	0.0067	0.898	0.732	6.177
0.2486	0.0112	0.898	0.652	5.467
0.2504	0.0177	0.898	0.546	4.980
0.0426	0.0055	0.898	0.378	4.026
0.0438	0.0079	0.898	0.277	3.459
0.0390	0.0123	0.898	0.148	2.383
0.0429	0.0199	0.898	0.085	1.755
0.0435	0.0320	0.898	0.043	1.162
0.0444	0.0490	0.898	0.022	0.794
BLANK 1			0.855	
BLANK 5			0.904	

APPENDIX V. Shower/Handwash Mixture Isotherm Data

TABLE V-1. 580-26 GAC TOC ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.2-8.7
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2475	0.0030	260.46	251.89	709.09
0.2499	0.0069	260.46	251.03	342.53
0.2487	0.0163	260.46	236.54	366.03
0.0432	0.0065	260.46	207.41	353.32
0.0414	0.0148	260.46	163.77	271.26
0.0431	0.0214	260.46	133.73	254.83
0.0420	0.0341	260.46	52.00	256.64
0.0428	0.0463	260.46	33.74	209.88
0.0422	0.0519	260.46	31.70	185.72
0.0416	0.1013	260.46	24.37	97.00
0.0419	0.2182	260.46		
0.0416	0.3285	260.46	10.43	31.67
0.0419	0.5050	260.46	11.05	20.69
0.0418	0.8033	260.46	11.26	12.96
0.0416	1.1680	260.46	10.51	8.90
BLANK 1			266.23	
BLANK 2		281.44		
BLANK 3			267.00	
BLANK 4		286.44		
BLANK 5			265.38	
BLANK 6		274.14		

TABLE V-2. 580-26 GAC TOC ISOTHERM, DILUTE SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.9
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Dilute Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2516	0.0028	115.12	112.31	252.50
0.2479	0.0073	115.12	104.99	344.00
0.2491	0.0165	115.12	96.09	287.30
0.0374	0.0068	115.12	68.16	258.58
0.0427	0.0150	115.12	32.05	236.69
0.0388	0.0225	115.12	17.16	168.72
0.0430	0.0327	115.12	13.37	133.87
0.0426	0.0441	115.12	12.47	99.04
0.0429	0.0517	115.12	11.10	86.28
0.0426	0.1091	115.12	8.19	41.72
0.0427	0.2131	115.12	7.85	21.49
0.0425	0.3231	115.12	8.80	13.98
0.0422	0.5219	115.12	7.77	8.67
0.0425	0.8013	115.12	8.41	5.66
0.0418	1.2040	115.12	12.30	3.57
BLANK 1			113.25	
BLANK 2		125.20		
BLANK 3			113.94	
BLANK 4		124.35		
BLANK 5			103.71	
BLANK 6		124.13		

TABLE V-3. 580-26 GAC METHYLENE CHLORIDE TRACER ISOTHER, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.8
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0424	0.0106	1.144	1.105	0.156
0.0431	0.0364	1.144	0.964	0.213
0.0436	0.0696	1.144	0.781	0.228
0.0426	0.0953	1.144	0.615	0.237
0.0425	0.1835	1.144	0.417	0.168
0.0425	0.2562	1.144	0.187	0.159
0.0419	0.3527	1.144	0.151	0.118
0.0426	0.4909	1.144	0.099	0.091
BLANK 1			1.153	
BLANK 5			1.134	

TABLE V-4. 580-26 GAC METHYLENE CHLORIDE TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.4
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0433	0.0362	8.112	7.768	0.411
0.0428	0.0485	8.112	7.250	0.760
0.0429	0.0690	8.112	6.353	1.093
0.0433	0.0949	8.112	5.512	1.188
0.0421	0.1326	8.112	4.246	1.229
0.0429	0.1868	8.112	3.093	1.152
0.0418	0.2588	8.112	2.057	0.979
0.0420	0.3693	8.112	1.259	0.779
0.0415	0.4964	8.112	0.790	0.612
BLANK 1			8.096	
BLANK 5			8.128	

TABLE V-5. 580-26 GAC CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.7
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0431	0.0139	0.813	0.751	0.192
0.0440	0.0356	0.813	0.551	0.324
0.0430	0.0501	0.813	0.381	0.371
0.0427	0.0682	0.813	0.224	0.369
0.0424	0.0954	0.813	0.115	0.310
0.0426	0.1317	0.813	0.063	0.243
0.0430	0.1839	0.813	0.036	0.182
0.0420	0.2668	0.813	0.017	0.125
0.0431	0.3584	0.813	0.009	0.097
0.0414	0.4972	0.813	0.005	0.067
BLANK 1			0.905	
BLANK 3			0.912	
BLANK 5			0.909	

TABLE V-6. 580-26 GAC CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	580-26
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.9
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0427	0.0049	8.979	8.850	1.131
0.0430	0.0068	8.979	8.652	2.079
0.0434	0.0104	8.979	8.528	1.875
0.0430	0.0367	8.979	6.381	3.042
0.0428	0.0495	8.979	4.989	3.445
0.0428	0.0699	8.979	2.889	3.725
0.0424	0.0953	8.979	1.686	3.242
0.0427	0.1335	8.979	0.896	2.583
0.0431	0.1871	8.979	0.521	1.950
0.0424	0.2591	8.979	0.257	1.426
0.0428	0.3629	8.979	0.157	1.040
0.0426	0.4978	8.979	0.080	0.761
BLANK 1			9.279	
BLANK 3			9.470	

TABLE V-7. APA GAC TOC ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.2-7.8
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2508	0.0038	260.46	255.40	338.03
0.2499	0.0077	260.46	244.74	509.78
0.2491	0.0171	260.46	234.86	373.10
0.0434	0.0070	260.46	206.98	330.97
0.0425	0.0148	260.46	195.49	186.17
0.0425	0.0207	260.46	159.98	205.72
0.0421	0.0310	260.46	98.70	219.69
0.0424	0.0447	260.46	39.83	209.24
0.0415	0.0510	260.46	42.14	177.89
0.0418	0.1061	260.46	24.48	92.99
0.0419	0.2045	260.46	23.63	48.50
0.0411	0.3278	260.46	16.78	30.53
0.0369	0.5031	260.46	13.97	18.10
0.0411	0.5966	260.46	13.61	17.00
0.0420	0.8016	260.46	8.29	13.23
0.0422	1.1753	260.46	8.31	9.04
BLANK 1			261.69	
BLANK 2		276.41		
BLANK 3			263.61	
BLANK 4		280.59		

TABLE V-8. APA GAC TOC ISOTHERM, DILUTE SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-8.6
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Dilute Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2477	0.0034	115.12	115.29	-12.25
0.2495	0.0077	115.12	112.66	80.15
0.2476	0.0154	115.12	99.40	252.43
0.0430	0.0074	115.12	75.01	234.24
0.0428	0.0153	115.12	36.52	219.53
0.0423	0.0208	115.12	21.60	189.95
0.0437	0.0315	115.12	13.20	141.16
0.0428	0.0425	115.12	11.15	104.75
0.0428	0.0514	115.12	6.28	90.76
0.0429	0.1054	115.12	3.43	45.47
0.0429	0.2048	115.12	3.73	23.32
0.0422	0.3196	115.12	3.24	14.77
0.0419	0.5055	115.12	3.97	9.22
0.0423	0.7928	115.12	3.27	5.97
0.0411	1.1902	115.12	4.89	3.80

BLANK 1		113.41
BLANK 2	126.21	
BLANK 3		116.52
BLANK 4	126.81	
BLANK 5		116.47
BLANK 6	126.57	

TABLE V-9. APA GAC METHYLENE CHLORIDE TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-7.8
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0433	0.0504	1.044	0.959	0.073
0.0428	0.0683	1.044	0.863	0.114
0.0435	0.1329	1.044	0.553	0.161
0.0428	0.1843	1.044	0.381	0.154
0.0427	0.2548	1.044	0.207	0.140
0.0421	0.3557	1.044	0.111	0.111
0.0425	0.4917	1.044	0.071	0.084
BLANK 1			1.039	
BLANK 5			1.048	

TABLE V-10. METHYLENE CHLORIDE TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.1
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0433	0.0270	8.103	7.816	0.461
0.0423	0.0363	8.103	7.562	0.630
0.0436	0.0487	8.103	7.295	0.723
0.0424	0.0701	8.103	6.622	0.896
0.0429	0.0977	8.103	5.959	0.941
0.0417	0.1338	8.103	4.795	1.031
0.0374	0.1856	8.103	2.906	1.048
0.0425	0.2584	8.103	2.118	0.984
0.0414	0.3574	8.103	1.175	0.803
0.0419	0.4935	8.103	0.774	0.622
BLANK 1			8.093	
BLANK 5			8.113	

TABLE V-11. APA GAC CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0433	0.0077	0.813	0.801	0.068
0.0427	0.0108	0.813	0.768	0.179
0.0428	0.0366	0.813	0.590	0.261
0.0433	0.0523	0.813	0.476	0.279
0.0433	0.0716	0.813	0.317	0.300
0.0425	0.0961	0.813	0.184	0.278
0.0437	0.1342	0.813	0.075	0.240
0.0430	0.1869	0.813	0.030	0.180
0.0436	0.2554	0.813	0.012	0.137
0.0429	0.3524	0.813	0.005	0.098
0.0427	0.4944	0.813	0.003	0.070
BLANK 1			0.832	
BLANK 3			0.833	
BLANK 5			0.843	

TABLE V-12. APA GAC CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	APA
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-7.1
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0432	0.0052	8.979	8.794	1.550
0.0434	0.0071	8.979	8.925	0.328
0.0448	0.0097	8.979	8.801	0.821
0.0435	0.0367	8.979	7.049	2.289
0.0386	0.0495	8.979	5.559	2.663
0.0438	0.0684	8.979	4.433	2.912
0.0385	0.0957	8.979	2.104	2.769
0.0432	0.1335	8.979	1.389	2.456
0.0428	0.1843	8.979	0.623	1.942
0.0367	0.2585	8.979	0.171	1.251
0.0429	0.3535	8.979	0.112	1.077
0.0420	0.4918	8.979	0.051	0.763
BLANK 1			8.916	
BLANK 3			9.155	

TABLE V-13. XAD-4 RESIN TOC ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.2-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2482	0.0023	260.46	236.76	2595.41
0.2499	0.0049	260.46	244.16	831.69
0.2502	0.0106	260.46	221.75	909.90
0.0423	0.0053	260.46	199.75	487.55
0.0432	0.0098	260.46	180.28	354.87
0.0427	0.0144	260.46	165.26	281.97
0.0431	0.0215	260.46	143.70	233.72
0.0434	0.0286	260.46	142.18	179.55
0.0435	0.0343	260.46	125.00	171.87
0.0436	0.0715	260.46	57.77	123.52
0.0427	0.1477	260.46	39.40	63.88
0.0426	0.2249	260.46	34.14	42.86
0.0435	0.3444	260.46	30.26	29.05
0.0428	0.5387	260.46	30.79	18.24
0.0433	0.8197	260.46	26.41	12.36
BLANK 1			241.82	
BLANK 2		272.65		
BLANK 3			242.83	
BLANK 4		272.65		
BLANK 5			238.76	
BLANK 6		277.79		

TABLE V-14. XAD-4 RESIN TOC ISOTHERM, DILUTE SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.3
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Dilute Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.2501	0.0019	112.15	114.27	-279.41
0.2489	0.0059	112.15	106.78	226.21
0.2498	0.0116	112.15	101.33	232.11
0.0424	0.0056	112.15	84.30	212.43
0.0429	0.0110	112.15	73.72	149.94
0.0421	0.0148	112.15	67.26	127.48
0.0432	0.0232	112.15	41.35	131.98
0.0421	0.0311	112.15	36.49	102.28
0.0431	0.0390	112.15	30.47	90.16
0.0426	0.0776	112.15	20.42	50.29
0.0427	0.1546	112.15	17.49	26.12
0.0428	0.2321	112.15	16.44	17.64
0.0438	0.3712	112.15	13.45	11.64
0.0426	0.5766	112.15	14.01	7.26
0.0388	0.9132	112.15	13.38	4.20

BLANK 1		110.40
BLANK 2	123.94	
BLANK 3		104.91
BLANK 4	124.33	
BLANK 5		110.61
BLANK 6	125.36	

TABLE V-15. XAD-4 RESIN METHYLENE CHLORIDE TRACER ISOTEHRM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.1-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0428	0.0053	7.619	7.528	0.735
0.0389	0.0378	7.619	6.657	0.991
0.0433	0.0534	7.619	6.277	1.088
0.0427	0.0721	7.619	5.728	1.121
0.0437	0.1409	7.619	4.246	1.046
0.0429	0.1994	7.619	3.242	0.942
0.0383	0.2728	7.619	2.082	0.778
0.0435	0.3878	7.619	1.682	0.666
0.0431	0.5273	7.619	1.196	0.525
BLANK 1			7.589	
BLANK 5			7.648	

TABLE V-16. XAD-4 RESIN METHYLENE CHLORIDE TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Methylene Chloride
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0395	0.0279	0.982	0.951	0.044
0.0431	0.0397	0.982	0.949	0.036
0.0435	0.0565	0.982	0.880	0.079
0.0435	0.0758	0.982	0.809	0.099
0.0433	0.1069	0.982	0.689	0.119
0.0440	0.1466	0.982	0.582	0.120
0.0427	0.2068	0.982	0.417	0.117
0.0437	0.2856	0.982	0.298	0.105
0.0438	0.3959	0.982	0.215	0.085
0.0436	0.5543	0.982	0.153	0.065
BLANK 1			0.959	
BLANK 5			1.004	

TABLE V-17. XAD-4 RESIN CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND	Chloroform
ADSORBENT TYPE	XAD-4
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 mesh
TEMPERATURE, Deg C	23
pH	6.0-6.5
EQUILIBRATION TIME, days	7
BACKGROUND WATER MATRIX	Shower/Handwash filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0437	0.0264	8.979	6.279	4.474
0.0432	0.0346	8.979	5.403	4.474
0.0388	0.0485	8.979	4.171	3.847
0.0434	0.0685	8.979	3.412	3.528
0.0428	0.0952	8.979	2.111	3.089
0.0432	0.1308	8.979	1.387	2.508
0.0436	0.1828	8.979	0.830	1.944
0.0429	0.2526	8.979	0.489	1.443
0.0427	0.3494	8.979	0.289	1.063
0.0432	0.5087	8.979	0.189	0.747
BLANK 1			8.772	
BLANK 3			8.817	
BLANK 5			8.769	

TABLE V-18. XAD-4 RESIN CHLOROFORM TRACER ISOTHERM, SHOWER/HANDWASH MIXTURE

CHEMICAL COMPOUND.. Chloroform
ADSORBENT TYPE.. XAD-4
ISOTHERM TYPE.. Virgin
PARTICLE SIZE.. 200x400 mesh
TEMPERATURE, Deg C... 23
pH... 6.0-6.5
EQUILIBRATION TIME, days..................................... 7
BACKGROUND WATER MATRIX............................... Shower/Handwash
filtered and MCV'd

Bottle Volume (Liters)	Dry Weight (Grams)	Initial Conc. (mg/L)	Eq. Liq-Phase Conc. (mg/L)	Eq. Sol-Phase Conc. (mg/g)
0.0435	0.0286	0.813	0.721	0.140
0.0424	0.0389	0.813	0.632	0.197
0.0395	0.0536	0.813	0.517	0.218
0.0426	0.1087	0.813	0.248	0.221
0.0430	0.1468	0.813	0.163	0.190
0.0431	0.2040	0.813	0.100	0.151
0.0438	0.2892	0.813	0.059	0.114
0.0436	0.3941	0.813	0.035	0.086
0.0394	0.5552	0.813	0.022	0.056
BLANK 1			0.793	
BLANK 3			0.791	
BLANK 5			0.781	

APPENDIX VI. Urine Distillate Isotherm Data

TABLE VI-1. 580-26 GAC TOC ISOTHERM, TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.3-7.3
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2511	0.0036	12.75	10.48	156.80
0.2504	0.0055	12.75	10.04	123.33
0.2502	0.0113	12.75	9.41	73.96
0.2500	0.0229	12.75	8.82	42.93
0.0429	0.0273	12.75	5.47	11.44
0.0425	0.0365	12.75	6.23	7.58
0.0438	0.0586	12.75	5.62	5.33
0.0431	0.1475	12.75	3.35	2.75
0.0430	0.4490	12.75	2.69	0.96
0.0421	0.5413	12.75	2.44	0.80
Blank 1		12.82		
Blank 2		12.77		
Blank 3		12.68		
Blank 4		12.73		

TABLE VI-2. 580-26 GAC TOC ISOTHERM, DILUTE TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.5-7.3
EQUILIBRATION TIME, Days	11
BACKGROUND WATER MATRIX	Dilute Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2490	0.0041	5.90	4.22	101.62
0.2513	0.0055	5.90	4.18	78.88
0.2499	0.0236	5.90	3.18	28.84
0.0429	0.0367	5.90	1.47	5.17
0.0427	0.0601	5.90	1.34	3.24
0.0428	0.1475	5.90	1.01	1.42
Blank 1		5.90		
Blank 2		5.99		
Blank 3		5.86		
Blank 4		5.85		

TABLE VI-3. 580-26 GAC SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH 3.89-4.68	3.9-4.7
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2523	0.0047	379.8	349.7	1619.9
0.2521	0.0118	377.3	229.7	3162.0
0.2517	0.0222	374.9	114.0	2951.5
0.2493	0.0555	370.0	38.7	1489.1
0.2516	0.0815	367.5	20.2	1072.0

Blank 1	392.9
Blank 2	366.7
Blank 3	376.1
Blank 4	358.9
Blank 5	353.0
Blank 6	337.5

TABLE VI-4. 580-26 GAC SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-6.0
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2495	0.0037	6943.8	6232.6	48079.6
0.2517	0.0117	6760.0	4694.7	44539.1
0.2497	0.0217	6576.2	2818.4	43145.8
0.2508	0.0378	6392.3	1496.3	32476.1
0.2508	0.0563	6208.5	764.3	24265.0
0.2504	0.0826	6024.7	381.5	17109.9
0.2503	0.1089	6024.7	196.3	13390.6
0.2503	0.1364	5984.4	108.7	10783.7
0.0430	0.0366	5944.2	48.4	6916.5
Blank 1		6772.7		
Blank 2		7114.9		
Blank 3		5846.5		
Blank 4		6202.8		
Blank 5		5823.4		

TABLE VI-4. 580-26 GAC SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND		Toluene
ADSORBENT TYPE		580-26 GAC
ISOTHERM TYPE		Virgin
PARTICLE SIZE		200x400 Mesh
TEMPERATURE, Deg C		21 +/- 1
pH	3.80-4.35	3.8-4.4
EQUILIBRATION TIME, Days		11
BACKGROUND WATER MATRIX		Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2522	0.0029	447.1	362.2	7466.7
0.2507	0.0040	441.4	301.9	8840.1
0.2512	0.0061	435.7	201.5	9592.9
0.2514	0.0080	430.0	154.5	8646.8
0.2510	0.0116	424.3	78.1	7510.2
0.2523	0.0246	418.6	15.8	4126.3
0.2509	0.0375	413.2	6.2	2724.7
0.2520	0.0521	407.8	2.8	1958.2
0.2488	0.0776	402.5	1.6	1284.4
Blank 1		382.4		
Blank 2		447.1		
Blank 3		414.4		
Blank 4		422.9		
Blank 5		390.3		
Blank 6		393.2		

TABLE VI-6. 580-26 GAC SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-4.4
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Litersl)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2492	0.0038	7480.7	5449.1	134706.6
0.2498	0.0160	7355.5	2209.0	80247.1
0.2504	0.0418	7230.0	374.1	41042.5
0.2486	0.0636	7167.0	122.0	27537.4
0.0434	0.0215	7021.5	30.3	14128.1
0.0436	0.0313	6991.9	12.0	9733.2
0.0430	0.0448	6962.4	13.1	6663.7
0.0430	0.0670	6932.8	8.9	4444.6
0.0429	0.0961	6903.3	6.2	3078.7
Blank 1		7492.3		
Blank 2		7469.0		
Blank 3		7166.7		
Blank 4		7050.7		
Blank 5		7010.0		
Blank 6		6796.6		

TABLE VI-7. 580-26 GAC SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-4.5
EQUILIBRATION TIME, Days	13
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2506	0.0041	104.4	1.3	6378.8
0.2520	0.0054	104.4	1.2	4784.0
0.5000	0.0041	104.4	4.2	12073.5
0.4967	0.0057	104.4	8.9	8275.2
Blank 1		101.1		
Blank 2		105.4		
Blank 3		102.5		
Blank 4		111.5		
Blank 5		101.0		
Blank 6		105.1		

TABLE VI-8. 580-26 GAC SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-4.0
EQUILIBRATION TIME, Days	13
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2517	0.00435	925.7	22.1	52317.8
0.2507	0.00672	925.7	8.0	34244.4
0.5010	0.00375	925.7	161.5	101977.5
0.4988	0.00583	925.7	59.4	74128.6
Blank 1		926.5		
Blank 2		927.3		
Blank 3		928.4		
Blank 4		953.5		
Blank 5		920.6		
Blank 6		906.9		

TABLE VI-9. APA GAC TOC ISOTHERM, TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.1-6.1
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered and MCV'd

BOTTLE VOLUME Liters	DRY WEIGHT Grams	INITIAL CONC. mg/L	EQ. LIQ-PHASE CONC. mg/L	EQ. SOL-PHASE CONC. mg/g
0.2503	0.0040	12.74	10.45	141.69
0.2507	0.0057	12.74	10.32	106.03
0.2495	0.0210	12.74	8.89	45.75
0.2504	0.0702	12.74	5.85	24.57
0.0427	0.0406	12.74	5.21	7.92
0.0424	0.1242	12.74	3.14	3.27
0.0425	0.2007	12.74	3.17	2.03
0.0421	0.3177	12.74	2.75	1.32
0.0412	0.5054	12.74	2.98	0.79
Blank 1		12.74		
Blank 2		12.77		
Blank 3		12.70		
Blank 4		12.73		

TABLE VI-10. APA GAC TOC ISOTHERM, DILUTE TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	4.0-6.1
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Dilute Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2517	0.0059	5.90	4.62	54.54
0.2500	0.0207	5.90	2.93	35.94
0.0438	0.0399	5.90	1.69	4.62
0.0433	0.0730	5.90	1.75	2.46
0.0431	0.1235	5.90	1.68	1.47
0.0433	0.3146	5.90	1.31	0.63
0.0416	0.5040	5.90	1.13	0.39
Blank 1		5.90		
Blank 2		5.86		
Blank 3		5.88		
Blank 4		5.94		

TABLE VI-11. APA GAC SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-5.3
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME Liters	DRY WEIGHT Grams	INITIAL CONC. ug/L	EQ. LIQ-PHASE CONC. ug/L	EQ. SOL-PHASE CONC. ug/g
0.2498	0.0039	393.9	375.4	1198.0
0.2504	0.0158	393.9	240.3	2430.9
0.2531	0.0333	393.9	102.9	2210.1
0.2505	0.0545	393.9	36.6	1642.3
0.2517	0.0807	393.9	17.7	1173.1
0.2507	0.1187	393.9	15.5	799.4
Blank 1		384.0		
Blank 2		405.7		
Blank 3		368.7		
Blank 4		576.7		
Blank 5		383.2		
Blank 6		427.7		

TABLE VI-12. APA GAC SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-5.4
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2504	0.0177	7177.3	4697.7	35073.1
0.2532	0.0324	7140.4	2745.3	34305.2
0.2505	0.0555	7103.4	1345.1	25998.3
0.2517	0.0814	7066.5	692.5	19706.5
0.2507	0.1174	7029.5	315.6	14337.8
0.2485	0.1573	7029.5	169.8	10833.4
0.0427	0.0385	7001.1	78.6	7683.2
0.0433	0.0548	6972.7	42.7	5476.7
Blank 1		7264.0		
Blank 2		7164.6		
Blank 3		7011.3		
Blank 4		7047.7		
Blank 5		6879.1		
Blank 6		6895.9		

TABLE VI-13. APA GAC SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-4.9
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2513	0.0044	389.1	310.4	4444.8
0.2503	0.0057	389.1	272.4	5093.2
0.2507	0.0077	389.1	194.7	6319.9
0.2510	0.0122	389.1	109.6	5769.3
0.2504	0.0185	389.1	49.6	4598.2
0.2508	0.0251	389.1	22.4	3661.5
0.2514	0.0349	389.1	9.6	2733.3
0.2499	0.0507	389.1	4.5	1895.0
0.2484	0.0744	389.1	1.7	1294.1
Blank 2		357.7		
Blank 3		405.0		
Blank 4		406.3		
Blank 6		387.5		

TABLE VI-14. APA GAC SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	4.0-5.4
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2480	0.0037	7852.9	7008.0	55951.1
0.2496	0.0108	7838.0	4572.2	75179.7
0.2509	0.0179	7823.2	2947.4	68205.2
0.2490	0.0296	7808.4	1471.3	53365.1
0.2504	0.0405	7793.5	782.1	43338.4
0.2504	0.0558	7778.7	382.3	33196.7
0.2497	0.0707	7778.7	199.7	26777.4
0.2500	0.0853	7745.0	141.8	22269.4
0.0423	0.0222	7711.3	51.3	14626.4
0.0428	0.0303	7677.5	24.9	10818.2
0.0428	0.0388	7643.8	10.1	8414.5
0.0437	0.0521	7610.1	6.5	6375.1
Blank 1		8032.6		
Blank 2		7673.1		
Blank 3		7831.7		
Blank 4		7725.7		
Blank 5		7850.4		
Blank 6		7369.8		

TABLE VI-15. APA GAC SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-3.9
EQUILIBRATION TIME, Days	11
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.4981	0.0029	105.8	15.4	15795.5
0.5000	0.0037	105.8	9.6	12876.8
0.4989	0.0043	105.8	7.4	11350.2
Blank 1		111.6		
Blank 2		105.6		
Blank 3		102.1		
Blank 4		107.9		
Blank 5		103.7		
Blank 6		103.6		

TABLE VI-16. APA GAC SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-3.9
EQUILIBRATION TIME, Days	11
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2510	0.0031	928.0	95.3	66444.5
0.2500	0.0049	928.0	31.9	45579.9
0.2513	0.0063	928.0	17.3	36377.6
0.2516	0.0071	928.0	10.0	32633.8
0.2501	0.0101	928.0	4.3	22816.8
0.4981	0.0040	928.0	205.5	89288.0
Blank 1		940.9		
Blank 2		943.5		
Blank 3		902.9		
Blank 4		936.3		
Blank 5		919.1		
Blank 6		925.5		

TABLE VI-17. XAD-4 RESIN TOC ISOTHERM, TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-4.8
EQUILIBRATION TIME, Days	11
BACKGROUND WATER MATRIX	Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2511	0.0045	12.79	12.00	43.78
0.2508	0.0059	12.79	11.97	34.78
0.2506	0.0125	12.79	11.51	25.70
0.2488	0.0292	12.79	11.05	14.81
0.2505	0.0692	12.79	10.51	8.25
0.0385	0.0884	12.79	9.30	1.52
0.0436	0.1440	12.79	9.19	1.09
0.0423	0.2677	12.79	9.08	0.59
0.0428	0.4907	12.79	8.17	0.40
0.0412	0.8512	12.79	7.56	0.25
0.0401	1.3728	12.79	4.58	0.24
Blank 1		12.71		
Blank 2		12.85		
Blank 3		12.74		
Blank 4		12.86		

TABLE VI-18. XAD-4 RESIN TOC ISOTHERM, DILUTE TREATED URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	4.0-5.5
EQUILIBRATION TIME, Days	11
BACKGROUND WATER MATRIX	Dilute Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2512	0.0090	6.01	5.47	14.88
0.2517	0.0154	6.01	5.44	9.30
0.0436	0.0366	6.01	4.66	1.61
0.0436	0.0982	6.01	4.19	0.81
0.0429	0.1646	6.01	3.45	0.67
0.0418	0.5650	6.01	2.57	0.25
0.0410	0.9206	6.01	1.72	0.19

Blank 1	5.98
Blank 2	6.02
Blank 3	5.98
Blank 4	6.06

TABLE VI-19. XAD-4 RESIN SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-4.7
EQUILIBRATION TIME, Days	13
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2514	0.0068	324.9	249.4	2781.7
0.2505	0.0258	314.0	125.0	1832.1
0.2530	0.0388	303.1	90.4	1388.6
0.2490	0.0922	292.3	36.5	690.8
0.2499	0.1489	281.4	33.0	417.0
0.2498	0.2701	270.5	20.0	231.7
Blank 1		324.3		
Blank 2		325.4		
Blank 3		278.5		
Blank 4		262.4		
Blank 5		239.2		
Blank 6		256.0		

TABLE VI-20. XAD-4 RESIN SPIKE ISOTHERM, TCE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-5.6
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2508	0.0053	6123.1	5103.1	48427.8
0.2523	0.0233	5971.4	3404.3	27804.6
0.2509	0.0412	5819.7	2197.4	22038.7
0.2509	0.0796	5668.0	1191.9	14097.4
0.2502	0.1424	5516.3	587.1	8657.9
0.2497	0.2547	5364.6	250.9	5014.4
0.2511	0.3893	5212.9	149.0	3265.8
0.0435	0.1080	5061.2	78.3	2006.6
0.0426	0.1787	4909.5	46.8	1158.6
0.0427	0.2974	4757.8	23.9	680.3
0.0429	0.5025	4606.2	16.8	391.5

Blank 1	6057.9
Blank 2	6188.3
Blank 3	2809.1
Blank 4	4663.7
Blank 5	4456.7
Blank 6	4452.2

TABLE VI-1. XAD-4 RESIN SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	3.9-4.6
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Urine Distillate Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2516	0.0722	487.8	37.2	1571.3
0.2482	0.0922	487.8	35.8	1216.8
0.2490	0.1308	487.8	22.9	885.0
0.0422	0.0404	487.8	10.9	498.9
0.0431	0.0518	487.8	9.6	398.2

Note: Not many bottles since some were broken when tumbler came open.

Blank 1	506.6
Blank 2	494.9
Blank 3	490.4
Blank 5	490.4
Blank 6	456.5

TABLE VI-22. XAD-4 RESIN SPIKE ISOTHERM, TOLUENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND		Toluene
ADSORBENT TYPE		XAD-4 Resin
ISOTHERM TYPE		Virgin
PARTICLE SIZE		0.3-1.2 mm
TEMPERATURE, Deg C		21 +/- 1
pH	3.77-9.78	3.8-9.8
EQUILIBRATION TIME, Days		13
BACKGROUND WATER MATRIX		Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2508	0.0045	6994.7	6012.9	54831.1
0.2499	0.0143	6820.4	4247.9	44837.9
0.2506	0.0325	6646.1	2406.2	32727.5
0.2509	0.0626	6471.8	1100.6	21519.5
0.2500	0.1026	6297.5	523.8	14070.1
0.2495	0.1742	6123.2	259.0	8401.4
0.0437	0.0522	6123.2	112.9	5027.6
0.0432	0.0731	5944.9	70.5	3470.2
0.0382	0.1126	5766.6	40.1	1942.7
0.0430	0.1814	5588.3	27.3	1317.9
0.0429	0.2950	5410.0	17.7	784.1
0.0422	0.4891	5231.7	8.3	450.7
Blank 1			6904.1	
Blank 2			7085.3	
Blank 3			6325.5	
Blank 4			5920.9	
Blank 5			5220.4	
Blank 6			5242.9	

TABLE VI-23. XAD-4 RESIN SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	3.8-6.2
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2511	0.0019	106.9	50.4	7486.6
0.2501	0.0031	106.9	36.8	5710.9
0.2511	0.0044	106.9	25.9	4626.3
0.2511	0.0068	106.9	17.0	3309.0
0.2513	0.0103	106.9	9.4	2385.6
0.2510	0.0134	106.9	7.9	1852.1
0.2513	0.0170	106.9	5.9	1491.5
0.2506	0.0254	106.9	3.6	1019.5
0.5002	0.0017	106.9	71.8	10070.6
Blank 1		110.3		
Blank 2		107.0		
Blank 3		107.2		
Blank 4		106.2		
Blank 5		102.9		
Blank 6		107.7		

TABLE VI-24. XAD-4 RESIN SPIKE ISOTHERM, NAPHTHALENE IN URINE DISTILLATE

LIQUID-PHASE SPIKED ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH 3.8-6.6	3.8-6.6
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Urine Distillate Filtered & MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2488	0.0015	949.0	608.5	54726.4
0.2505	0.0035	949.0	378.8	40903.5
0.2510	0.0091	949.0	148.4	22150.6
0.2510	0.0114	949.0	101.5	18699.2
0.2511	0.0136	949.0	82.8	15941.3
0.2509	0.0197	949.0	48.5	11452.5
0.2502	0.0257	949.0	28.1	8963.9
0.2502	0.0355	949.0	21.3	6545.7
0.2512	0.0474	949.0	14.4	4951.7
0.5009	0.0015	949.0	741.0	67304.4
Blank 1		970.9		
Blank 2		926.7		
Blank 3		940.4		
Blank 4		972.6		
Blank 5		936.2		
Blank 6		947.0		

APPENDIX VII. Humidity Condensate Isotherm Data

TABLE VII-1. 580-26 TOC ISOTHERM, HUMIDITY CONDNENSATE WATER

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.2-7.6
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humdity Condensate, Nondilute Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2486	0.0060	58.48	57.81	27.61
0.2531	0.0113	58.48	57.16	29.63
0.2535	0.0187	58.48	54.77	50.31
0.2524	0.0392	58.48	54.83	23.52
0.2494	0.0785	58.48	52.91	17.69
0.0438	0.0289	58.48	52.07	9.72
0.0435	0.0587	58.48	46.13	9.14
0.0426	0.1288	58.48	44.71	4.56
0.0423	0.3268	58.48	33.34	3.25
0.0423	0.4945	58.48	31.01	2.35
0.0421	0.9892	58.48	21.13	1.59
Blank 1		58.78		
Blank 2		54.63		
Blank 3		57.15		
Blank 4		59.52		

TABLE VII-2. 580-26 GAC TOC ISOTHERM DILUTE HUMIDITY CONDENSATE WATER

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.2-7.4
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humdity Condensate, Diluted Filtered and MCV'd

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2532	0.0056	29.96	28.34	72.76
0.2523	0.0115	29.96	28.23	38.05
0.2526	0.0188	29.96	27.05	39.12
0.2557	0.0391	29.96	26.78	20.81
0.0429	0.0291	29.96	25.58	6.46
0.0430	0.0583	29.96	24.37	4.13
0.0428	0.1289	29.96	22.31	2.54
0.0423	0.4947	29.96	15.33	1.25
0.0415	0.9889	29.96	12.59	0.73
Blank 1		29.81		
Blank 2		30.25		
Blank 3		30.15		
Blank 4		29.61		

TABLE VII-3. 580-26 GAC SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.2 - 6.7
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2507	0.0044	551.7	447.2	5994.0
0.2496	0.0122	551.7	281.9	5512.3
0.2469	0.0224	551.7	135.7	4575.8
0.2503	0.0380	551.7	58.0	3248.6
0.2500	0.0562	551.7	25.7	2339.2
0.2500	0.0819	551.7	11.9	1647.0
0.0428	0.0226	551.7	4.8	1033.7
BLANK1		554.00		
BLANK2		569.60		
BLANK3		541.20		
BLANK4		546.50		
BLANK5		513.70		
BLANK6		547.10		

TABLE VII-4. 580-26 GAC SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	5.9-6.5
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2470	0.0046	9941.6	8612.1	71881.8
0.2512	0.0117	9941.6	6672.4	70075.5
0.2443	0.0375	9941.6	2550.2	48099.8
0.2487	0.0559	9941.6	1556.8	37294.5
0.2480	0.0841	9941.6	757.6	27076.0
0.0417	0.0223	9941.6	312.3	17969.4
0.0425	0.0274	9941.6	204.6	15097.0
0.0419	0.0370	9941.6	105.8	11125.0
0.0420	0.0530	9941.6	52.5	7831.6
BLANK1		9464.30		
BLANK2		10375.10		
BLANK3		9794.70		
BLANK4		4421.50		
BLANK5		8867.00		
BLANK6		10132.40		

TABLE VII-5. 580-26 GAC SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.5-7.3
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2496	0.0032	488.7	334.8	12063.5
0.2509	0.0064	488.7	180.0	12159.3
0.2495	0.0088	488.7	115.9	10620.6
0.2503	0.0118	488.7	69.1	8869.6
0.2475	0.0179	488.7	32.7	6300.7
0.0426	0.0045	488.7	17.0	4489.2
0.0432	0.0062	488.7	7.5	3365.3
0.0434	0.0080	488.7	4.4	2639.5
BLANK 1		504.3		
BLANK 2		507.0		
BLANK 3		521.1		
BLANK 4		469.0		
BLANK 5		460.7		
BLANK 6		470.0		

TABLE VII-6. 580-26 GAC SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.2-7.4
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2481	0.0042	9446.7	7205.0	133315.3
0.2518	0.0101	9446.7	4696.7	118066.7
0.2516	0.0184	9446.7	2710.8	92245.9
0.2520	0.0280	9446.7	1264.8	73615.0
0.2508	0.0411	9446.7	763.2	52974.8
0.2502	0.0577	9446.7	412.8	39172.5
0.2497	0.0712	9446.7	244.2	32276.6
0.2510	0.0864	9446.7	164.9	26962.8
0.0427	0.0300	9446.7	33.7	13401.8
0.0431	0.0382	9446.7	21.7	10619.6
0.0427	0.0516	9446.7	16.7	7804.7
BLANK 1		9353.7		
BLANK 2		9573.1		
BLANK 3		9460.9		
BLANK 4		7991.0		
BLANK 5		8948.7		
BLANK 6		9399.1		

TABLE VII-7. 580-26 GAC SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.6-7.0
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.9872	0.00027	102.4	73.8	104956.7
0.9828	0.00057	102.4	68.4	58834.5
0.9859	0.00071	102.4	68.0	47939.4
0.9899	0.00148	102.4	44.8	38656.9
1.0447	0.00237	102.4	36.8	28892.1
1.0448	0.00312	102.4	26.6	25386.5
0.5003	0.00240	102.4	13.3	18557.6
0.4976	0.00333	102.4	6.8	14289.5
0.2498	0.00187	102.4	4.4	13064.2
0.2489	0.00363	102.4	1.5	6922.1
BLANK 1		102.1		
BLANK 2		101.3		
BLANK 3		113.3		
BLANK 4		98.9		
BLANK 5		100.6		
BLANK 6		98.3		

TABLE VII-8. 580-26 GAC SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	580-26 GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.5-7.3
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
1.0431	0.00063	1016.8	855.8	267622.4
0.9914	0.00296	1016.8	480.1	179896.8
0.9889	0.00505	1016.8	249.5	150286.6
0.4982	0.00360	1016.8	160.7	118313.2
0.5002	0.00595	1016.8	76.5	78981.3
0.2496	0.00500	1016.8	21.0	49719.8
0.2509	0.00704	1016.8	13.5	35754.4
0.2504	0.01043	1016.8	9.5	24191.5
0.2501	0.01354	1016.8	8.0	18629.3
0.0424	0.00368	1016.8	4.1	11653.7
BLANK 1		1005.2		
BLANK 2		1026.7		
BLANK 3		998.8		
BLANK 4		1009.7		
BLANK 5		1096.2		
BLANK 6		963.9		

TABLE VII-9. APA GAC TOC ISOTHERM, TREATED HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	5.9-6.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate, MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
.2506	.0040	63.27	61.90	84.59
.2507	.0105	63.27	61.70	37.52
.2493	.0201	63.27	60.90	29.29
.2499	.0396	63.27	59.60	23.14
.2504	.0594	63.27	58.40	20.50
.2506	.0805	63.27	58.20	15.78
.2511	.1390	63.27	56.42	12.36
.0425	.0844	63.27	50.74	6.30
.0429	.1277	63.27	48.84	4.85
.0428	.2105	63.27	44.91	3.73
.0421	.4574	63.27	36.60	2.45
.0416	1.2437	63.27	23.64	1.33
Blank 1		63.42		
Blank 2		63.12		
Blank 3		63.27		

TABLE VII-10. APA GAC TOC ISOTHERM, DILUTE TREATED HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	5.9-6.9
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate, Diluted, MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2500	0.0042	27.25	26.58	39.28
0.2496	0.0101	27.25	26.06	29.41
0.2501	0.0205	27.25	25.05	26.87
0.2484	0.0394	27.25	24.28	18.70
0.2472	0.0598	27.25	24.48	11.45
0.2500	0.0801	27.25	23.91	10.41
0.2487	0.1396	27.25	23.49	6.69
0.0428	0.0846	27.25	20.74	3.29
0.0427	0.1285	27.25	19.90	2.44
0.0422	0.2106	27.25	17.42	1.97
0.0414	0.4578	27.25	12.96	1.29
0.0384	1.2470	27.25	7.52	0.61
Blank 1		27.22		
Blank 2		26.93		
Blank 3		27.80		
Blank 4		27.04		

TABLE VII-11. APA GAC SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.2-7.0
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2478	0.0041	557.9	521.0	2245.5
0.2486	0.0167	557.9	278.9	4162.1
0.2494	0.0298	557.9	150.4	3414.8
0.2487	0.0523	557.9	61.1	2363.4
0.2470	0.0820	557.9	26.6	1600.1
0.2478	0.1184	557.9	13.8	1138.7
0.2476	0.1550	557.9	7.2	879.4
BLANK1		583.4		
BLANK2		553.0		
BLANK3		533.8		
BLANK4		567.5		
BLANK5		566.4		
BLANK6		543.0		

TABLE VII-12. APA GAC SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	5.9-7.0
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2488	0.0043	9940.4	9299.8	37377.2
0.2491	0.0166	9940.4	6400.0	53243.5
0.2452	0.0314	9940.4	4415.0	43090.4
0.2511	0.0558	9940.4	1509.6	37912.3
0.2471	0.0818	9940.4	1379.9	25849.7
0.2448	0.1174	9940.4	644.5	19376.3
0.2490	0.1520	9940.4	457.9	15530.0
0.0424	0.0390	9940.4	200.5	10583.3
0.0417	0.0557	9940.4	133.0	7330.7
0.0421	0.0762	9940.4	62.4	5454.9
0.0420	0.1051	9940.4	46.0	3955.0
0.0413	0.1488	9940.4	30.6	2753.9
BLANK1		9514.4		
BLANK2		9747.9		
BLANK3		8822.6		
BLANK4		9946.1		
BLANK5		10130.4		
BLANK6		10363.3		

TABLE VII-13. APA GAC SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.6-7.4
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2501	0.0089	432.8	201.1	6547.1
0.2508	0.0150	432.8	78.0	5924.6
0.2511	0.0189	432.8	57.2	4991.3
0.0432	0.0047	432.8	22.9	3784.1
0.0430	0.0068	432.8	12.2	2671.9
0.0420	0.0080	432.8	5.7	2254.7
0.0424	0.0098	432.8	4.1	1845.8
0.0427	0.0121	432.8	2.5	1514.7
0.0425	0.0183	432.8	1.7	1001.0
0.0433	0.0216	432.8	1.4	865.6
BLANK1		465.0		
BLANK2		438.0		
BLANK3		473.9		
BLANK4		393.8		
BLANK5		453.0		
BLANK6		373.1		

TABLE VII-14. APA GAC SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2508	0.0048	8956.9	7485.5	77377.7
0.2504	0.0111	8956.9	5703.5	73205.9
0.2505	0.0182	8956.9	3737.4	71899.2
0.2504	0.0299	8956.9	1783.4	60041.3
0.2524	0.0411	8956.9	1158.2	47844.4
0.2511	0.0547	8956.9	676.1	38047.7
0.2499	0.0719	8956.9	417.2	29655.4
0.2496	0.0863	8956.9	267.1	25145.2
0.0430	0.0231	8956.9	100.4	16510.5
0.0432	0.0302	8956.9	50.1	12721.8
0.0428	0.0387	8956.9	42.4	9876.8
0.0425	0.0534	8956.9	16.6	7126.8
BLANK1		9184.3		
BLANK2		9452.9		
BLANK3		9008.4		
BLANK4		9049.8		
BLANK5		8089.3		
BLANK6		7403.8		

TABLE VII-15. APA GAC SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.7-7.2
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
1.0580	0.00036	98.7	98.6	245.6
1.0310	0.00092	98.7	85.6	14703.8
1.0459	0.00174	98.7	65.5	20003.3
1.0496	0.00268	98.7	48.1	19793.4
1.0536	0.00359	98.7	35.8	18456.5
0.4970	0.00309	98.7	13.0	13776.3
0.5004	0.00386	98.7	7.5	11824.0
0.4977	0.00447	98.7	6.8	10236.9
0.2525	0.00297	98.7	2.9	8139.1
BLANK 1		98.7		
BLANK 2		102.1		
BLANK 3		98.8		
BLANK 4		97.5		
BLANK 5		97.7		
BLANK 6		97.3		

TABLE VII-16. APA GAC SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	APA GAC
ISOTHERM TYPE	Virgin
PARTICLE SIZE	200x400 Mesh
TEMPERATURE, Deg C	21 +/- 1
pH	6.5-7.3
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
1.0435	0.00087	1046.6	941.8	126260.5
0.4999	0.00228	1046.6	519.6	115591.0
0.4980	0.00388	1046.6	295.1	96420.5
0.2506	0.00211	1046.6	282.7	90731.4
0.2512	0.00359	1046.6	72.0	68142.8
0.2499	0.00455	1046.6	36.5	55500.4
0.2502	0.00597	1046.6	22.8	42897.6
0.2495	0.00840	1046.6	10.2	30784.9
BLANK 1		1061.7		
BLANK 2		1032.9		
BLANK 3		1056.5		
BLANK 4		991.6		
BLANK 5		1044.3		
BLANK 6		1037.4		

TABLE VII-17. XAD-4 RESIN TOC ISOTHERM, TREATED HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.6-7.4
EQUILIBRATION TIME, Days	7
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2517	0.0043	62.3	60.8	87.9
0.2511	0.0065	62.3	60.1	84.4
0.2505	0.0124	62.3	61.0	26.3
0.2505	0.0311	62.3	60.1	17.7
0.2486	0.0700	62.3	59.2	11.0
0.0423	0.0342	62.3	60.2	2.6
0.0427	0.0915	62.3	57.9	2.1
0.0422	0.1503	62.3	56.1	1.7
0.0419	0.2746	62.3	53.9	1.3
0.0378	0.5078	62.3	50.5	0.9
0.0401	0.9076	62.3	46.9	0.7
0.0393	1.3948	62.3	43.6	0.5
BLANK 1		62.6		
BLANK 2		62.0		
BLANK 3		62.8		
BLANK 4		62.0		

TABLE VII-18. XAD-4 RESIN TOC ISOTHERM, DILUTE TREATED HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TOC
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	7.0-7.3
EQUILIBRATION TIME, Days	7
BACKGROUND WATER MATRIX	Humidity Condensate, Diluted MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (mg/L)	EQ. LIQ-PHASE CONC. (mg/L)	EQ. SOL-PHASE CONC. (mg/g)
0.2505	0.0038	26.93	26.83	6.19
0.2457	0.0072	26.93	26.59	11.60
0.2493	0.0140	26.93	26.49	7.85
0.2505	0.0376	26.93	26.13	5.33
0.2498	0.0840	26.93	25.60	3.95
0.0426	0.0392	26.93	24.94	2.17
0.0429	0.1009	26.93	24.12	1.19
0.0429	0.1695	26.93	23.27	0.93
0.0428	0.2965	26.93	22.78	0.60
0.0428	0.5508	26.93	21.69	0.41
0.0406	1.0588	26.93	19.40	0.29
0.0388	1.6608	26.93	18.13	0.21
BLANK 1		27.21		
BLANK 2		26.81		
BLANK 3		26.97		
BLANK 4		26.71		

TABLE VII-19. XAD-4 RESIN SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.8-7.4
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2504	0.00177	596.4	547.7	6897.2
0.2515	0.00700	590.0	484.0	3810.8
0.2511	0.01591	583.6	358.2	3557.5
0.2491	0.02118	577.3	325.6	2959.9
0.0428	0.00813	570.9	124.3	2352.3
0.0429	0.01283	564.5	76.1	1633.3
0.0432	0.01715	558.1	57.1	1261.7
0.0421	0.02814	551.7	35.5	772.4
0.0428	0.03468	545.3	22.4	645.3
0.0428	0.05586	539.0	13.4	402.7
0.0437	0.07618	532.6	11.8	298.8
0.0434	0.12188	526.2	6.7	185.0
BLANK 1		576.8		
BLANK 2		590.2		
BLANK 3		602.6		
BLANK 4		567.5		
BLANK 5		533.8		
BLANK 6		518.7		

TABLE VII-20. XAD-4 RESIN SPIKE ISOTHERM, TCE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	TCE
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.8-7.3
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2505	0.00595	8866.1	8144.1	30422.8
0.2519	0.01847	8771.1	6206.1	34983.3
0.2515	0.04090	8676.1	3921.1	29237.5
0.2472	0.09068	8581.2	1614.7	18990.3
0.2514	0.15204	8486.2	900.1	12543.9
0.2497	0.23658	8391.2	515.5	8312.5
0.2500	0.42647	8391.2	291.0	4748.4
0.0428	0.11070	8298.3	152.8	3149.3
0.0429	0.18164	8205.3	93.3	1915.9
0.0431	0.32362	8112.4	47.1	1074.2
0.0425	0.51275	8019.4	29.1	662.3
0.0413	0.88745	7926.5	16.6	368.1
BLANK 1		8567.8		
BLANK 2		8866.1		
BLANK 3		8664.9		
BLANK 4		8391.2		
BLANK 5		7984.9		
BLANK 6		7868.0		

TABLE VII-21. XAD-4 RESIN SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.7-7.4
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2483	0.0022	494.1	443.2	5781.8
0.2502	0.0037	488.9	409.9	5286.6
0.2499	0.0147	483.7	228.8	4332.1
0.0426	0.0054	478.4	102.3	2947.8
0.0387	0.0072	473.2	62.8	2221.0
0.0428	0.0107	468.0	45.3	1688.0
0.0428	0.0168	468.0	32.2	1111.2
0.0439	0.0241	460.3	17.7	806.9
0.0431	0.0349	452.6	12.1	544.6
0.0434	0.0477	444.9	9.2	396.6
0.0429	0.0749	437.2	5.5	246.9
0.0420	0.1217	429.5	4.3	146.8
BLANK 1		495.0		
BLANK 2		493.2		
BLANK 3		473.2		
BLANK 4		462.7		
BLANK 5		431.7		
BLANK 6		427.3		

TABLE VII-22. XAD-4 RESIN SPIKE ISOTHERM, TOLUENE IN HUMIDITY CONDENSATE

LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Toluene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.6-7.4
EQUILIBRATION TIME, Days	14
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.2512	0.0042	9496.8	8757.4	43825.5
0.2500	0.0131	9496.8	6768.3	52061.5
0.2495	0.0316	9496.8	4318.3	40864.2
0.2502	0.1622	9496.8	553.7	13800.7
0.0431	0.0479	9496.8	232.9	8332.4
0.0418	0.0651	9496.8	167.1	5997.5
0.0430	0.1186	9496.8	88.8	3406.7
0.0430	0.1668	9496.8	51.7	2435.7
0.0421	0.2773	9496.8	36.6	1435.8
0.0422	0.4561	9496.8	18.8	877.8
BLANK 1		9176.7		
BLANK 2		9659.6		
BLANK 3		9491.6		
BLANK 4		9307.2		
BLANK 5		9771.3		
BLANK 6		9574.5		

TABLE VII-23. XAD-4 RESIN SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.7-7.1
EQUILIBRATION TIME, Days	10
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.4988	0.0015	99.5	85.9	4435.8
0.0430	0.0013	99.5	12.2	2972.2
0.2499	0.0019	99.5	42.3	7470.5
0.2619	0.0032	99.5	70.3	2408.3
0.0441	0.0008	99.5	22.4	4230.6
0.0430	0.0015	99.5	8.7	2615.8
0.0428	0.0020	99.5	5.4	1985.5
0.0437	0.0023	99.5	5.7	1815.3
0.0429	0.0030	99.5	4.2	1352.2
0.0423	0.0047	99.5	2.6	870.7
BLANK 1		102.6		
BLANK 2		97.9		
BLANK 3		99.0		
BLANK 4		89.3		
BLANK 5		103.9		
BLANK 6		104.4		

TABLE VII-24. XAD-4 RESIN SPIKE ISOTHERM, NAPHTHALENE IN HUMIDITY CONDENSATE

SPIKED LIQUID-PHASE ISOTHERM DATA

CHEMICAL COMPOUND	Naphthalene
ADSORBENT TYPE	XAD-4 Resin
ISOTHERM TYPE	Virgin
PARTICLE SIZE	0.3-1.2 mm
TEMPERATURE, Deg C	21 +/- 1
pH	6.8-7.2
EQUILIBRATION TIME, Days	12
BACKGROUND WATER MATRIX	Humidity Condensate MCV'd and Filtered

BOTTLE VOLUME (Liters)	DRY WEIGHT (Grams)	INITIAL CONC. (ug/L)	EQ. LIQ-PHASE CONC. (ug/L)	EQ. SOL-PHASE CONC. (ug/g)
0.4997	0.0021	990.3	822.3	39052.9
0.2511	0.0032	990.3	416.8	44666.8
0.2509	0.0046	990.3	336.0	35349.1
0.0431	0.0013	990.3	200.0	26102.4
0.0428	0.0024	990.3	72.7	16504.4
0.0423	0.0033	990.3	40.3	12174.7
0.0427	0.0042	990.3	27.4	9738.9
0.0428	0.0053	990.3	17.4	7919.3
0.0424	0.0066	990.3	13.1	6240.2
0.0426	0.0100	990.3	7.9	4177.8
0.0431	0.0114	990.3	6.8	3731.1
0.0424	0.0166	990.3	7.8	2512.5
BLANK 1		1021.0		
BLANK 2		1008.9		
BLANK 3		1018.8		
BLANK 4		968.8		
BLANK 5		962.3		
BLANK 6		961.8		

APPENDIX VIII. FCA MODEL

```
c   gafca3.for - program fits initial concentrations for any number of
c   fictive components using any number of TOC, dilute TOC, and tracer
c   isotherms.  important to note that the tracer here is a tracer
c   added to the mixture and not singled out of the mixture.  the TOC
c   of the tracer isotherms is assumed to be that of the concentrated
c   TOC isotherm.  the parameters are the initial concentrations of
c   nfcs-1 fictive components.
c
c   the program uses a genetic algorithm as the search routine
c
c   program last modified 5/12/96 by john l. bulloch
c   program originally written by john l. bulloch
c
c   program modifications by Anisa N. Ali for Master's Thesis 6/96 - 12/96
c
c
c
c#############################################################################
c
      program gafortran
c
c This is version 1.6.1, last updated on 3/22/96.
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c David L. Carroll
c University of Illinois
c 306 Talbot Laboratory
c 104 S. Wright St.
c Urbana, IL  61801
c
c e-mail: carroll@uxh.cso.uiuc.edu
c Phone:  217-333-4741
c fax:    217-244-0720
c
c This genetic algorithm (GA) driver is free for public use.  My only
c request is that the user reference and/or acknowledge the use of this
c driver in any papers/reports/articles which have results obtained
c from the use of this driver. I would also appreciate a copy of such
c papers/articles/reports, or at least an e-mail message with the
c reference so I can get a copy.  Thanks.
c
c This program is a FORTRAN version of a genetic algorithm driver.
```

```
c This code initializes a random sample of individuals with different
c parameters to be optimized using the genetic algorithm approach, i.e.
c evolution via survival of the fittest. The selection scheme used is
c tournament selection with a shuffling technique for choosing random
c pairs for mating. The routine includes binary coding for the
c individuals, jump mutation, creep mutation, and the option for
c single-point or uniform crossover. Niching (sharing) and an option
c for the number of children per pair of parents has been added.
c An option to use a micro-GA was recently added.
c
c For companies wishing to link this GA driver with an existing code,
c I am available for some consulting work. Regardless, I suggest
c altering this code as little as possible to make future updates
c easier to incorporate.
c
c Any users new to the GA world are encouraged to read David Goldberg's
c "Genetic Algorithms in Search, Optimization and Machine Learning,"
c Addison-Wesley, 1989.
c
c Other associated files are:  gafca3.inp
c                              restart.ga
c                              params.f
c
c I have provided a sample subroutine "func", but ultimately
c the user must supply this subroutine "func" which should be your
c function evaluator. You should be able to run the code with the
c sample subroutine "func" and the provided gafca3.inp file and obtain
c the optimal function value of 40.0 at generation 59 with the
c micro-GA enabled (this is only 295 function evaluations!).
c
c The code is presently set for a maximum population size of 200,
c 22 chromosomes (binary bits) and 8 parameters. These values can be
c changed in params.f as appropriate for your problem. Correspondingly
c you will have to change a few 'write' and 'format' statements if you
c change nchrome and/or nparam. In particular, if you change nchrome
c and/or nparam, then you should change the 'format' statement numbers
c 1050, 1075, 1275, and 1500 (see ReadMe file).
c
c Please feel free to contact me with questions, comments, or errors
c (hopefully none of latter).
c
c Disclaimer: this program is not guaranteed to be free of error
c (although it is believed to be free of error), therefore it should
c not be relied on for solving problems where an error could result in
c injury or loss. If this code is used for such solutions, it is
```

```
c entirely at the user's risk and the author disclaims all liability.
c
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c    Variables added by john bulloch for fictive component analysis
c
c
c    bn     = bottle number for do loop counters
c    c0molar= molar concentrations of fictive components entering
c             iast for each new generation
c    cdata  = equilibrium concentrations for input isotherm data
c             mg/L TOC or mg/L tracer
c    ctot   = equilibrium TOC concentration for isotype 1 or 2 isotherms
c             predicted from model
c    cpres  = percent residual in liquid phase concentration, TOC
c             or tracer depending
c    cres   = liquid phase concentration residuals, TOC or tracer
c    czero  = initial TOC concentration.  necessary for isotype=1,
c             isotype=2, or isotype=3 isotherm
c    czerod = initial dilute TOC concentration, for isotype=2 isotherm
c    czerot = initial concentration of each tracer component, mg/L
c    errel  = error limit criteria for convergence in DNEQNF
c    foc    = fraction organic carbon for fictive component
c    funcval= 100-sdev for each individual in each generation
c    in     = isotherm number for do loop counters
c    itmax  = maximum number of iterations in DNEQNF
c    n      = number of components in IAST calculation
c    ndata  = number of data points per isotherm
c    nfcs   = desired number of fictive components
c    numisos= total number of isotherms being fit
c    par    = input parameters for iast
c    qpres  = percent residual in solid phase concentration, TOC
c             or tracer dependent
c    qres   = solid phase residuals, TOC or tracer dependent
c    qtot   = equilibrium solid phase TOC concentration for
c             isotype 1 or 2 isotherms predicted from model
c    sdev   = sample deviation for each individual in each generation
c    isotype   = input descriptor defining isotherm isotype, isotype 1 = TOC,
c             isotype 2 = dilute TOC, isotype 3 = tracer
c    v      = volume of filling solution per isotherm point, L
c    x      = solid phase equilibrium concentrations predicted from
c             iast
c    xguess = solid phase equilibrium concentration initial guesses
c             input to iast
```

```
c    xk     = freundlich K for fictive component, (mg/g)(L/mg)^1/n
c             on input, changed to (mmol/g)(L/mmol)^1/n after calling
c             subroutine k2molar
c    xkt    = freundlich K for tracer, (mg/g)(L/mg)^1/n on input,
c             changed to (mmol/g)(L/mmol)^1/n after calling k2molar
c    xm     = mass of adsorbent per isotherm bottle, input as mg and
c             converted to g by program1
c    xmw    = molecular weight for fictive component
c    xmwt   = molecular weight for tracer
c    xn     = freundlich K for fictive component
c    xnonad = nonadsorbing TOC concentration portion of czero
c    xnt    = Freundlich 1/n for tracer
c    zz     = factor used to calculate xguess values for DNEQNF
c
c
c    subroutines added for fictive component analysis
c
c    subroutine input - reads input data for fictive component analysis
c    subroutine k2molar - converts input K in mass units to molar
c    subroutine erset - external IMSL subroutine to set procedure
c                   for errors in DNEQNF
c    subroutine iastpars - set up IAST parameters for each individual
c    subroutine dneqnf - external IMSL subroutine to solve IAST eqns.
c    subroutine fcn - set up series of IAST equations
c    subroutine residual - calculate residuals for each individual
c    subroutine objfun - calculate sdev for each individual
c    subroutine func - calculate funcval for each individual
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
      implicit double precision (a-h,o-z)
      integer bn, isotype, gennum, qneg
      save
c
      include 'params.f'
      dimension parent(indmax,nparmax),child(indmax,nparmax)
      dimension fitness(indmax),nposibl(nparmax),nichflg(nparmax)
      dimension iparent(indmax,nchrmax),ichild(indmax,nchrmax)
      dimension g0(nparmax),g1(nparmax),ig2(nparmax)
      dimension paramsm(nparmax),paramav(nparmax),ibest(nchrmax)
      dimension parmax(nparmax),parmin(nparmax),pardel(nparmax)
      dimension cdata(maxisos,maxdat),isotype(maxisos),ndata(maxisos),
     &qdata(maxisos,maxdat)
      dimension ctot(maxisos,maxdat),qtot(maxisos,maxdat)
      dimension foc(nparmax),xk(nparmax),xmw(nparmax),xn(nparmax)
```

```
      dimension c0molar(nparmax),par(50),czerot(maxisos)
      dimension cpres(maxisos,maxdat),cres(maxisos,maxdat)
      dimension qpres(maxisos,maxdat),qres(maxisos,maxdat)
      dimension x(nparmax),xguess(nparmax)
      dimension xkt(maxisos),xnt(maxisos),xmwt(maxisos)
      dimension v(maxisos,maxdat),xm(maxisos,maxdat)
      dimension cout(indmax,nparmax),bestpar(nparmax)
c
      common / ga1   / npopsiz,nowrite
      common / ga2   / nparam,nchrome
      common / ga3   / parent,iparent
      common / ga4   / fitness
      common / ga5   / g0,g1,ig2
      common / ga6   / parmax,parmin,pardel,nposibl
      common / ga7   / par
c
C
      EXTERNAL FCN,DNEQNF,ERSET
C
      namelist / ga   / irestrt,npopsiz,pmutate,maxgen,idum,pcross,
     +          itourny,ielite,icreep,pcreep,iunifrm,iniche,
     +          iskip,iend,nchild,nparam,parmin,parmax,nposibl,
     +          nowrite,nichflg,microga
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c  Genetic Algorithm Input variable definitions:
c
c  irestrt  = 0 for a new GA run, or for a single function evaluation
c           = 1 for a restart continuation of a GA run.
c  npopsiz  The population size of a GA run (typically 100 works well).
c           For a single calculation, set equal to 1.
c  nparam   Number of parameters (groups of bits) of each individual.
c           Make sure that nparam matches the number of values in the
c           parmin, parmax and nposibl input arrays.
c  maxgen   The maximum number of generations to run by the GA.
c           For a single function evaluation, set equal to 1.
c  idum     The initial random number seed for the GA run.  Must equal
c           a negative integer, e.g. idum=-1000.
c  pmutate  The jump mutation probability.  Typically set = 1/npopsiz.
c  pcreep   The creep mutation probability.  Typically set this
c           = (nchrome/nparam)/npopsiz.
c  pcross   The crossover probability.  For single-point crossover, a
c           value of 0.6 or 0.7 is recommended.  For uniform crossover,
c           a value of 0.5 is suggested.
```

```
c itourny  No longer used.  The GA is presently set up for only
c          tournament selection.
c ielite   = 0 for no elitism (best individual not necessarily
c             replicated from one generation to the next).
c          = 1 for elitism to be invoked (best individual replicated
c             into next generation); elitism is recommended.
c iunifrm  = 0 for single-point crossover
c          = 1 for uniform crossover; uniform crossover is recommended.
c iniche   = 0 for no niching
c          = 1 for niching; niching is recommended.
c nchild   = 1 for one child per pair of parents (this is what I
c             typically use).
c          = 2 for two children per pair of parents (2 is more common
c             in GA work).
c iskip    = 0 for normal GA run (this is standard).
c          = number in population to look at a specific individual or
c            set of individuals.  Setting iskip-0 is only used for
c            debugging purposes.
c iend     = 0 for normal GA run (this is standard).
c          = number of last population member to be looked at in a set
c            of individuals.  Setting iend-0 is only used for debugging
c            purposes and is commonly used in conjunction with iskip.
c nowrite  = 0 to write detailed mutation and parameter adjustments
c          = 1 to not write detailed mutation and parameter adjustments
c parmin   = array of the minimum allowed values of the parameters
c parmax   = array of the maximum allowed values of the parameters
c nposibl  = array of integer number of possibilities per parameter.
c            For optimal code efficiency set nposibl=2**n, i.e. 2, 4,
c            8, 16, 32, 64, etc.
c nichflg  = array of 1/0 flags for whether or not niching occurs on
c            a particular parameter.  Set to 0 for no niching on
c            a parameter, set to 1 for niching to operate on parameter.
c            The default value is 1, but the implementation of niching
c            is still controlled by the flag iniche.
c microga  = 0 for normal conventional GA operation
c          = 1 for micro-GA operation (this will automatically reset
c            some of the other input flags).  I recommend using
c            npopsiz=5 when microga=1.
c
c For single function evaluations, set npopsiz=1, maxgen=1, & irestrt=0.
c
c My newest favorite choice of GA parameters is:
c   microga=1, npopsiz=5, inunifrm=1
c I've gotten roughly a factor of 4 improvement in the number of
c function evaluations using the uniform crossover micro-GA!
```

```
c (The single-point crossover micro-GA was not as good as with
c uniform crossover.)
c
c For those wishing to use the more conventional GA techniques,
c my old favorite choice of GA parameters was:
c    iunifrm=1, iniche=1, ielite=1, itourny=1, nchild=1
c For most problems I have dealt with, I get good performance using
c    npopsiz=100, pcross=0.5, pmutate=0.01, pcreep=0.02, maxgen=26
c or
c    npopsiz= 50, pcross=0.5, pmutate=0.02, pcreep=0.04, maxgen=51
c Any negative integer for idum should work.  I typically arbitrarily
c choose idum=-10000 or -20000.
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c Code variable definitions (those not defined above):
c
c best     = the best fitness of the generation
c child    = the floating point parameter array of the children
c cpu      = cpu time of the calculation
c creep    = +1 or -1, indicates which direction parameter creeps
c del      = square root of del2
c del2     = sum of the squares of the normalized multidimensional
c            distance between member j and all other members of
c            the population
c delta    = del/nparam
c diffrac  = fraction of total number of bits which are different
c            between the best and the rest of the micro-GA population.
c            Population convergence arbitrarily set as diffrac<0.05.
c fbar     = average fitness of population
c fitness  = array of fitnesses of the parents
c fitsum   = sum of the fitnesses of the parents
c g0       = lower bound values of the parameter array to be optimized.
c            The number of parameters in the array should match the
c            dimension set in the above parameter statement.
c g1       = the increment by which the parameter array is increased
c            from the lower bound values in the g0 array.  The minimum
c            parameter value is g0 and the maximum parameter value
c            equals g0+g1*(2**g2-1), i.e. g1 is the incremental value
c            between min and max.
c ig2      = array of the number of bits per parameter, i.e. the number
c            of possible values per parameter.  For example, ig2=2 is
c            equivalent to 4 (=2**2) possibilities, ig2=4 is equivalent
c            to 16 (=2**4) possibilities.
c ig2sum   = sum of the number of possibilities of ig2 array
```

```
c ibest   = binary array of chromosomes of the best individual
c ichild  = binary array of chromosomes of the children
c icount  = counter of number of different bits between best
c           individual and other members of micro-GA population
c icross  = the crossover point in single-point crossover
c indmax  = maximum # of individuals allowed, i.e. max population size
c iparent = binary array of chromosomes of the parents
c istart  = the generation to be started from
c jbest   = the member in the population with the best fitness
c jelite  = a counter which tracks the number of bits of an individual
c           which match those of the best individual
c jend    = used in conjunction with iend for debugging
c jstart  = used in conjunction with iskip for debugging
c kount   = a counter which controls how frequently the restart
c           file is written
c kountmx = the maximum value of kount before a new restart file is
c           written; presently set to write every fifth generation.
c           Increasing this value will reduce I/O time requirements
c           and reduce wear and tear on your storage device
c kelite  = kelite set to unity when jelite=nchrome, indicates that
c           the best parent was replicated amongst the children
c mate1   = the number of the population member chosen as mate1
c mate2   = the number of the population member chosen as mate2
c nchrmax = maximum # of chromosomes (binary bits) per individual
c nchrome = number of chromosomes (binary bits) of each individual
c ncreep  = # of creep mutations which occurred during reproduction
c nmutate = # of jump mutations which occurred during reproduction
c nparmax = maximum # of parameters which the chromosomes make up
c paramav = the average of each parameter in the population
c paramsm = the sum of each parameter in the population
c parent  = the floating point parameter array of the parents
c pardel  = array of the difference between parmax and parmin
c rand    = the value of the current random number
c sigshar = floating point equivalent of nparam
c sumshar = the scaling factor to be applied to the fitness of each
c           individual based on a triangular sharing function
c npossum = sum of the number of possible values of all parameters
c time0   = clock time at start of run
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
      kountmx=5
      irestrt=0
      itourny=0
      ielite=0
```

```
      iunifrm=0
      iniche=0
      iskip=0
      iend=0
      nchild=1
      do 2 i=1,nparam
         nichflg(i)=1
 2    continue
      microga=0
c     TIME0=SECNDS(0.0)
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c     starting section added by john bulloch
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
      OPEN (UNIT=24, FILE='gafca3.out', STATUS='UNKNOWN')
      OPEN (UNIT=30, FILE='testing.out')
      write(24,*)'opened output file gafca3.out'
      OPEN (UNIT=23, FILE='gafca3.inp', STATUS='OLD')
      READ (23, NML = ga)
      CLOSE (23)
c
c     opening fitting data file and reading data
c
      OPEN (UNIT=25, FILE='gafca3.dat', STATUS='OLD')
c
c     calling subroutine to read input data
c
      call input(cdata,czero,czerod,errel,foc,itmax,numisos,xk,
     &xkt,xm,xmw,xmwt,xn,xnt,nfcs,ndata,isotype,xnonad,v,zz,czerot)
c
c     calling subroutine to convert Freundlich K units to molar values
c        when it returns, xk is in molar units
c
      call k2molar(nfcs,numisos,isotype,xk,xkt,xmw,xmwt,xn,xnt)
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c     end of section added by john bulloch
c
```

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c
      itourny=1
      if (itourny.eq.0) nchild=2
      if (npopsiz.gt.indmax) then
         write(6,1600) npopsiz
         write(24,1600) npopsiz
         close(24)
         stop
      endif
      if (nparam.gt.nparmax) then
         write(6,1700) nparam
         write(24,1700) nparam
         close(24)
         stop
      endif
c
c  If using the microga option, reset some input variables
      if (microga.ne.0) then
         pmutate=0.0
         pcreep=0.0
         itourny=1
         ielite=1
         iniche=0
         nchild=1
         if (iunifrm.eq.0) then
           pcross=1.0
         else
           pcross=0.5
         endif
      endif
c
c  Set up the g0, g1 and ig2 arrays for the parameters
      do 3 i=1,nparam
         g0(i)=parmin(i)
         pardel(i)=parmax(i)-parmin(i)
         g1(i)=pardel(i)/dble(nposibl(i)-1)
 3    continue
      do 6 i=1,nparam
         do 7 j=1,40
           n2j=2**j
           if (n2j.ge.nposibl(i)) then
             ig2(i)=j
```

```
            goto 8
          endif
          if (j.ge.40) then
            write(6,2000)
            write(24,2000)
            close(24)
            stop
          endif
 7      continue
 8      continue
 6    continue
c
c  Count the total number of chromosomes (bits) required
      nchrome=0
      npossum=0
      ig2sum=0
      do 9 i=1,nparam
           nchrome=nchrome+ig2(i)
           npossum=npossum+nposibl(i)
           ig2sum=ig2sum+(2**ig2(i))
 9    continue
      if (nchrome.gt.nchrmax) then
           write(6,1800) nchrome
           write(24,1800) nchrome
           close(24)
           stop
      endif
c
c  Initialize random number generator
      call ran3(idum,rand)
c
      if(irestrt.eq.0) then
c  Initialize the random distribution of parameters in the individual
c  parents when irestrt=0.
           istart=1
           do 10 i=1,npopsiz
             do 15 j=1,nchrome
               call ran3(1,rand)
               iparent(i,j)=1
               if(rand.lt.0.5) iparent(i,j)=0
 15          continue
 10        continue
           if (npossum.lt.ig2sum) call possibl(parent,iparent)
      else
c  If irestrt.ne.0, read from restart file.
```

```
        OPEN (UNIT=25, FILE='restart.ga', STATUS='OLD')
        rewind 25
        read(25,*) istart,npopsiz
        do 1 j=1,npopsiz
          read(25,*) k,(iparent(j,l),l=1,nchrome)
 1      continue
        CLOSE (25)
    endif
c
    if(irestrt.ne.0) call ran3(idum-istart,rand)
    kount=0
    do 20 i=istart,maxgen+istart-1
        gennum=i
        write (6,1111) i
        write (24,1111) i
        fitsum=0.0
        best=-100000000000.d0
        do 29 n=1,nparam
          paramsm(n)=0.0
29      continue
        write(24,1050)
        jstart=1
        jend=npopsiz
        if(iskip.ne.0) jstart=iskip
        if(iend.ne.0) jend=iend
c
c   starting loop where changes implemented for fitting data
c
          do 30 j=jstart,jend
          call decode(j,parent,iparent)
          if(iskip.ne.0 .and. iend.ne.0 .and. iskip.eq.iend)
   +    write(6,1075) j,(iparent(j,k),k=1,nchrome),
   +            (parent(j,kk),kk=1,nparam),0.0
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c    starting section added by john bulloch
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c  Entering loop which calculates IAST prediction and residuals
c  for each bottle based on individual j.
c
```

```
         call erset (4, 1, 0)
c
         do 31 in = 1,numisos
              do 39 bn = 1,ndata(in)
c         write(6,*)'parent(',j,1,') = ',parent(j,1)
c         write(6,*)'parent(',j,2,') = ',parent(j,2)
c         write(6,*)'parent(',j,3,') = ',parent(j,3)
c    write(6,*)'calling IASTPARS for IN = ',in,' andbn = ',bn
c
    call iastpars(bn,czero,czerod,czerot,c0molar,foc,in,j,n,
   &nfcs,isotype,v,xk,xkt,xm,xmw,xmwt,xn,xnt,xnonad,gennum, maxgen,
   &cout)
c
c    write(6,*)'exited IASTPARS for IN = ',in,' andbn = ',bn
c
c
c         if (in .eq. 2) then
c         do 3000 kn = 1,n
c           write(6,*)'kmolar',kn,' = ',par(kn)
c           write(6,*)'xn',kn,' = ',par(10+kn)
c           write(6,*)'c0molar',kn,' = ',par(20+kn)
c 3000       continue
c         endif
c         if (bn .eq. 1) then
c           write(6,*)'m',kn,' = ',par(30)
c           write(6,*)'v',kn,' = ',par(40)
c         endif
c         write(6,*)'IAST parameters set up'
c
           L=0
           ZZ=0.50D0
C
C        CALCULATE INITIAL GUESSES ON Q's
C
 32        IF (bn .EQ. 1) THEN
                DO 37 id=1,n
                  xguess(id)=ZZ*par(20+id)*V(in,1)/xM(in,1)
c            write(6,*)'xguess',id,' = 'xguess(id)
 37         CONTINUE
            ELSE
                DO 38 id=1,n
                  xguess(id)=zz*x(id)
 38          CONTINUE
            ENDIF
c
```

```
c           write(6,*)'callingdneqnf for bottle',k
c           write(6,*)'L = ',L
             call dneqnf(fcn,errel,n,itmax,xguess,x,fnorm)
C
C     PRINT *, 'FNORM = ', FNORM
C
C    CORRECTING FOR ERRORS IN INITIAL GUESSES
C
                              qneg=0
                              do 200 k=1,n
                               if      (x(k). lt. 0.d0) then
                               qneg=1
                              endif
 200                           continue
            IF (IERCD() .EQ. 3.or.qneg.eq.1) THEN

c             write(6,*)'problem with initial guesses'
                 IF (L .EQ. 0) THEN
                   ZZ=0.90D0
                   L=L+1
                   GOTO 32
                 ENDIF
                 IF (L .EQ. 1) THEN
                   ZZ=0.10D0
                   L=L+1
                   GOTO 32
                 ENDIF
                 IF (L .EQ. 2) THEN
                   ZZ=1.20D0
                   L=L+1
                   GOTO 32
                 ENDIF
           IF (L .EQ. 3) THEN
                   ZZ=0.30D0
                   L=L+1
                   GOTO 32
                 ENDIF
                 IF (L .EQ. 4) THEN
                   ZZ=0.70D0
                   L=L+1
                   GOTO 32
                 ENDIF
                 IF (L .EQ. 5) THEN
                   WRITE (24,5100) xM(in,bn)
```

```
                  ENDIF
              ENDIF
C
c
              call residual(bn,c0molar,cdata,cpres,cres,ctot,
   &czero,czerod,czerot,foc,in,nfcs,qdata,qpres,qres,qtot,isotype,
   &v,x,xm,xmw,xmwt,xnonad)
c


 39          continue
 31       continue
c
c

c



c  Call subroutine objfun to calculate objective function for
c  isotherm using individual j.
c
c
    call objfun(bn,cpres,cres,in,j,ndata,numisos,qpres,qres,sdev)
c
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c    end of section added by john bulloch
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c
c  Call function evaluator, write out individual and fitness, and add
c  to the summation for later averaging.
c
             call func(j,funcval,sdev)
c
             fitness(j)=funcval
             if (i .eq. maxgen) then
             write(24,1075) j,(iparent(j,k),k=1,nchrome),
     +              (cout(j,kk),kk=1,nfcs),fitness(j)
             endif
```

```
          fitsum=fitsum+fitness(j)
          do 22 n=1,nparam
            paramsm(n)=paramsm(n)+parent(j,n)
 22       continue
c
c  Check to see if fitness of individual j is the best fitness.
          if (fitness(j).gt.best) then
            best=fitness(j)
               do 26 m=1,nparam
            bestpar(m)=parent(j,m)
 26            continue
            jbest=j
            do 24 k=1,nchrome
                 ibest(k)=iparent(j,k)
 24          continue
          endif
 30     continue
c
c  Compute parameter and fitness averages.
        fbar=fitsum/dble(npopsiz)
        do 23 n=1,nparam
          paramav(n)=paramsm(n)/dble(npopsiz)
 23     continue
c




c  Write output information
        if (npopsiz.eq.1) then
          write(24, 1075) 1,(iparent(1,k),k=1,nchrome),
    +      (parent(1,k),k=1,nparam),fitness(1)
          write(24,*) ' Average Values:'
          write(24,1275) (parent(1,k),k=1,nparam),fbar
        else
          write(24,1275) (paramav(k),k=1,nparam),fbar
        endif
        write(6,1100) fbar
        write(24,1100) fbar
        write(6,1200) best
        write(24,1200) best
        if(npopsiz.eq.1 .or. iskip.ne.0) then
          close(24)
          stop
```

```
        endif
c
c  Implement "niching" through Goldberg's multidimensional phenotypic
c  sharing scheme with a triangular sharing function.  To find the
c  multidimensional distance from the best individual, normalize all
c  parameter differences.
        if (iniche.ne.0) then
          sigshar=0.0
          do 33 jj=1,nparam
            sigshar=sigshar+dble(nichflg(jj))
 33       continue
          if (sigshar.eq.0.0) then
            write(6,1900)
            write(24,1900)
            close(24)
            stop
          endif
          do 34 ii=1,npopsiz
            sumshar=0.0
            do 35 j=1,npopsiz
                 del2=0.0
                 do 36 k=1,nparam
                   if (nichflg(k).ne.0) then
                        del2=del2+
   +               ((parent(j,k)-parent(ii,k))/pardel(k))**2.0
                   endif
 36              continue
                 del=dsqrt(del2)
                 delta=del/sigshar
                 sumshar=sumshar+1-delta
 35           continue
            fitness(ii)=fitness(ii)/sumshar
 34       continue
        endif
c
c  Enter main crossover and mutation loop.
        ncross=0
        ipick=npopsiz
        do 45 j=1,npopsiz,nchild
c
c##### Tournament Selection Implementation Section #####
c  If tournament selection is chosen (i.e. itourny=1), then
c  implement "tournament" selection for selection of new population.
            if(itourny.eq.1) then
              call select(mate1,ipick)
```

```
             call select(mate2,ipick)
c          write(3,*) mate1,mate2,fitness(mate1),fitness(mate2)
             do 46 n=1,nchrome
                  ichild(j,n)=iparent(mate1,n)
                  if(nchild.eq.2) ichild(j+1,n)=iparent(mate2,n)
 46         continue
           endif
c#####
c
c  Now perform crossover between the randomly selected pair.
c
           if (iunifrm.eq.0) then
c  Single-point crossover at a random chromosome point.
             call ran3(1,rand)
             if(rand.gt.pcross) goto 69
             ncross=ncross+1
             call ran3(1,rand)
             icross=2+dint(dble(nchrome-1)*rand)
             do 50 n=icross,nchrome
                  ichild(j,n)=iparent(mate2,n)
                  if(nchild.eq.2) ichild(j+1,n)=iparent(mate1,n)
 50         continue
           else
c  Perform uniform crossover between the randomly selected pair.
             do 60 n=1,nchrome
                  call ran3(1,rand)
                  if(rand.le.pcross) then
                    ncross=ncross+1
                    ichild(j,n)=iparent(mate2,n)
                    if(nchild.eq.2) ichild(j+1,n)=iparent(mate1,n)
                  endif
 60         continue
           endif
 69       continue
 45     continue
c
c  Now perform random mutation if a random number is less than pmutate.
c  Perform random creep mutation if a different random number is less
c  than pcreep.  If running micro-GA, skip mutation.
         nmutate=0
         ncreep=0
         if (microga.ne.0) goto 79
         do 70 j=1,npopsiz
           do 75 k=1,nchrome
c  Jump mutation
```

```
            call ran3(1,rand)
            if (rand.le.pmutate) then
                nmutate=nmutate+1
                if(ichild(j,k).eq.0) then
                  ichild(j,k)=1
                else
                  ichild(j,k)=0
                endif
                if (nowrite.eq.0) write(6,1300) j,k
                if (nowrite.eq.0) write(24,1300) j,k
            endif
 75        continue
c  Creep mutation (one discrete position away).
          if (icreep.ne.0) then
            do 76 k=1,nparam
                call ran3(1,rand)
                if(rand.le.pcreep) then
                  call decode(j,child,ichild)
                  ncreep=ncreep+1
                  creep=1.0
                  call ran3(1,rand)
                  if (rand.lt.0.5) creep=-1.0
                  child(j,k)=child(j,k)+g1(k)*creep
                  if (child(j,k).gt.parmax(k)) then
                      child(j,k)=parmax(k)-1.0*g1(k)
                  elseif (child(j,k).lt.parmin(k)) then
                      child(j,k)=parmin(k)+1.0*g1(k)
                  endif
                  call code(j,k,child,ichild)
                  if (nowrite.eq.0) write(6,1350) j,k
                  if (nowrite.eq.0) write(24,1350) j,k
                endif
 76          continue
          endif
 70     continue
 79     continue

        write(6,1250) ncross,nmutate,ncreep
        write(24,1250) ncross,nmutate,ncreep
c
c  Write child array back into parent array for new generation.  Check
c  to see if the best parent was replicated; if not, and if ielite=1,
c  then reproduce the best parent into a random slot.
        if (npossum.lt.ig2sum) call possibl(child,ichild)
        kelite=0
```

```
      do 94 j=1,npopsiz
        jelite=0
        do 95 n=1,nchrome
          iparent(j,n)=ichild(j,n)
          if (iparent(j,n).eq.ibest(n)) jelite=jelite+1
          if (jelite.eq.nchrome) kelite=1
 95     continue
 94   continue
      if (ielite.ne.0 .and. kelite.eq.0) then
        call ran3(1,rand)
        irand=1+dint(dble(npopsiz)*rand)
        do 96 n=1,nchrome
          iparent(irand,n)=ibest(n)
 96     continue
        write(24,1260) irand
      endif
c
c##### micro-GA Implementation Section #####
c  If running a micro-GA, check for convergence of micro population.
c  If converged, start a new generation with best individual and fill
c  the remainder of the population with new randomly generated parents.
      if (microga.ne.0) then
c  Count number of different bits from best member in micro-population
        icount=0
        do 81 j=1,npopsiz
          do 82 n=1,nchrome
              if(iparent(j,n).ne.ibest(n)) icount=icount+1
 82       continue
 81     continue
c  If icount less than 5% of number of bits, then consider population
c  to be converged.  Restart with best individual and random others.
        diffrac=dble(icount)/dble((npopsiz-1)*nchrome)
        if (diffrac.lt.0.05) then
          do 87 n=1,nchrome
              iparent(1,n)=ibest(n)
 87       continue
          do 88 j=2,npopsiz
              do 89 n=1,nchrome
                call ran3(1,rand)
                iparent(j,n)=1
                if(rand.lt.0.5) iparent(j,n)=0
 89           continue
 88       continue
          if (npossum.lt.ig2sum) call possibl(parent,iparent)
          write(6,1375) i
```

```
                write(24,1375) i
              endif
            endif
c#####
c
c  Write to restart file.
            kount=kount+1
            if(i.eq.maxgen+istart-1 .or. kount.eq.kountmx) then
              OPEN (UNIT=25, FILE='restart.ga', STATUS='OLD')
              rewind 25
              write(25,*) i+1,npopsiz
              do 80 j=1,npopsiz
                write(25,1500) j,(iparent(j,l),l=1,nchrome)
 80          continue
              CLOSE (25)
              kount=0
            endif
c         CPU = SECNDS(TIME0)
c         write(6,1400) cpu
c         write(24,1400) cpu
 20   continue
c 999  continue
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c          calculate the concentration values for the best fit for maximum
c          generation
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
          do 104 m=1,nparam
                  parent(1,m)= bestpar(m)
 104      continue
c



          do 100 in = 1,numisos
           do 105 bn = 1,ndata(in)
          j=1
     call iastpars(bn,czero,czerod,czerot,c0molar,foc,in,j,n,
    &nfcs,isotype,v,xk,xkt,xm,xmw,xmwt,xn,xnt,xnonad,gennum, maxgen,
    &cout)

          L=0
          ZZ=0.5d0
```

```
C        CALCULATE INITIAL GUESSES ON Q's
C
 102       IF (bn .EQ. 1) THEN
             DO 110 id=1,n
                   xguess(id)=ZZ*par(20+id)*V(in,1)/xM(in,1)
c              write(6,*)'xguess',id,' = ',xguess(id)
 110          CONTINUE
             ELSE
                 DO 115 id=1,n
                   xguess(id)=zz*x(id)
 115           CONTINUE
             ENDIF
c
c          write(6,*)'callingdneqnf for bottle',k
c          write(6,*)'L = ',L
             call dneqnf(fcn,errel,n,itmax,xguess,x,fnorm)
C
C     PRINT *, 'FNORM = ', FNORM
C
C    CORRECTING FOR ERRORS IN INITIAL GUESSES
C
                         qneg =0
                         do 202 k=1,n
                          if       (x(k). lt. 0.d0) then
                          qneg=1
                         endif
 202                      continue
             IF (IERCD() .EQ. [illegible]     qneg.eq.1) THEN

c             write(6,*)'problem with initial guesses'
                 IF (L .EQ. 0) THEN
                   ZZ=0.90D0
                   L=L+1
                   GOTO 102
                 ENDIF
                 IF (L .EQ. 1) THEN
                   ZZ=0.10D0
                   L=L+1
                   GOTO 102
                 ENDIF
                 IF (L .EQ. 2) THEN
                   ZZ=1.20D0
                   L=L+1
                   GOTO 102
```

```
          ENDIF
      IF (L .EQ. 3) THEN
           ZZ=0.30D0
           L=L+1
           GOTO 102
          ENDIF
          IF (L .EQ. 4) THEN
           ZZ=0.70D0
           L=L+1
           GOTO 102

           ENDIF


           IF (L .EQ. 5) THEN
            WRITE (24,5100) xM(in,bn)




          ENDIF
        ENDIF
C
c
            call residual(bn,c0molar,cdata,cpres,cres,ctot,
   &czero,czerod,czerot,foc,in,nfcs,qdata,qpres,qres,qtot,isotype,
   &v,x,xm,xmw,xmwt,xnonad)
c
 105          continue
 100      continue
c


c       call objfun(bn,cpres,cres,in,j,ndata,numisos,qpres,qres,sdev)
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc



ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c  writing output for isotherm bottle data to output file.
c  including expermimental isotherm data and model isotherm data
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
```

```
        do 120 in=1,numisos


    write (24,5995) in
        if (in.lt.3) then

        write (24,6000)
        else
        write (24,6001)
        endif
 6000   format ('C data (mg TOC/L)',2x,'C model (mg TOC/L)',2x,
   &'q data (mg TOC/g)',2x,'q model (mg TOC/g)')

 6001 format ('C data (mg/L)',5x,'C model (mg/L)',10x,
   &'q data (mg/g)',10x,'q model (mg/g)')

                do 125 bn=1,ndata(in)
        write (24,6005) cdata(in,bn),ctot(in,bn),qdata(in,bn),qtot(in,bn)
 6005 format (f10.4,10x,f10.4,10x,f10.4,10x,f10.4)

 125            continue
 120            continue
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
   CLOSE (24)
c
 1111 format(//'################# Generation',i5,' #################')
 1050 format(1x,' #     Binary Code',8x,'Param1 Param2')
 1075 format(i3,1x,50i1,30x,6(1x,F10.3),1x,f15.6)
 1100 format(1x,'Average Function Value of Generation=',f15.6)
 1200 format(1x,'Maximum Function Value              =',f15.6/)
 1250 format(/'  Number of Crossovers      =',i5/
   +       '  Number of Jump Mutations  =',i5/
   +       '  Number of Creep Mutations =',i5)
 1260 format('  Elitist Reproduction on Individual ',i4)
 1275 format(/' Average Values:',65x,5(1x,f10.3),1x,f15.6/)
 1300 format('*** Jump mutation performed on individual  ',i4,
   +     ', chromosome ',i3,' ***')
 1350 format('*** Creep mutation performed on individual ',i4,
   +     ', parameter  ',i3,' ***')
 1375 format(//'%%%%%%% Restart micro-population at generation',
   +     i5,' %%%%%%%')
c 1400 format(2x,'CPU time for generation=',e10.4)
 1500 format(i5,3x,22i2)
 1600 format(1x,'ERROR: npopsiz > indmax.  Set indmax = ',i6)
```

```
 1700 format(1x,'ERROR: nparam > nparmax.  Set nparmax = ',i6)
 1800 format(1x,'ERROR: nchrome > nchrmax.  Set nchrmax = ',i6)
 1900 format(1x,'ERROR: iniche=1 and all values innichflg array = 0'/
     +       1x,'      Do you want to niche or not?')
 2000 format(1x,'ERROR: You have a parameter with a number of '/
     +       1x,'   possibilities > 2**40!  If you really desire this,'/
     +       1x,'   change the DO loop 7 statement and recompile.')
c 3000 format(1x,'Inital solid phase multiplier = ',T50,f10.3/)
c 3010 format(1x,'Stopping tolerance for DNEQNF = ')
 5100 FORMAT(1X,'THERE IS A PROBLEM WITH THE INITIAL
CONCENTRATIONS
     & THAT THE PROGRAMS FIXING ROUTINE DID NOT HELP.
DOSAGE=',F10.4)
 5995   format (//'ISOTHERM',2x,i2)
c
      stop
      end
c
c#######################################################################
c
      subroutine ran3(idum,rand)
c
c  Returns a uniform random deviate between 0.0 and 1.0.  Set idum to
c  any negative value to initialize or reinitialize the sequence.
c  This function is taken from W.H. Press', "Numerical Recipes" p. 199.
c
      implicit double precision (a-h,m,o-z)
      save
c       implicit real*4(m)
      parameter (mbig=4000000.,mseed=1618033.,mz=0.,fac=1./mbig)
c      parameter (mbig=1000000000,mseed=161803398,mz=0,fac=1./mbig)
c
c  According to Knuth, any large mbig, and any smaller (but still large)
c  mseed can be substituted for the above values.
      dimension ma(55)
      data iff /0/
      if (idum.lt.0 .or. iff.eq.0) then
          iff=1
          mj=mseed-dble(iabs(idum))
          mj=dmod(mj,mbig)
          ma(55)=mj
          mk=1
          do 11 i=1,54
            ii=mod(21*i,55)
            ma(ii)=mk
```

```
            mk=mj-mk
            if(mk.lt.mz) mk=mk+mbig
            mj=ma(ii)
 11      continue
          do 13 k=1,4
            do 12 i=1,55
              ma(i)=ma(i)-ma(1+mod(i+30,55))
              if(ma(i).lt.mz) ma(i)=ma(i)+mbig
 12        continue
 13      continue
          inext=0
          inextp=31
          idum=1
      endif
      inext=inext+1
      if(inext.eq.56) inext=1
      inextp=inextp+1
      if(inextp.eq.56) inextp=1
      mj=ma(inext)-ma(inextp)
      if(mj.lt.mz) mj=mj+mbig
      ma(inext)=mj
      rand=mj*fac
      return
      end
c
c##############################################################################
      subroutine select(mate,ipick)
c
c  This routine selects the better of two possible parents for mating.
c
      implicit double precision (a-h,o-z)
      save
c
      include 'params.f'
      common / ga1   / npopsiz,nowrite
      common / ga2   / nparam,nchrome
      common / ga3   / parent,iparent
      common / ga4   / fitness
      dimension parent(indmax,nparmax),iparent(indmax,nchrmax)
      dimension fitness(indmax)
c
      if(ipick+1.gt.npopsiz) call shuffle(ipick)
      ifirst=ipick
      isecond=ipick+1
      ipick=ipick+2
```

```
      if(fitness(ifirst).gt.fitness(isecond)) then
         mate=ifirst
      else
         mate=isecond
      endif
c     write(3,*)'select',ifirst,isecond,fitness(ifirst),fitness(isecond)
c
      return
      end
c
c#######################################################################
      subroutine shuffle(ipick)
c
c  This routine shuffles the parent array and its corresponding fitness
c
      implicit double precision (a-h,o-z)
      save
c
      include 'params.f'
      common / ga1   / npopsiz,nowrite
      common / ga2   / nparam,nchrome
      common / ga3   / parent,iparent
      common / ga4   / fitness
      dimension parent(indmax,nparmax),iparent(indmax,nchrmax)
      dimension fitness(indmax)
c
      ipick=1
      do 10 j=1,npopsiz-1
         call ran3(1,rand)
         iother=j+1+dint(dble(npopsiz-j)*rand)
         do 20 n=1,nchrome
            itemp=iparent(iother,n)
            iparent(iother,n)=iparent(j,n)
            iparent(j,n)=itemp
 20      continue
         temp=fitness(iother)
         fitness(iother)=fitness(j)
         fitness(j)=temp
 10   continue
c
      return
      end
c
c#######################################################################
      subroutine decode(i,array,iarray)
```

```
c
c  This routine decodes a binary string to a real number.
c
     implicit double precision (a-h,o-z)
     save
c
     include 'params.f'
     common / ga2   / nparam,nchrome
     common / ga5   / g0,g1,ig2
     dimension array(indmax,nparmax),iarray(indmax,nchrmax)
     dimension g0(nparmax),g1(nparmax),ig2(nparmax)
c
     l=1
     do 10 k=1,nparam
          iparam=0
          m=l
          do 20 j=m,m+ig2(k)-1
            l=l+1
            iparam=iparam+iarray(i,j)*(2**(m+ig2(k)-1-j))
 20     continue
          array(i,k)=g0(k)+g1(k)*dble(iparam)
 10   continue
c
     return
     end
c
c####################################################################
     subroutine code(j,k,array,iarray
c
c  This routine codes a parameter into a binary string.
c
     implicit double precision (a-h,o-z)
     save
c
     include 'params.f'
     common / ga2   / nparam,nchrome
     common / ga5   / g0,g1,ig2
     dimension array(indmax,nparmax),iarray(indmax,nchrmax)
     dimension g0(nparmax),g1(nparmax),ig2(nparmax)
c
c  First, establish the beginning location of the parameter string of
c  interest.
     istart=1
     do 10 i=1,k-1
          istart=istart+ig2(i)
```

```
 10   continue
c
c  Find the equivalent coded parameter value, and back out the binary
c  string by factors of two.
      m=ig2(k)-1
      if (g1(k).eq.0.0) return
      iparam=nint((array(j,k)-g0(k))/g1(k))
      do 20 i=istart,istart+ig2(k)-1
         iarray(j,i)=0
         if ((iparam+1).gt.(2**m)) then
           iarray(j,i)=1
           iparam=iparam-2**m
         endif
         m=m-1
 20   continue
c     write(3,*)array(j,k),iparam,(iarray(j,i),i=istart,istart+ig2(k)-1)
c
      return
      end
c
c#######################################################################
c
      subroutine possibl(array,iarray)
c
c  This subroutine determines whether or not all parameters are within
c  the specified range of possibility.  If not, the parameter is
c  randomly reassigned within the range.  This subroutine is only
c  necessary when the number of possibilities per parameter is not
c  optimized to be 2**n, i.e. if npossum < ig2sum.
c
      implicit double precision (a-h,o-z)
      save
c
      include 'params.f'
      common / ga1   / npopsiz,nowrite
      common / ga2   / nparam,nchrome
      common / ga5   / g0,g1,ig2
      common / ga6   / parmax,parmin,pardel,nposibl
      dimension array(indmax,nparmax),iarray(indmax,nchrmax)
      dimension g0(nparmax),g1(nparmax),ig2(nparmax),nposibl(nparmax)
      dimension parmax(nparmax),parmin(nparmax),pardel(nparmax)
c
      do 10 i=1,npopsiz
         call decode(i,array,iarray)
         do 20 j=1,nparam
```

```
          n2ig2j=2**ig2(j)
          if(nposibl(j).ne.n2ig2j .and. array(i,j).gt.parmax(j)) then
            call ran3(1,rand)
            irand=dint(dble(nposibl(j))*rand)
            array(i,j)=g0(j)+dble(irand)*g1(j)
            call code(i,j,array,iarray)
            if (nowrite.eq.0) write(6,1000) i,j
            if (nowrite.eq.0) write(24,1000) i,j
          endif
 20     continue
 10   continue
c
 1000 format('*** Parameter adjustment to individual     ',i4,
   +       ', parameter  ',i3,' ***')
c
    return
    end
c
c
c
c
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c     subroutines following this point written by john bulloch
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c
c
c#########################################################################
c
c     *******************************************************************
c     * SUBROUTINE INPUT reads all input data from data file and        *
c     * converts input masses from mg to g units.                       *
c     *                                                                 *
c     * Variables internal to subroutine:                               *
c     *                                                                 *
c     *   i = do loop counter                                           *
c     *******************************************************************
c
c
    subroutine input(cdata,czero,czerod,errel,foc,itmax,numisos,xk,
```

```
     &xkt,xm,xmw,xmwt,xn,xnt,nfcs,ndata,isotype,xnonad,v,zz,czerot)
c
      implicit double precision (a-h,o-z)
      integer bn, isotype, ndata
c
      include 'params.f'
      dimension v(maxisos,maxdat),xm(maxisos,maxdat)
      dimension foc(nparmax),xk(nparmax),xmw(nparmax),xn(nparmax)
      dimension isotype(maxisos),ndata(maxisos),cdata(maxisos,maxdat)
      dimension xkt(maxisos),xnt(maxisos),xmwt(maxisos)
      dimension czerot(maxisos)
c
c     reading input and writing input values to gafca3.out
c
      read(25,*)nfcs,numisos,zz,errel,itmax
      write(24,*)'Inital solid phase multiplier = ',zz
      write(24,*)'Stopping tolerance for DNEQNF = ',errel
      write(24,*)'Maximum number iterations for DNEQNF = ',itmax
      write(24,*)
      write(24,*)'Input Component Data'
      write(24,*)'K(mg/g), 1/n, MW, FOC'
      do 10 i = 1,nfcs
          read(25,*)xk(i),xn(i),xmw(i),foc(i)
c        write(24,*)xk(i),xn(i),xmw(i),foc(i)
 10   continue
c     write(24,*)
c
      do 20 in = 1,numisos
c
         read(25,*)isotype(in), ndata(in)
c
         if (isotype(in) .eq. 1) then
           read(25,*)czero,xnonad
         else if (isotype(in) .eq. 2) then
           read(25,*)czero,czerod,xnonad
         else
           read(25,*)czero,xnonad,xkt(in),xnt(in),xmwt(in),czerot(in)
         endif
c
         do 25 bn = 1,ndata(in)
           read(25,*)v(in,bn),xm(in,bn),cdata(in,bn)
           xm(in,bn) = xm(in,bn)/1000.0d0
 25      continue
 20      continue
c
```

```
c
c        write (24,*) 'input:czerot(3)=',czerot(3)
c        print *, 'input:czerot(4)=',czerot(4)
c         do 27 i=3,4
c          tracer(i) = czerot(i)
c 27       continue
c     write(24,*)'Initial TOC = ',czero,' with nonadsorbing = ',xnonad
c     write(24,*)'Input Data'
c     write(24,*)'Bottle Volume, Mass Adsorbent, Liquid Phase TOC Data'
c
      return
      end
c
c####################################################################
c
c     ***************************************************************
c     * SUBROUTINE k2molar converts freundlich K values input in      *
c     * units of (mg/g)(L/mg)^1/n to (mmol/g)(L/mmol)^1/n.           *
c     *                                                  *
c     * Variables internal to subroutine:                      *
c     *                                                  *
c     *   i = do loop counter                            *
c     ***************************************************************
c
c
      subroutine k2molar(nfcs,numisos,isotype,xk,xkt,xmw,xmwt,xn,xnt)
c
      implicit double precision (a-h,o-z)
      integer isotype
      save
c
      include 'params.f'
      dimension isotype(maxisos)
      dimension xk(nparmax),xmw(nparmax),xn(nparmax)
      dimension xkt(maxisos),xnt(maxisos),xmwt(maxisos)
c
c     changing fictive components xk's from mass to molar units
c
      do 10 i=1,nfcs
       xk(i)=xk(i)*xmw(i)**(xn(i)-1.0d0)
 10   continue
c
c     changing tracer's xkt's from mass to molar units
c
      do 15 in = 1,numisos
```

```
          if (isotype(in) .eq. 3) then
            xkt(in)=xkt(in)*xmwt(in)**(xnt(in)-1.0d0)
          endif
 15   continue
c
      return
      end
c
c##########################################################################
c
c     ********************************************************************
c     * SUBROUTINE  sets up parameters for IAST solution for   *
c     * each individual of each generation.                  *
c     *                                     *
c     * Variables internal to subroutine:                    *
c     *                                     *
c     *  cotr = intermediate variable used in scaling procedure      *
c     *        if final fictive component comes out less than zero   *
c     *  csum = sum of TOC from each fictive component              *
c     *  i = do loop counter                        *
c     *  skal = skaling factor used of intial concentration of       *
c     *        final fictive component comes out less than zero      *
c     ********************************************************************
c
c
      subroutine iastpars(bn,czero,czerod,czerot,c0molar,foc,in,j,n,
     &nfcs,isotype,v,xk,xkt,xm,xmw,xmwt,xn,xnt,xnonad,gennum,maxgen,
     &cout)
c
      implicit double precision (a-h,o-z)
      integer bn, isotype, gennum
c
      include 'params.f'
c
      dimension v(maxisos,maxdat),xm(maxisos,maxdat)
      dimension isotype(maxisos),czerot(maxisos)
      dimension xkt(maxisos),xnt(maxisos),xmwt(maxisos)
      dimension parent(indmax,nparmax),cout(indmax,nparmax)
      dimension iparent(indmax,nchrmax)
      dimension par(50),c0molar(nparmax),c0toc(nparmax)
      dimension foc(nparmax),xk(nparmax),xmw(nparmax),xn(nparmax)

c
      common / ga3   / parent,iparent
      common / ga7   / par
```

```
c
      csum = 0.0d0
      do 10 i = 1,nfcs-1
          c0toc(i) = parent(j,i)*foc(i)
          c0molar(i) = parent(j,i)/xmw(i)
          csum = csum + c0toc(i)
 10   continue
      c0toc(nfcs)=(czero-csum-xnonad)
c
c     Correcting initial concentrations if c0toc(nfcs) less than 0.0d0
c
c      print*,'before conc. corrections'
c      do 11 i=1,nfcs
c      print*, 'c0toc(',i,')=',c0toc(i)
c 11   continue


      if (c0toc(nfcs) .lt. 0.0d0) then
          c0toc(nfcs)=(czero-xnonad)/10.0d0
          c0tr = xnonad
          do 20 i = 1,nfcs
            c0tr = c0tr + c0toc(i)
 20       continue
c
c     skal is the scaling factor if c0toc(nfcs) IS LESS THAN 0
c
          skal = (czero - xnonad)/(c0tr - xnonad)
          do 25 jn = 1,nfcs
            c0toc(jn) = c0toc(jn)*skal
 25       continue
      endif


      do 27 i=1,nfcs
          cout(j,i)=c0toc(i)
 27   continue
c
c     entering parameters in form for dneqnf and fcn depending on
c     the isotype of isotherm currently being calculated
c
      if (isotype(in) .eq. 1) then
          do 30 i = 1,nfcs
            c0molar(i)=c0toc(i)/foc(i)/xmw(i)
            par(i)=xk(i)
            par(10+i)=1.0d0/xn(i)
```

```
            par(20+i)=c0molar(i)
 30      continue
          par(30)=xm(in,bn)
          par(40)=v(in,bn)
          n=nfcs
     else if (isotype(in) .eq. 2) then
          do 35 i = 1,nfcs
c          write(6,*)'czerod = ',czerod
            c0molar(i)=c0toc(i)/foc(i)/xmw(i)*(czerod/czero)
            par(i)=xk(i)
            par(10+i)=1.0d0/xn(i)
            par(20+i)=c0molar(i)
 35      continue
          par(30)=xm(in,bn)
          par(40)=v(in,bn)
          n=nfcs
     else
          do 40 i = 1,nfcs
            c0molar(i)=c0toc(i)/foc(i)/xmw(i)
            par(i)=xk(i)
            par(10+i)=1.0d0/xn(i)
            par(20+i)=c0molar(i)
 40      continue
          par(nfcs+1)=xkt(in)
          par(nfcs+11)=1.0d0/xnt(in)
          par(nfcs+21)=czerot(in)/xmwt(in)
          par(30)=xm(in,bn)
          par(40)=v(in,bn)
          n=nfcs+1
     endif
c
     return
     end
c
c###########################################################################
c
c    *******************************************************************
c    * SUBROUTINE FCN sets up set of IAST equations for              *
c    * each individual of each generation.                      *
c    *                                                  *
c    * Variables internal to subroutine:                   *
c    *                                                  *
c    *   i = do loop counter                          *
c    *******************************************************************
c
```

```
c
      subroutine fcn(x,f,n)
c
      implicit double precision (a-h,o-z)
c
      include 'params.f'
c
      dimension x(nparmax),f(nparmax),par(50)
c
      common / ga7   / par
c
      QT=0.0D0
      QNQ=0.0D0
      DO 10 I=1,N
       QT=QT+X(I)
       QNQ=QNQ+PAR(10+I)*X(I)
 10    CONTINUE
       IF(QNQ.LE.0.0D0)    QNQ=0.0D0
      DO 20 I=1,N
       F(I)=PAR(20+I)-PAR(30)/PAR(40)*X(I)-X(I)/QT*(QNQ/PAR(10+I)/
     $PAR(I))**PAR(10+I)
 20    CONTINUE
c
      RETURN
      END
c
c######################################################################
c
c     ***          ********************************************************
c     * SUBROUTINE RESIDUAL calculates the liquid and solid phase      *
c     * residuals or percent residuals.                         *
c     *                                               *
c     * Variables internal to subroutine:                        *
c     *                                               *
c     *  delta = intermediate value in calculations             *
c     *  i = do loop counter                                *
c     *****************************************************************
c
c
      subroutine residual(bn,c0molar,cdata,cpres,cres,ctot,
     &czero,czerod,czerot,foc,in,nfcs,qdata,qpres,qres,qtot,isotype,
     &v,x,xm,xmw,xmwt,xnonad)
c
      implicit double precision (a-h,o-z)
      integer bn, isotype
```

```
c
      include 'params.f'
c
      dimension v(maxisos,maxdat),xm(maxisos,maxdat)
      dimension isotype(maxisos),czerot(maxisos)
      dimension foc(nparmax),xmw(nparmax)
      dimension cdata(maxisos,maxdat),qdata(maxisos,maxdat)
      dimension x(nparmax),xmwt(maxisos)
      dimension c0molar(nparmax),ctoc(nparmax),qtoc(nparmax)
      dimension cpres(maxisos,maxdat),cres(maxisos,maxdat)
      dimension qpres(maxisos,maxdat),qres(maxisos,maxdat)
      dimension ctot(maxisos,maxdat),qtot(maxisos,maxdat)
c
c      calculate the equilibrium toc concentrations
c
c           write (24,*) 'czerot(3)=',czerot(3)
c           print *, 'tracer(3)=',tracer(3)
      if (isotype(in) .eq. 1) then
           qtot(in,bn)=0.0D0
           ctot(in,bn)=0.0D0
           do 10 i=1,nfcs
             ctoc(i)=(c0molar(i)-xm(in,bn)/v(in,bn)*x(i))*xmw(i)*foc(i)
             qtoc(i)=x(i)*xmw(i)*foc(i)
             qtot(in,bn)=qtoc(i)+qtot(in,bn)
             ctot(in,bn)=ctoc(i)+ctot(in,bn)
 10        continue
           ctot(in,bn)=ctot(in,bn)+xnonad
C
C      setting residuals or %residuals for minimization for isotype 1
C
           delta=czero-cdata(in,bn)
           qdata(in,bn)=delta*v(in,bn)/xm(in,bn)
           qres(in,bn)=(delta)*v(in,bn)/xm(in,bn)-qtot(in,bn)
           CRES(in,bn)=cdata(in,bn)-ctot(in,bn)
           QPRES(in,bn)=QRES(in,bn)/((delta)*v(in,bn)/xm(in,bn))
           CPRES(in,bn)=CRES(in,bn)/cdata(in,bn)



      else if (isotype(in) .eq. 2) then
           qtot(in,bn)=0.0D0
           ctot(in,bn)=0.0D0
           do 20 i=1,nfcs
             ctoc(i)=(c0molar(i)-xm(in,bn)/v(in,bn)*x(i))*xmw(i)*foc(i)
             qtoc(i)=x(i)*xmw(i)*foc(i)
```

```
         qtot(in,bn)=qtoc(i)+qtot(in,bn)
         ctot(in,bn)=ctoc(i)+ctot(in,bn)
 20    continue
        ctot(in,bn)=ctot(in,bn)+xnonad*(czerod/czero)

C
C   setting residuals or %residuals for minimization isotype 2
C
        delta=czerod-cdata(in,bn)
        qdata(in,bn)=delta*v(in,bn)/xm(in,bn)
        qres(in,bn)=(delta)*v(in,bn)/xm(in,bn)-qtot(in,bn)
        CRES(in,bn)=cdata(in,bn)-ctot(in,bn)
        QPRES(in,bn)=QRES(in,bn)/((delta)*v(in,bn)/xm(in,bn))
        CPRES(in,bn)=CRES(in,bn)/cdata(in,bn)

   else if (isotype(in) .eq. 3) then
        qtot(in,bn)=0.0D0
        ctot(in,bn)=0.0D0

c
c     no toc summing required for isotype 3 (tracer) isotherms
c
c       write (24,*) 'x(7)=', x(nfcs+1)

        delta=czerot(in)-cdata(in,bn)
        qdata(in,bn)=delta*v(in,bn)/xm(in,bn)
        ctot(in,bn)=czerot([illegible]xm(in,bn)/v(in,bn)*x(nfcs+1)*xmwt(in))
        qtot(in,bn)=x(nfcs[illegible]xmwt(in)
        qres(in,bn)=qdata([illegible])-qtot(in,bn)
        CRES(in,bn)=cdata(in,bn)-ctot(in,bn)
        QPRES(in,bn)=QRES(in,bn)/qdata(in,bn)
        CPRES(in,bn)=CRES(in,bn)/cdata(in,bn)
c
       else
   endif
c
   return
   end
c
c#######################################################################
c
c   ******************************************************************
c   * SUBROUTINE OBJFUN calculates the sample deviation for each    *
c   * individual of each generation.                        *
c   *                                        *
```

```
c   * Variables internal to subroutine:                    *
c   *                                          *
c   *  ssq1 = sum of the squares of percent residuals in liquid    *
c   *  ssq2 = sum of the squares of percent residuals in solid     *
c   *  nptsfit = sum of number of data in each isotherm          *
c   *******************************************************************
c
c
      subroutine objfun(bn,cpres,cres,in,j,ndata,numisos,
     &qpres,qres,sdev)
c
      implicit double precision (a-h,o-z)
      integer bn
      save
c
      include 'params.f'
      dimension cpres(maxisos,maxdat),cres(maxisos,maxdat)
      dimension qpres(maxisos,maxdat),qres(maxisos,maxdat)
      dimension ndata(maxisos)
c
      nptsfit=0
      sdev = 0.0d0
      ssq1 = 0.0d0
      ssq2 = 0.0d0
      do 10 in = 1,numisos
          do 15 bn = 1,ndata(in)
            ssq1=ssq1+(cpres(in,bn))**2.0d0
            ssq2=ssq2+(qpres(in,bn))**2.0d0
 15     continue
      nptsfit=nptsfit+ndata(in)
 10   continue
c     write(30,*)'ssq1 = ',ssq1
      sdev=((1.0d0/dble(nptsfit-1))*(ssq1+ssq2)**0.50d0)*100.0d0
c     sdev=((1.0d0/dble(nptsfit-1))*(ssq2)**0.50d0)*100.0d0

      if (j .eq. 1) then
          write(30,*)'sdev = ',sdev
      endif
c
      return
      end
c
c###########################################################################
c
c    *******************************************************************
```

```
c    * SUBROUTINE FUNC calculates the fitness (100-sdev) for each     *
c    * individual of each generation.                        *
c    *                                       *
c    ********************************************************************
c
c
     subroutine func(j,funcval,sdev)
c
     implicit double precision (a-h,o-z)
     save
c
     funcval=100.0d0-sdev
     if (j .eq. 1) then
          write(30,*)'fitness = 'funcval
     endif
c
     return
     end
c
c###########################################################################
```

Input Data File: gafca3.dat

```
6,1,0.5D-1,1.0d-4,100
0.00001,1.0,106.,.703
.4,.7,1.06,.703
2.5,.61,96.5,.742
10.0,.54,100.,.73
50.0,.46,355.,.711
500.0,.34,257.5,.757
3,4
145.08,26.6,180.31,.71,165.85,.888,          PCE
.043,5.0,.432
.0428,6.9,.284
.0424,10.8,.141
.0432,17.7,.052
```

Output File: gafca3.out

```
################ Generation 100 ################
 #    Binary Code      Param1 Param2
 1 01101011010111010101001101000010001101100010010001
25.842    28.251    13.225    35.404    8.834    6.924    43.496620
 2 00011110111011110111011001000000011000111110110111
5.868    36.206    20.139    4.904    45.880    5.483    44.402482
 3 10100000111011110100000100100010101100111101001101
24.092    28.326    2.848    26.885    32.021    4.307    43.361937
 4 11010000111000001100110011011111011011001011010101
24.823    15.577    25.823    27.042    21.798    3.417    41.183871
 5 00011111110111001000101100000000100000101111001000
5.592    20.077    32.715    11.933    43.103    5.061    42.328684
 6 10100100110001000010101011011100001001001011000010
33.583    3.364    37.383    1.905    36.388    5.857    39.135890
 7 11001111101110001001010101110111010100101101011100
24.766    27.004    10.991    26.337    25.953    3.430    43.008019
 8 11000110111100111101000100001100001111000001100101
47.713    49.754    4.245    3.740    6.131    6.898    45.602580
 9 11111010110000000100011110111111110001110111011010
37.991    .152    19.790    38.035    18.159    4.354    39.037207
10 00001100100011001100001110001110000000011111101100
2.747    11.207    13.163    29.265    55.784    6.314    41.733596
11 00100000111011011000010001100010110110000110001101
6.395    35.540    14.428    36.905    19.602    5.611    44.374385
12 00100010001000100111010101011110110101011111010010
5.545    22.465    14.761    30.695    40.328    4.686    42.808644
13 10100111110111111000111101000101011111111110000101
21.900    16.450    33.656    12.981    29.742    3.751    41.313911
14 10100101011111110000110101101111101001110110010011
19.246    29.350    26.399    28.270    11.868    3.347    43.190122
15 01111100101111110101100111000110010001000111001011
17.602    35.804    23.316    21.287    16.408    4.063    44.066593
16 11100001111001010101111001110100011010110001010101
38.369    25.367    41.485    4.721    3.653    4.884    42.407620
17 10011111110100111110000001001101110000111010110011
33.511    16.677    1.052 . 24.561    36.651    6.028    41.965513
18 1110100011101101111101001000000000110100000001100000
48.168    38.027    15.727    5.588    5.024    5.947    44.257467
19 00000101111000110001001010001111100001111011000101
1.079    26.316    8.071    43.986    33.637    5.392    43.468140
20 01000110101001000001100000000110000000100000010111
16.122    32.987    30.955    30.514    1.330    6.571    43.947626
```

```
 21 0100101010100010011001011011111000101111111011 1100
 12.185    22.489    15.839    23.734    39.534    4.700     42.708129
 22 00110100010010000101111101110100011000111001101011
 11.106    7.068     55.469    5.463     33.267    6.108     39.931720
 23 01111100111001100110001001101110000110110110000001
 25.259    31.080    8.281     28.331    19.710    5.818     43.769930
 24 01011010000011100010010011110100110111010100000110
 27.878    17.501    25.910    17.771    20.520    8.901     42.169402
 25 00110100111011101010001111100101001001011010101110
 10.717    37.888    13.348    15.453    35.237    5.838     44.612571
 26 01100000110000011011001110101110001010011100100111
 21.155    1.476     13.559    31.390    44.616    6.283     40.569117
 27 00011110111101010010001110110111110101011100111001
 4.567    31.558    9.288    37.821    30.979    4.267     43.880918
 28 01101011111001011010000101100100011101101010101110
 24.810    34.654    5.408     7.054     39.938    6.616     44.287922
 29 10001000000100001011100101000111010010110101111100
 22.924    11.252    26.376    36.889    16.196    4.844     40.698032
 30 11010110100100100111110111110101110001000011100011
 34.940    12.013    38.383    19.114    9.349     4.681     40.251890
 31 00011001101101101110110110011110101101011000100101
 3.674    31.627    33.115    25.922    20.001    4.140     43.663716
 32 11011010000010100100011111010101010110010010000110
 47.533    8.940    28.825    19.529    7.388     6.265     39.773709
 33 00100010111100010000100010101110110000111011111111
 5.256    29.642    22.148    27.758    29.330    4.346     43.546911
 34 10101100010011110100011111000010001000111000101011
 30.225    10.704    22.966    24.918    24.624    5.042     40.564126
 35 00000101011111011111010000000110110100100100110011
 1.012    47.759    13.073    36.132    14.964    5.539     45.594456
 36 11110001000100010101011110111011110101101100100101
 30.775    8.843    16.646    32.554    25.992    3.669     40.161867
 37 01100000001001011100000111010011000101011100111 0101
 21.292    10.176    13.601    31.872    35.182    6.357     41.134459
 38 01101110010100101000111111010110000111000111110001
 17.507    11.751    42.445    22.260    19.954    4.563     40.554813
 39 00000010001111100111000100010000000100110000110111
 .747    93.264    6.701    1.843    5.194    10.731    49.190973
 40 10110110000000100110011100010101111000000010001 11001
 25.019    2.612    32.863    34.259    19.777    3.950     38.976714

 Average Values:                                      68.322    76.126    67.999
 77.262    81.456    42.528307

 Average Function Value of Generation=    42.528307
```

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Maximum Function Value          =     49.190973


 Number of Crossovers      = 984
 Number of Jump Mutations  = 972
 Number of Creep Mutations =   0
 Elitist Reproduction on Individual   24


ISOTHERM   1
C data (mg TOC/L)  C model (mg TOC/L)  q data (mg TOC/g)  q model (mg TOC/g)
    .4320            .1053           3.9216          6.7316
    .2840            .0774           3.7466          5.0278
    .1410            .0499           2.9327          3.2904
    .0520            .0313           2.0404          2.0910
```